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CHAPTER P-1 NOMENCLATURE OF ORGANIC COMPOUNDS

P-10 Introduction

For nomenclature purposes, a structure containing at least one carbon atom is considered to be an organic compound. The formation of a systematic name for an organic compound requires selection and then naming of a parent structure. This basic name may then be modified by prefixes, infixes, and, in the case of a parent hydride, suffixes, which convey precisely the structural changes required to generate the compound in question from the parent structure. In contrast to such systematic names, there are traditional names which are widely used in industry and academic circles. Examples are acetic acid, benzene and pyridine. Therefore, when they meet the requirements of utility and when they fit into the general pattern of systematic nomenclature, these traditional names are retained.

A major new principle is elaborated in these Recommendations. The concept of ‘preferred IUPAC names’ is developed and systematically applied. Up to now, the nomenclature developed and recommended by IUPAC has emphasized the generation of unambiguous names in accord with the historical development of the subject. In 1993, due to the explosion in the circulation of information and the globalization of human activities, it was deemed necessary to have a common language that will prove important in legal situations, with manifestations in patents, export-import regulations, environmental and health and safety information, etc. However, rather than recommend only a single ‘unique name’ for each structure, we have developed rules for assigning ‘preferred IUPAC names’, while continuing to allow alternatives in order to preserve the diversity and adaptability of the nomenclature to daily activities in chemistry and in science in general.

Thus, the existence of preferred IUPAC names does not prevent the use of other names to take into account a specific context or to emphasize structural features common to a series of compounds. Preferred IUPAC names belong to ‘**preferred IUPAC nomenclature’** Any name other than a preferred IUPAC name, as long as it is unambiguous and follows the principles of the IUPAC recommendations herein, is acceptable as a ‘general’ IUPAC name, in the context of **‘general’ IUPAC nomenclature**.

The concept of preferred IUPAC names is developed as a contribution to the continuing evolution of the IUPAC nomenclature of organic compounds. This book (Recommendations 2004) covers and extends the principles, rules and conventions described in two former publications: *Nomenclature of Organic Chemistry*, 1979 Edition (ref. 1) and *A Guide to IUPAC Nomenclature of Organic Compounds, Recommendations 1993* (ref. 2). In a few instances, the 1979 rules and the 1993 recommendations have been modified to achieve consistency within the entire system. In case of divergence among the various recommendations, Recommendations 2004 prevail.

P-11 Scope of nomenclature for organic compounds

For nomenclature purposes we consider all compounds containing carbon as organic compounds. Oxygen and nitrogen are two elements usually associated with carbon to form the system of functions or characteristic groups. Other elements, among them the halogens and sulfur, complete the basic core of elements found in organic compounds. Substitutive nomenclature was first applied to compounds containing this set of atoms. The success of this type of nomenclature was such that it was extended to all elements of Groups 14, 15, 16, 17 and, in Group 13, to boron; it is now fully extended to all elements of Group 13.

Table 1.1 Elements included in these recommendations

Groups	13	14	15	16	17
	B boron	C carbon	N nitrogen	O oxygen	F fluorine
	Al aluminium	Si silicon	P phosphorus	S sulfur	Cl chlorine
	Ga gallium	Ge germanium	As arsenic	Se selenium	Br bromine
	In indium	Sn tin	Sb antimony	Te tellurium	I iodine
	Tl thallium	Pb lead	Bi bismuth	Po polonium	As astatine

The ending ‘ane’, characteristic of alkanes, was borrowed from methane, ethane, etc., and glued to terms forming the roots of the names of the various elements, for example sulfane, H_2S; phosphane, PH_3; silane, SiH_4; alumane, AlH_3. The resulting names constitute the basis of substitutive nomenclature; this treatment of parent hydrides is called **generalized ‘ane’ nomenclature** because all the rules applicable to alkanes are applicable to all hydrides of the elements of Groups 13, 14, 15, 16 and 17. The nomenclature of hydrides of carbon may be conveniently termed **‘carbane nomenclature’**; whereas the term **‘heterane nomenclature’** covers the hydrides of elements other than carbon. Names of mononuclear parent hydrides are listed in Table 2.1 in Chapter 2.

Organometallic compounds, i.e., compounds in which one or more carbon atom(s) is (are) directly attached to a metal atom, were always regarded as organic compounds for nomenclature purposes. This association is maintained in these recommendations (see P-69), for the metals, semimetals, and nonmetals included in Groups 13, 14, 15, 16, and 17. The nomenclature for other organic derivatives of the elements in Groups 1 through 12 is considered as part of the nomenclature of inorganic compounds.

The construction of systematic names is based on general nomenclature operations and rules, and on operations and rules specific to different types of nomenclature. These aspects are discussed in the following sections.

P-12 Preferred, preselected and retained IUPAC names

P-12.1 ‘Preferred IUPAC names’ are names that are preferred among two or more names for the same structure generated from two or more recommended IUPAC rules or the many synonyms that have been coined and used over the years.

Preferred IUPAC names, or PINs, for short, are names selected according to the set of principles, conventions, and rules given herein. They originate from the strict application of the rules; in this sense, they can be referred to as ‘single names’. All preferred IUPAC names are identified by the parenthetical abbreviation ‘(PIN)’ following the name. Names used in the past, but now discarded or no longer recommended, are sometimes mentioned as a link to past rules and recommendations and are identified by words such as ‘not’ or ‘formerly’ or phrases like ‘no longer recommended’.

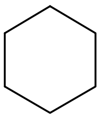
It is necessary to select a preferred alternative in many instances in the construction of the names of organic compounds. Preferred IUPAC names are given to parent structures and to characteristic groups denoted by prefixes and suffixes. They also result from the choice to be made among the different types of nomenclature, for example, substitutive nomenclature, functional class nomenclature and multiplicative nomenclature; and among the different types of operations, for example substitutive, additive and subtractive.

Most commonly, a **parent structure** is a **parent hydride**, i.e., a structure containing, in addition to one or more hydrogen atoms, a single atom of an element, for example, methane; or a number of atoms (alike or different) linked together to form an unbranched chain, for example, pentane; or a monocyclic or polycyclic ring system, for example, cyclohexane and quinoline. Methane is a retained name (see P-12.3) that is preferred to the systematic name ‘carbane’, a name never recommended to replace methane, but used to derive the names ‘carbene’ and carbyne for the radicals **:**CH_2 and **:**CH·, respectively. The name ‘pentane’ is formed by application of P-21.2.1 and is marked as the preferred IUPAC name, or PIN, even though no rule has been cited giving an alternative name. The same reasoning applies to cyclohexane, a IUPAC name resulting from the application of P-22.1.1. The name ‘quinoline’ is a retained name that is preferred to the systematic alternative fusion names ‘1-benzopyridine’ and ‘benzo[*b*]pyridine’.

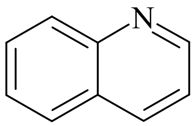
Examples:

CH_4 methane (preferred IUPAC name or PIN, a retained name)
carbane

$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3$ pentane (preferred IUPAC name or PIN)

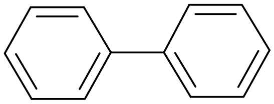


cyclohexane (PIN)

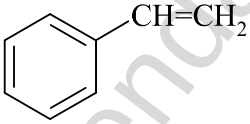


quinoline (PIN, a retained name)
1-benzopyridine (a systematic fusion name)
benzo[*b*]pyridine (a systematic fusion name)

It is sometimes convenient to employ parent hydrides of more complex structure, such as ring or ring-chain assemblies, for example biphenyl and styrene. The name ‘1,1′-biphenyl’ results from the application of Rule P-28.2.1; it is the preferred IUPAC name and the locants 1,1′ are compulsory; the name ‘biphenyl’, without locants, can be used in general IUPAC nomenclature. The name ‘styrene’ is a retained name and is preferred to the systematic substitutive names ‘vinylbenzene’, ‘ethenylbenzene’, ‘phenylethene’ and ‘phenylethylene’, that are acceptable in general IUPAC nomenclature as being clear and unambiguous.



1,1′-biphenyl (PIN)
biphenyl



styrene (PIN, a retained name)
vinylbenzene
ethenylbenzene
phenylethene
phenylethylene

A special class of parent structures having retained names (see P-12.3) is called **functional parents**, for example acetone and acetic acid. These two names are preferred IUPAC names; the corresponding systematic alternatives, propan-2-one and ethanoic acid, may be used in general IUPAC nomenclature.

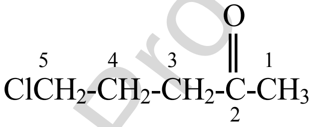
$CH_3\text{-}CO\text{-}CH_3$

acetone (PIN)
propan-2-one

$CH_3\text{-}COOH$

acetic acid (PIN)
ethanoic acid

In order to generate the parent structure from a compound to be named, various formal **operations** must be carried out. For example, in naming the structure below, the parent hydride ‘pentane’ is formally derived by replacing the oxygen and chlorine atoms by the appropriate number



$$\mathrm{Cl\overset{5}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\underset{2}{\overset{O}{\overset{\|}{C}}}\text{-}\overset{1}{C}H_3}$$

of hydrogen atoms. For constructing the name, the formal operation is reversed; the suffix ‘one’ and the prefix ‘chloro’, indicating **substitution** of the hydrogen atoms of pentane, are attached to the name of the parent hydride to give the name ‘5-chloropentan-2-one’. Suffixes and prefixes can represent a number of different types of formal operations on the parent structure. Frequently, the suffix or prefix denotes the attachment of a characteristic group (functional group), for example, ‘one’ or ‘oxo’ for =O. A prefix may also describe a group derived from a parent hydride, for example ‘pentyl’, from pentane, for $CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2–$.

The **substitutive operation**, described in P-13.1, is the operation used most extensively in organic nomenclature. Indeed, the comprehensive nomenclature system based largely on the application of this operation to parent structures is, for convenience, termed **substitutive nomenclature**, although this nomenclature also involves many of the other types of operations described in P-13. Substitutive nomenclature is the set of **substitutive names and principles, conventions, and rules used for name construction**. Examples of substitutive and other nomenclature operations are shown in Table 1.2

Another type of nomenclature expresses the principal characteristic group not as a suffix but as a term denoting the functional class cited in a name as a separate word; in Table 1.2, the name ‘ethyl propyl ether’ is a typical **functional class name** based on the functional class name ‘ether’. The corresponding substitutive name ‘1-ethoxypropane’ is constructed by using the prefix ‘ethoxy’ and the parent hydride name ‘propane’.

Substitutive and functional class names are written differently. Generally, substitutive names are unitary names that combine prefixes, names of parent hydrides, endings and suffixes in one word. On the contrary, a functional class name is written as separate words, even though the part describing the parent hydride or the modified parent hydride is the result of the same operations used to construct substitutive names.

The great majority, if not all, of organic compounds can be named in accordance with the principles of substitutive and functional class operations. However, in these recommendations, where there is a choice, names obtained by the substitutive operation are preferred IUPAC names. In Table 1.2, examples 1, 2 and 3 illustrates this preference. The substitutive names ethoxypropane and 2-chloropentan-2-one are preferred to the functional class names based on the names of the corresponding class, ether and ketone, ethyl propyl ether and 2-chloropropyl methyl ketone. On the contrary, a functional class name is preferred for the ester trimethyl phosphite over the substitutive name trimethoxyphosphane. Esters, along with acid halides and anhydrides are preferably named by using functional class nomenclature; substitutive nomenclature is not adapted to naming these classes.

Other types of operations are widely used, alone or along with substitutive nomenclature. **The skeletal replacement operation** (often referred to as ‘a’ replacement) is used as a necessary complement in order to introduce heteroatoms into cyclic hydrocarbons and to avoid the proliferation of prefixes in names for acyclic systems. For example, the name formed by skeletal replacement ‘2,5,8,11-tetraoxatridecane’ is preferred to the substitutive name ‘1-ethoxy-2-[2-(methoxyethoxy)ethoxy]ethane’. **Additive** and **subtractive operations** have been extended for naming radicals and ions. They are the sole method for modification of the degree of hydrogenation, by adding or subtracting pairs of hydrogen atoms. Examples 5 and 6 illustrate the preference for substitutive operations over additive or subtractive operations. **The conjunctive operation** eliminates hydrogen atoms from two different compounds and then combines them; this method is used to name parent hydrides composed of repeated identical units or to link rings and chains under specific conditions. Example 7 in Table 1.2 illustrates such an operation; in IUPAC nomenclature,
however, a substitutive name is always preferred to a conjunctive name, for example ‘1*H*-indol-1-ylacetic acid’ is preferred to ‘1*H*-indole-1-acetic acid’.

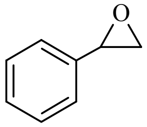
Table 1.2 Nomenclature operations

CH_3-CH_2-O-CH_2-CH_2-CH_3
1

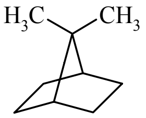
CH_3-CHCl-CH_2-CO-CH_3
2

$P(OCH_3)_3$
3

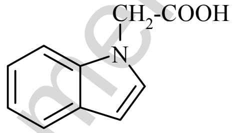
CH_3-O-CH_2-CH_2-O-CH_2-CH_2-O-CH_2-CH_2-O-CH_2-CH_3
4



5



6



7

Formula	Parent Structure (Class Name)	Operation	Name	Reference
1	propane (ether)	substitutive functional class	1-ethoxypropane (PIN) ethyl propyl ether	P-13.1 P-13.3.3.2
2	pentane (ketone)	substitutive functional class	4-choropentan-2-one (PIN) 2-chloropropyl methyl ketone	P-13.1 P-13.3.3.2
3	phosphane (phosphite)	substitutive functional class	trimethoxyphosphane trimethyl phosphite (PIN)	P-13.1 P-13.3.3.2
4	ethane tridecane	substitutive skeletal ('a') replacement	1-ethoxy-2-[2-(methoxyethoxy)ethoxy]ethane 2,5,8,11-tetraoxatridecane (PIN)	P-13.1 P-13.2.1
5	oxirane styrene + oxide	substitutive additive	2-phenyloxirane (PIN) styrene oxide	P-13.1 P-13.3.3.1
6	bornane bicycloheptane	substitutive substitutive	10-norbornane 7,7-dimethylbicyclo[2.2.1]heptane (PIN)	P-13.4.4.3 P-13.1
7	acetic acid acetic acid + indole	substitutive conjunctive	1*H*-indol-1-ylacetic acid (PIN) 1*H*-indole-1-acetic acid	P-13.2 P-13.5.2

A nomenclature embraces the major operations along with the principles, conventions and rules necessary to construct names of a particular type. Substitutive nomenclature and functional class nomenclature have been discussed above. Replacement nomenclature and conjunctive nomenclature also require specific principles, conventions and rules. On the contrary, additive and subtractive operations do not correspond to nomenclatures in their own right, but are necessary complements to other nomenclatures.

It is very important to recognize that, in general, the rules of the nomenclature of organic compounds are written in terms of classical valence bonding and do not imply electronic configurations of any kind.

Principles and general rules are described in this Chapter. Substitutive nomenclature is then elaborated in Chapter 2 (parent hydride names), in Chapter 3 (endings, suffixes and prefixes), and in Chapter 4 (rules for name construction). Chapter 5 describes the construction of preferred IUPAC names. In Chapter 6 the naming of compounds arranged in classes and groups is described. In Chapter 7, nomenclature for radicals, ions and related species is discussed. Chapter 8 describes isotopic modifications of organic compounds. Chapter 9 deals with configuration and conformation specification and Chapter 10 covers natural products.

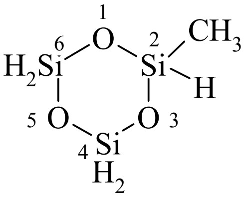
Several topics discussed in these recommendations have been published recently as fully comprehensive documents: radicals and ions (ref. 3), fused and bridged fused ring systems (ref. 4), phane nomenclature (refs. 5,6), the von Baeyer system for polycyclic compounds (ref. 7), spiro compounds (ref. 8), natural products (ref. 9), and fullerenes (ref. 10). They are not reproduced *in extenso* in these recommendations. Rather, the principles, conventions and rules are discussed in a less rigorous manner. Readers should use the full publications to deal with more complex cases; these publications are not superseded unless specifically noted in boxed comments. Again, all modifications made to achieve consistency are clearly signaled in these Recommendations and prevail over any former rules or interpretations.

P-12.2 'Preselected names' are names chosen among two or more names for noncarbon-containing (inorganic) parents to be used as the basis for preferred IUPAC names for organic derivatives in the nomenclature of organic compounds.

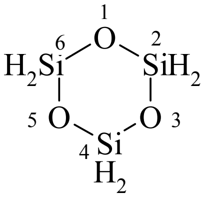
In the context of substitutive organic nomenclature, we need to select names for parent hydrides or other parent structures that do not contain carbon, in order to name organic derivatives. The names chosen here for this purpose are termed 'preselected'. Each non-carbon-containing parent capable of substitution or functionalization by carbon-containing groups is assigned a unique 'preselected' name to be used as the basis for deriving a preferred IUPAC name. Parent names identified here as 'preselected' may not necessarily emerge as preferred IUPAC names in the context of inorganic chemical nomenclature.

All names listed in Table 2.1, with the exception of methane (carbane), are preselected names, and the concept is illustrated by the following two examples.

CH_3-SnH_2-$[SnH_2]_{11}$-SnH_3	SnH_3-$[SnH_2]_{11}$-SnH_3
1-methyltridecastannane (PIN)	tridecastannane (preselected name)
$(CH_3$-$O)_3PO$	$(HO)_2P(O)$-OH
trimethyl phosphate (PIN)	phosphoric acid (preselected name)



2-methyl-1,3,5,2,4,6-trioxatrisilinane (PIN)
2-methylcyclotrisiloxane



1,3,5,2,4,6-trioxatrisilinane (preselected name; see P-22.2.2.1.6)
cyclotrisiloxane (P-22.2.5)

P-12.3 'Retained names' are traditional or common well-established names that may be used either as preferred IUPAC name or as an allowed alternatives in general nomenclature, for example, naphthalene, benzoic acid and pyridine.

P-12.4 Methodology

In this book, names of parent structures, characteristic groups and their prefixes, and organic compounds are systematically identified as preferred IUPAC names or preselected IUPAC names; preferred IUPAC stereodescriptors are described and used in Chapter 9. To facilitate the construction of the names of organic compounds, preferred prefixes for use in generating preferred IUPAC names are listed in Appendix 2 along with other recommended prefixes to be used in general nomenclature.

P-13 Operations in nomenclature of organic compounds

The operations described in this section all involve structural modifications, and are classified first according to the type of modification, for example 'replacement'; and then according to the way in which the modification is expressed, for example 'by use of replacement infixes'. The structures to which the various modifications are applied can be regarded as parent structures, and the modifications are expressed by suffixes, affixes, infixes and prefixes, or by a change of the endings.

P-13.1 The substitutive operation
P-13.2 The replacement operation
P-13.3 The additive operation
P-13.4 The subtractive operation
P-13.5 The conjunctive operation
P-13.6 The multiplicative operation
P-13.7 The fusion operation
P-13.8 Operations used only in the nomenclature of natural products

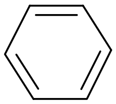
P-13.1 The substitutive operation

The substitutive operation involves the exchange of one or more hydrogen atoms for another atom or group of atoms. This process is expressed by a suffix or a prefix denoting the atom or group being introduced.

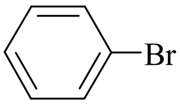
Examples:

$CH_3\text{-}CH_3 \longrightarrow CH_3\text{-}CH_2\text{-}SH$

ethane (PIN) ethanethiol (PIN)
(substitutive suffix = 'thiol')



benzene (PIN)



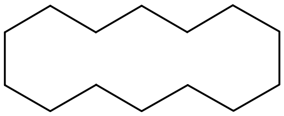
bromobenzene (PIN)
(substitutive prefix = 'bromo')

P-13.2 The replacement operation

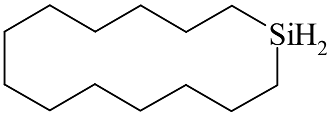
The replacement operation involves the exchange of one group of atoms or a single nonhydrogen atom for another. This can be expressed in several ways, as shown in the following subsections.

P-13.2.1 By replacement ('a') prefixes that represent the element being introduced. This type of replacement is called 'skeletal replacement'. The most important type in the nomenclature of organic compounds is replacement of carbon atoms by O, S, Se, Te, N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, or Tl.

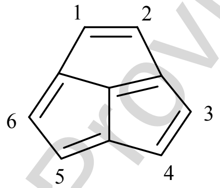
Examples:



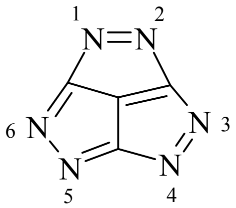
cyclotetradecane (PIN)



silacyclotetradecane (PIN)
(replacement prefix = 'sila')



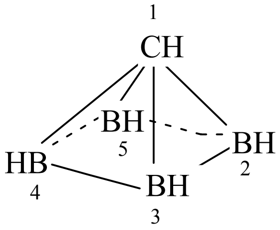
cyclopenta[*cd*]pentalene (PIN)



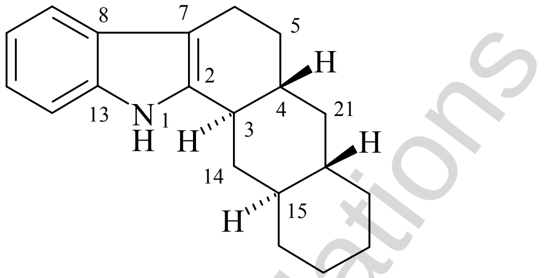
1,2,3,4,5,6-hexaazacyclopenta[*cd*]pentalene (PIN)
(replacement prefix = 'aza')

In specific instances, a heteroatom may be replaced by a carbon atom or another heteroatom. The former is exemplified in the nomenclature of cyclic polyboranes (see I-11.4.3.2, ref. 11) and both are found in natural products (see RF-5, ref. 9 and P-101.4) and must be applied only when specifically prescribed because the nomenclature of organic compounds is normally based on carbon atoms.

Examples:



1-carba-*nido*-pentaborane(5) (PIN)
(replacement prefix = ‘carba’;
carbon replacing boron)



(4β)-1*H*-4-carbayohimban (PIN)
(replacement prefix = ‘carba’; carbon
replacing nitrogen; see P-94.2)

P-13.2.2 By prefixes or infixes signifying replacement of oxygen atoms or oxygen-containing groups. This type of replacement is called ‘functional replacement’. The affixes represent the group(s) being introduced. Functional replacement nomenclature is described in P-15.5.

Examples:

$(CH_3)_2P(O)\text{-}OCH_3 \longrightarrow (CH_3)_2P(=NH)\text{-}OCH_3$

methyl dimethylphosphinate (PIN)

methyl *P*,*P*-dimethylphosphinimidate (PIN)
methyl *P*,*P*-dimethyl(imidophosphinate)
(replacement infix = ‘imid(o)’;
=NH replacing =O)

$C_6H_5\text{-}P(O)(OH)_2 \longrightarrow C_6H_5\text{-}P(\equiv N)\text{-}OH$

phenylphosphonic acid (PIN)

phenylphosphononitridic acid (PIN)
phenyl(nitridodophosphonic acid)
(replacement infix = ‘nitrid(o)’;
≡N replacing both =O and −OH)

The affixes ‘thio’, ‘seleno’, and ‘telluro’ indicate replacement of an oxygen atom of a characteristic group by another chalcogen atom.

Examples:

$C_6H_5\text{-}COOH \longrightarrow C_6H_5\text{-}C\{O,Se\}H$

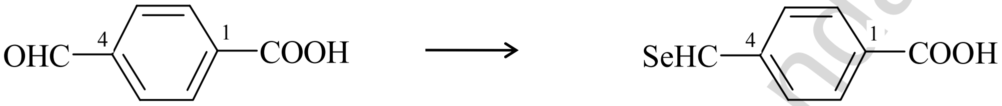
benzoic acid

benzenecarboselenoic acid (PIN)
selenobenzoic acid
(replacement prefix = ‘selen(o)’;
selenium replacing either =O or −O−)

$CH_3\text{-}[CH_2]_4\text{-}COOH \longrightarrow CH_3\text{-}[CH_2]_4\text{-}C(S)SH$

hexanoic acid (PIN)

hexanedithioic acid (PIN)
hexane(dithioic) acid
(replacement infix = ‘thi(o)’;
S replaces both =O and −O−)

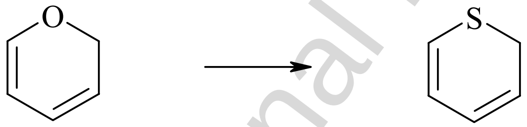


4-formylbenzoic acid (PIN)

4-methaneselenoylbenzoic acid (PIN)
4-(selenoformyl)benzoic acid
(replacement prefix = ‘selen(o)’;
Se replaces =O)

In specific instances, the prefixes ‘thio’, ‘seleno’, and ‘telluro’, indicate a skeletal modification. This replacement occurs with the cyclic parent hydrides having retained names, i.e., morpholine (see Table 2.3), pyran (see Table 2.2), chromene, isochromene, and xanthene (see Table 2.7), chromane and isochromane (see Table 3.1).

Example:



2*H*-pyran (PIN)
2*H*-oxine

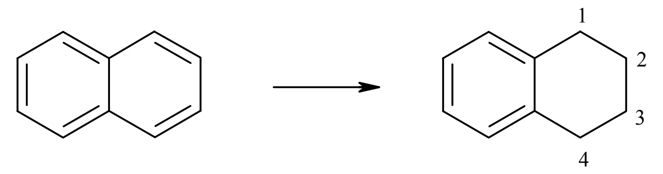
2*H*-thiopyran (PIN)
2*H*-thiine
(replacement prefix = ‘thio’;
S replacing O)

P-13.3 The additive operation

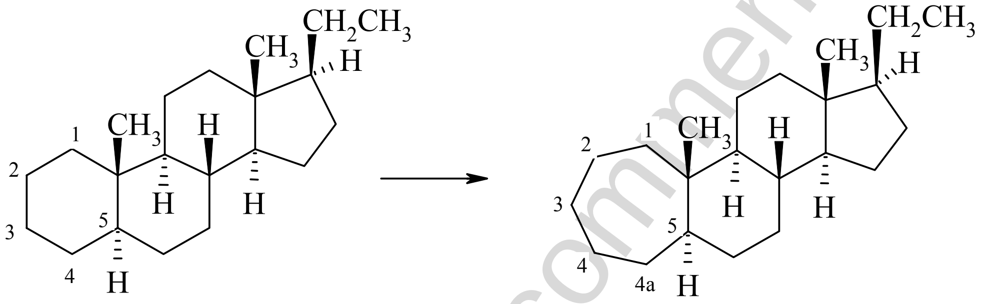
The additive operation involves the formal assembly of a structure from its component parts without loss of any atoms or groups. This operation can be expressed in several ways, as shown in the following subsections.

P-13.3.1 By an additive prefix

Examples:

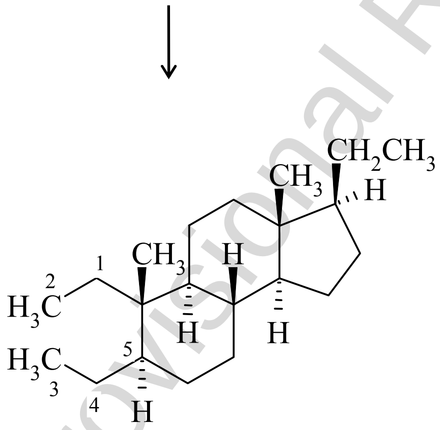


naphthalene (PIN) 1,2,3,4-tetrahydronaphthalene (PIN)
('hydro' = prefix designating addition of one hydrogen atom)

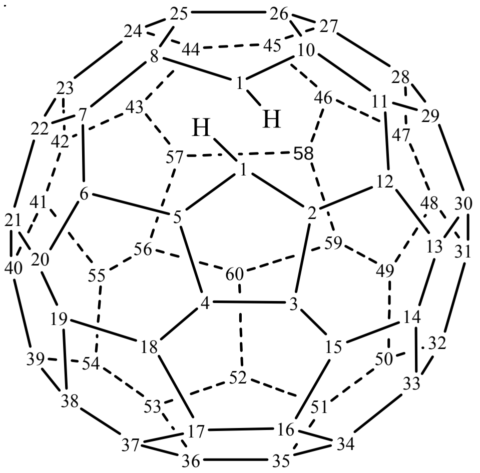


5α -pregnane (PIN)

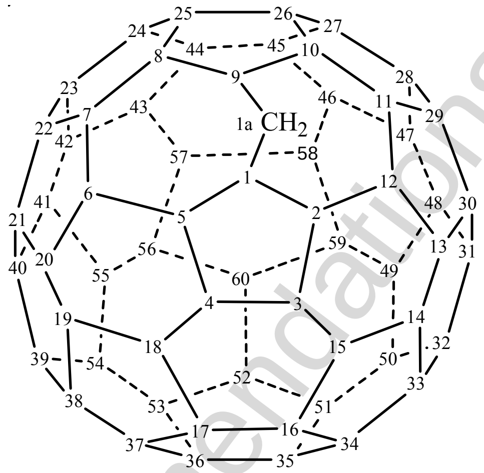
4a-homo-5α -pregnane (PIN)
('homo' = addition of a methylene, CH_2, group, which in this case expands a ring, see P-101.3.2.1)



2,3-seco-5α -pregnane (PIN)
('seco' = addition of two hydrogen atoms following the cleavage of a bond)



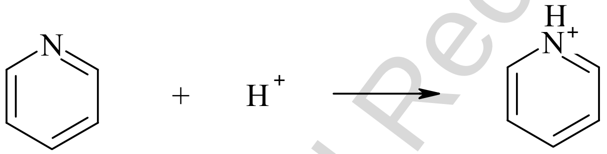
1,9-seco(C_{60}-I_h)[5,6]fullerene (PIN)



1a*H*-1(9)a-homo(C_{60}-I_h)[5,6]fullerene (PIN)

P-13.3.2 By an additive suffix

Examples:



pyridine (PIN)

pyridinium (PIN)
(‘ium’ = suffix designating the addition of one H^+)

BH_3 + H^- ⟶ BH_4^-

borane (preselected name)

boranuide (preselected name)
(‘uide’ = suffix designating the addition of one H^-)

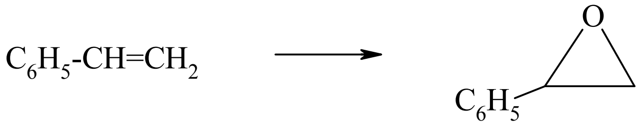
P-13.3.3 By a separate word

P-13.3.3.1 With the name of a neutral parent structure

Examples:

CH_3-C≡N ⟶ CH_3-C≡NO

acetonitrile (PIN) acetonitrile oxide (PIN)



styrene
ethenylbenzene (PIN)

styrene oxide
2-phenyloxirane (PIN)

P-13.3.3.2 With one or more substituent prefix name(s)

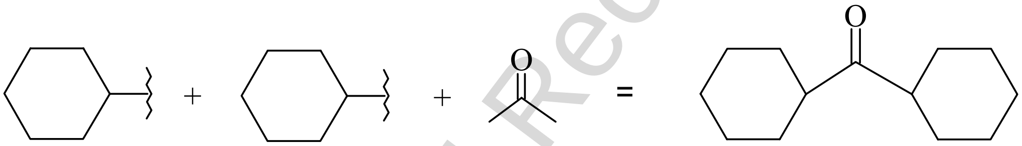
Here the separate word is a class or subclass name representing the characteristic group or the kind of characteristic group to which the substituents are linked (see also functional class nomenclature, P-15.2).

Examples:

$CH_3–$ + $–OH$ $\longrightarrow$ $CH_3\text{-}OH$

methyl (PIN) alcohol

methyl alcohol
methanol (PIN)



cyclohexyl (PIN) cyclohexyl (PIN) ketone

dicyclohexyl ketone
dicyclohexylmethanone (PIN)

$CH_3–$ + $C_6H_5–$ + $–O–$ $\longrightarrow$ $CH_3\text{-}O\text{-}C_6H_5$

methyl (PIN) phenyl (PIN) ether

methyl phenyl ether
anisole (PIN)
methoxybenzene

$C_6H_5\text{-}CH_2–$ + $–CN$ $\longrightarrow$ $C_6H_5\text{-}CH_2\text{-}CN$

benzyl (PIN) cyanide

benzyl cyanide
phenylacetonitrile (PIN)

P-13.3.4 By adding substituent groups, in an operation called ‘concatenation’

Examples:

$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2–$ + $–O–$ $\longrightarrow$ $CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}O–$

pentyl (PIN) oxy pentyloxy (PIN)

Cl– + –CO– ⟶ Cl-CO–

chloro (preselected name) carbonyl (PIN) chlorocarbonyl
carbonochloridoyl (PIN)

–NH– + $–CH_2-CH_2–$ + –NH– ⟶ $–NH-CH_2-CH_2-NH–$

azanediyl (preselected name) ethane-1,2-diyl (PIN) azanediyl (preselected name) ethane-1,2-diylbis(azanediyl) (PIN)

P-13.3.5 By adding molecular entities together

Chemical species AB in which two molecular entities A and B are combined directly with no loss of atoms from either A or B can be named by citing the names of A and B linked with an 'em' dash.

Example:

CO + BH_3 ⟶ $CO \bullet BH_3$

carbon monoxide (PIN) borane (preselected name) carbon monoxide—borane (PIN)

P-13.4 The subtractive operation

The subtractive operation involves the removal of an atom or group implicit in a name. This operation can occur with no other change, with introduction of unsaturation, or with formation of substituent groups, radicals, or ions. Several prefixes are used to indicate subtractive operations of many kinds in natural products. Subtraction can be expressed in several ways as shown in the following subsections.

P-13.4.1 By a suffix

Examples:

CH_4 – $H^\bullet$ ⟶ $CH_3^\bullet$ or $CH_3–$

methane (PIN) monohydrogen methyl (PIN; a radical or substituent group; the suffix 'yl' indicates loss of one hydrogen atom)

CH_3-CH_3 – H^+ ⟶ $CH_3-CH_2^-$

ethane (PIN) hydron ethanide (PIN: the suffix 'ide' indicates loss of a hydron, i.e., a hydrogen cation)

$CH_3-CH_2-CH_2-CH_3$ – H^- ⟶ $CH_3-CH_2-\overset{2}{C}H^+-\overset{1}{C}H_3$

butane (PIN) hydride butan-2-ylium (PIN; the suffix 'ylium' indicates loss of a hydride ion)

P-13.4.2 By a change in ending

Examples:

$C_6H_5\text{-}SO_2\text{-}OH$ – H^+ $\longrightarrow$ $C_6H_5\text{-}SO_2\text{-}O^-$

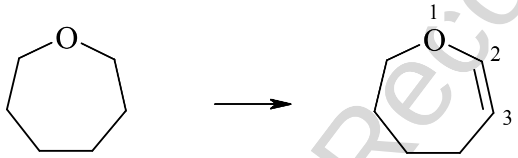
benzenesulfonic acid (PIN) hydron benzenesulfonate (PIN;the ending -ate indicates loss of a hydron, i.e., a hydrogen cation, from an ‘ic acid’)

$CH_3\text{-}CH_2\text{-}CH_3$ – H_2 $\longrightarrow$ $CH_3\text{-}\overset{2}{C}H\text{=}\overset{1}{C}H_2$

Propane (PIN) hydrogen prop-1-ene (PIN;the ending ‘ene’ indicates loss of 2 hydrogen atoms)

P-13.4.3 By a prefix

Example:



oxepane (PIN) 2,3-didehydrooxepane (PIN; the prefix ‘didehydro’ indicates loss of 2 hydrogen atoms)

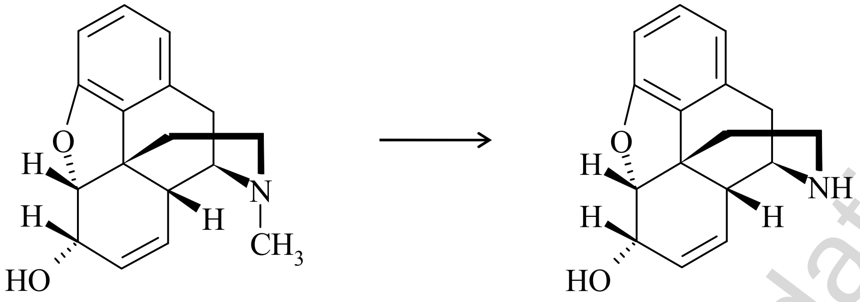
P-13.4.4 Prefixes used only in the nomenclature of natural products

In the nomenclature of natural products several prefixes are used to indicate the loss of a group, i.e., the exchange of a group for hydrogen. The subtraction of the elements of water with concomitant bond formation can also be regarded as a subtractive operation. Subtraction can be expressed as illustrated in the following subsections.

P-13.4.4.1 By the prefixes ‘de’ and ‘des’

P-13.4.4.1.1 The prefix ‘de’ (not ‘des’), followed by the name of a group or atom (other than hydrogen), denotes removal (or loss) of that group and addition of the necessary hydrogen atoms, i.e., exchange of that group with hydrogen atoms.

Example:

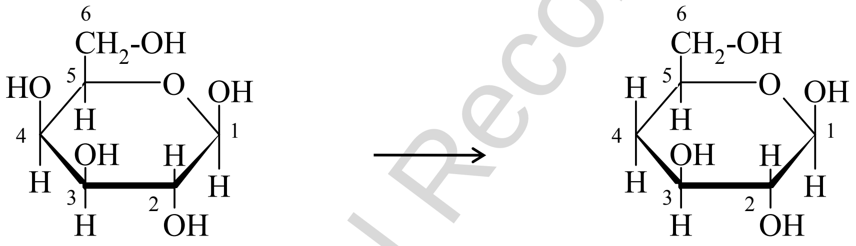


morphine (PIN)

demethylmorphine
(exchange of methyl for H)
17-normorphine (PIN)

As an exception, ‘deoxy’, when applied to hydroxy compounds, denotes the removal of an oxygen atom. ‘Deoxy’ is extensively used as a subtractive prefix in carbohydrate nomenclature (see P-93.6).

Example:



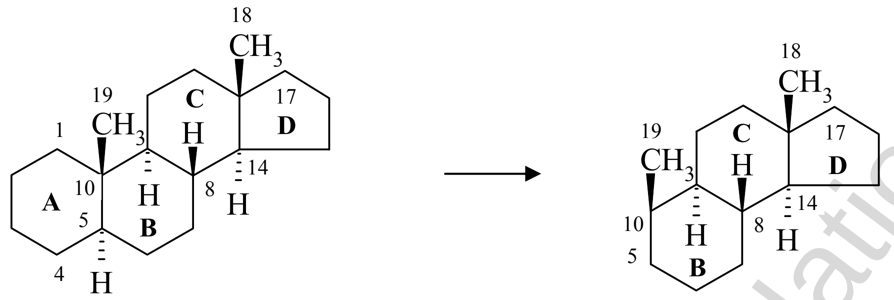
β-D-galactopyranose (PIN)

4-deoxy-β-D-*xylo*-hexopyranose (PIN)
(not 4-deoxy-β-D-galactopyranose)

P-13.4.4.1.2 The prefix ‘des’ signifies removal of an amino acid residue of a polypeptide, with rejoining of the chain (see P-103.5) or the removal of a terminal ring of a stereoparent (see P-101.3.6).

Examples:

oxytocin (PIN) ⟶ des-7-proline-oxytocin (PIN)
(removal of the proline residue at position 7)



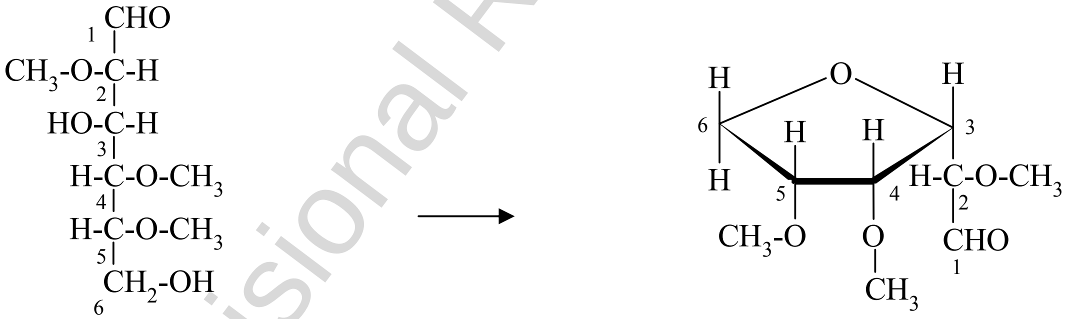
5α-androstane (PIN)

des-*A*-androstane
(3a*S*,5a*R*,6*R*,9a*R*,9b*S*)-3a,6-dimethyldodecahydrocyclopenta[*a*]naphthalene (PIN)

P-13.4.4.2 By the prefix ‘anhydro’

Intramolecular ethers, formally arising by elimination of water from two hydroxy groups of a single molecule of a monosaccharide (aldose or ketose) or monosaccharide derivative, is indicated by the detachable prefix ‘anhydro’ preceded by a pair of locants identifying the two hydroxy groups involved. The prefix ‘anhydro’ is placed in a name in accordance with the principles of alphabetical order (see P-102.5.5.7.1).

Example:



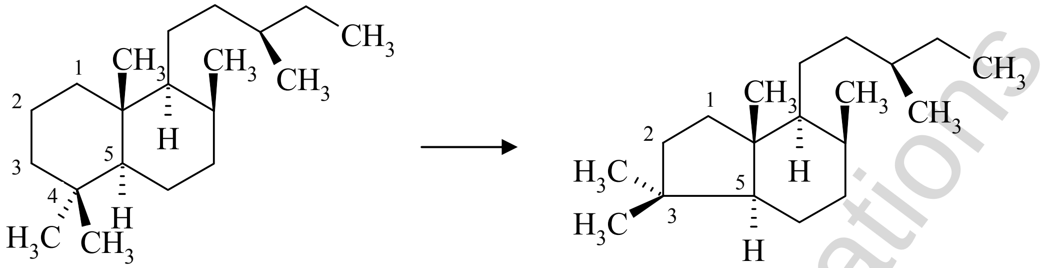
2,4,5-tri-*O*-methyl-D-mannitol (PIN)

3,6-anhydro-2,4,5-tri-*O*-methyl-D-mannitol (PIN)
(the prefix ‘anhydro’ describes removal of water from 2 ‘OH’ groups in the same molecule)

P-13.4.4.3 By the prefix ‘nor’

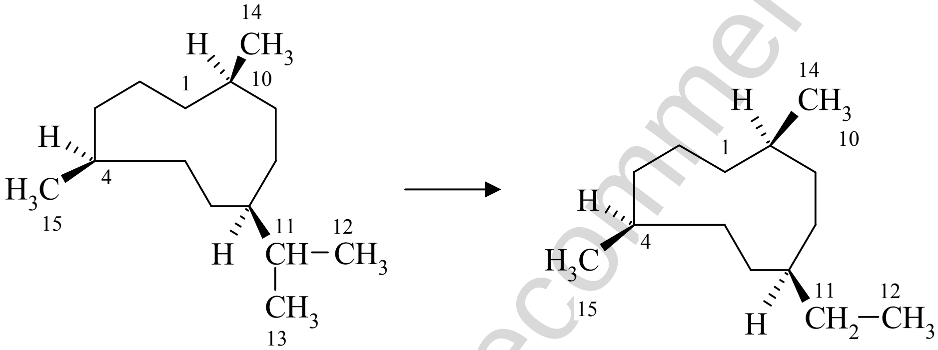
The prefix ‘nor’ is used to indicate removal of an unsubstituted saturated skeletal atom from a ring or a chain of a stereoparent parent structure with its attached hydrogen atom(s). It can also indicate the loss of a –CH= group from a mancude ring in a stereoparent parent structure (see P-101.3.1).

Examples:



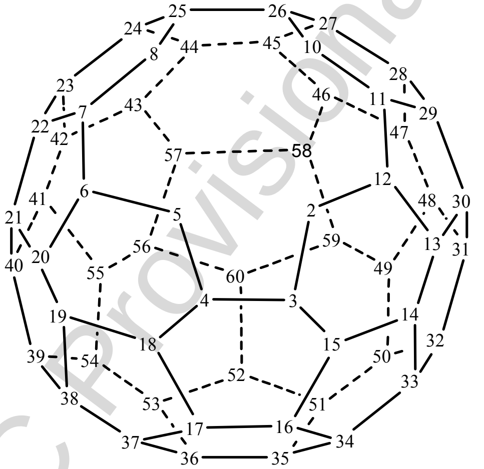
labdane (PIN)

3-norlabdane (PIN; ring contraction by removal of a methylene, $-CH_2-$, group)



germacrane (PIN)

13-norgermacrane (removal of a side chain methylene, $-CH_2-$, group)
(1*R*,4*s*,7*S*)-1-ethyl-4,7-dimethylcyclodecane (PIN, see P-101.3.1.1)



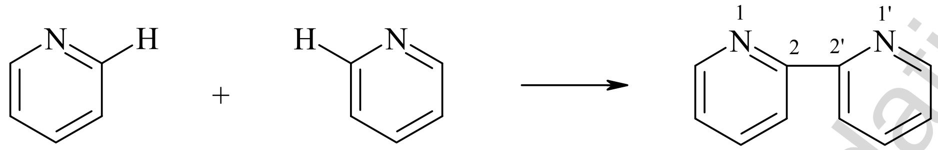
1,9-dinor(C_{60}-I_h)[5,6]fullerene (PIN)

P-13.5 The conjunctive operation

The conjunctive operation involves the formal construction of a name for a compound from the names of its components with subtraction of the same number of hydrogen atoms from each component at each site of the junction. This operation is expressed as noted in the following subsections.

P-13.5.1 By placing a multiplicative prefix ‘bi’, ‘ter’, ‘quater’, etc., before the name of the corresponding parent hydride.

Example:

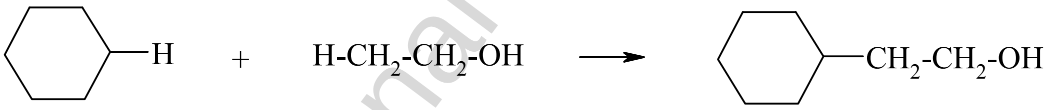


pyridine (PIN) pyridine (PIN) 2,2′-bipyridine (PIN)

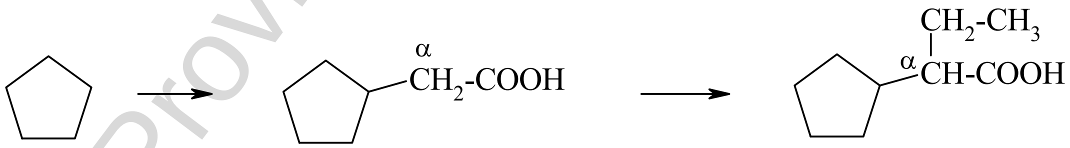
P-13.5.2 By juxtaposition of component names (conjunctive nomenclature)

This method is used by Chemical Abstracts Service. It is not recommended for constructing preferred IUPAC names; substitutive nomenclature is the recommended operation. This method is most commonly used when the two components to be joined are a ring or a ring system and a carbon chain (or chains) substituted by the principal characteristic group of the compound. In this method, both the principal characteristic group and the ring, or ring system, must terminate the chain; the rest of the structure attached to the chain, if any, is described by substituent prefixes, the location of which is indicated by Greek letter locants, α, β, etc. (α designates the atom next to the principal characteristic group).

Examples:



cyclohexane (PIN) ethanol (PIN) cyclohexaneethanol
2-cyclohexylethanol (PIN)

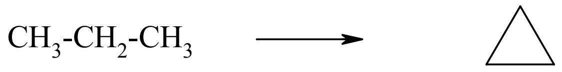


cyclopentane (PIN) cyclopentaneacetic acid
2-cyclopentylacetic acid (PIN)
α-ethylcyclopentaneacetic acid
2-cyclopentylbutanoic acid (PIN)

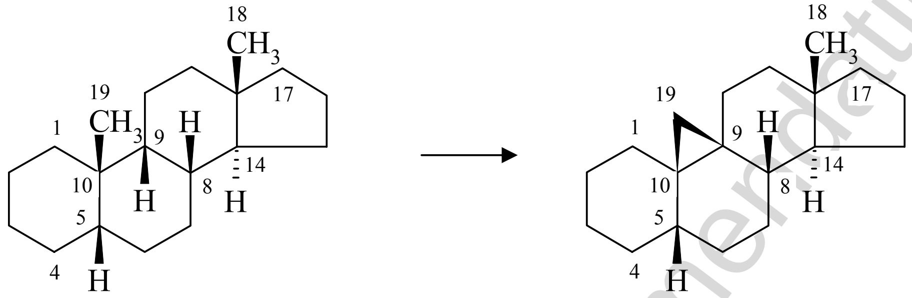
P-13.5.3 Ring formation

The formation of a ring by means of a direct link between any two atoms of a parent structure with loss of one hydrogen atom from each is indicated by the prefix ‘cyclo’.

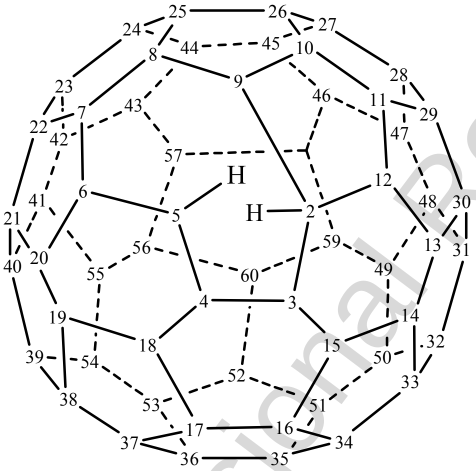
Examples:



propane (PIN) cyclopropane (PIN)



5β,9β-androstane (PIN) 9,19-cyclo-5β,9β-androstane (PIN; see P-101.3.3)

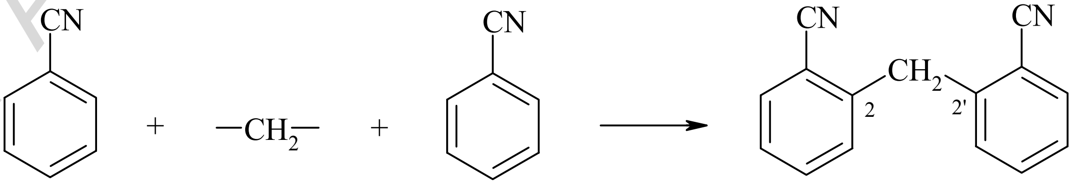


2*H*-2,9-cyclo-1-nor(C_{60}-I_h)[5,6]fullerene (PIN)

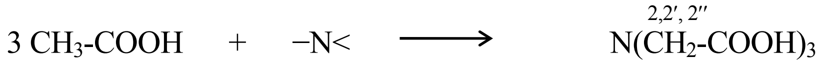
P-13.6 The multiplicative operation

This operation is used to name assemblies of identical units linked by di- or polyvalent substituent groups. Identical units are functionalized parent hydrides, functional parents and rings or ring systems. It is in fact substitutive nomenclature in which identical parent compounds are interconnected by a substituent group.

Examples:

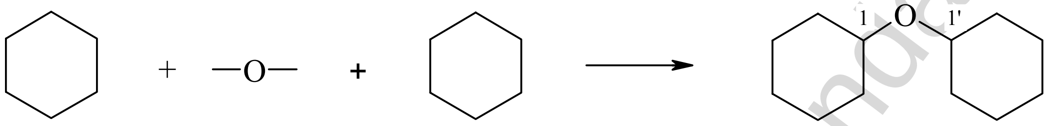


benzonitrile (PIN) methylene (PIN) benzonitrile (PIN) 2,2′-methylenedibenzonitrile (PIN)



$$3\ CH_3\text{-}COOH \quad + \quad -N< \quad \longrightarrow \quad \overset{2,2',2''}{N(CH_2\text{-}COOH)_3}$$

acetic acid (PIN) nitrilo (PIN) 2,2′,2″-nitrilotriacetic acid
N,*N*-bis(carboxymethyl)glycine (PIN)

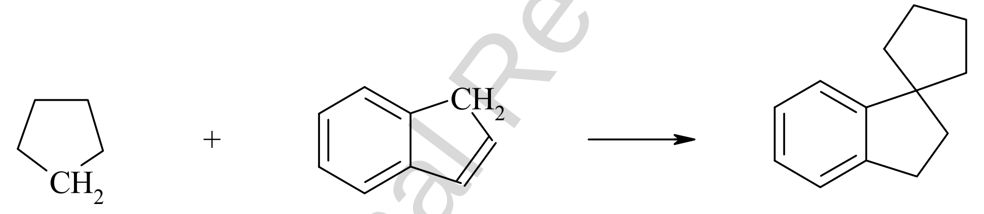


cyclohexane (PIN) oxy (PIN) cyclohexane (PIN) 1,1′-oxydicyclohexane (PIN)

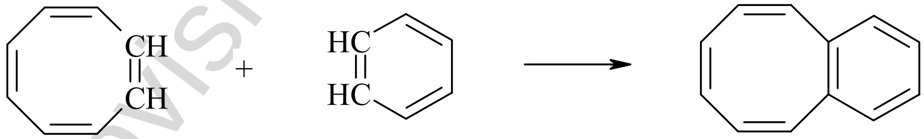
P-13.7 The fusion operation

The fusion operation involves the union of two rings or ring systems so that atoms or atoms and bonds are common to each. Spiro systems have one atom in common; fused ring systems have both atoms and bonds in common,

Examples:



cyclopentane (PIN) indene (PIN) spiro[cyclopentane-1,1′-indene] (PIN)



[8]annulene
cyclooctatetraene (PIN) benzene (PIN) benzo[8]annulene (PIN)

P-13.8 Operations used only in the nomenclature of natural products

The nomenclature of natural products and related compounds, described in Chapter 9, has its own principles, conventions and rules. In addition to the replacement, additive, subtractive, and conjunctive operations shared with systematic nomenclature, other operations are used only to modify parent structures, most of which are cyclic systems. These operations involve rearrangement of single bonds, and moving double bonds, and are denoted by the nondetachable prefixes ‘abeo’ and ‘*retro’* respectively. The use of these prefixes and others is described and exemplified in Chapter 10.

P-14 General rules

P-14.0 Introduction

Rules described in this section are of general application for naming types of compounds and individual compounds. They must be closely followed to construct preferred IUPAC names as well as names for general use.

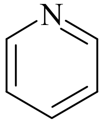
P-14.1 Bonding number

The concept of a standard valence state is fundamental to organic nomenclature. Since most organic names are derived by formal exchange of atoms or groups for hydrogen atoms of a parent structure, it is necessary to know exactly how many hydrogen atoms are implied by the name of the parent structure. For example, does the name phosphane refer to PH_3 or PH_5? This is a problem when an element can occur in more than one valence state; in such cases, the standard state is normally not specified, but any other valence state is noted by citation of an appropriate **bonding number**. More details are given in the publication 'Treatment of Variable Valence in Organic Nomenclature (Lambda Convention)' (ref. 12). In these Recommendations, this convention is called simply the 'λ-convention'.

P-14.1.1 Definition.

The bonding number '*n*' of a skeletal atom is the sum of the total number of bonding equivalents (valence bonds) of that skeletal atom to adjacent skeletal atoms if any in a parent hydride and the number of hydrogen atoms.

Examples:

H_2S	for S, $n = 2$
H_6S	for S, $n = 6$
$(C_6H_5)_3PH_2$	for P, $n = 5$
	for N, $n = 3$

P-14.1.2 Standard bonding numbers. The bonding number of a skeletal atom is standard when it has the value given in Table 1.3.

Table 1.3 Standard bonding numbers for the elements of Groups 13, 14, 15, 16, and 17

Standard bonding number (n)	Elements				
3	B	Al	Ga	In	Tl
4	C	Si	Ge	Sn	Pb
3	N	P	As	Sb	Bi
2	O	S	Se	Te	Po
1	F	Cl	Br	I	At

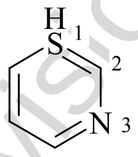
P-14.1.3 Nonstandard bonding numbers

A nonstandard bonding number of a **neutral** skeletal atom in a parent hydride is indicated by the symbol λ^n, cited in conjunction with an appropriate locant. Note that the 'n' in the symbol 'λ^n' is italicized but the numbers in a specific symbol, e.g., λ^4, are not (for the use of italicized 'n' in λ^n see the General rules for symbols in physical quantities, Section 1.3 in ref. 13).

Examples:

CH_3-SH_5
methyl-λ^6-sulfane (PIN)

$(C_6H_5)_3PH_2$
triphenyl-λ^5-phosphane (PIN)



1λ^4,3-thiazine (PIN)

P-14.2 Multiplying prefixes

Three types of multiplying prefixes are used in names to denote multiplicity of identical features in structures (characteristic groups, substituent groups or terms) and correspondingly of affixes (suffixes and prefixes) in names. They are always placed before the part of the name to which they relate.

P-14.2.1 Basic multiplying prefixes denote simple features and, in general, are the first choice among prefixes to specify multiplicity (ref. 14). They are listed in Table 1.4.

Table 1.4 Basic numerical terms (multiplying prefixes)

Number	Numerical Term	Number	Numerical Term	Number	Numerical Term	Number	Numerical Term
1	mono, hen	11	hendeca	101	henhecta	1001	henkilia
2	di, do	20	icosa	200	dicta-	2000	dilia
3	tri	30	triaconta	300	tricta-	3000	trilia
4	tetra	40	tetraconta	400	tetracta	4000	tetralia
5	penta	50	pentaconta	500	pentacta	5000	pentalia
6	hexa	60	hexaconta	600	hexacta	6000	hexalia
7	hepta	70	heptaconta	700	heptacta	7000	heptalia
8	octa	80	octaconta	800	octacta	8000	octalia
9	nona	90	nonaconta	900	nonacta	9000	nonalia
10	deca	100	hecta	9000	nonalia		

P-14.2.1.1 The prefix mono

P-14.2.1.1.1 When alone, the numerical term for the number 1 is 'mono' and that for 2 is 'di'. In association with other numerical terms, the number 1 is represented by 'hen' (except in the case of 'undeca') and the number 2 by 'do' (except in the cases of 'dicta' and 'dilia'). The numerical term for the number 11 is 'undeca'.

P-14.2.1.1.2 The prefix 'mono' is not used in systematically formed names to indicate the presence of one nomenclatural feature, for example suffixes, prefixes, endings. It is used in functional class nomenclature to designate a monoester of a diacid, for example phthalic acid monomethyl ester, and in terminology, to emphazise singleness, for example, monocyclic and mononuclear in contrast to bicyclic and polynuclear.

P-14.2.1.2 Derivation of basic numerical terms

After 'undeca-' (number eleven), composite numerical terms are formed systematically by citing the basic terms in the order opposite to that of the constituent digits in the arabic numbers. The composite terms are formed by direct joining of the basic terms, without hyphen(s). The letter 'i' in 'icosa' is elided after a vowel.

Examples:

486 hexaoctacontatetracta
| 6 | 80 | 400 |

14	tetradeca	21	henicosa	22	docosa
23	tricosa	24	tetracosa	41	hentetraconta
52	dopentaconta	111	undecahecta		
363	trihexacontatricta				

P-14.2.2 Numerical terms for complex features

Multiplying prefixes for complex entities, such as substituted substituents, are formed by adding the ending 'kis' to the basic multiplying prefix ending in 'a', 'tetrakis', 'pentakis', etc. (ref. 14). The prefixes 'bis' and 'tris' correspond to 'di' and 'tri'. The basic prefix 'mono' has no counterpart in this series.

Examples:

2	bis	3	tris	4	tetrakis
231	hentriacontadictakis				

P-14.2.3 Multiplying prefixes for naming assemblies of identical units

Latin based prefixes are used to denote the number of repeated identical units in unbranched assemblies: 'bi', 'ter', 'quater',

2	bi	5	quinque	8	octi
3	ter	6	sexi	9	novi
4	quater	7	septi	10	deci

The list has been completed from 11 to 9999. The prefixes are formed by changing the ending 'a' of basic numerical prefixes into 'i', for example, 'undeci' for 11, 'hexadeci' for 16, 'tetraconti' for 40.

P-14.3 Locants and numbering

P-14.3.1 Types of locants

Traditional types of locants are arabic numbers, i.e., 1, 2, 3; primed locants, i.e., 1′, 1‴, 2″; locants including a lower case Roman letter, i.e., 3a, 3b; italicized Roman letters, i.e., *O*, *N*, *P*; Greek letters, i.e., α, β, γ; and compound locants, i.e., 1(10), 5(17).

Composite locants, for example, 3^2 and $2a^1$, have been developed in recent years for various purposes and are included in these recommendations. They are used in Phane Nomenclature to indicate positions in amplificants (see P-26.4.3); for numbering in ring assemblies, (see P-29.3); for numbering polyanhydrides (see P-65.4.7.1.2); to denote interior positions in fused ring systems (see P-25.3.3.3); in von Baeyer descriptors for spiro ring systems (see P-24.2.2); and in numbering natural products, for example, amino acids (see P-103.2.2). Although not included in these recommendations, they are also used in steroid and tetrapyrrole nomenclature.

Primes are added to differentiate between the same locant in the same or different parts of the structure, for example, 1′, 2″, *N*′, and α′. In locants consisting of two or more characters, primes are generally added to the primary character. For example, in locants including a lower case Roman letter, used in fused rings, primes are added following the arabic number, for example, 3′a and $2'a^1$; this format follows the principle that in locants for fusion positions in a fused ring system a letter follows the previous peripheral locant. For composite locants used in phane nomenclature, the prime follows the superatom locant, as in $2'^{3}$ and $2'^{4a}$.

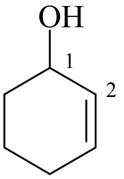
P-14.3.2 Position of locants

Locants (numerals and/or letters) are placed immediately before that part of the name to which they relate, except in the case of the traditional contracted names when locants are added at the front of their names.

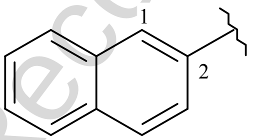
Examples:

$$\overset{6}{CH_3}\text{-}\overset{5}{CH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{CH}{=}\overset{2}{CH}\text{-}\overset{1}{CH_3}$$

hex-2-ene (PIN)
(not 2-hexene)



cyclohex-2-en-1-ol (PIN)
(not 2-cyclohexen-1-ol)



naphthalen-2-yl (PIN)
2-naphthyl
(not naphth-2-yl)

P-14.3.3 Omission of locants

The practice of omitting locants when there is no ambiguity is widespread. However for designating preferred IUPAC names it is necessary to be prescriptive about when omission of locants is permissible. Thus, in preferred IUPAC names, if any locants are essential for defining the structure, then all locants should be cited. For example, the omission of the locant ‘1’ in 2-chloroethanol, while permissible in general usage, is not allowed in the preferred IUPAC name 2-chloroethan-1-ol. Also, in preferred IUPAC multiplicative names and in preferred IUPAC names for ring assemblies locants are always cited, e.g., 1,1′-oxydibenzene and 1,1′-biphenyl.

Locants are omitted in preferred IUPAC names in the following cases.

P-14.3.3.1 Terminal locants in names for mono- and dicarboxylic acids derived from acyclic hydrocarbons and their corresponding acyl halides, amides, nitriles, and aldehydes are never cited (however, see P-15.4.3.1).

Examples:

$HOOC\text{-}CH_2\text{-}CH_2\text{-}COOH$	butanedioic acid (PIN)
$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}$	pentanoyl (PIN)

P-14.3.3.2 The locant ‘1’ is omitted:

(a) in substituted mononuclear parent hydrides;

Examples:

CH_3Cl chloromethane (PIN)

SiH_2Cl_2 dichlorosilane (preselected name)

$(CH_3)_3Al$ trimethylalumane (PIN)

(b) in monosubstituted homogeneous chains consisting of only two identical atoms;

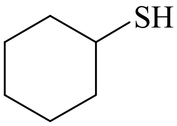
Examples:

$CH_3\text{-}CH_2\text{-}OH$ ethanol (PIN)

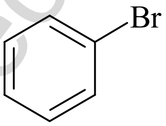
$NH_2{-}NH\text{-}Cl$ chlorohydrazine (preselected name)

(c) in monosubstituted homogeneous monocyclic rings;

Examples:



cyclohexanethiol (PIN)



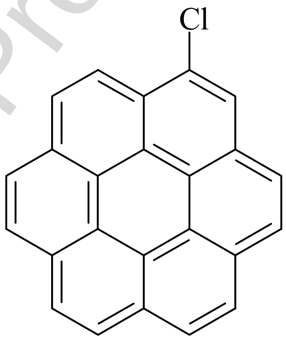
bromobenzene (PIN)

(d) in monosubstituted symmetrical parent hydrides or parent compounds where there is only one kind of substitutable hydrogen;

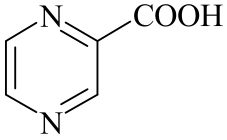
Examples:

$CH_3\text{-}NH_2\text{-}CO\text{-}NH_2$ methylurea (PIN)

$Cl\text{-}SiH_2\text{-}O\text{-}SiH_3$ chlorodisiloxane (preselected name)



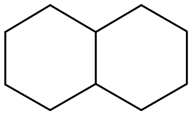
chlorocoronene (PIN)



pyrazinecarboxylic acid (PIN)

P-14.3.3.3 All locants are omitted in compounds in which all substitutable positions are completely substituted or modified in the same way. The prefix ‘per-’ is no longer recommended. In case of partial substitution or modification, all numerical prefixes must be indicated.

Examples:



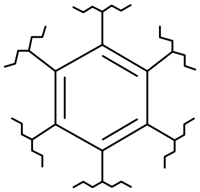
decahydronaphthalene (PIN)

$CF_3\text{-}CF_2\text{-}CF_2\text{-}COOH$

heptafluorobutanoic acid (PIN)

$\overset{3}{C}F_3\text{-}\overset{2}{C}F_2\text{-}\overset{1}{C}H_2\text{-}OH$

2,2,3,3,3-pentafluoropropan-1-ol (PIN)



benzenehexayl (PIN)

P-14.3.4 Lowest set of locants

The lowest set of locants is defined as the set that, when compared term by term with other locant sets, each cited in order of increasing value, has the lowest term at the first point of difference; for example, the locant set ‘2,3,5,8’ is lower than ‘3,4,6,8’ and ‘2,4,5,7’.

Primed locants are placed immediately after the corresponding unprimed locants in a set arranged in ascending order; locants consisting of a number and a lower-case letter are placed immediately after the corresponding numeric locant with or without prime and are followed by locants having superscripts.

Examples:

2 is lower than 2′

3 is lower than 3a

8a is lower than 8b

4′ is lower than 4a

4′a is lower than 4″a

1^2 is lower than 1^3

1^4 is lower than 2′

3a is lower than $3a^1$

Italic capital and lower-case letter locants are lower than Greek letter locants, which, in turn, are lower than numerals.

Example:

'*N*, α,1,2' is lower than '1,2,4,6'

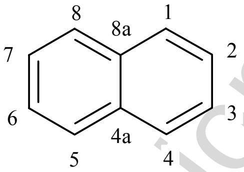
P-14.4 Numbering

When several structural features appear in cyclic and acyclic compounds, low locants are assigned to them in the following decreasing order of seniority.

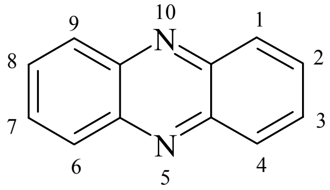
> Two important changes have been made to the 1979 recommendations (ref 1).
>
> (1) heteroatoms in chains are now considered as part of the parent hydride; as such, they have seniority over suffixes for numbering;
>
> (2 hydro/dehydro prefixes are now classified as detachable prefixes, but are not included in the category of alphabetized detachable prefixes.

(a) fixed numbering of a ring or ring system;

Examples:



naphthalene (PIN)



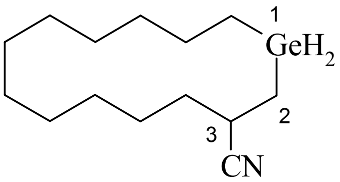
phenazine (PIN)

(b) heteroatoms in chains and in rings and ring systems;

Examples:

$$\overset{1}{CH_3}\text{-}\overset{2}{S}\text{-}\overset{3}{CH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{5}{O}\text{-}\overset{6}{CH_2}\text{-}\overset{7}{CH_2}\text{-}\overset{8}{S}\text{-}\overset{9}{CH_2}\text{-}\overset{10}{CH_2}\text{-}\overset{11}{SiH_2}\text{-}\overset{12}{CH_2}\text{-}\overset{13}{CH_2}\text{-}\overset{14}{COOH}$$

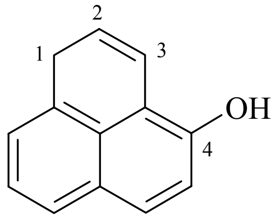
5-oxa-2,8-dithia-11-silatetradecan-14-oic acid (PIN)



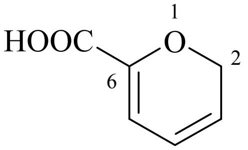
1-germacyclotetradecane-3-carbonitrile (PIN)

(c) indicated hydrogen;

Examples:



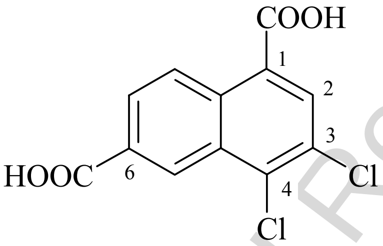
1*H*-phenalen-4-ol (PIN)



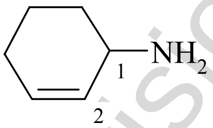
2*H*-pyran-6-carboxylic acid (PIN)

(d) principal characteristic groups and free valences (suffixes);

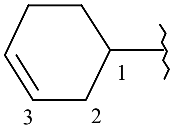
Examples:



3,4-dichloronaphthalene-1,6-dicarboxylic acid (PIN)



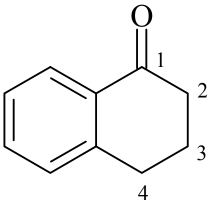
cyclohex-2-en-1-amine (PIN)



cyclohex-3-en-1-yl (PIN)

(e) added hydrogen;

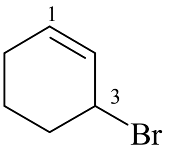
Example:



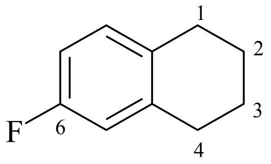
3,4-dihydronaphthalen-1(2*H*)-one (PIN)

(f) saturation/unsaturation (hydro/dehydro prefixes and ‘ene’ and ‘yne’ endings);

Examples:



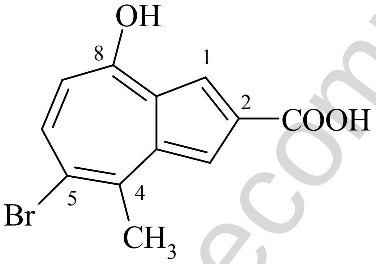
3-bromocyclohex-1-ene (PIN)



6-fluoro-1,2,3,4-tetrahydronaphthalene (PIN)

(g) detachable alphabetized prefixes, all considered together in a series of increasing numerical order;

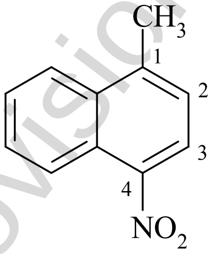
Example:



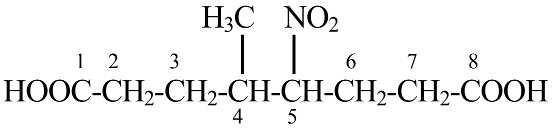
5-bromo-8-hydroxy-4-methylazulene-2-carboxylic acid (PIN)

(h) lowest locants for the substituent cited first as a prefix in the name;

Examples:



1-methyl-4-nitronaphthalene (PIN)

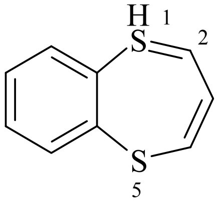


$$\mathrm{HOO\overset{1}{C}\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\underset{4}{\overset{\overset{H_3C}{|}}{C}}H\text{-}\underset{5}{\overset{\overset{NO_2}{|}}{C}}H\text{-}\overset{6}{C}H_2\text{-}\overset{7}{C}H_2\text{-}\overset{8}{C}OOH}$$

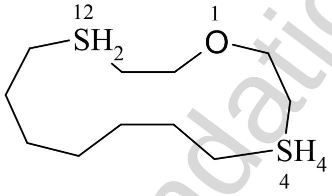
4-methyl-5-nitrooctanedioic acid (PIN)

(i) When a choice is needed between the same skeletal atom in different valence states, the one in a nonstandard valence state is assigned the lower locant. If a further choice is needed between the same skeletal atom in two or more nonstandard valence states, the one in the higher valence state is assigned the lower locant;

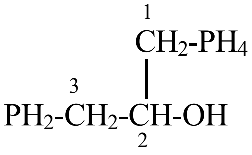
Examples:



1λ^4,5-benzodithiepine (PIN)



1-oxa-4λ^6,12λ^4-dithiacyclotetradecane (PIN)



$$\begin{array}{l} \qquad\qquad\quad \overset{1}{C}H_2\text{-}PH_4 \\ \qquad\qquad\quad | \\ PH_2\text{-}\overset{3}{C}H_2\text{-}\underset{2}{C}H\text{-}OH \end{array}$$

1-(λ^5-phosphanyl)-3-phosphanylpropan-2-ol (PIN)
(λ^5-phosphanyl is cited before phosphanyl and
is given the lower locant)

(j) When there is a choice between equivalent numberings in an isotopically unmodified compound, the starting point and the direction of numbering of the analogous isotopically substituted compound are chosen so as to give lowest locants to the modified atoms or groups considered together in one series in increasing numerical order. If a choice still remains, the lower locant is given to the nuclide of higher atomic number. In the case of different nuclides of the same element, the lower locant is assigned to the nuclide of higher mass number.

Examples:

$\overset{1}{C}H_3\text{-}{}^{14}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_3$

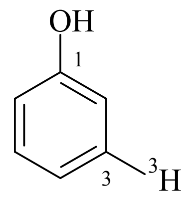
(2-^{14}C)butane (PIN)
[not (3-^{14}C)butane]

$\overset{1}{C}H_3\text{-}\overset{2}{C}{}^2H_2\text{-}{}^{14}\overset{3}{C}H_2\text{-}\overset{4}{C}H_3$

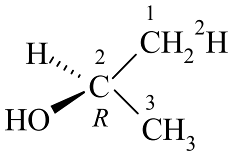
(3-^{14}C,2,2-$^2H_2$)butane (PIN)
[not (2-^{14}C,3,3-$^2H_2$)butane]

$\overset{1}{C}H_3\text{-}{}^{14}\overset{2}{C}H_2\text{-}\overset{3}{C}H{}^2H\text{-}\overset{4}{C}H_3$

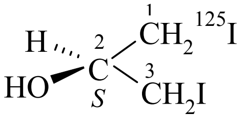
(2-^{14}C,3-$^2H_1$)butane (PIN)
[not (3-^{14}C,2-$^2H_1$)butane]



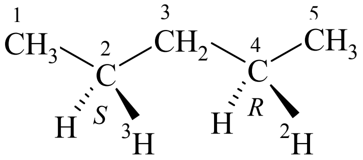
(3-^{3}H)phenol (PIN)



(R)-(1-^{2}H$_{1}$)propan-2-ol (PIN)



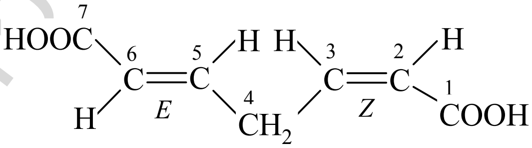
(S)-1,3-(1-^{125}I)diiodopropan-2-ol (PIN)



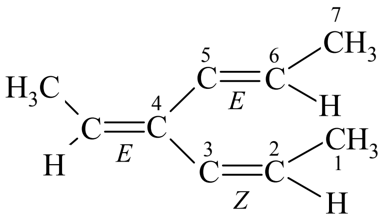
(2S,4R)-(4-^{2}H$_{1}$,2-^{3}H$_{1}$)pentane (PIN)
[not (2R,4S)-(2-^{2}H$_{1}$,4-^{3}H$_{1}$)pentane; isotopic modifications have seniority for low locants over stereodescriptors described in (k) below]

(k) When there is a choice for lower locants related to the presence of stereogenic centers or stereoisomers, the lower locant is assigned to CIP stereodescriptors *Z*, *R*, *R*$_{a}$, *R*$_{p}$, *M* , and *r* CIP stereodescriptors, that are preferred to non-CIP stereodescriptors *cis* or *r*, *c* (see P-92 for CIP and non-CIP stereodescriptors).

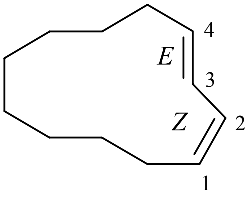
Examples:



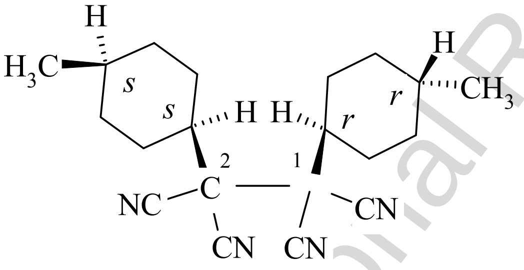
(2Z,5E)-hepta-2,5-dienedioic acid (PIN)
(the chain is numbered by assigning the low locant to the ‘Z’ double bond)



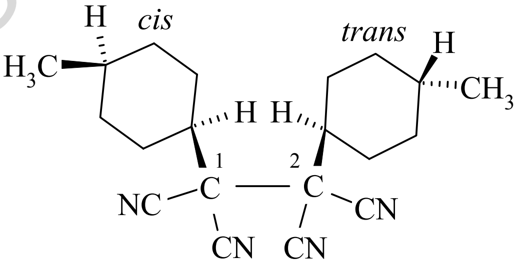
(2*Z*,4*E*,5*E*)-4-ethylidenehepta-2,5-diene (PIN)
(low locants are assigned to the longest chain, then to the '*Z*' double bond)



(1*Z*,3*E*)-cyclododeca-1,3-diene (PIN)



I

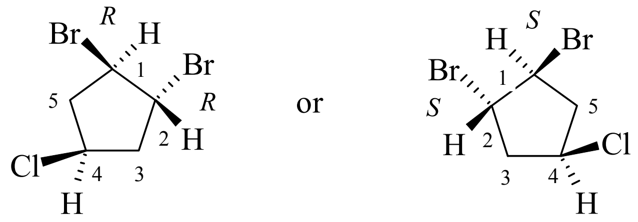


II

1-[(1*r*4*r*)-4-methylcyclohexyl-2-[(1*s*,4*s*)-4-methylcyclohexyl]ethane-1,1,2,2-tetracarbonitrile **(I)** (PIN)
(the substituent denoted by the '*r*' stereodescriptor receives the lowest locant, '1'; the use of CIP stereodescriptor generates the preferred IUPAC name)

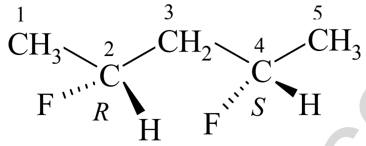
1-(*cis*-4-methylcyclohexyl)-2-(*trans*-4-methylcyclohexyl)ethane-1,1,2,2-tetracarbonitrile **(II)**
(the '*cis*' substituent receives the lowest locant, '1')

.

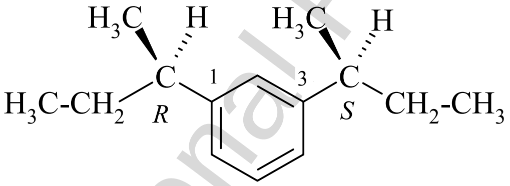


rel-(1*R*,2*R*)-1,2-dibromo-4-chlorocyclopentane (PIN)
1*r*,2*t*-dibromo-4-*c*-chlorocyclopentane

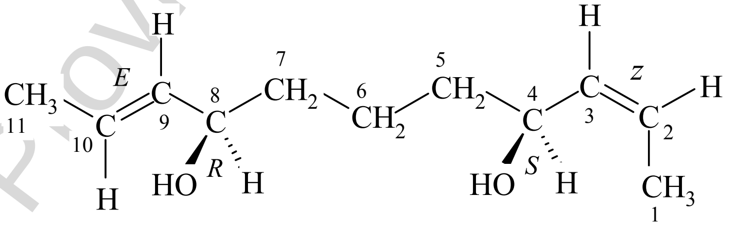
(the preferred IUPAC name is denoted by CIP stereodescriptors; in the second name, the relative configuration is expressed by the non CIP stereodescriptors 1*r*,2*t*,4*c* rather than 1*r*,2*t*,4*t*, because a ‘*cis*’ arrangement, denoted by ‘*c*’, has priority over a ‘*trans*’ arrangement, denoted by ‘*t*’, in position ‘4’)



(2*R*,4*S*)-2,4-difluoropentane (PIN)



1-[(2*R*)-butan-2-yl]-3-[(2S)-butan-2-yl]benzene (PIN)



(2*Z*,4*S*,8*R*,9*E*)-undeca-2,9-diene-4,8-diol (PIN)

(the choice is between ‘*E*’ and ‘*Z*’ for position ‘2’, not between ‘*R*’ and ‘*S*’ for position ‘4’)

P-14.5 Alphanumerical order

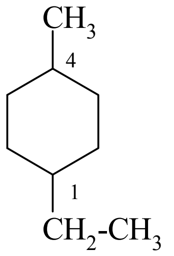
> Alphanumerical order has been commonly called ‘alphabetical order’. As it does imply ordering both letters and numbers, in a strict sense it is best called ‘alphanumerical order’ in order to convey the message that both letters and numbers are involved.

Alphanumerical order is used to establish the order of citation of detachable prefixes and the numbering of a chain, ring, or ring system by giving the lowest possible locants to nondetachable prefixes.

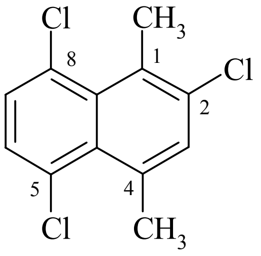
Alphanumerical order is applied as follows in organic nomenclature. Letters are considered first (all Roman letters before any italic letters), unless used as locants or part of a compound or composite locant, for example, ‘*N*-‘ or ‘4a’). If there is a further choice, numerical locants are considered in order from lowest to highest

P-14.5.1 Simple prefixes (i.e., those describing atoms and unsubstituted substituents) are arranged alphabetically; multiplying prefixes, if necessary, are then inserted and do not alter the alphabetical order already established.

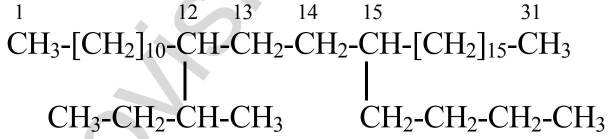
Examples:



1-ethyl-4-methylcyclohexane (PIN)



2,5,8-trichloro-1,4-dimethylnaphthalene (PIN)

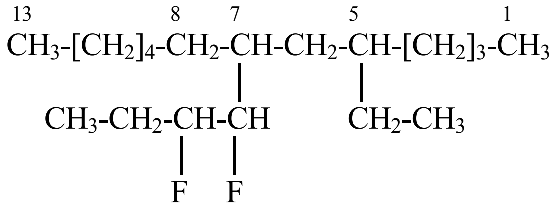


$$\overset{1}{CH_3}\text{-}[CH_2]_{10}\text{-}\underset{CH_3\text{-}CH_2\text{-}CH\text{-}CH_3}{\overset{12}{CH}}\text{-}\overset{13}{CH_2}\text{-}\overset{14}{CH_2}\text{-}\underset{CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3}{\overset{15}{CH}}\text{-}[CH_2]_{15}\text{-}\overset{31}{CH_3}$$

12-(butan-2-yl)-15-butylhentriacontane (PIN)
(butyl is not treated as butan-1-yl; see also P-56.2.2)

P-14.5.2 The name of a prefix for a substituted substituent is considered to begin with the first letter of its complete name.

Example:

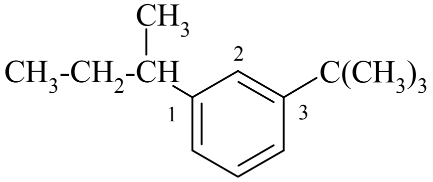


$CH_3\text{-}[CH_2]_4\text{-}CH_2\text{-}CH(CH(F)\text{-}CH(F)\text{-}CH_2\text{-}CH_3)\text{-}CH_2\text{-}CH(CH_2\text{-}CH_3)\text{-}[CH_2]_3\text{-}CH_3$

7-(1,2-difluorobutyl)-5-ethyltridecane (PIN)

P-14.5.3 When an alphanumerical ordering is required and Roman letters do not permit a decision for the order of citation, italicized letters are considered.

Example:

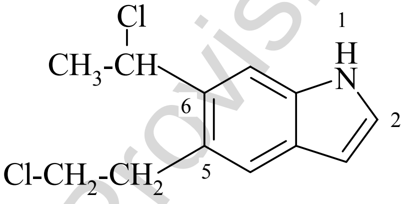


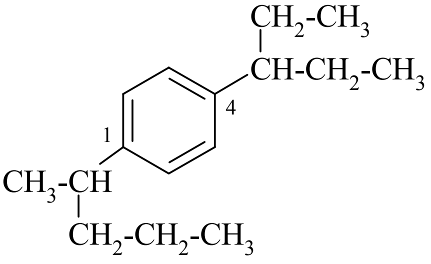
1-*sec*-butyl-3-*tert*-butylbenzene
1-(butan-2-yl)-3-*tert*-butylbenzene (PIN)

Similarly, *as*-indacen-1-yl is senior to *s*-indacen-1-yl and naphtho[1,2-*f*]quinolin-2-yl is senior to naphtho[1,2-*g*]quinolin-1-yl (‘*f*’ before ‘*g*’).

P-14.5.4 When two or more prefixes consist of identical Roman letters, priority for order of citation is given to the group that contains the lowest locant at the first point of difference.

Examples:



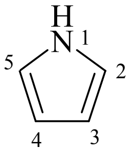


6-(1-chloroethyl)-5-(2-chloroethyl)indole (PIN) 1-(pentan-2-yl)-4-(pentan-3-yl)benzene (PIN)

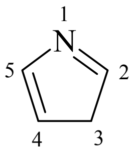
P-14.6 Indicated and added hydrogen

Under certain circumstances it is necessary to indicate in the name of a mancude ring or ring system, i.e., one that contains the maximum number of noncumulative double bonds, one or more positions where no multiple bond is attached. This is done by specifying the presence of an ‘extra’ hydrogen atom at such positions by citation of the appropriate numerical locant followed by an italicized capital ‘*H*’.

Examples:



1*H*-pyrrole (PIN)
pyrrole

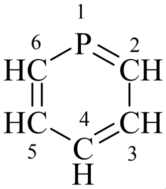


3*H*-pyrrole (PIN)

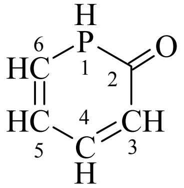
In the first example, the 'indicated hydrogen' locates one hydrogen atom in position '1' of the pyrrole ring; and in the second, the 'indicated hydrogen' indicates an 'extra' hydrogen' atom at position '3' , i.e., one hydrogen atom more than the number present if there were a double bond in the ring at that position. Indicated hydrogen of this type normally precedes the name of a parent hydride. Indicated hydrogen may be omitted (see P-25-7-1.3). 1*H*-Pyrrole is usually called just 'pyrrole'. However, when locants are present in a preferred IUPAC name, indicated hydrogen atoms must be cited.

A second type of indicated hydrogen, called 'added hydrogen' describes hydrogen atoms added to a specified structure as the consequence of the addition of a suffix or a prefix describing a structural modification. 'Added hydrogen' is normally cited in parentheses after the locant of the structural feature to which it refers.

Example:



phosphinine (PIN)

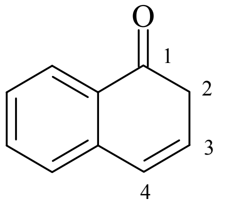


phosphinin-2(1*H*)-one (PIN)

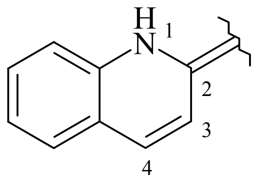
'Added hydrogen' is used to introduce a free valence, a radical or an ionic center, or a principal characteristic group into a fully unsaturated heteromonocyclic compound or fused polycyclic system in the absence of, or lack of sufficient hydrogen atoms, to accommodate the operation at the site of the operation. Such substituted compounds are named by using a suffix to denote an operation on either a –CH= group or a =C< atom, or on equivalent heteroatoms such as –N= or =Si<, or groups such as –SiH=.

Detailed procedures for using both 'indicated hydrogen' and 'added hydrogen' are discussed in P-58.3.3.3.

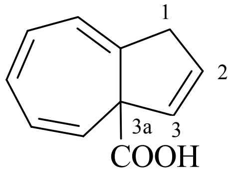
Examples:



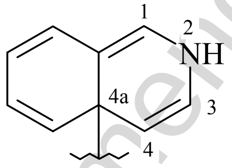
naphthalene-1(2*H*)-one (PIN)



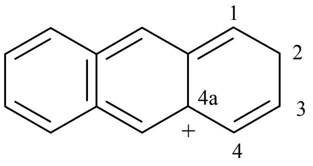
quinolin-2(1*H*)-ylidene (PIN)



azulene-3a(1*H*)-carboxylic acid (PIN)



isoquinolin-4a(2*H*)-yl (PIN)



anthracen-4a(2*H*)-ylium (PIN)

P-15 Types of nomenclature

P-15.0 Introduction
P-15.1 Substitutive nomenclature
P-15.2 Functional class nomenclature
P-15.3 Multiplicative nomenclature
P-15.4 Skeletal replacement (‘a’) nomenclature
P-15.5 Functional replacement nomenclature
P-15.6 Conjunctive nomenclature

P-15.0 Introduction

‘Nomenclature’, in chemistry, is a system by which names are formed using various nomenclatural operations in accordance with a set of principles, rules and conventions. There are fundamentally two types of nomenclature: (1) substitutive nomenclature, the principal nomenclature used in organic chemistry and is the basis of IUPAC preferred organic names; and (2) additive nomenclature used in inorganic chemistry for generating binary and coordination names. These two types are applied to name organic compounds and inorganic compounds, thus making nomenclature a matter of choice between these two types of compounds. For example, $SiCl_4$ can be named silicon tetrachloride (binary name), tetrachloridosilicon (coordination name), and tetrachlorosilane (substitutive name). Although coordination nomenclature is not discussed in these recommendations, it is used in the nomenclature of organometallic compounds belonging to Groups 1 and 2, for example dimethylmagnesium. Binary names are used for salts composed of an anionic or cationic organic part, for example sodium acetate and methanaminium chloride. Preferred IUPAC names (PINs) are recommended when there is a choice within the limits of the nomenclature of organic compounds, but not between coordination and/or binary names and substitutive names.

The nomenclature of organic compounds is considered as the set of different types of nomenclature based on the various operations described in P-13. The term nomenclature is usually associated with more than one operation. **Substitutive nomenclature** may be regarded as based on substitutive, additive, and subtractive operations. **Functional class nomenclature** is essentially based on additive operations, but includes substituent groups formed by substitutive nomenclature. **Multiplicative nomenclature** is a subtype of substitutive nomenclature based on cyclic parent structures, functionalized or not; functionalized acyclic parent structures; or heteroacyclic parent structures. **Skeletal replacement nomenclature** usually refers to replacement by ‘a’ terms and is thus often called just **‘a’ nomenclature**. Similarly, **conjunctive nomenclature** is restricted to conjunction operations involving rings or ring systems substituted by a principal group named substitutively or having a retained name.

The term nomenclature is not associated with one operation. In this case, names are formed by simply describing the type of operation, for example subtractive operation in the formation of double bonds and functional replacement operation in the replacement of oxygen atoms by chalcogen or nitrogen atoms.

The term nomenclature also applies to families or classes of compounds, for instance **Nomenclature of Radicals and Ions**, **Phane Nomenclature** for naming compounds composed of chains and/or ring systems and **Fullerene Nomenclature** to describe all operations necessary to name polycyclic carbon cage compounds and their derivatives. This term is also used to describe families of compounds of natural origin, for example **Nomenclature of Natural Products** is based on the concept of stereoparents. The nomenclature of carbohydrates, of α-amino-acids, peptides, lipids, and of some other compounds of biochemical significance, is generally considered to be **Biochemical Nomenclature** and, as such, is published comprehensively separately.

P-15.1 Substitutive nomenclature

Substitutive nomenclature is based on the choice of a compound having substitutable hydrogen atoms, called a parent hydride, and its substitution by structural fragments represented by suffixes and prefixes to generate names can be represented as follows:

prefixes—parent hydride—suffixes

A complete substitutive name is indicated schematically in **Fig. 1**. It includes the parent hydride, the different kinds of suffixes, prefixes, and endings, and the order in which they are placed in a name.

PREFIXES			PARENT	ENDINGS	SUFFIXES	
Detachable Prefixes	Hydro/ dehydro prefixes	Non- detachable prefixes	NAME OF PARENT	Endings ane/ene/yne	Functional Suffixes	Cumulative Suffixes

Fig. 1 Order of components in substitutive names

P-15.1.1 Order of suffixes

Suffixes are of two kinds depending on the operation used to generate them. **Functional suffixes** are used for characteristic groups expressing classes, for example ketones, acids, amines, etc.. **Cumulative suffixes** designate radicals, ions, radical ions, and related species, as well as substituent groups.

Functional suffixes are **exclusive suffixes**, as the presence of one denoting the principal characteristic group excludes all other functional suffixes; the modifications normally signaled by those suffixes must be designated as prefixes. To the contrary, cumulative suffixes can be present in any number and kind in a name and can even be associated with functional suffixes.

Functional suffixes are attached only to the name of the parent hydride. Cumulative suffixes are attached to the name of the parent hydride or to a functional suffix, if present.

Examples:

CH_4	$\longrightarrow$	$CH_4^{+\bullet}$
methane (PIN) (parent hydride)		methaniumyl (PIN) ('iumyl' is a cumulative suffix)

CH_3-CH_3	$\longrightarrow$	CH_3-CH_2-NH_2	$\longrightarrow$	CH_3-CH_2-NH_3^+
ethane (PIN) (parent hydride)		ethanamine (PIN) ('amine' is a functional suffix)		ethanaminium (PIN) ('ium' is a cumulative suffix)

P-15.1.2 Position of endings

The modification of the ending 'ane' to 'ene' or 'yne' in acyclic, cyclic and polycyclic parent hydrides is used to describe the subtractive operation that forms double and triple bonds.

P-15.1.3 Prefixes and their order in names

There are different kinds of prefixes in substitutive names:

P-15.1.3.1 Nondetachable prefixes
P-15.1.3.2 Hydro/dehydro prefixes
P-15.1.3.3 Detachable or alphabetized prefixes

Nondetachable, hydro/dehydro, and detachable prefixes are cited in names as indicated in Fig. 1.

P-15.1.3.1 Nondetachable prefixes

Nondetachable prefixes are permanently attached to the name of the parent structure in a given order, which normally matches the order of operations used to modify the parent structure. Prefixes describing the first operation are attached directly to the name of the parent structure; those resulting from a second operation are placed in front of those already introduced, and so on (this technique may be termed 'advancing backwards' from the name of the parent structure). The order is precisely prescribed for each category, as indicated below:

P-15.1.3.1.1 Nondetachable prefixes creating new parent structures:

(a) alicyclic rings and ring systems: ‘cyclo’, ‘bicyclo’, ‘tricyclo’, etc.; ‘spiro’, ‘dispiro’, etc.

(b) fused ring systems by fusion prefixes: ‘benzo’, ‘naphtho’, ‘imidazo’, etc.

(c) bridged fused ring systems by addition of bridge prefixes: ‘methano’, ‘epoxy’, etc.

(d) spiro compounds formed by combining cyclic compounds (a), (b), and/or (c).

P-15.1.3.1.2 Replacement of atoms other than hydrogen by other atoms.

This type of replacement, called ‘skeletal replacement’, is essentially the replacement of carbon atoms by heteroatoms; it takes place with cyclic and acyclic hydrocarbons and generates new parent compounds by using ‘a’ prefixes, i.e., ‘oxa’, ‘aza’, ‘thia’, etc.

P-15.1.3.1.3 Indicated hydrogen

Under certain circumstances it is necessary to indicate in the name of a ring or ring system that contains the maximum number of noncumulative double bonds one or more positions where no double bond is attached. This is done by specifying the presence of an ‘extra’ hydrogen atom at such positions by citation of the appropriate numerical locant followed by an italicized capital *H*. Indicated hydrogen is considered a nondetachable prefix and is introduced last, that is, last before the detachable prefixes.

P-15.1.3.2 ‘Hydro’ and ‘dehydro’ prefixes

> These two prefixes are considered as detachable but are not included in the category of alphabetized detachable prefixes described in P-15.1.3.3. In names, they occupy a place between nondetachable prefixes and alphabetized detachable prefixes. These prefixes are used to express modifications of the degree of hydrogenation and are treated like the endings ‘ene’ and ‘yne’, which fulfill the same function. In names, the prefix ‘dehydro’ precedes the prefix ‘hydro’, when both are present. Simple numerical terms, such as ‘di-’‘tetra-’, etc., are used with ‘dehydro’

P-15.1.3.3 Detachable (alphabetized) prefixes

These prefixes describe substituent groups denoting characteristic groups or groups derived from parent hydrides and are cited before ‘hydro-dehydro’ prefixes, if present (see P-15.1.3.2), or nondetachable prefixes, if present, as indicated in Fig. 1. They are alphabetized in accordance with P-14.5.

P-15.1.4 Other components of substitutive names

In addition to the components described above, the following nomenclatural indicators are added, as required:

P-15.1.4.1 Multiplying prefixes placed before suffixes and prefixes to indicate multiple occurrence;

P-15.1.4.2 Locants used to indicate positions of the parent structure at which modifications represented by suffixes, prefixes, and endings occur;

P-15.1.4.3 Stereodescriptors placed at the front of the complete name or name fragment.

P-15.1.5 Construction of substitutive names

This subsection describes the formation of substitutive names and the application of four general rules: numbering, locants, multiplying prefixes, and alphanumerical order. These four rules are applied in constructing names of most organic compounds. In the first set of examples, alkanes and branched alkanes are used. In the second set, the general rule of numbering is exemplified by saturated and unsaturated acyclic compounds denoted by suffixes. The full question of name construction is considered in P-46.

P-15.1.5.1 Naming alkanes and branched alkanes

(a) The names of alkanes are either retained names, which are methane, ethane, propane, and butane; or are formed systematically by adding the ending ‘ane’ to a basic multiplying prefix, with elision of the final letter ‘a’ of the multiplicative term (See Chapter 2).

Examples:

CH_4
methane (PIN)

CH_3-CH_3
ethane (PIN)

$CH_3-CH_2-CH_3$
propane (PIN)

$CH_3-CH_2-CH_2-CH_3$
butane (PIN)

$CH_3-CH_2-CH_2-CH_2-CH_3$
pentane (PIN)

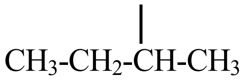
$CH_3-[CH_2]_8-CH_3$
decane (PIN)

(b) Monovalent substituent groups derived from unbranched acyclic hydrocarbons (alkanes) by the removal of one hydrogen atom from a terminal carbon atom (subtractive operation) are named by replacing the ending ‘ane’ of the name of the hydrocarbon by ‘yl’ (see P-19-3.2.1) or, if one hydrogen atom is removed from a nonterminal carbon atom of a chain, by replacing the final ‘e’ of the name of the hydrocarbon by ‘yl’ (see P-29-3.2.2) (‘yl’ is a cumulative suffix, see P-15.1).

Examples:

$CH_3-CH_2-CH_2-CH_2-$
butyl (PIN)

$CH_3-CH_2-CH_2-CH_2-CH_2-$
pentyl (PIN)

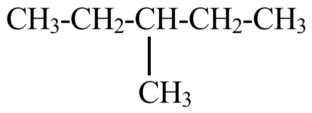


$CH_3-CH_2-\overset{|}{C}H-CH_3$

butan-2-yl (PIN)

(c) A saturated branched acyclic hydrocarbon is formed by substituting one or more substituent groups, formed as described in (b), into the longest chain present in the formula (substitutive operation); it is named by prefixing the designations of the side chains, as formed in (b), to the name of the longest chain [see (d) for numbering].

Example:

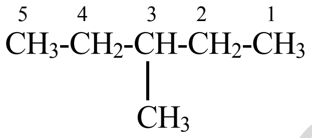


$CH_3\text{-}CH_2\text{-}CH(CH_3)\text{-}CH_2\text{-}CH_3$

3-methylpentane (PIN)

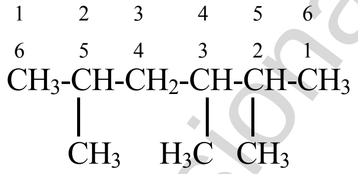
(d) The longest chain is numbered from one end to the other by arabic numbers, the direction being so chosen as to give the lower locants possible to the substituent groups (side chains) [see P-14.4(g)]. The lower set of locants is defined as the set that, when compared term by term with other locant sets cited in order of increasing magnitude, has the lower term at the first point of difference (see P-14.3.4). The locants are placed immediately in front of the part of the name to which they refer. Identical substituent groups are indicated by the appropriate multiplying prefix 'di', 'tri', etc. (see P-14.2). This rule is applied regardless of the nature of the substituent groups.

Examples:



$\overset{5}{C}H_3\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H(CH_3)\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_3$

3-methylpentane (PIN)



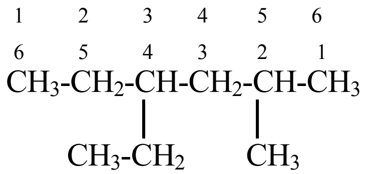
$CH_3\text{-}CH(CH_3)\text{-}CH_2\text{-}CH(CH_3)\text{-}CH(CH_3)\text{-}CH_3$

incorrect numbering
correct numbering

2,3,5-trimethylhexane (PIN)
(not 2,4,5-trimethylhexane; the locant set 2,3,5 is lower than 2,4,5)

(e) If two or more different substituent groups are present, they are cited in names in alphanumerical order (see P-14.4). When two or more substituent groups occupy equivalent positions, the one to be assigned the lower locant is that one cited first in the name.

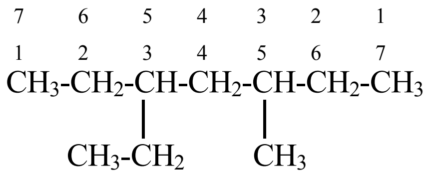
Examples:



$$\mathrm{\overset{1}{\underset{6}{CH_3}}\text{-}\overset{2}{\underset{5}{CH_2}}\text{-}\overset{3}{\underset{4}{CH}}(CH_2\text{-}CH_3)\text{-}\overset{4}{\underset{3}{CH_2}}\text{-}\overset{5}{\underset{2}{CH}}(CH_3)\text{-}\overset{6}{\underset{1}{CH_3}}}$$

incorrect numbering
correct numbering

4-ethyl-2-methylhexane (PIN)
(not 3-ethyl-5-methylhexane; the locant set 2,4 is lower than 3,5)



$$\mathrm{\overset{7}{\underset{1}{CH_3}}\text{-}\overset{6}{\underset{2}{CH_2}}\text{-}\overset{5}{\underset{3}{CH}}(CH_2\text{-}CH_3)\text{-}\overset{4}{\underset{4}{CH_2}}\text{-}\overset{3}{\underset{5}{CH}}(CH_3)\text{-}\overset{2}{\underset{6}{CH_2}}\text{-}\overset{1}{\underset{7}{CH_3}}}$$

incorrect numbering
correct numbering

3-ethyl-5-methylheptane (PIN)
(not 5-ethyl-3-methylheptane; the lower locant must be assigned to the substituent group that is cited first)

P-15.1.5.2 The numbering rule

The following examples illustrate the rule for numbering described in P-14.4. This rule establishes an order of priority among different nomenclatural features for assignment of the lowest possible locants.

(a) Alcohols are named by attaching the suffix ‘ol’ to the name of the parent hydride, with elision of the final letter ‘e’ in the parent hydride, if present. When alone in the structure, the characteristic group(s) must receive the lowest locant(s) possible, which is (are) cited immediately in front of the suffix (see P-14.3.2).

Example:

$$\mathrm{\overset{3}{CH_3}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CH_2}\text{-}OH}$$

propan-1-ol (PIN)

(b) Alkenes are acyclic branched or unbranched hydrocarbons having one double bond. When one double bond is present, an unbranched alkene is named by changing the ending ‘ane’ in the name of the alkane having the same number of carbon atoms to the ending ‘ene’ (see P-31). The double bond is assigned the lower locant possible, which is placed immediately in front of the ending ‘ene’ (see P-14.3.2)

Example:

$$\mathrm{\overset{1}{CH_2}{=}\overset{2}{CH}\text{-}\overset{3}{CH_2}\text{-}\overset{4}{CH_3}}$$

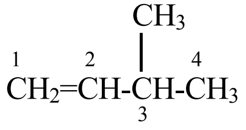
but-1-ene (PIN)

(c) When several nomenclatural features are present in a structure, lowest locants are assigned in accordance with P-14.4. For example, in a cyclic unsaturated alcohol having one substituent group, lowest locants are assigned in the order: (i) characteristic group cited as suffix (-ol); (ii) unsaturation (‘ene’ ending, for example); (iii) detachable alphabetized prefixes (a methyl group, for instance). The following examples illustrate the application of the rule.

Examples:

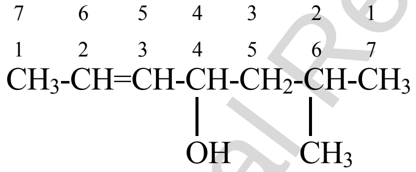
$$\overset{4}{CH_2}=\overset{3}{CH}-\overset{2}{CH_2}-\overset{1}{CH_2}-OH$$

but-3-en-1-ol (PIN)



$$\overset{1}{CH_2}=\overset{2}{CH}-\underset{3}{\overset{CH_3}{CH}}-\overset{4}{CH_3}$$

3-methylbut-1-ene (PIN)



$$CH_3-CH=CH-\underset{OH}{CH}-CH_2-\underset{CH_3}{CH}-CH_3$$

incorrect numbering: 7 6 5 4 3 2 1
correct numbering: 1 2 3 4 5 6 7

6-methylhept-2-en-4-ol (PIN)
(not 2-methylhept-5-en-4-ol)

P-15.2 Functional class nomenclature

P-15.2.0 Introduction

Functional class nomenclature was quite important in early days of organic chemistry when many compounds were named using class names. The procedures were identical with those of substitutive nomenclature except that suffixes were never used. Substituent groups, called ‘radicals’ in early nomenclature, were used in association with a name denoting the class; this nomenclature was called ‘radicofunctional nomenclature’. With time, substitutive nomenclature replaced functional class nomenclature in all but a few instances. In the context of IUPAC preferred names, substitutive nomenclature is the primary way for naming organic compounds; functional class nomenclature is reduced to a strict minimum.

The notion of functional class nomenclature is also applied to compounds that are named using a class name, but not necessarily preceded by a substituent group name. To that purpose, ‘functional modifiers’ are used to indicate a functional change, for example the change of acid to anhydride, as acetic anhydride, or the formation of derivatives of ketones, for example, butan-2-one oxime.

It is convenient to classify the main operation involved in functional class nomenclature as an additive one, as is done in P-13.3.3.2. However it is also possible (and probably more relevant from a historical point of view) to regard the process as one of specifying the substituent groups (‘radicals’) present in compounds for which a class name is given. For instance, the name ‘methyl alcohol’ (for CH_3-OH) consists of the name ‘methyl’ for the substituent group CH_3– and the class name ‘alcohol’ (for R-OH).

Functional class nomenclature is discussed in relation to the traditional use of substituent group names and the use of functional modifiers. Some names are formed on the basis of a class name, but are not considered as belonging to the functional class nomenclature. They are called ‘descriptive’ names and are never considered as IUPAC preferred names. The order of seniority of classes is discussed in the context of IUPAC preferred names.

P-15.2.1 Functional class nomenclature using substituent group names

P-15.2.1.1 Names are formed by expressing the functional class name of the compound as one word and the remainder of the molecule, a monovalent substituent or acyl group as separate word, placed in front of the class name.

Examples:

CH_3-CH_2-CO-O-CH_3	methyl propanoate (PIN)
CH_3-CO-Cl	acetyl chloride (PIN)
C_6H_5-CO-CN	benzoyl cyanide (PIN)
C_6H_5-CH_2-NCS	benzyl isothiocyanate (isothiocyanatomethyl)benzene (PIN)
C_6H_5-NC	phenyl isocyanide isocyanobenzene (PIN)
CH_3-OH	methyl alcohol methanol (PIN)
C_6H_5-N_3	phenyl azide azidobenzene (PIN)

P-15.2.1.2 When the functional class name refers to a characteristic group that is divalent, the two substituent groups attached to it are each named. When different, they are written as separate words, being in alphanumerical order.

Examples:

CH_3-CH_2-CO-CH_2-CH_3	diethyl ketone pentan-3-one (PIN)
CH_3-CH_2-CO-CH_3	ethyl methyl ketone (not methyl ethyl ketone) butan-2-one (PIN)

P-15.2.2 Functional class nomenclature using functional modifiers

Many derivatives of principal characteristic groups or functional parent compounds (see P-34) may be named by modifiers consisting of one or more separate words placed after the name of the parent structure. This method is most useful in an indexing environment, but it is the sole method used for naming acyclic anhydrides in the context of IUPAC preferred names.

P-15.2.2.1 For IUPAC preferred names, functional class modifiers are used to generate IUPAC preferred names for acyclic anhydrides. Substitutive nomenclature is preferred to the use of other modifiers.

Examples:

CH_3-CO-O-CO-CH_3	acetic anhydride (PIN) (the term ‘acid’ is replaced by ‘anhydride’)
CH_3-CH_2-CH=N-OH	propanal oxime (the term ‘oxime’ is added to the name of the carbonyl compound) *N*-propylidenehydroxylamine (PIN)

P-15.2.2.2 Functional modifers are still acceptable for general nomenclature purposes, but substitutive names are preferred IUPAC names for azines, hydrazones, semicarbazones, carbohydrazones, acetals, and hemiacetals.

Examples:

CH_3-CH_2-CH=N-NH_2	propanal hydrazone propylidenehydrazine (PIN)
$(CH_3)_2$C=N-NH-CO-NH_2	acetone semicarbazone 2-(propan-2-ylidene)hydrazinecarboxamide (PIN)
CH_3-CH_2-CH(O-CH_3)$_2$	propanal dimethyl acetal 1,1-dimethoxypropane (PIN)
CH_3-CH_2-CH_2-CO-OCH_3	butanoic acid methyl ester methyl butanoate (PIN)

P-15.2.3 Rules for functional class nomenclature

Functional class nomenclature is used in place of substitutive nomenclature to name acyclic anhydrides. When two classes are present and both named by functional class nomenclature, the senior class must be chosen in accordance with the seniority order of classes (see P-41). The relevant order for acid functional classes is acids, anhydrides, esters, acyl halides. The senior class is expressed by functional class nomenclature and the lower ranking classes are expressed by prefixes, as usual, in that part of the name that is constructed by substitutive nomenclature.

Examples:

$\mathrm{Cl\text{-}\overset{4}{C}O\text{-}CH_2\text{-}CH_2\text{-}\overset{1}{C}OOH}$

4-chloro-4-oxobutanoic acid (PIN)
4-(chlorocarbonyl)propanoic acid
4-carbonochloridoylpropanoic acid
(acid senior to acyl halide)

$\mathrm{Cl\text{-}\overset{4}{C}O\text{-}CH_2\text{-}CH_2\text{-}\overset{1}{C}OO\text{-}CH_3}$

methyl 4-chloro-4-oxobutanoate (PIN)
methyl 4-(chlorocarbonyl)propanoate
methyl 4-carbonochloridoylpropanoate
(ester senior to acyl halide)

$\mathrm{NC\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}Cl}$

2-cyanoacetyl chloride (PIN)
(acyl chloride senior to nitrile)

$\mathrm{CH_3O\text{-}\overset{4}{C}H_2\text{-}CH_2\text{-}CH_2\text{-}\overset{1}{C}O\text{-}OCH_3}$

methyl 4-methoxybutanoate (PIN)
(ester senior to ether)

Functional class names for polyfunctional compounds are not recommended. Substitutive nomenclature is preferred.

Example:

$\mathrm{HO\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}O\text{-}\overset{1}{C}H_3}$

4-hydroxybutan-2-one (PIN; substitutive name)
2-hydroxyethyl methyl ketone (functional class name)

P-15.3 Multiplicative nomenclature

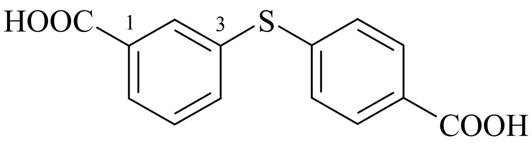
P-15.3.0 Introduction

Assemblies involving two or more identical parent structures linked by di- or polyvalent substituent groups can be named in two ways:

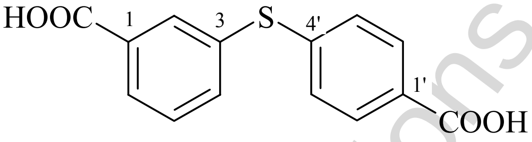
(a) by regular substitutive nomenclature in which one of the parent structures is chosen and the remainder of the structure is substituted into it; and,

(b) by multiplicative nomenclature, a form of substitutive nomenclature through which a multiplicity of parent structures can be recognized.

The following compound can be named 3-[(4-carboxyphenyl)sulfanyl]benzoic acid by simple substitutive nomenclature [numbering shown in **(I)**], a name that recognizes only one benzoic acid group as the parent structure.



(I)



(II)

Alternatively, it can be named 3,4′-sulfanediyldibenzoic acid (PIN) [numbering shown in **(II)**] using multiplicative nomenclature, a name that recognizes both benzoic acid groups in the parent structure.

> This method was reserved for naming compounds having characteristic groups expressed as suffixes or implied by a retained name and heteroacyclic parent hydrides. It is now recommended that it be extended to cyclic structures with or without characteristic groups. Chains composed only of carbon atoms are excluded from this type of nomenclature; the traditional approach, based on substitutive nomenclature, is recommended. The system has also been expanded by allowing substitution on the central unit of a multiplying group and the use of nonsymmetrical central units, under specific conditions

P-15.3.1 General methodology

Assemblies of identical units (parent structures) linked by di- or polyvalent substituent groups are named by multiplicative nomenclature when the identical units are:

(a) cyclic parent hydrides, mancude or saturated;

(b) mononuclear or polynuclear acyclic parent hydrides with the exception of acyclic hydrocarbons, saturated or unsaturated; or

(c) cyclic or acyclic parent hydrides substituted by characteristic groups expressed as suffixes.

Names are formed in accordance with the number of occurrences of identical parent structures and the symmetry properties of the linking multiplicative substituent in relation to the parent structures. The resulting multiplicative name must be unambiguous.

P-15.3.2 Assemblies linked by symmetrical substituent groups
P-15.3.3 Assemblies linked by unsymmetrical substituent groups
P-15.3.4 Multiple occurrences of identical parent structures

P-15.3.2 Assemblies linked by symmetrical substituent groups

P-15.3.2.1 When a compound contains identical units as defined in P-15.3.1 linked by a symmetrical di- or polyvalent substituent group, it may be named by stating successively:

(a) the locants for the positions of substitution of the di- or polyvalent multiplicative substituent substituent group into the identical units (locant 1 is omitted when alone in the name of a mononuclear parent hydride);

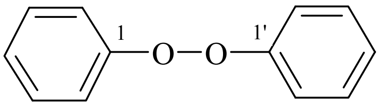
(b) the name of the di- or polyvalent multiplicative substituent group;

(c) the numerical prefix di , tri, etc., with no elision of the final vowel before identical units;

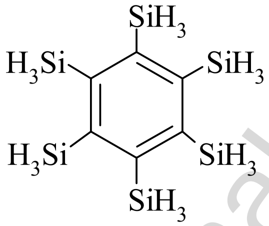
(d) the name of one of the identical units including the principal characteristic group, if any, enclosed in appropriate enclosing marks.

The numbering of the identical units is retained; when there is a choice, the points of substitution by the di- or polyvalent substituent groups on the parent structures are numbered as low as possible. Primes, double primes, etc. are used to distinguish among the locants of the identical units. Retained and systematically formed names are used for the identical units. Unsubstituted parent structures are enclosed in parentheses; parent structures substituted by atoms or groups expressed as prefixes are enclosed in square brackets.

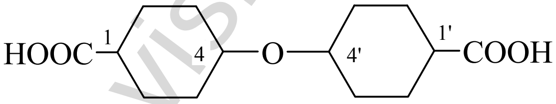
Examples:



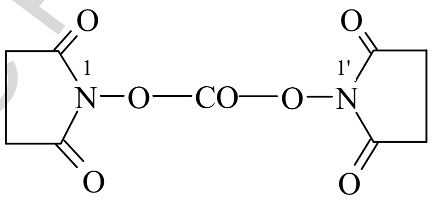
1,1′-peroxydibenzene (PIN)
1,1′-dioxydibenzene



benzenehexaylhexakis(silane) (PIN)

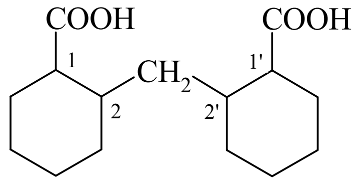


4,4′-oxydi(cyclohexane-1-carboxylic acid) (PIN)

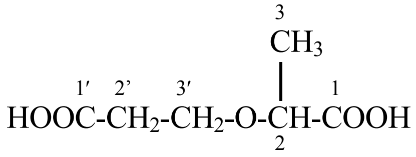


1,1′-[carbonylbis(oxy)]di(pyrrolidine-2,5-dione) (PIN)

P-15.3.2.2 If there is a choice, the greater number of primes is given to the locants of the unit having the higher numbered point of attachment to the di- or polyvalent multiplicative substituent group.
Examples:



2,2′-methylenedi(cyclohexane-1-carboxylic acid) (PIN)



$$\overset{1'}{HOOC}\text{-}\overset{2'}{CH_2}\text{-}\overset{3'}{CH_2}\text{-}O\text{-}\underset{2}{CH}(\overset{3}{CH_3})\text{-}\overset{1}{COOH}$$

2,3′-oxydipropanoic acid (PIN)

P-15.3.2.3 Simple multiplicative substituent groups.

Any simple polyvalent substituent (see P-29-1 for definitions) may be used as a multiplicative substituent:

$–CH_2–$	methylene (PIN)
–O–	oxy (PIN)
–S–	sulfanediyl (PIN) (thio is no longer recommended)
–OO–	peroxy (PIN) dioxy
–SS–	disulfanediyl (PIN) (dithio is no longer recommended)
–N<	nitrilo (PIN)
$–C_6H_4–$	phenylene (1,2- ;1,3- ;1,4-isomers) (PIN)
$–OC\text{-}CH_2\text{-}CH_2\text{-}CO–$	butanedioyl (PIN) succinyl

The following names derived from the parent hydride name ‘azane’ are recommended for some multiplicative substituent groups derived from NH_3.

–NH–	azanediyl (PIN; no longer imino; only =NH remains as imino)
–N=	azanylylidene (PIN;no longer nitrilo; only –N< remains as nitrilo)

Examples:

$\overset{2,2',2''}{\mathrm{N}}(CH_2\text{-}COOH)_3$	2,2′,2″-nitrilotriacetic acid (not 2,2′,2″-azanetriyltriacetic acid) *N*,*N*-bis(carboxymethyl)glycine (PIN)
$\overset{3,3'}{\mathrm{O}}(CH_2\text{-}CH_2\text{-}COOH)_2$	3,3′-oxydipropanoic acid (PIN)
$\overset{2,2',2''}{\mathrm{P}}(CH_2\text{-}COOH)_3$	2,2′,2″-phosphanetriyltriacetic acid (PIN)

Substitution is allowed on simple multiplicative substituent groups generating compound multiplicative substituent groups (see P-35.3).

Examples:

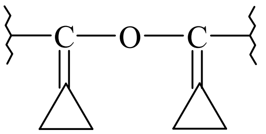
ClCH<	chloromethylene (PIN)
Me-N<	methylazanediyl (PIN) (no longer methylimino)

P-15.3.2.4 Multipart symmetrical di- and polyvalent multiplicative substituent groups

Concatenation is the method used for formation of multipart di- and polyvalent multiplicative substituent groups. In such substituent groups, the central substituent is cited first, then, in order and in the direction of one of the identical units, the successive di- or polyvalent substituent groups are cited.

Examples:

$–O\text{-}CH_2\text{-}O–$	methylenebis(oxy) (PIN) (not methylenedioxy; dioxy is −OO−)
$–CH_2\text{-}O\text{-}CH_2–$	oxybis(methylene) (PIN)
$–H_2C\text{-}NH\text{-}CO\text{-}CH_2\text{-}CO\text{-}NH\text{-}CH_2–$	propanedioylbis(azanediylmethylene) (PIN) malonylbis(azanediylmethylene)

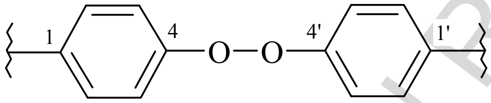


[oxybis(cyclopropylidenemethylene)] (PIN)
(note that if the suffix ‘ylidene’ were not limited to the indication of double bonds, the name given would be ambiguous. It could refer to a structure in which the cyclopropane bonds went to both a CH_2 group and an oxygen atom)

Numbering of the components of a multipart di- or trivalent multiplicative substituent group, when necessary, is achieved by attributing lowest locants to the atoms that are at the end of the component nearest to the parent structure.

Examples:

$-\overset{1}{\text{C}}\text{HCl-}\overset{2}{\text{C}}\text{H}_2\text{–O-}\overset{2'}{\text{C}}\text{H}_2\text{-}\overset{1'}{\text{C}}\text{HCl–}$ oxybis(1-chloroethane-2,1-diyl) (PIN)
oxybis(1-chloroethylene)



peroxydi-4,1-phenylene (PIN)

$\text{HOOC-}\overset{2}{\text{C}}\text{H}_2\text{-O-CH}_2\text{-CH}_2\text{-O-CH}_2\text{-CH}_2\text{-O-}\overset{2''}{\text{C}}\text{H}_2\text{-COOH}$

2,2′ -[oxybis(ethane-2,1-diyloxy)]diacetic acid (PIN)

$\text{HO}\overset{14}{\text{O}}\text{C-}\overset{13}{\text{C}}\text{H}_2\text{-}\overset{12}{\text{O}}\text{-}\overset{11}{\text{C}}\text{H}_2\text{-}\overset{10}{\text{C}}\text{H}_2\text{-}\overset{9}{\text{O}}\text{-}\overset{8}{\text{C}}\text{H}_2\text{-}\overset{7}{\text{C}}\text{H}_2\text{-}\overset{6}{\text{O}}\text{-}\overset{5}{\text{C}}\text{H}_2\text{-}\overset{4}{\text{C}}\text{H}_2\text{-}\overset{3}{\text{O}}\text{-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{1}{\text{C}}\text{OOH}$

2,2′-[ethane-1,2-diylbis(oxyethane-2,1-diyloxy)]diacetic acid (multiplicative name)
3,6,9,12-tetraoxatetradecanedioic acid (PIN; see P-51.4)

P-15.3.2.5 Derivatives of assemblies of identical parent structures

When assemblies named in accordance with Rule P-15.3.2.1 contain substituents on the identical parent structures, whether or not a principal characteristic group is present, these substituent groups are named by prefixes, which are cited in one of two ways.

P-15.3.2.5.1 Substituent groups on the identical parent structures are cited as prefixes associated with the identical parent structures when they fulfill the following two conditions:

(1) the linking bonds (single or multiple) between the central unit of the multiplicative substituent group and all subsequent structural units are identical; and

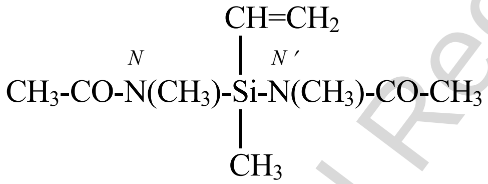
(2) the locants of all substituent groups on the identical parent structures cited as suffixes and prefixes are identical.

The identical parent structures, together with their prefixes and suffix are treated as a complex group, and the multiplicity of occurrences is designated by the appropriate numerical prefixes ‘bis’, ‘tris’, tetrakis’, etc.

Examples:

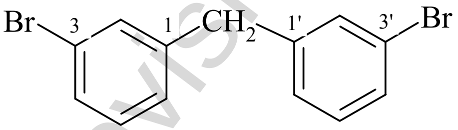
$F_3Si\text{-}\overset{1}{Si}F_2\text{-}CH_2\text{-}\overset{1'}{Si}F_2\text{-}SiF_3$ 1,1′-methylenebis(pentafluorodisilane) (PIN)

$(CH_3)_2\overset{N}{N}\text{-}O\text{-}\overset{N'}{N}(CH_3)_2$ *N*,*N* ′-oxybis(*N*-methylmethanamine)
tetramethyldiazoxane (PIN; see P-21.2.3.1;
diazoxane is a nonfunctional parent hydride)

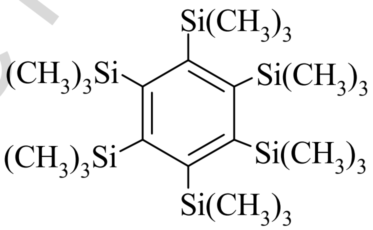


$CH_3\text{-}CO\text{-}\overset{N}{N}(CH_3)\text{-}\underset{\displaystyle CH_3}{\overset{\displaystyle CH{=}CH_2}{Si}}\text{-}\overset{N'}{N}(CH_3)\text{-}CO\text{-}CH_3$

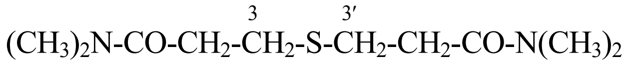
N,N′-[ethenyl(methyl)silanediyl]bis(*N*-methylacetamide)
1,1′-(2-ethenyl-1,2,3-trimethyldisilazane-1,3-diyl)bis(ethan-1-one) (PIN)
(a pseudo ketone; disilazane is a nonfunctional parent hydride)



1,1′-methylenebis(3-bromobenzene) (PIN)

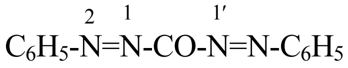


benzenehexaylhexakis(trimethylsilane) (PIN)



$(CH_3)_2N\text{-}CO\text{-}CH_2\text{-}\overset{3}{C}H_2\text{-}S\text{-}\overset{3'}{C}H_2\text{-}CH_2\text{-}CO\text{-}N(CH_3)_2$

3,3′-sulfanediylbis(*N*,*N*-dimethylpropanamide) (PIN)

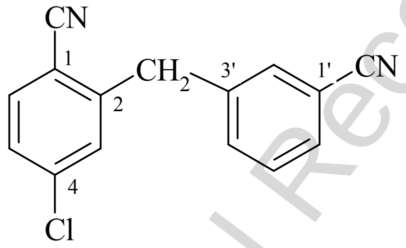


$C_6H_5\text{-}\overset{2}{N}{=}\overset{1}{N}\text{-}CO\text{-}\overset{1'}{N}{=}N\text{-}C_6H_5$

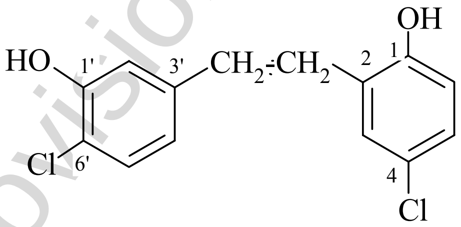
1,1′-carbonylbis(2-phenyldiazene) (PIN)

P-15.3.2.5.2 When the conditions defined in P-15.3.2.5.1 above are not met, the substituent groups other than those identified by suffixes, if present, are cited as prefixes at the front of the name of the assembly. These prefixes are assigned the lowest locants available after priority has been given to the principal characteristic groups, and the linking di- or polyvalent substituent groups.

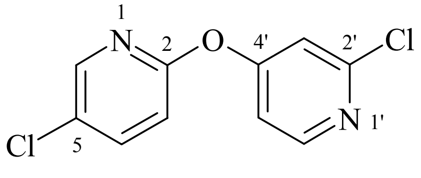
Examples:



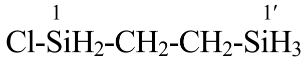
4-chloro-2,3′-methylenedibenzonitrile (PIN)



4,6′-dichloro-2,3′-(ethane-1,2-diyl)diphenol (PIN)

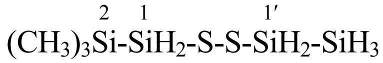


2′,5-dichloro-2,4′-oxydipyridine (PIN)



$\mathrm{Cl\text{-}\overset{1}{Si}H_2\text{-}CH_2\text{-}CH_2\text{-}\overset{1'}{Si}H_3}$

1-chloro-1,1′-(ethane-1,2-diyl)bis(silane) (PIN)

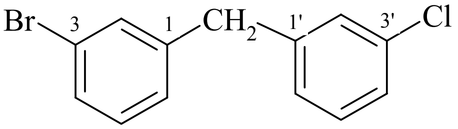


$\mathrm{(CH_3)_3\overset{2}{Si}\text{-}\overset{1}{Si}H_2\text{-}S\text{-}S\text{-}\overset{1'}{Si}H_2\text{-}SiH_3}$

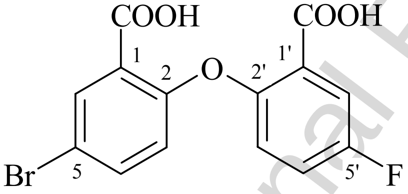
2,2,2-trimethyl-1,1′-(disulfanediyl)bis(disilane) (PIN)

P-15.3.2.5.3 When a choice is possible, unprimed locants are assigned to the identical parent structure having the substituent cited first in alphanumeric order.

Examples:



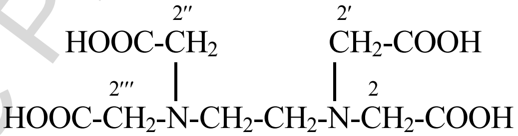
3-bromo-3′-chloro-1,1′-methylenedibenzene (PIN)



5-bromo-5′-fluoro-2,2′-oxydibenzoic acid (PIN)

P-15.3.2.6 When more than two identical parent structures are present, priming is used to distinguish each locant of the identical parent structures located at one end of the multiplying substituent, then at the other end, as required.

Example:

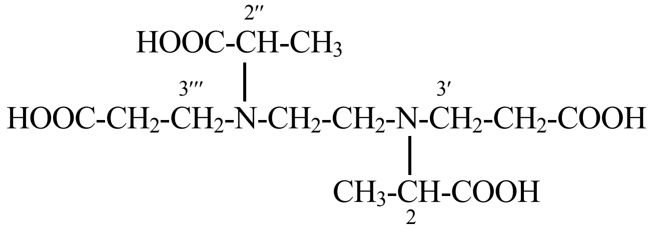


$$\mathrm{HOOC\text{-}\overset{2'''}{C}H_2\text{-}\overset{\substack{\overset{2''}{HOOC\text{-}CH_2}\\ |}}{N}\text{-}CH_2\text{-}CH_2\text{-}\overset{\substack{\overset{2'}{CH_2\text{-}COOH}\\ |}}{N}\text{-}\overset{2}{C}H_2\text{-}COOH}$$

2,2′,2′′,2′′′-(ethane-1,2-diyldinitrilo)tetraacetic acid
N,*N*′-ethane-1,2-diylbis[*N*-(carboxymethyl)glycine] (PIN)

If there is a choice, the greater number of primes is given to the locants of the identical parent structure having the higher numbered point of attachment to each end of the polyvalent multiplicative substituent group.

Example:



$$\begin{array}{c} \mathrm{HOOC\text{-}\overset{2''}{C}H\text{-}CH_3} \\ | \\ \mathrm{HOOC\text{-}CH_2\text{-}\overset{3'''}{C}H_2\text{-}N\text{-}CH_2\text{-}CH_2\text{-}N\text{-}\overset{3'}{C}H_2\text{-}CH_2\text{-}COOH} \\ | \\ \mathrm{CH_3\text{-}\underset{2}{C}H\text{-}COOH} \end{array}$$

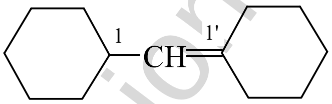
2,2′′,3′,3′′′-(ethane-1,2-diyldinitrilo)tetrapropanoic acid
N,*N*′-ethane-1,2-diylbis[*N*-(2-carboxyethyl)alanine] (PIN)

P-15.3.3 Assemblies linked by unsymmetrical substituent groups

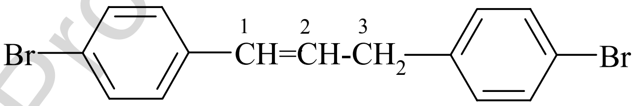
This method constitutes an addition to the nomenclature of assemblies as previously recommended.

P-15.3.3.1 Multiplicative nomenclature can also be used to name assemblies of identical parent structures linked by unsymmetrical substituent groups provided that all parent structures have identical locants assigned to the characteristic groups cited as suffixes and substituent groups cited as prefixes. This method is identical with that described in P-15.3.2.4.1. Unprimed, primed, double primed, etc., locants for attachment points of the unsymmetrical substituent group to the identical parent structures are cited in increasing order of the locants of the unsymmetrical substituent group.

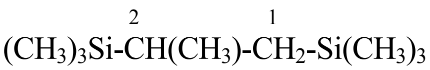
Examples:



1,1′-methanylylidenedicyclohexane (PIN)

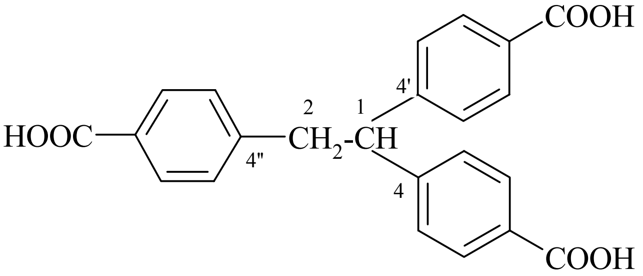


1,1′-(prop-1-en-1,3-diyl)bis(4-bromobenzene) (PIN)



$$\mathrm{(CH_3)_3Si\text{-}\overset{2}{C}H(CH_3)\text{-}\overset{1}{C}H_2\text{-}Si(CH_3)_3}$$

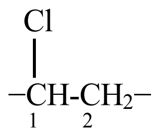
(propane-1,2-diyl)bis(trimethylsilane) (PIN)



4,4′,4″-ethane-1,1,2-triyltribenzoic acid (PIN)

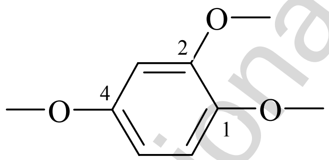
P-15.3.3.2 Unsymmetrical central substituent groups are allowed if they are formed from a basic multivalent substituent group to which subsequent groups are attached by identical bonds (single or multiple). There is no limit to the number of individual groups in the full central substituent used as a multiplier.

P-15.3.3.2.1 Examples of allowed unsymmetrical multiplicative substituent groups:

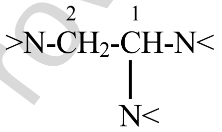


$$\overset{\text{Cl}}{\underset{1}{-\text{CH}}}-\underset{2}{\text{CH}_2}-$$

(1-chloroethane-1,2-diyl) (PIN)



[1,2,4-benzenetriyltris(oxy)] (PIN)



$$>\text{N}-\overset{2}{\text{CH}_2}-\underset{\text{N}<}{\overset{1}{\text{CH}}}-\text{N}<$$

(ethane-1,1,2-triyltrinitrilo) (PIN)

P-15.3.3.2.2 Disallowed unsymmetrical multiplicative substituent groups:

(a) Unsymmetrical substituent groups consisting of two different components:

Examples: $-\text{CH}_2\text{-OO}-$ $-\text{CH}_2\text{-NH}-$

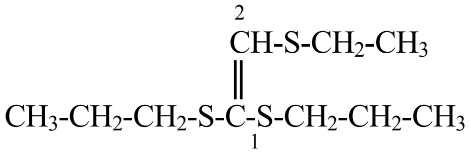
(b) Unsymmetrical substituent groups having terminal atoms with different bonding orders:

Example: $-CH\text{-}CH{=}N\text{-}CH_2\text{-}CH{=}$

(c) Unsymmetrical multipart substituent groups;

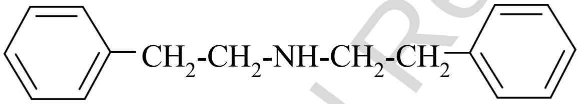
Example: $-O\text{-}CH_2\text{-}CH_2\text{-}S-$

P-15.3.4 Examples of multiplicative names that are not allowed



$$CH_3\text{-}CH_2\text{-}CH_2\text{-}S\text{-}\overset{\overset{2}{CH}\text{-}S\text{-}CH_2\text{-}CH_3}{\overset{\|}{\underset{1}{C}}}\text{-}S\text{-}CH_2\text{-}CH_2\text{-}CH_3$$

2-(ethylsulfanyl)-1,1-bis(propylsulfanyl)ethene (PIN; substitutive name)
(not 1,1′-{[(2-ethylsulfanyl)ethene-1,1-diyl]bis(sulfanyl)}dipropane;
multiplication of alkanes is not allowed; see P-15.1.2.1)



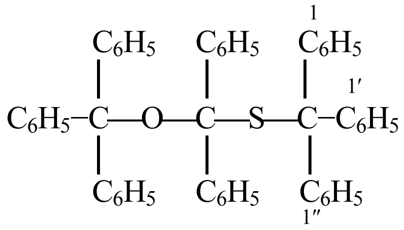
2-phenyl-*N*-(2-phenylethyl)ethan-1-amine (PIN)
(functionality expressed by a suffix is senior to a multiplicative name based on a parent cyclic hydrocarbon)

P-15.3.5 Multiple occurrences of identical parent structures

When more than two identical parent structures occur in the whole structure, the following rules are to be followed. It should be noted that preferred IUPAC names are formed by using Phane Nomenclature when four rings are present, two being terminal, in a system containing a minimum of seven nodes (see P-52.5.3.2) and that skeletal replacement (‘a’) nomenclature is used when the conditions for its use are met (see P-15.4.3.2).

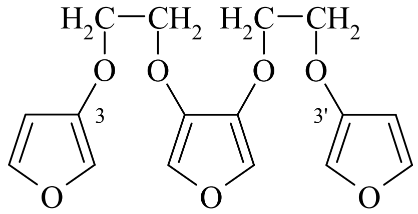
P-15.3.5.1 A maximum number of parent structures must be expressed

Example:



$$(C_6H_5)_3C-O-C(C_6H_5)_2-S-C(C_6H_5)_3$$

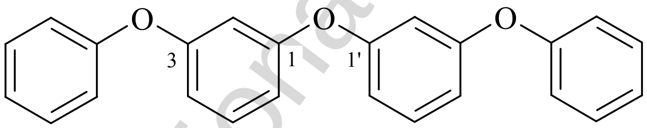
1,1′,1″-({[diphenyl(triphenylmethoxy)methyl]sulfanyl}methanetriyl)tribenzene (PIN)



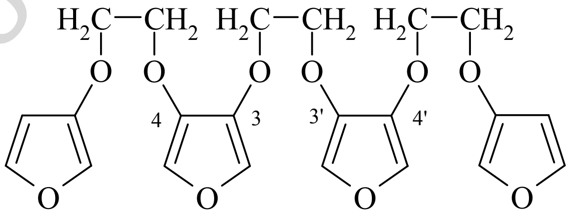
3,3′-[furan-3,4-diylbis(oxyethane-2,1-diyloxy)]difuran (PIN)

P-15.3.5.2 When the parent structure occurs more than three times in the whole structure, the two parent structures to be multiplied are those nearer to the central unit of the multiplicative substituent group; the other parent structures are substituted into the multiplied structure.

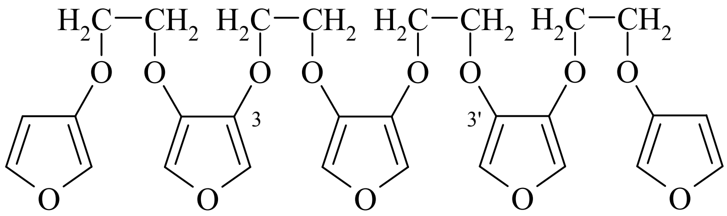
Examples:



1,1′-oxybis(3-phenoxybenzene) (multiplicative name)
2,4,6-trioxa-1,7(1),3,5(1,3)-tetrabenzenaheptaphane (PIN; phane name, see P-51.4)



3,3′-[ethane-1,2-diylbis(oxy)]bis{4-[2-(furan-3-yloxy)ethoxy]furan} (multiplicative name)
2,5,7,10,12,15-hexaoxa-1,16(3),6,11(3,4)-tetrafuranahexadecaphane (PIN; phane name, see P-51.4)



3,3′-[furan-3,4-diylbis(oxyethane-2,1-diyloxy)]bis{4-[2-(furan-3-yloxy)ethoxy]furan} (multiplicative name)

2,5,7,10,12,15,17,20-octaoxa-1,21(3), 6,11,16,21(3,4)-pentafuranahenicosaphane (PIN; phane name, see P-51.4)

P-15.4 Skeletal replacement (‘a’) nomenclature

P-15.4.0 Introduction.

Skeletal replacement nomenclature is a subset of the replacement operation that also includes functional replacement nomenclature (see P-13.2). Functional replacement nomenclature is discussed in P-15.5. Just as functional replacement is considered a nomenclature, skeletal replacement is also considered a nomenclature.

In the nomenclature of organic compounds, skeletal replacement based on the replacement of carbon atoms by other atoms included in the general scope of the nomenclature of organic compounds is described under the title of skeletal replacement (‘a’) nomenclature, because the heteroatoms replacing carbon atoms are denoted by nondetachable prefixes ending in ‘a’. Skeletal replacement (‘a’) nomenclature also includes replacement of boron atoms by other atoms, including carbon, (see P-68.1.1.3.4) and the replacement of heteroatoms by other atoms, including carbon, to modify fundamental structures of natural products as described in P-101.4. Skeletal replacement denoted by methods other than ‘a’ prefixes is described for the replacement of nitrogen atoms by phosphorus and arsenic atoms in certain heterocycles (see Table 2.7) and oxygen atoms by sulfur, selenium and tellurium atoms in other specific heterocycles (see Table 2.6).

This section deals primarily with skeletal replacement in hydrocarbon parent hydrides. Skeletal replacement (‘a’) nomenclature is used in two ways:

(a) to generate names for heterocyclic parent hydrides by replacing carbon atoms in corresponding cyclic hydrocarbons; and

(b) to generate simpler names for heteroacyclic structures than those formed by substitutive nomenclature when four or more heterounits (usually heteroatoms) are present, for example, in naming polyamines, polyethers, etc.

P-15.4.1 General rules

P-15.4.1.1 Nondetachable prefixes, called ‘a’ prefixes, are used to designate replacing skeletal atoms with their standard bonding number. Those related to these recommendations are listed in Table 1.5.

Table 1.5 Skeletal replacement ‘a’ prefixes

Standard Bonding Numbers	3		4		3		2		1	
	B	bora	C	carba	N	aza	O	oxa	F	fluora
	Al	alumina	Si	sila	P	phospha	S	thia	Cl	chlora
	Ga	galla	Ge	germa	As	arsa	Se	selena	Br	broma
	In	inda	Sn	stanna	Sb	stiba	Te	tellura	I	ioda
	Tl	thalla	Pb	plumba	Bi	bisma	Po	polona	At	astata

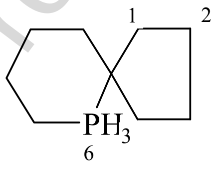
P-15.4.1.2 For naming and numbering purposes, the following decreasing order of seniority is followed: F > Cl > Br > I > At > O > S > Se > Te > Po > N > P > As > Sb > Bi > C > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

P-15.4.1.3 Names are formed by citing the ‘a’ terms (see Table 1.5) as prefixes to the name of the parent structure with the same number of skeletal atoms in the order given in P-15.4.1.2. The numerical prefixes ‘di’, ‘tri’, ‘tetra’, etc., are used to indicate a multiplicity of identical replacing atoms. The final letter ‘a’ of the ‘a’ term and the final letters ‘a’ and ‘i’ of a multiplying prefix are not elided when followed by a vowel.

P-15.4.1.4 Numbering is based first on the numbering of the acyclic or cyclic parent structure, and then low locants are assigned on the basis of the seniority order of the ‘a’ prefixes given in P-15.4.1.2. Once a structure modified by skeletal replacement (‘a’) prefixes has been named and numbered, it is considered to be a new parent hydride.

P-15.4.1.5 The symbol λ^n is used to describe heteroatoms having nonstandard bonding numbers (P-14.1.3). In names, it is placed immediately after the locant (without an intervening hyphen) denoting the heteroatom.

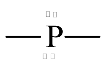
Example:



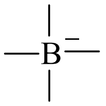
6λ^5-phosphaspiro[4.5]decane (PIN)

P-15.4.1.6 Derived skeletal replacement (‘a’) prefixes are used to designate anionic and cationic heteroatoms.

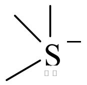
Examples:



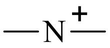
posphanida (PIN)



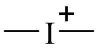
boranuida (PIN)



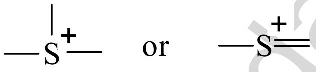
sulfanuida (PIN)
λ^4-sulfanida



azanylia (PIN)



iodonia (PIN)



thionia (PIN)

These prefixes are used when skeletal replacement (‘a’) nomenclature is recommended to name ionic parent structures. This question and the selection of preferred IUPAC names are fully discussed in P-73.4.

P-15.4.2 Skeletal replacement (‘a’) nomenclature for rings and ring systems

Skeletal replacement (‘a’) nomenclature is used to modify rings and ring systems. Such rings and ring systems differ in the modalities of application of the general rules for naming and numbering parent hydrides; therefore, these rings and ring systems are described at the end of each section that describes their naming and numbering before the replacement operation occurs.

(a) cycloalkanes having more than ten skeletal carbon atoms, in P-22.2.3;

(b) di- and polycycloalkanes of the von Baeyer type, in P-23.2;

(c) spiro compounds, in P-24.2.4;

(d) fusion systems, in P-25.5.1;

(e) phane parent hydrides, in P-26.5;

(f) fullerenes, in P-27.

P-15.4.3 Skeletal replacement (‘a’) nomenclature for chains

A major modification to Rule C-0.6 (ref. 1) has been made to skeletal replacement (‘a’) nomenclature as applied to chains. In these recommendations, skeletal replacement (‘a’) nomenclature generates new acyclic parent hydrides whose numbering is fixed as it is for rings and ring systems. Then suffixes, endings, and prefixes are added in accordance with this fixed numbering.

P-15.4.3.1 Name formation

P-15.4.3.1.1 Names are formed by placing ‘a’ prefixes in front of the name of the unbranched parent structure formed in accord with their seniority order given in P-15.4.1.2. Multiplicative prefixes ‘di’, ‘tri’, ‘tetra’, etc, indicate a multiplicity of identical heteroatoms, and locants are used to designate their positions.

Unbranched chains are numbered continuously from one end to the other so as to give a lower set of locants to heteroatoms considered together as a set without regard to kind, and then, if there is a choice, to heteroatoms cited first in the seniority order given in P-15.4.1.2.

Examples:

$$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{8}{\mathrm{S}}\text{-}\overset{9}{\mathrm{CH_2}}\text{-}\overset{10}{\mathrm{CH_3}}$$

8-thia-2,4,6-trisiladecane (PIN)
(the locant set' 2,4,6,8' is lower than '3,5,7,9')

$$\overset{9}{\mathrm{CH_3}}\text{-}\overset{8}{\mathrm{SiH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{O}}\text{-}\overset{1}{\mathrm{CH_3}}$$

2-oxa-4,6,8-trisilanonane (PIN)
(the heteroatom locant sets, '2,4,6,8', are identical;
therefore, the low locant is given to 'O' over 'Si')

P-15.4.3.1.2 Free valences of substituent groups receive locants according to the fixed numbering of the heterochain.

Example:

$$\overset{1}{\mathrm{CH_3}}\text{-}\ \overset{2}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{8}{\mathrm{SiH_2}}\text{-}\overset{9}{\mathrm{CH_2}}\text{-}\overset{10}{\mathrm{CH_2}}\text{–}$$

2,4,6,8-tetrasiladecan-10-yl (PIN)
(Note: 'decan-10-yl' not 'dec-10-yl'; see P-29.2.1)

$$\overset{1}{\mathrm{CH_3}}\text{-}\ \overset{2}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{|}{\underset{5}{\mathrm{C}}}\mathrm{H}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{8}{\mathrm{SiH_2}}\text{-}\overset{9}{\mathrm{CH_2}}\text{-}\overset{10}{\mathrm{CH_3}}$$

2,4,6,8-tetrasiladecan-5-yl (PIN)

P-15.4.3.1.3 Characteristic groups cited as suffixes are given locants in accordance with the fixed numbering of the heterochain.

Examples:

$$\overset{9}{\mathrm{CH_3}}\text{-}\ \overset{8}{\mathrm{SiH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{SiH_2}}\text{-}\overset{1}{\mathrm{C}}\mathrm{OOH}$$

2,4,6,8-tetrasilanonanoic acid (PIN)
(locant 1 is omitted; see P-14.3.3.1)

$$\overset{1}{\mathrm{CH_3}}\text{-}\ \overset{2}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{8}{\mathrm{SiH_2}}\text{-}\overset{9}{\mathrm{CH_2}}\text{-}\overset{10}{\mathrm{CH_2}}\text{-OH}$$

2,4,6,8-tetrasiladecan-10-ol (PIN)

1 2 3 4 5 6 7 8 9 10

CH_3- SiH_2-CH_2-SiH_2-CH_2-SiH_2-CH_2-SiH_2-CH_2-COOH

2,4,6,8-tetrasiladecan-10-oic acid (PIN)

P-15.4.3.1.4 Double and triple bonds are given locants in accordance with the fixed numbering of the heterochain, and, if there is a choice, according to the general priorities for multiple bonds (see P-31.1.2).

Example:

1 2 3 4 5 6 7 8 9 10

CH_3- SiH_2-CH_2-SiH_2-CH_2-SiH_2-CH_2-SiH_2-CH=CH_2

2,4,6,8-tetrasiladec-9-ene (PIN)

P-15.4.3.1.5 Heteroatoms with nonstandard valences

(a) A nonstandard bonding number of a neutral skeletal heteroatom in a parent hydride is indicated by the symbol λ^n, where '*n*' is the bonding number following the appropriate locant (see P-14.1.3).

Example:

1 2 3 4 5 6 7 8 9 10 11 12

CH_3-O-CH_2-CH_2-O-CH_2-CH_2-O-CH_2-CH_2-SH_2-CH_3

2,5,8-trioxa-11λ^4-thiadodecane (PIN)
('O' is preferred to 'S' for low locant)

(b) When there is a choice, low locants are assigned to heteroatoms having a higher bonding number.

Example:

1 2 3 4 5 6 7 8 9 10 11 12

CH_3-SH_2-CH_2-CH_2-S-CH_2-CH_2-S-CH_2-CH_2-S-CH_3

2λ^4,5,8,11-tetrathiadodecane (PIN)

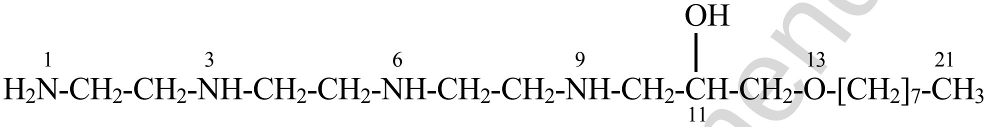
P-15.4.3.1.6 The use of anionic and cationic skeletal replacement ('a') prefixes is discussed in P-72.4 and P-73.4, respectively.

P-15.4.3.2 General conditions for use of skeletal replacement ('a') nomenclature

Skeletal replacement ('a') nomenclature is used in place of substitutive or multiplicative nomenclature when the following conditions are fulfilled.

P-15.4.3.2.1 Skeletal replacement ('a') nomenclature must be used when at least four heteroatoms or units are present in a unbranched chain containing at least one carbon atom and none of the heteroatoms constitute all or part of the principal characteristic group of the compound. A heterounit is a set of heteroatoms having a name of its own as, −SS−, disulfanediyl; $SiH_2SiOSiH_2$−, disiloxane-1,3-diyl; –SOS–, dithioxanediyl; but not –$OSiH_2O$–, nor _–OSO– that correspond to three consecutive units 'oxysilanediyloxy' and 'oxysulfanesiyloxy', respectively. Acids such as carbonic acid or phosphorus, arsenic and antimony acids, when representing the parent compound or the principal group, are not considered as units. In presence of a characteristic group having seniority for citation as a suffix, the group –O-P(O)(OCH_3)-O– is composed of three units (see third example below).

Examples:

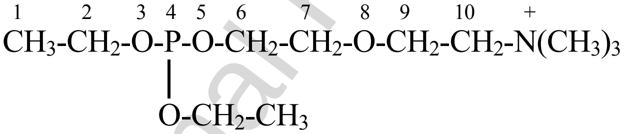


$$\mathrm{H_2N{-}CH_2{-}CH_2{-}NH{-}CH_2{-}CH_2{-}NH{-}CH_2{-}CH_2{-}NH{-}CH_2{-}\overset{OH}{C}H{-}CH_2{-}O{-}[CH_2]_7{-}CH_3}$$

1-amino-13-oxa-3,6,9-triazahenicosan-11-ol (PIN)

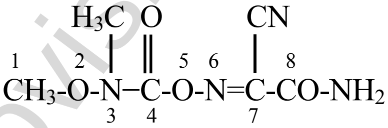
$$\mathrm{F{-}CO{-}NH{-}S{-}NH{-}CH_2{-}O{-}N{=}CH{-}CH{=}N{-}O{-}CH_2{-}NH{-}S{-}NH{-}CO{-}F}$$

6,11-dioxa-3,14-dithia-2,4,7,10,13,15-hexaazahexadeca-7,9-dienedioyl difluoride (PIN)
(an acyclic dioyl fluoride is preferred to a multiplied carbamoyl difluoride)



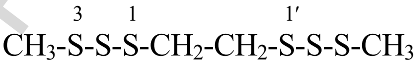
$$\mathrm{CH_3{-}CH_2{-}O{-}\underset{O{-}CH_2{-}CH_3}{P}{-}O{-}CH_2{-}CH_2{-}O{-}CH_2{-}CH_2{-}\overset{+}{N}(CH_3)_3}$$

4-ethoxy-*N*,*N*,*N*-trimethyl-3,5,8-trioxa-4-phosphadecan-10-aminium (PIN)



$$\mathrm{CH_3{-}O{-}\overset{H_3C}{N}{-}\overset{O}{\overset{\|}{C}}{-}O{-}N{=}\overset{CN}{C}{-}CO{-}NH_2}$$

7-cyano-3-methyl-4-oxo-2,5-dioxa-3,6-diazaoct-6-en-8-amide (PIN)



$$\mathrm{CH_3{-}S{-}S{-}S{-}CH_2{-}CH_2{-}S{-}S{-}S{-}CH_3}$$

1,1′-(ethane-1,2-diyl)bis(3-methyltrisulfane) (PIN)
(not 2,3,4,7,8,9-hexathiadecane; trisulfane, HS-S-SH, is a parent hydride and is not allowed to be a heterounit)

$(CH_3)_3C\text{-OO-Si}(CH_3)_2\text{-O-CO-}CH_2\text{-}CH_3$

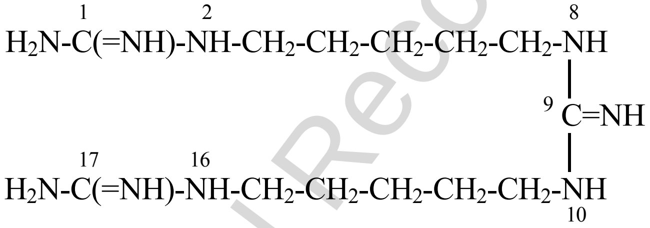
(*tert*-butylperoxy)dimethylsilyl propanoate (PIN)
(not 3,4,6-trioxa-5-silaoctan-7-one; only two heterounits are present: –OO– and –Si–; the principal characteristic group is an ester and the –O– is a part of it)

$CH_3\text{-O-PH(O)-O-}CH_2\text{-O-}CH_3$

methoxymethyl methyl phosphonate (PIN)
(not 2,4,6-trioxa-3λ^5-phosphan-3-one; the principal characteristic group, an ester, must be expressed, leaving only one heterounit, −O−)

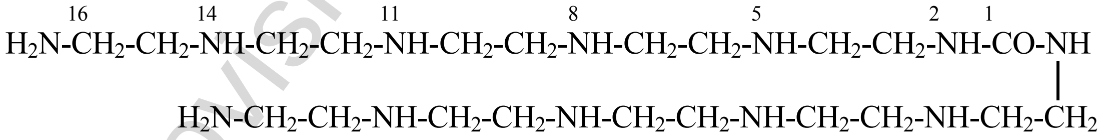
P-15.4.3.2.2 The same number of characteristic groups that would be expressed as suffixes in substitutive names must be present in skeletal replacement ('a') names.

Examples:



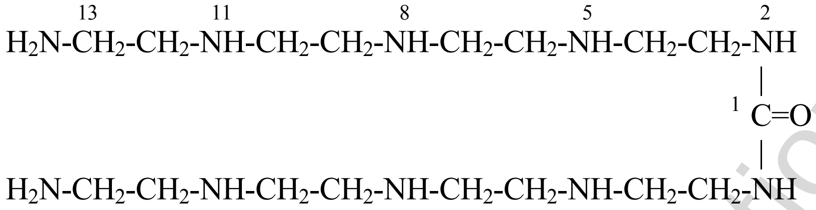
$$\begin{array}{l}
\overset{1}{}H_2N\text{-}C(=NH)\text{-}\overset{2}{NH}\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}\overset{8}{NH} \\
\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad | \\
\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\ {}^{9}C{=}NH \\
\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad | \\
H_2N\text{-}\overset{17}{C}(=NH)\text{-}\overset{16}{NH}\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}\underset{10}{NH}
\end{array}$$

9-imino-2,8,10,16-tetraazaheptadecanediimidamide (PIN)
(a diimidamide expressed as a principal characteristic group is senior to a carbonimidic diamide)

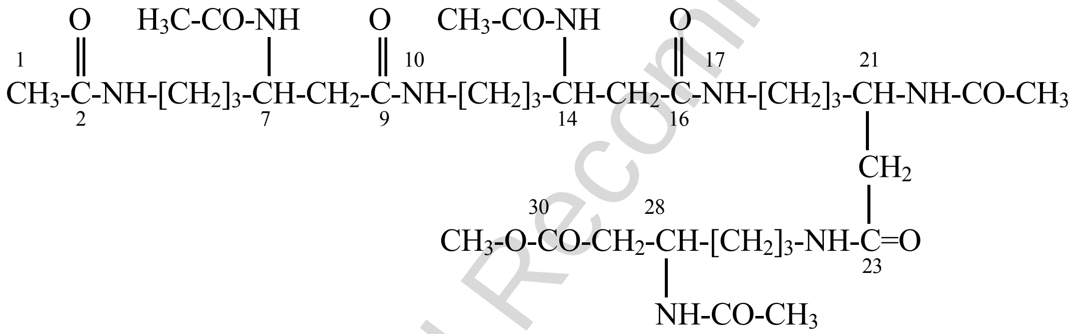


$$\begin{array}{r}
H_2N\text{-}\overset{16}{CH_2}\text{-}CH_2\text{-}\overset{14}{NH}\text{-}CH_2\text{-}CH_2\text{-}\overset{11}{NH}\text{-}CH_2\text{-}CH_2\text{-}\overset{8}{NH}\text{-}CH_2\text{-}CH_2\text{-}\overset{5}{NH}\text{-}CH_2\text{-}CH_2\text{-}\overset{2}{NH}\text{-}\overset{1}{CO}\text{-}NH \\
| \\
H_2N\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2
\end{array}$$

16-amino-*N*-(14-amino-3,6,9,12-tetraazatetradecan-1-yl)-2,5,8,11,14-pentaazahexadecanamide (PIN)
[an amide expressed as a principal characteristic group is senior to urea, a carbonic diamide, or an amine expressed as a principal characteristic group; since four heteroatoms are also present in the *N*-substituent group, it must also be named by skeletal replacement ('a') nomenclature]



13-amino-*N*-(2-{2-[(2-{[2-(2-aminoethyl)amino]ethyl}amino)ethyl]amino}ethyl)-2,5,8,11-tetraazatridecanamide (PIN)
(an amide expressed as a characteristic group is senior to urea, a carbonic diamide, and to an amine expressed as a characteristic group; since only three heteroatoms are present in the *N*-substituent group, it must be named substitutively)



methyl 7,14,21,28-tetrakis(acetamido)-2,9,16,23-tetraoxo-3,10,17,24-tetraazatriacontan-30-oate (PIN; an ester is senior to an amide or a ketone)

P-15.4.3.2.3 The chain must be terminated by C or one of the following heteroatoms: P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, or Tl.

Examples:

$\overset{1}{H_3Si}\text{-}\overset{2}{O}\text{-}CH_2\text{-}\overset{4}{S}\text{-}\overset{5}{SiH_3}$

2-oxa-4-thia-1,5-disilapentane (PIN)

P-15.5 Functional replacement nomenclature

P-15.5.1 Definition

Functional replacement nomenclature is a method by which oxygen atoms of characteristic groups and in functional parent compounds are replaced by halogen, chalcogen and/or nitrogen atoms.

P-15.5.2 General methodology

The replacement of oxygen atoms or hydroxy groups by other atoms or groups can be described by prefixes attached to, or infixes inserted into, names of characteristic groups, parent hydrides and functional parent compounds having retained or systematic names. A list of prefixes and infixes is given in Table 1.6. Prefixes and infixes are used for designating the replacing atom(s) −OO−, S, Se, and Te. For example, thio indicates the replacement of oxygen atoms by sulfur in the suffixes sulfonothioyl and carbothioyl and in the functional parent thioacetic acid. Similarly, peroxo or peroxy indicates the replacement of an oxygen atom by a −OO− group in the suffix peroxoic acid and in the name peroxyacetic acid.

Table 1.6 Prefixes and infixes in functional replacement nomenclature

Prefix	Infix	Replaced atom or group	Replacing atom or group
amido	amido	–OH	$–NH_2$
azido	azido	–OH	$–N_3$
bromo	bromido	–OH	–Br
chloro	chlorido	–OH	–Cl
cyanato	cyanatido	–OH	–OCN
cyano	cyanido	–OH	–CN
dithioperoxy*	dithioperoxo*	–O–	–S-S–
fluoro	fluorido	–OH	–F
hydrazido	hydrazido	–OH	$–NH-NH_2$
hydrazono	hydrazono	=O	$=N-NH_2$
imido	imido	=O	=NH
iodo	iodido	–OH	–I
isocyanato	isocyanatido	–OH	–NCO
isocyano	isocyanido	–OH	–NC
isothiocyanato*	isothiocyanatido*	–OH	–NCS
nitrido	nitrido	=O and –OH	≡N
peroxy	peroxo	–O–	–O-O–
seleno	seleno	=O or –OH	=Se or –SeH

telluro	telluro	=O or –OH	=Te or –TeH
thio	thio	=O or –OH	=S or –S–
thiocyanato*	thiocyanatido*	–OH	–SCN
thioperoxy*	thioperoxo*	–O–	–OS– or –SO–

* Selenium and tellurium analogues are named using ‘seleno’ and ‘telluro’ instead of ‘thio’.

P-15.5.3 Scope of functional replacement nomenclature

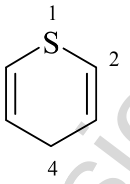
Prefixes and infixes are used in accordance with specific rules describing replacement in:

P-15.5.3.1 Heterocyclic parent hydrides
P-15.5.3.2 Characteristic groups expressed as suffixes in substitutive nomenclature
P-15.5.3.3 Characteristic groups expressed as prefixes in substitutive nomenclature
P-15.5.3.4 Functional parents

P-15.5.3.1 Replacement in heterocyclic parent hydrides

Prefixes are used to modify a limited group of parent hydrides as follows. See Table 2.3 for pyran, Table 2.4 for morpholine, Table 2.11 for chromene, isochromene and xanthene, and Table 3.2 for chromane and isochromane.

Example:



4*H*-thiopyran (PIN)
4*H*-thiine

P-15.5.3.2 Replacement in characteristic groups expressed as suffixes

Replacement in suffixes is limited to –OO–, =S and –S–, =Se and –Se–, =Te and –Te–, =NH and =NNH$_2$ and any combination of these affixes. Suffixes including a carbon atom and those corresponding to sulfonic and sulfinic acids and their analogues are modified by infixes. Other suffixes are modified by prefixes. For examples and the order of seniority of suffixes modified by functional replacement see Tables 4.4 and 4.5 and Appendix 2.

Examples:

–CO-OOH	carboperoxoic acid
–CO-SH	carbothioic *S*-acid

$-CS\text{-}OH$	carbothioic *O*-acid
$-C(=NH)\text{-}OH$	carboximidic acid
$-SO\text{-}OOH$	sulfinoperoxoic acid
$-S(=NNH_2)\text{-}OH$	sulfinohydrazonic acid
$-(C)O\text{-}SH$	thioic acid
$-(C)S\text{-}NH_2$	thioamide (no contraction to thiamide)
$=S$	thione
$-SeH$	selenol

P-15.5.3.3 Functional replacement in prefixes

Functional replacement is used to modify prefixes containing oxygen atoms by the prefixes ‘thio’, ‘seleno’, and ‘telluro’. Prefixes are described in appropriate sections of Chapter 6 and listed in Appendix 1.

Examples:

$-C\{O/S\}H$	thiocarboxy (PIN)
$=S$	thioxo sulfanylidene (PIN)

P-15.5.3.4 Functional replacement in functional parents

Functional replacement is used to modify carboxylic acids and oxoacids, by prefixes and suffixes according to specific rules given in P-15.5.3.4.1 and P-15.5.3.4.2 below. It is also used to modify two retained names expressing functional parent structures, urea and semicarbazone, as described in P-15.5.3.4.3 below. Functional replacement is not used to replace oxygen atoms in ketones, alcohols, and derivatives such as acetals and ketals, etc.; systematic names are recommended instead.

Examples:

$CH_3\text{-}CS\text{-}CH_3$	propane-2-thione (PIN) (not thioacetone)
$C_6H_5\text{-}SH$	benzenethiol (PIN) (not thiophenol)

P-15.5.3.4.1 In general nomenclature, retained names of monocarboxylic acids may be modified by the prefixes peroxy, thio, seleno and telluro to indicate the replacement of an oxygen atom by the replacing atom(s) $-OO-$, $-S-$ or $=S$, $-Se-$ or $=Se$, and $-Te-$ or $=Te$ (see P-65.1.1.4.2.2).

Examples:

CH_3-CO-SH	CH_3-CH_2-CS-OH
thioacetic *S*-acid ethanethioic *S*-acid (PIN)	thiopropionic *O*-acid propanethioic *O*-acid (PIN)

C_6H_5-CS-SH

dithiobenzoic acid
benzenecarbodithioic acid (PIN)

P-15.5.3.4.2 Names of mononuclear and polynuclear oxoacids are modified by prefixes and infixes listed in Table 1.6 according to the rules described in P-67.

Example:

CH_3-P(=NH)(OH)(SH)

methylphosphonimidothioic acid (PIN)

P-15.5.3.4.3 Retained names of acyclic polynitrogen functional parent compounds described in P-68.3.1 are modified by prefixes thio, seleno and telluro.

Examples:

H_2N-CS-NH_2	H_2N-NH-CS-NH_2
thiourea (PIN) carbonothioic diamide	thiosemicarbazide hydrazinecarbothioamide (PIN)

P-15.6 Conjunctive nomenclature

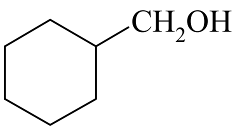
P-15.6.0 Introduction

Conjunctive nomenclature is based essentially on the conjunctive operation, by which a compound is formally constructed by subtracting the same number of hydrogen atoms from each component at each site where joined. It is traditionally reserved for naming compounds having a principal group attached to an acyclic component that is also directly attached by a carbon-carbon bond to a cyclic component. This method can be used in general nomenclature as an alternative to substitutive nomenclature, but it is not recommended for generating preferred IUPAC names. Its principles, conventions and rules have been established for Chemical Abstracts index nomenclature They are briefly discussed in this section. Its limitations are dealt with in P-15.6.2.

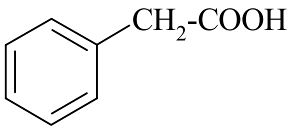
P-15.6.1 Name formation

P-15.6.1.1 Names are formed by juxtaposition of component names. The name of the cyclic component is cited first followed by the systematic or retained name of the component to which the principal characteristic group is attached.

Examples:



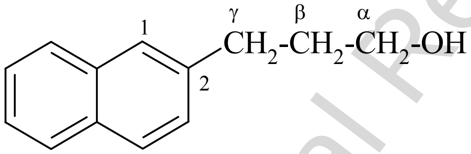
cyclohexanemethanol
cyclohexylmethanol (PIN)



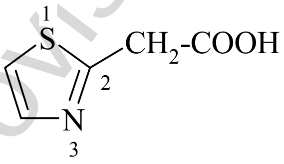
benzeneacetic acid
phenylacetic acid (PIN)

P-15.6.1.2 When necessary, the position of attachment of the side chain to the cyclic component is given by the appropriate locant placed before the name of the cyclic component, unless locants for structural features referring to the cyclic component, such as heteroatoms and indicated hydrogen, are already there; in this case the locant follows the name of the cyclic component chain. Since the acyclic component must terminate at the cyclic component, it is not necessary to give its locant of attachment. Carbon atoms of the side chain are indicated by Greek letters proceeding from the principal characteristic group to the cyclic component; these locants are used in the name only to locate other substituents on the side chain. The carbon atom of the characteristic group (in acids, aldehydes, nitriles, etc.) is omitted when allocating Greek letter locants.

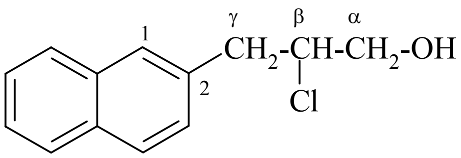
Examples:



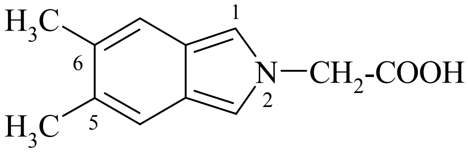
2-naphthalenepropanol
3-(naphthalen-2-yl)propan-1-ol (PIN)
3-(2-naphthyl)propan-1-ol



1,3-thiazole-2-acetic acid
1,3-thiazol-2-ylacetic acid (PIN)



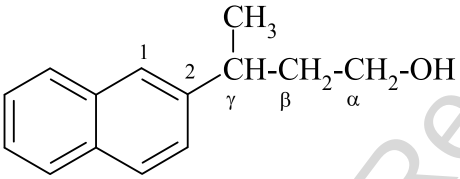
β-chloro-2-naphthalenepropanol
2-chloro-3-(naphthalen-2-yl)propan-1-ol (PIN)



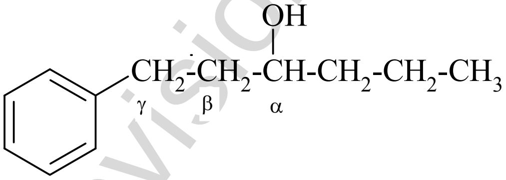
5,6-dimethyl-2*H*-isoindole-2-acetic acid
(5,6-dimethyl-2*H*-isoindol-2-yl)acetic acid (PIN)

P-15.6.1.3 For all purposes in conjunctive nomenclature the side chain is considered to extend only from the principal group to the cyclic component. Any other chain members, even those extending the side chain terminally, are named as substituents, appropriate prefixes and locants being placed before the name of the cyclic component.

Examples:



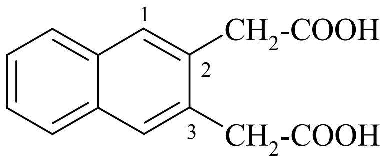
γ-methyl-2-naphthalenepropanol
3-(naphthalen-2-yl)butan-2-ol (PIN)
3-(2-naphthyl)butan-2-ol



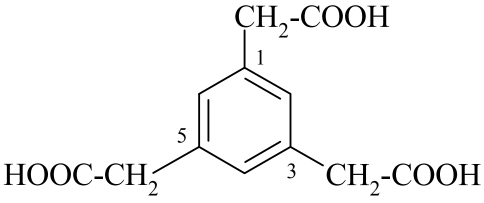
α-propylbenzenepropanol
1-phenylhexan-3-ol (PIN)

P-15.6.1.4 When a cyclic component carries at least two identical side chains, multiplying prefixes ‘di’, ‘tri’, etc. are used to indicate their number; these prefixes are placed before the name of the side chain.

Examples:



2,3-naphthalenediacetic acid
2,2′-naphthalene-2,3-diyldiacetic acid (PIN)



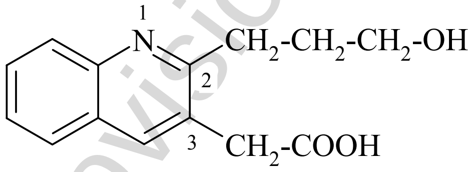
1,3,5-benzenetriacetic acid
benzene-1,3,5-triyltriacetic acid (PIN)

P-15.6.1.5 When different side chains are attached to a cyclic component:

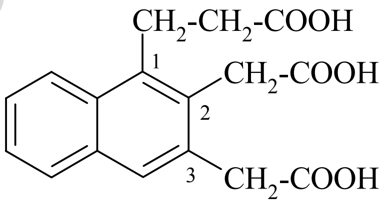
(a) the chain that contains the principal characteristic group is chosen for naming by the conjunctive method; or

(b) if there is more than one side chain containing the principal characteristic group, the conjunctive name that expresses the greater number of the principal characteristic group is chosen. When necessary, side chains are selected by applying the seniority order for selecting the principal chain (see P-44.3).

Examples:



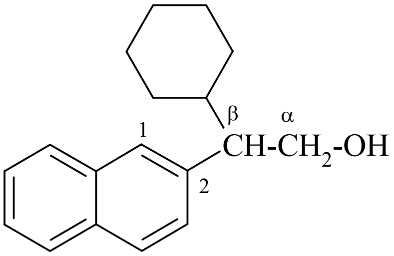
2-(3-hydroxypropyl)-3-quinolineacetic acid
[2-(3-hydroxypropyl)quinolin-3-yl]acetic acid (PIN)
(a carboxylic acid is senior to an alcohol)



1-(2-carboxyethyl)-2,3-naphthalenediacetic acid
[1-(2-carboxyethyl)naphthalen-2,3-diyl]diacetic acid (PIN)

P-15.6.1.6 When the side chain is linked to two different cyclic components, the senior ring or ring system is selected in accord with the seniority order of rings and ring systems (see P-44.2).

Example:



β-cyclohexyl-2-naphthaleneethanol
2-cyclohexyl-2-(naphthalen-2-yl)ethan-1-ol (PIN)
(naphthalene is senior to cyclohexane)

P-15.6.2 Limitations of conjunctive nomenclature

Conjunctive nomenclature is not used when:

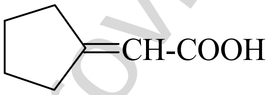
(a) a double bond links the acyclic component and a ring system;

(b) a double bond or a heteroatom is present in the side chain;

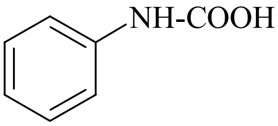
(c) two identical characteristic groups are located on the side chain;

(d) characteristic groups having priority for citation as principal groups are located on the cyclic component or when two or more characteristic groups of the same kind are located on the ring or ring system. In such cases, substitutive nomenclature is used.

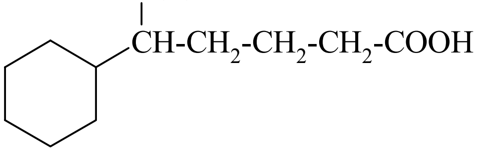
Examples:



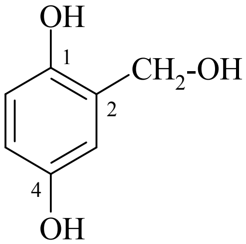
cyclopentylideneacetic acid (PIN)



phenylcarbamic acid (PIN)



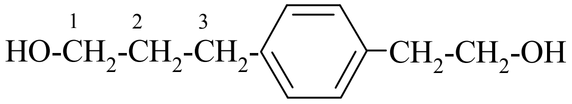
2-cyclohexylhexanedioic acid (PIN)



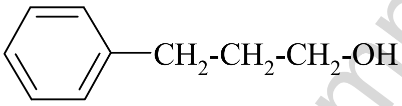
2-(hydroxymethyl)benzene-1,4-diol (PIN)

P-15.6.3 Analysis for construction of conjunctive names

Example 1:



Principal group	–OH	ol
Parent:		
ring:	C_6H_6	benzene
chain:	$CH_3-CH_2-CH_3$	propane
Parent including suffix		



benzenepropanol

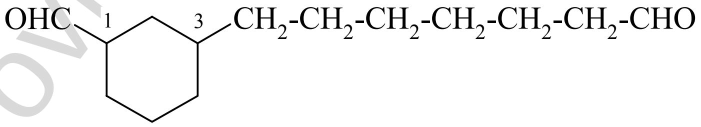
Prefix:	$-CH_2-CH_2-OH$	
Prefix components:	–OH	hydroxy
	$-CH_2-CH_3$	ethyl

Prefix name: 2-hydroxyethyl

Together with other rules, this analysis leads to the conjunctive and substitutive names:

4-(2-hydroxyethyl)benzenepropanol
3-[4-(2-hydroxyethyl)phenyl]propan-1-ol (PIN)

Example 2



Principal group:	–CHO	carbaldehyde or al
Parent:	ring	cyclohexane
	chain	heptane
Parent including suffix	ring + chain	cyclohexaneheptanal (a conjunctive name)
Prefix:	–CHO	formyl

Together with other rules this analysis leads to the names:

3-formylcyclohexaneheptanal
7-(3-formylcyclohexyl)heptanal (PIN)

P-16 Name writing

P-16.0 Introduction

Names are written in accordance with a symbolism specific to the nomenclature of organic compounds in order to avoid ambiguity and to establish an unequivocal relationship between a name and the corresponding structure. The recommended symbolism is particularly important in the formation of IUPAC preferred names. As usual, IUPAC recognizes the needs of other languages to introduce modifications specific to a particular language, but it is hoped that, whenever possible, the following conventions will be applied to construct IUPAC names for general use as well as for IUPAC preferred names.

In the 1979 and 1993 recommendations, names were written with a capital initial letter. This practice has been abandoned in recent publications in order to ensure that names of organic compounds are not considered as proper nouns; the usual practice to capitalize letters at the beginning of a sentence must however be respected.

P-16.1 Spelling

The spelling of elements is that given in the IUPAC *Nomenclature of Inorganic Chemistry* (ref. 11), for example, sulfur not sulphur, aluminium not aluminum, and caesium not cesium.

P-16.2 Punctuation

P-16.2.1 Commas are used:

(a) to separate locants, numerals, or italicized letters;

Examples: 1,2-dibromoethane (PIN, P-61.3.1)

N,*N*-diethylfuran-2-carboxamide (PIN, P-66.1.1.3.1.1)

(b) to separate numbers, as well as italicized letters, in fusion descriptors when they indicate the presence of separate attached components; however, italicized letters denoting *peri*-fused junctions are not separated by commas.

Examples: dibenzo[*a*,*j*]anthracene (PIN, P-25.3.3.1.1)

6*H*-pyrrolo[3,2,1-*de*]acridine (PIN, P-25.3.1.3)

P-16.2.2 Full stops

Full stops are used to separate numbers that denote lengths of bridges in polyalicyclic names constructed according to the von Baeyer system (see P-23.2.5.1) and of chain lengths between spiro atoms in von Baeyer spiro names (see P-24.2.1).

Examples: bicyclo[3.2.1]octane (PIN, P-23.2.3)

6-oxaspiro[4.5]decane (PIN, P-24.2.4.1.1)

P-16.2.3 Colons and semicolons

Colons separate related sets of locants; if a higher level of separation is required, semicolons are used.

Examples: benzo[1″,2″:3,4;4″,5″:3′,4′]dicyclobuta[1,2-*b*:1′,2′-*c*′]difuran (PIN, P-25.3.7.3)

$1^1,2^1:2^2,3^1$-tercyclopropane (PIN, P-28.3.1)

P-16.2.4 Hyphens

P-16.2.4.1 Hyphens are used in substitutive names:

(a) to separate locants from words or word fragments;

Example: 2-chloro-2-methylpropane (PIN, P-61.3.1)

(b) after parentheses, if the final parenthesis is followed by a locant;

Examples: 1-(chloromethyl)-4-nitrobenzene (PIN, P-61.5.1)

N-(2-aminomethyl)-*N*,*N*′,*N*′-trimethylethane-1,2-diamine (P-62.2.1.3)

(c) to separate adjacent locants from a subsequent opening enclosing mark:

Examples: 1-(1,2,3,4-tetrahydroquinolin-1-yl)ethan-1-one (PIN, P-64.3.2)

N-acetyl-*N*-(3-chloropropanoyl)benzamide (PIN, P-66.1.2.1)

P-16.2.4.2 No hyphen is placed before a numerical prefix cited in front of a compound substituent enclosed by parentheses, even if that substituent begins with locants;

Example: *N*,1-bis(4-chlorophenyl)methanimine (PIN, P-62.3.1.2)

P-16.2.4.3 Hyphens in fusion names. Hyphens separate the two parts of a fusion descriptor, i.e., numbers and italicized letters.

Example: naphtho[1,2-*a*]azulene (PIN, P-25.3.1.3)

P-16.2.4.4 Hyphens related to stereodescriptors

Hyphens separate stereodescriptors from the rest of the name or the part of a name to which they relate.

Example: (2*E*)-but-2-ene (PIN, P-92.1.7.2)

P-16.2.5 A long hyphen (em dash)

An em dash is used to separate the names of components in adducts;

Example: carbon monoxide—borane (PIN, P-13.3.5)

P-16.2.6 Spaces are a very important type of punctuation for many kinds of names in the English language. If a space is required in a name, it must be used. On the other hand, the use of spaces where they are not required, for example, in substitutive names that must be written continuously from one end to the other using hyphens to connect the different parts, may be misleading. Spaces are used in:

(a) names of acids and salts:

Examples: acetic acid (PIN, P-65.1.1.1)

calcium diacetate (PIN, P-65.6.2.1)

(b) functional class names,

Examples: ethyl acetate (PIN, P-65.6.3.2.1)

2-(chlorocarbonothioyl)benzoyl cyanide (PIN, P-65.5.3)

butyl ethyl sulfoxide (P-63.6)
[ethanesulfonylbutane (PIN)]

(c) names formed using a class modifier,

Examples: cyclohexanone ethyl methyl ketal (P-66.6.5.1.1)
[1-ethoxy-1-methoxycyclohexane (PIN)]

pentan-2-one oxime (P-68.3.1.1.2)
[*N*-pentan-2-ylidenehydroxylamine (PIN)]

(d) additive names

Examples: ethylene oxide (P-63.5)
[oxirane (PIN)]

trimethylphosphane oxide (PIN, P-74.2.1.4)

P-16.3 Numerical (multiplicative) prefixes

Numerical prefixes are derived from Greek and Latin number names (see P-14.3) and are the principal method for describing a multiplicity of identical features of a structure in chemical names.

P-16.3.1 The basic numerical prefixes 'di', 'tri', 'tetra', etc. are used to indicate a multiplicity of substituent suffixes, conjunctive components, replacement affixes, simple (i.e., unsubstituted) substituent prefixes, and simple (i.e., unsubstituted) functional modification terms provided that there is no ambiguity (see also P-16.3.2).

Examples:

diol

dicarboxylic acid

tricyclohexyl

di(tridecyl)

diamido

diaza

di(propan-2-yl)

di(tetradecane-1,14-diyl)

tetra(2-naphthyl)
[tetra(naphthalen-2-yl) (PIN)]

dioxime

dibenzenesulfonate

di(isoxazol-3-yl)
[di([1,2-oxazol-3-yl) (PIN)]

benzene-1,3,5-triacetic acid (P-15.6.1.4)
[benzene-1,3,5-triyltriacetic acid (PIN)]

di(cyclohexane-1-carboxylic acid)

P-16.3.2 The numerical prefixes 'bis', 'tris', 'tetrakis', etc., are used to indicate a multiplicity of complex (i.e., substituted) substituent prefixes or functional modifiers.

Examples:

bis(2-aminoethyl) (PIN)

ethane-1,2-diylbis(oxymethylene) (PIN)

bis(2-chloropropan-2-yl) (PIN)

bis(phenylhydrazone)
[bis(phenylhydrazinylidene)(PIN)]

These prefixes are also used when the use of 'di', 'tri', etc.:

(a) indicates another structure; or,

(b) is (or could be) ambiguous; this usually happens when an analogue of the term being multiplied begins with a basic numerical prefix.

Examples:

(a) tris(methylene) (PIN) indicates three methylene ($-CH_2-$) groups;. trimethylene [propane-1,3-diyl (PIN)] describes the multiplicative substitutive group $-[CH_2]_3-$;

(b) tris(decyl) (PIN) indicates three decyl ($C_{10}H_{11}$–) groups; tridecyl (PIN) describes the $C_{13}H_{14}$– substitutive group;

(c) bisoxy) (PIN) indicates two oxy (–O–) groups; dioxy has been used to mean both a –OO– group (peroxy, PIN) and two oxy (–O–) (PIN) groups

(d) bis(benzo[*a*]anthracen-1-yl) (PIN)

(e) benzo[1,2-*c*:3,4-*c*′]bis[1,2,5]oxadiazole (PIN)

(f) ethane-1,2-diylbis(azanediyl) (PIN)

P-16.3.3 The numerical prefixes 'bi', 'ter', 'quater', etc. are used mainly in naming ring assemblies (see P-28).

Examples: 1,1′-biphenyl (PIN, P-28.2.3)

$1^2,2^2{:}2^6,3^2{:}3^6,4^2$-quaterpyridine (PIN, P-28.3.1)

P-16.3.4 The prefix 'mono' is usually omitted in names of organic compounds. However, it is used to indicate that only one characteristic group of a parent structure has been modified. The ending 'kis' is never associated with 'mono'.

Example: monoperoxyphthalic acid (P-65.1.4.2)
2-carboxybenzenecarboperoxoic acid (PIN)

P-16.4 Enclosing marks

Parentheses, ( ), (also called 'curves' or 'round brackets'), brackets, [ ], (also called 'square brackets'), and braces { }, (also called 'curly brackets') are used in chemical nomenclature to set off parts of a name dealing with specific structural features in order to convey the structure of a compound as clearly as possible. It is important to note that they are used differently in names of organic and inorganic compounds.

All enclosing marks is recommended in preferred IUPAC names. In general nomenclature, when there is no possible ambiguity, enclosing marks may be omitted to simplify a name.

P-16.4.1 Parentheses (also called curves or round brackets)

P-16.4.1.1 Parentheses are used around complex (substituted) prefixes; after the numerical multiplicative prefixes 'bis', 'tris', etc.; and to enclose a multiplied parent structure consisting of a parent hydride and a substituent suffix even though preceded by a simple prefix, such as 'di', 'tri', etc..

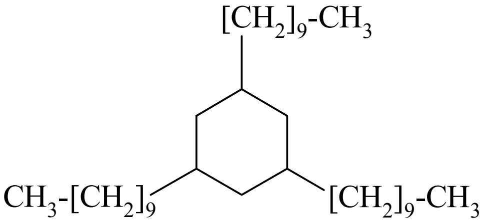
Examples:

$Cl\text{-}CH_2\text{-}SiH_3$

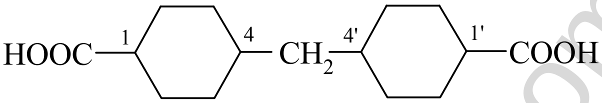
(chloromethyl)silane (PIN)

$(HO\text{-}CH_2\text{-}CH_2\text{-}O)_2CH\text{-}COOH$

bis(2-hydroxyethoxy)acetic acid (PIN)



1,3,5-tris(decyl)cyclohexane (PIN)
(not 1,3,5-tridecylcyclohexane)



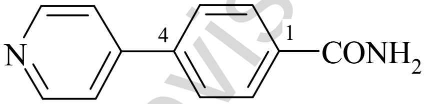
4,4′-methylenedi(cyclohexane-1-carboxylic acid) (PIN)

$H\{S/O\}C\text{-}CH_2\text{-}CH_2\text{-}C\{O/S\}H$

butanebis(thioic acid) (PIN)

P-16.4.1.2 Parentheses are used around simple substituent prefixes to separate locants of the same type referring to different structural elements, even though only one may be expressed.

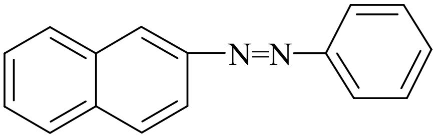
Example:



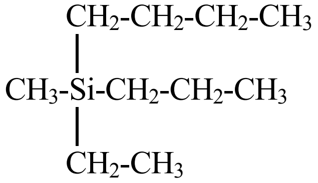
4-(pyridin-4-yl)benzamide (PIN)
4-(4-pyridyl)benzamide

P-16.4.1.3 Parentheses are placed around prefixes denoting simple substituent groups in front of parent hydrides when no locants are necessary and around prefixes defining simple substituent groups qualified by locants. A minimum of parentheses must be used. Enclosing marks are never used around the name of the first cited simple substituent group.

Examples:



naphthalen-2-yl(phenyl)diazene (PIN)
2-naphthyl(phenyl)diazene

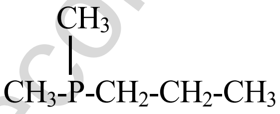


$$\begin{array}{l} \quad\;\; CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3 \\ \quad\;\; | \\ CH_3\text{-}Si\text{-}CH_2\text{-}CH_2\text{-}CH_3 \\ \quad\;\; | \\ \quad\;\; CH_2\text{-}CH_3 \end{array}$$

butyl(ethyl)methyl(propyl)silane (PIN)

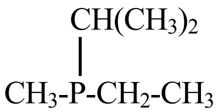
$CH_3\text{-}SiH_2Cl$

chloro(methyl)silane (PIN)



$$\begin{array}{l} \quad\;\; CH_3 \\ \quad\;\; | \\ CH_3\text{-}P\text{-}CH_2\text{-}CH_2\text{-}CH_3 \end{array}$$

ethyl(methyl)propylphosphane (PIN)



$$\begin{array}{l} \quad\;\; CH(CH_3)_2 \\ \quad\;\; | \\ CH_3\text{-}P\text{-}CH_2\text{-}CH_3 \end{array}$$

ethyl(methyl)propan-2-ylphosphane (PIN)
ethyl(isopropyl)methylphosphane

P-16.4.1.4 Parentheses are placed around the prefix denoting simple hydrocarbyl substituents adjacent to the name ‘amine’ in amines named by using the parent structure ‘amine’, when several different substituent groups are present. This requirement is necessary to insure the specificity of this kind of names of amines and to distinguish them from older names. Other parentheses are used as needed.

Examples: (2-chloroethyl)(propyl)amine (P-62.2.1.2.1)
[*N*-(2-chloroethyl)propan-1-amine (PIN)]

butyl(ethyl)(propyl)amine (P-62.2.1.2.1)
[*N*-ethyl-*N*-propylbutan-1-amine (PIN)]

butyl(ethyl)(methyl)amine (P-62.2.1.2.1)
[*N*-ethyl-*N*-methylbutan-1-amine (PIN)]

P-16.4.1.5 Parentheses are used to isolate the second locant of a compound locant, around locants denoting ring numbering in phane nomenclature, and to enclose fullerene identifiers.

Examples: bicyclo[8.5.1]hexadec-1(15)-ene (PIN, P-31.1.1.1)

1(1,3),4(1,4)-dibenzenacycloheptaphane (PIN, P-26.4.2.2)

(C_{60}-I_h)[5,6]fullerene (PIN, P-27.2.2)

P-16.4.1.6 Parentheses are used to enclose 'added hydrogen' and its locant, stereodescriptors such as '*E*', '*Z*', '*R*', '*S*', '*cis*', '*trans*', etc., and descriptors for isotopically substituted compounds;

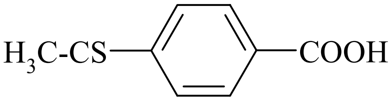
Examples: phosphinin-2(1*H*)-one (PIN, P-14.6)

(2*E*)-but-2-ene (PIN, P-92.1.7.2)

(^{13}C)methane (PIN, P-82.2.1)

P-16.4.1.7 Parentheses are used to avoid ambiguity.

Example:



4-(thioacetyl)benzoic acid
[4-ethanethioylbenzoic acid (PIN)]

P-16.4.1.8 Parentheses are used to enclose groups attached to a chain in linear formulas.

Examples:

CH_3-CH(SH)-CH_3 propane-2-thiol (PIN, P-63.1.5)

CH_3-CH(OH)-CO-CH_3 3-hydroxybutan-2-one (PIN, P-64.8)

P-16.4.2 Brackets (also called square brackets)

P-16.4.2.1 Brackets enclose descriptors denoting fusion sites in fused ring systems and enclose numbers denoting the length of bridges and chains connecting spiro atoms in names of polyalicyclic ring systems constructed according to von Baeyer methods. They also enclose ring assembly names when these are followed by a principal group suffix or a cumulative suffix and enclose names of components in von Baeyer spiro names.

Examples: naphtho[2,1-*a*]azulene (PIN, P-25.3.1.3)

bicyclo[3.2.1]octane (PIN, P-23.2.2)

spiro[4.5]decane (PIN, P-24.2.1)

[2,2′-bipyridin]-4-yl (PIN, P-29.3.5)

spiro[cyclohexane-1,1′-indene] (PIN, P-24.5.1)

P-16.4.2.2 Brackets enclose locants that describe structural features of components, such as double bonds in bridges and heteroatoms of component rings in names of fused ring systems.

Examples: 6,7-(prop[1]en[1]yl[3]ylidene)benzo[*a*]cyclohepta[*e*][8]annulene (PIN, P-25.4.3.3)

5*H*-pyrido[2,3-*d*][1,2]oxazine (PIN, P-25.3.2.4)

P-16.4.2.3 Brackets enclose the numerals that describe ring size in annulenes and fullerenes.

Examples: [10]annulene (P-22.1.2)
[cyclodeca-1,3,5,7,9-pentaene (PIN)]

(C_{60}-I_h)[5,6]fullerene (PIN, P-27.2.2)

P-16.4.2.4 Brackets enclose substituent prefixes in which parentheses have already been used.

Example: 4-[(hydroxyselanyl)methyl]benzoic acid (PIN, P-63.4.2,2)

P-16.4.2.5 Brackets are used to enclose descriptors for isotopically labeled compounds.

Example: [^{13}C]methane (PIN, P-83.1.3)

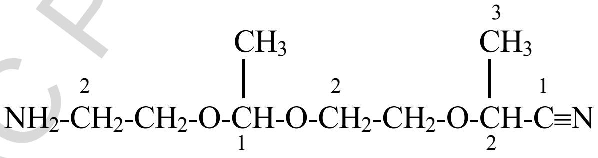
P-16.4.2.6 Brackets are employed in formulae to indicate repetition of a group in a chain.

Example: $CH_3\text{-}[CH_2]_{68}\text{-}CH_3$ heptacontane (PIN, P-21.2.1)

P-16.4.3 Braces (also called curly brackets)

P-16.4.3.1 Braces are used to enclose substituent prefixes in which brackets and parentheses have already been used.

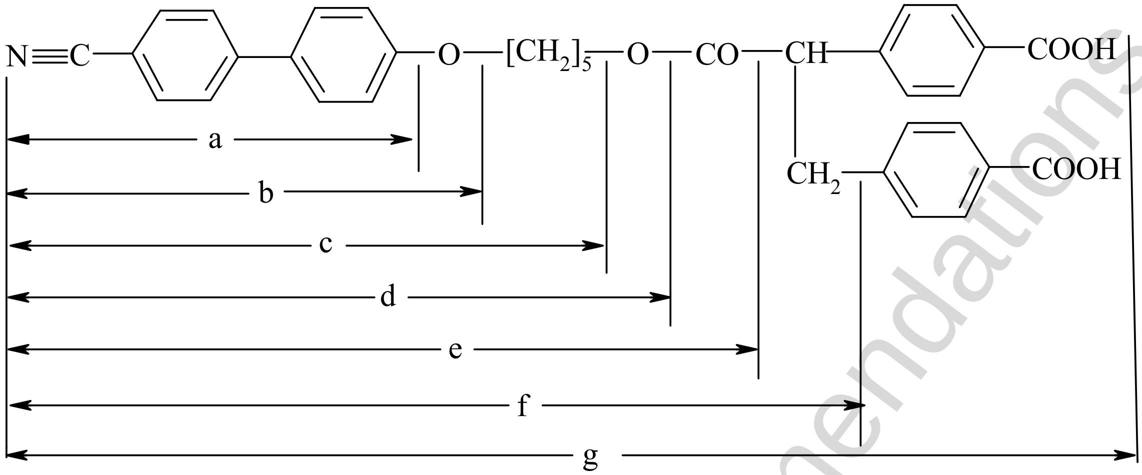
Example:



$$\mathrm{NH_2\text{-}\overset{2}{C}H_2\text{-}CH_2\text{-}O\text{-}\underset{1}{\overset{\overset{\displaystyle CH_3}{|}}{C}}H\text{-}O\text{-}\overset{2}{C}H_2\text{-}CH_2\text{-}O\text{-}\underset{2}{\overset{\overset{\overset{3}{CH_3}}{|}}{C}}H\text{-}\overset{1}{C}\equiv N}$$

2-{2-[1-(2-aminoethoxy)ethoxy]ethoxy}propanenitrile (PIN)

P-16.4.3.2 When additional enclosing marks are required, the nesting order is {[({[( )]})]}, etc., as illustrated in Fig. 1.2.



(a) = 4′-cyanobiphenyl-4-yl

(b) = (4′-cyanobiphenyl-4-yl)oxy

(c) = 5-[(4′-cyanobiphenyl-4-yl)oxy]pentyl

(d) = {5-[(4′-cyanobiphenyl-4-yl)oxy]pentyl}oxy

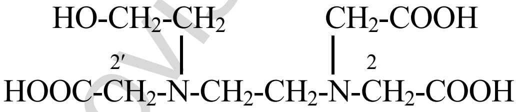
(e) = ({5-[(4′-cyanobiphenyl-4-yl)oxy]pentyl}oxy)carbonyl

(f) = 1-[({5-[(4′-cyanobiphenyl-4-yl)oxy]pentyl}oxy)carbonyl]ethane-1,2-diyl

(g) = 4,4′-{1-[({5-[(4′-cyanobiphenyl-4-yl)oxy]pentyl}oxy)carbonyl]ethane-1,2-diyl}dibenzoic acid (PIN)

FIG. 1.2 Nesting order of enclosing marks

Example:



$$\text{HOOC-}\overset{2'}{\text{CH}_2}\text{-}\overset{\overset{\text{HO-CH}_2\text{-CH}_2}{|}}{\text{N}}\text{-CH}_2\text{-CH}_2\text{-}\overset{\overset{\text{CH}_2\text{-COOH}}{|}}{\text{N}}\text{-}\overset{2}{\text{CH}_2}\text{-COOH}$$

2,2′-({2-[(carboxymethyl)(2-hydroxyethyl)amino]ethyl}azanediyl)diacetic acid
[*N*-(carboxymethyl)-*N*′-(2-hydroxyethyl)-*N*,*N*′-ethane-1,2-diyldiglycine (PIN)]

P-16.5 Italicization

Italicizing marks letters that are not involved in the primary stage of alphanumerical ordering. In manuscripts, italics are conventionally indicated by underlining when an italic font is not available.

P-16.5.1 Lower case italic letters are used in descriptors for fusion sites in names of fused ring systems.

Example: selenopheno[2,3-*b*]selenophene (PIN, P-25.3.1.3)

The letters *o*, *m*, and *p* have been used in place of *ortho*, *meta*, and *para*, respectively, to designate the 1,2- 1,3-, and 1,4- isomers of disubstituted benzene. This usage is strongly discouraged and is not used in preferred IUPAC names.

Examples: *o*-xylene (P-61.2.3)
[1,2-xylene (PIN)]

p-dinitrosobenzene (P-61.5.1)
[1,4-dinitrosobenzene (PIN)]

P-16.5.2 Italicized elements symbols, such as *O*, *N*, *As*, are locants indicating attachment of a substituent to these heteroatoms

Examples: *N*,*N*-diethylethanamine (PIN, P-62.2.1.2.1)

O-ethyl hexaneselenoate (PIN, P-65.6.3.2.4)

The italic element symbol *H* denotes indicated or added hydrogen.

Examples: 1*H*-azepine (PIN, P-22.2.2.1.4)

quinolin-2(1*H*)-one (PIN, P-64.3.1)

P-16.5.3 Italic terms, syllables and capital Roman letters are used in some structural descriptors and stereodescriptors, such as '*cis*', '*trans*', '*R*', '*S*', '*E*', '*Z*', '*r*', '*c*', '*t*', and '*retro*'.

Examples: *tert*-, but not 'iso' (P-29.6.3)

'*E*' and '*Z*' (P-92.1.7.1); '*cis*', and '*trans*' (P-92.2.1.1); '*r*', '*c*', and '*t*' (P-92.2.1.1); '*r*' and '*s*' (P-91.4)

'*R*' and '*S*' (P-92.1.1), '*R**' (spoken R-star), '*S**' (spoken S-star), '*rel*' (P-92.1.2)

'*meso*' (P-92.2.2.6), '*ambo*' (P-92.2.2.7), '*rac*' (P-92.1.3)

'*M*' and '*P*', 'R_a' and 'S_a', 'R_p' and 'S_p' (P-982.1.5)

'*TPY*-3', '*TS*-3', '*SS*-4', '*TBPY*', '*SPY*', and '*OC*' (P-92.1.9)

'*retro*', but not 'abeo', 'apo', 'cyclo', 'de', 'des', 'homo', 'nor' or 'seco' (P-101.3.1 through P-101.3.7)

P-16.6 Elision of vowels

P-16.6.1 Vowels are systematically elided as follows:

(a) the terminal letter 'e' in names of parent hydrides or endings 'ene' and 'yne' when followed by a suffix or 'en' ending beginning with 'a', 'e', 'i', 'o', 'u' or 'y';

Examples: pentanal (PIN, P-6.6.2.1)

cyclopentadec-1-en-4-yne (PIN, P-31.1.3.1)

methanium (PIN, P-73.1.1.2)

butan-2-one (PIN, P-64.2.2.1)

tetramethylboranuide (PIN, P-72.3)

sulfanyl (PIN, P-29.3.1)

(b) in Hantszch-Widman names, the final letter ‘a’ of an ‘a’ prefix when followed by a vowel;

Examples: 1,3-thiazole (PIN, P-22.2.2.1.2)
(not 1,3-thiaazaole)

1,6,2-dioxazepane (PIN, P-22.2.2.1.2)
(not 1,6,2-dioxaazaepane)

(c) the terminal letter ‘a’ in the names of numerical multiplicative affixes when followed by a suffix beginning with ‘a’ or ‘o’;

Examples: [1,1′-biphenyl]-3,3′,4,4′-tetramine (PIN, P-62.2.1.1.2)
(not [1,1′-biphenyl]-3,3′,4,4′-tetraamine)

benzenehexol (PIN, P-63.1.2)
(not benzenehexaol)

(d) the terminal letter ‘a’ of an element ‘a’ prefix in ‘a(ba)$_n$’ repeating unit names when followed by a vowel;

Examples: disilazane (preselected name, P-21.2.3.1)
(not disilaazane)

tetrastannoxane (preselected name, P-21.2.3.1)
(not tetrastannaoxane)

(e) the terminal letter ‘o’ of a functional replacement infix when followed by a vowel;

Example: *P*-phenylphosphonamidimidic acid (PIN, P-67.1.2.1)
(not *P*-phenylphosphonoamidoimidic acid)

(f) the terminal letter ‘o’ of ‘benzo’ in names of ‘benzoheterocycles’ formed by fusion of a benzene ring to a heteromonocycle whose name begins with a vowel [an exception to P-16.6.6(f)].

Examples: 3-benzoxepine (PIN, P-25.2.2.4)

4*H*-3,1-benzoxazine (PIN, P-25.2.2.4)

P-16.6.2 There is no elision of terminal vowels in the following cases:

(a) in conjunctive names

Example: benzeneacetic acid (P-15.6.1.1)
[phenylacetic acid (PIN)]

(b) from replacement or numerical multiplicative prefixes in skeletal replacement (‘a’) nomenclature;

Example: 2,4,6,8-tetrasilaundecane (PIN, P-15.4.1.3)

(c) from numerical multiplicative prefixes in multiplying parent compounds;

Example: 2,2′,2″,2‴-(ethane-1,2-diyldinitrilo)tetraacetic acid (P-15.3.2.6)
[*N*,*N*′-ethane-1,2-diylbis[*N*-(carboxymethyl)glycine (PIN)]

(d) from numerical multiplicative prefixes before substituent prefix names;

Example: 5,6,7,8-tetraiodo-1,2,3,4-tetrahydroanthracene-9-carboxylic acid (PIN, P-65.1.2.4)

(e) from component prefixes of compound and complex prefixes before following prefixes beginning with a vowel;

Examples: chloroamino (preselected name, P-34.3.1)

aminooxy (preselected name, P-68.3.1.1.1.5)

(f)) from prefixes designating attached components in fusion nomenclature; for example, the terminal letter ‘o’ of acenaphtho, benzo, perylo, phenanthro, and the terminal letter ‘a’ of anthra, cyclopropa, cyclobuta, are not elided before a vowel [see P-16.6.1(f) for an exception involving 'benzo'].

This recommendation is in accordance with P-25.3.1.3 (see below) and Rule R-2.4.1.1 in the 1993 Recommendations (ref. 2). Rule A-21.4 that recommended the elision in the 1979 Recommendations (ref. 1) is abrogated.

Examples: cyclopropa[*de*]anthracene (PIN, P-25.3.8.1)

naphtho[1,2-*a*]azulene (PIN, P-25.3.1.3)

P-16.7 Addition of vowels

P-16.7.1 For euphonic reasons, in functional replacement nomenclature the vowel ‘o’ is inserted between consonants.

Examples: ethanesulfonodiimidic acid (PIN, P-65.3.1.4)
(not ethanesulfondiimidic acid)

phenylphosphononitridic acid (PIN, P-67.1.1.2.2)
(not phenylphosphonnitridic acid)

P-16.7.2 For euphonic reasons, the letter ‘a’ is inserted between the root of the name for polyenes, polyynes, and polyenynes, and the numerical multiplying prefix ‘di’, ‘tri’, etc., preceding the ending ‘ene’ or ‘yne

Examples: buta-1,2-diene (PIN, P-31.1.1.2)
(not but-1,2-diene)

hexa-1,3-dien-5-yne (PIN, P-31.1.2.2.1)
(not hex-1,3-dien-5-yne)

P-16.8 Primes

P-16.8.1 Primes (′), double primes (″), triple primes (‴), etc., are used to differentiate identical locants, for example *N*,*N*′, 1,1′,1″. Such usage occurs:

(a) in multiplicative nomenclature to denote multiplied units and modify locants accordingly;

Example:

2,2′,2″-nitrilotriethanol (PIN, P-15.3.2.3)

(b) in spiro-fused compounds, to denote positions in polycyclic systems, identical or different;

Examples:

7,7′-spsirobi[bicycle[4.1.0]heptane] (PIN, P-24.3.1)

1*H*,1′*H*,1″*H*,3′*H*-2,2′:7,2″-dispiroter[naphthalene] (PIN, P-24.4.1)

spiro[cyclohexane-1,1′-indene] (PIN, P-24.5.1)

(c) in ring assemblies, to number identical ring components;

Examples:

1,1′-bi(cyclopropane) (PIN, P-28.2.1)

1,1′-biphenyl (PIN, P-28.2.3)

P-16.8.2 Primes also occur:

(a) in fusion nomenclature, to identify first and higher attached components, identical attached components and multiparent names;

Examples:

pyrido[1″,2″:1,2′]imidazo[4′,5′:5,6]pyrazino[2,3-*b*]phenazine (PIN, P-25.3.4.1.1)

difuro[3,2-*b*;2′,3′-*e*]pyridine (PIN, P-25.3.4.1.2)

cyclopenta[1,2-*b*:5,1-*b*′]bis[1,4]oxathiazine (PIN, P-25.3.4.1.3)

(b) in fullerenes *ortho*-fused to organic ring or ring systems, to identify positions in the nonfullerene component;

Example:

3′*H*-cyclopropa[1,9](C_{60}-I_h)[5,6}fullerene (PIN, P-27.6.1)

(c) in natural product nomenclature, to identify positions in ring(s) fused to a fundamental parent hydride;

Example:

benzo[2,3]-5α-androstane (PIN, P-101.5.1.1)

IUPAC Preferred Names
Chapter 2, Sect 20-24
September, 2004

CHAPTER P-2 PARENT HYDRIDES

P-20 Introduction

A parent hydride is the structure that is named before the addition of affixes denoting substituents to yield the name of a specific compound. Its name is understood to signify a definite population of hydrogen atoms attached to a skeletal structure. Acyclic parent hydrides are always saturated and unbranched, for example, pentane and trisilane. Cyclic parent hydrides are usually either fully saturated, for example, cyclopentane, cyclotrisiloxane, azepane, bicyclo[3.2.1]octane, and spiro[4.5]decane, or fully unsaturated, i.e., they contain the maximum number of noncumulative double bonds, for example, benzene, pyridine, 1,3-oxazole, 1*H*-phenalene, phenanthroline and benzo[*a*]acridine. Also, there are parent hydrides that are partially saturated, for example, spiro[1,3-dioxolane-2,1′-[1*H*]indene], and there are combinations of cyclic and acyclic hydrides, having traditional retained names, for example toluene.

Names of parent hydride names that do not contain skeletal carbon atoms, for example trisilane, are not designated as preferred IUPAC names in these recommendations. Instead they are called preselected, i.e., they are used to generate preferred IUPAC for derivatives substituted by organic (carbon-containing) substituents (see P-12.2). They may, however, become IUPAC preferred names depending on decisions of a team formed to decide IUPAC preferred names for inorganic (noncarbon-containing) compounds.

Names of parent hydrides are either traditional names that are retained or systematic names formed in accordance with specific rules. Rules and names must be unambiguous and clear. In order to achieve this goal and keep rules simple and concise, the rules for selecting preferred IUPAC names and preselected names of parent hydrides and prefixes denoting substituent groups derived from parent hydrides are not provided in this Chapter. These rules are given in Chapter 5.

P-21 Mononuclear and acyclic polynuclear parent hydrides

P-21.1 Mononuclear parent hydrides

P-21.1.1 Mononuclear hydrides with standard bonding numbers

P-21.1.1.1 Systematic names

The names of mononuclear hydrides of the elements for use as parents in naming organic compounds by substitutive nomenclature are given in Table 2.1. Most are formed systematically by combining the ‘a’ term of the element (with elision of the terminal letter ‘a’ before the ending ‘ane’, patterned after methane, for example, borane for BH_3, silane for SiH_4, etc.). There are important exceptions: methane, which is the retained name for CH_4, oxidane for H_2O, sulfane for H_2S, selane for H_2Se, tellane for H_2Te, polonane for H_2Po, and bismuthane for BiH_3 (see Table 2.1). The systematically formed names oxane, thiane, selenane, tellurane, polane, and bismane, are Hantzsch-Widman names designating the corresponding saturated six-membered rings with a single heteroatom. ‘Carbane’ has never been used in place of methane; it is not recommended.

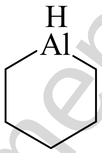
Table 2.1 Systematic names of mononuclear hydrides of Groups 13, 14, 15, 16 and 17 with normal bonding numbers
(all names except for methane are preselected)

Groups	13	14	15	16	17
	BH_3	CH_4	NH_3	OH_2	FH
	borane	methane	azane	oxidane	fluorane
	AlH_3	SiH_4	PH_3	SH_2	ClH
	alumane	silane	phosphane	sulfane	chlorane
	InH_3	GeH_4	AsH_3	SeH_2	BrH
	indigane	germane	arsane	selane	bromane
	GaH_3	SnH_4	SbH_3	TeH_2	IH
	gallane	stannane	stibane	tellane	iodane
	TlH_3	PbH_4	BiH_3	PoH_2	HAt
	thallane	plumbane	bismuthane	polane	astatane

The newly recommended names gallane and thallane are formed systematically. Alumane and indigane are exceptions. The name ‘aluminane’ could be ambiguous as it could designate the mononuclear hydride AlH_3 and the saturated six-membered ring with one aluminium atom that has a Hantzsch-Widman name denoted by the ending ‘-inane’. The name ‘alane’ has been used, but must also be discarded because its systematically derived substituent group, H_2Al-, would be named ‘alanyl’, the well entrenched name for the acyl group derived from the amino acid alanine. The name alumane has no negative connotation. The prefix ‘aluma’ is recommended for forming Hantszch-Widman names, and thus, the name ‘aluminane’ describes the saturated six-membered ring monocycle containing one aluminium atom (see P-22.2.2). The systematically formed name ‘indane’ cannot be used because it is already used to designate a partially saturated bicyclic fused hydrocarbon. Reich and Richter (ref . 15) called the element indium in 1863 after the indigo colored flame test, recognized as different than the color from caesium. Returning to the source indigo, ‘indigane’ could be an acceptable name; it is thus recommended for the hydride InH_3.

AlH_3

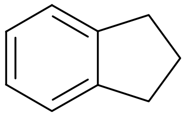
alumane (preselected name; see P-12.2)
(not alane)



aluminane (PIN)

InH_3

indigane (preselected name; see P-12.2)



indane
2,3-dihydro-1*H*-indene (PIN)

The monohydride names listed in Table 2.1 constitute the basis of ‘generalized ane nomenclature’. Substitutive nomenclature as applied to alkanes, cycloalkanes and polycycloalkanes has been systematically extended to hydrides of elements of Groups 13, 14, 15, 16, and 17. Generalized ‘ane‘ nomenclature is divided into ‘carbane nomenclature’, which covers the traditional substitutive nomenclature for carbon parent hydrides, and ‘heterane nomenclature’, which relates to atoms other than carbon, the ‘heteroatoms’ in the nomenclature of organic compounds.

P-21.1.1.2 Retained names

The names ‘phosphine’, PH_3, ‘arsine’, AsH_3, ‘stibine’, SbH_3, and ‘bismuthine’, BiH_3, are not retained.

The common names water, ammonia, the binary names for the hydracids of Group 17, for example hydrogen chloride, and binary names for the hydrides of Group 16, for example hydrogen sulfide, are retained. However, systematic alternatives to these common names, e.g. oxidane for water and azane for ammonia; and for the binary names of hydracids of Group 17 and the hydrides of Group 16, e.g., chlorane for hydrogen chloride and sulfane for hydrogen sulfide, are necessary for naming some derivatives and for generating names of radicals, ions, and polynuclear homologues.

P-21.1.2 Mononuclear parent hydrides with nonstandard bonding numbers

P-21.1.2.1 Systematic names

If the bonding number of the element differs from the standard one as defined in P-14.1 and exemplified in Table 2.1, the name of the hydride is modified by affixing the symbol λ^n, where '*n*' is the bonding number, to the name of the hydride (see P-14.1).

P-21.1.2.2 Retained names

The names 'phosphorane', PH_5; 'arsorane', AsH_5; 'stiborane', SbH_5; are retained for use in general nomenclature. However, the names 'sulfurane', H_4S; 'selenurane', H_4Se; 'iodinane', H_3I; 'persulfurane', H_6S; and 'periodinane, H_5I, which have been used in recent literature, are not recommended.

Examples:

H_3I

λ^3-iodane (preselected name; see P-12.2)
(not iodinane)

H_4S

λ^4-sulfane (preselected name; see P-12.2)
(not sulfurane)

SnH_2

λ^2-stannane (preselected name: see P-12.2)

PH_5

λ^5-phosphane (preselected name; see P-12.2)
phosphorane

AsH_5

λ^5-arsane (preselected name; see P-12.2)
arsorane

SbH_5

λ^5-stibane (preselected name; see P-12.2)
stiborane

P-21.2 Acyclic polynuclear parent hydrides

P-21.2.1 Hydrocarbons

The saturated unbranched acyclic hydrocarbons C_2H_6, C_3H_8, and C_4H_{10} have the retained names ethane, propane, and butane, respectively. Systematic names for the higher members of this series consist of a numerical term (see Table 1.4), followed by the ending 'ane' with elision of the terminal letter 'a' from the numerical term. The generic name for saturated acyclic hydrocarbons (branched or unbranched) is ‘alkane’. The chain is numbered from one end to the other with arabic numbers. Brackets are employed in formulas to indicate repetition of groups in chains.

Examples:

$\overset{7}{C}H_3\text{-}\overset{6}{C}H_2\text{-}\overset{5}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_3$

heptane (PIN)

$\overset{20}{C}H_3\text{-}[CH_2]_{18}\text{-}\overset{1}{C}H_3$

icosane (PIN)
(the Beilstein and CAS index name is ‘eicosane’)

$\overset{23}{C}H_3\text{-}[CH_2]_{21}\text{-}\overset{1}{C}H_3$

tricosane (PIN)

$\overset{70}{C}H_3\text{-}[CH_2]_{68}\text{-}\overset{1}{C}H_3$

heptacontane (PIN)

P-21.2.2 Homogeneous acyclic parent hydrides other than hydrocarbons and boron hydrides

A compound consisting of an unbranched chain containing two or more identical heteroatoms saturated with hydrogen atoms is named by citing the appropriate multiplying prefix from Table 1.4 (with no elision of the terminal vowel of the multiplying prefix) followed by the name of the appropriate hydride according to P-2.1. These names are preselected (see P-12.2).

Examples:

$\overset{2}{N}H_2\text{-}\overset{1}{N}H_2$

hydrazine (retained name, preselected; see P-12.2)
diazane

$\overset{9}{N}H_2\text{-}[NH]_7\text{-}\overset{1}{N}H_2$

nonaazane (preselected name; see P-12.2)

$\overset{5}{Si}H_3\text{-}\overset{4}{Si}H_2\text{-}\overset{3}{Si}H_2\text{-}\overset{2}{Si}H_2\text{-}\overset{1}{Si}H_3$

pentasilane (preselected name; see P-12.2)

$\overset{5}{P}H_2\text{-}\overset{4}{P}H\text{-}\overset{3}{P}H\text{-}\overset{2}{P}H\text{-}\overset{1}{P}H_2$

pentaphosphane (preselected name; see P-12.2)

P-21.2.3 Heterogeneous acyclic parent hydrides. There are two types to be considered.

P-21.2.3.1 Heterogeneous parent hydrides composed of alternating atoms
P-21.2.3.2 Heterogeneous parent hydrides formed by skeletal replacement (‘a’) nomenclature

P-21.2.3.1 Heterogeneous parent hydrides composed of alternating heteroatoms, i.e., [a(ba)*n* hydrides], excluding carbon atoms

Compounds containing an unbranched chain of alternating atoms terminated by two identical atoms of the element coming later in the seniority order F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn < Pb > B > Al > Ga > In > Tl may be named by citing successively a multiplying prefix denoting the number of atoms of the terminal element followed by the ‘a’ term for that element, then the ‘a’ term of the other element in the chain and the ending ‘ane’. The terminal letter ‘a’ of an ‘a’ term is elided when followed by a vowel; the terminal vowel of a numerical prefix is not elided even when the ‘a’ term begins with the same vowel. When nitrogen atoms are present, names of amines could be considered as alternative names but are not recommended. These parent hydrides have priority to receive preferred names, as long as they are used to name carbon containing compounds, i.e., they are preselected names.

Examples:

7 6 5 4 3 2 1
SnH_3-O-SnH_2-O-SnH_2-O-SnH_3

tetrastannoxane
(preselected name; see P-12.2)

7 6 5 4 3 2 1
AsH_2-NH-AsH-NH-AsH-NH-AsH_2

tetraarsazane
(preselected name; see P-12.2)

3 2 1
SiH_3-NH-SiH_3

disilazane (preselected name; see P-12.2)
(not *N*-silylsilanamine)

P-21.2.3.2 Heterogeneous parent hydrides formed by skeletal replacement (‘a’) nomenclature

Heterogeneous acyclic parent hydrides consisting of chains containing at least one carbon atom and at least four heteroatoms, alike or different, and terminating with C, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, or Tl are named by skeletal replacement (‘a’) nomenclature (see P-15.4.2.1).

Examples:

11 10 9 8 7 6 5 4 3 2 1
CH_3-O-CH_2-CH_2-O-CH_2-CH_2-O-CH_2-O-CH_3

2,4,8,10-tetraoxaundecane (PIN)

11 10 9 8 7 6 5 4 3 2 1
CH_3-O-CH_2-CH_2-O-CH_2-CH_2-SiH_2-CH_2-S-CH_3

7,10-dioxa-2-thia-4-silaundecane (PIN)

8 7 6 5 4 3 2 1
$CH_3\text{-}S\text{-}SiH_2\text{-}CH_2\text{-}CH_2\text{-}SiH_2\text{-}O\text{-}CH_3$

2-oxa-7-thia-3,6-disilaoctane (PIN)

P-21.2.4 Heteroatoms with nonstandard bonding numbers

P-21.2.4.1 Heteroatoms with nonstandard bonding numbers are denoted by the λ^n symbol which is placed after each appropriate locant (see P-14.1). Low numbering is first given to the heteroatoms in the usual manner without regard to nonstandard bonding numbers.

Examples:

1 2 3
$SH\text{-}SH_2\text{-}SH$

2λ^4-trisulfane (preselected name; see P-12.2)

3 2 1
$SH\text{-}S\text{-}SH_5$

1λ^6-trisulfane (preselected name; see P-12.2)

3 2 1
$PH_4\text{-}PH_3\text{-}PH_4$

1λ^5,2λ^5,3λ^5-triphosphane (preselected name; see P-12.2)
(not tri-λ^5-phosphane)

6 5 4 3 2 1
$SH\text{-}SH_2\text{-}S\text{-}S\text{-}SH_4\text{-}SH$

2λ^6,5λ^4-hexasulfane (preselected name; see P-12.2)

P-21.2.4.2 When a choice is needed between the same skeletal atom with two or more nonstandard bonding numbers, low locants are assigned in order of the decreasing value of the bonding number, for example λ^6 is assigned a lower locant than λ^4.

Examples:

6 5 4 3 2 1
$SH\text{-}SH_2\text{-}S\text{-}S\text{-}SH_4\text{-}SH$

2λ^6,5λ^4-hexasulfane (preselected name; see P-12.2)

12 11 10 9 8 7 6 5 4 3 2 1
$CH_3\text{-}S\text{-}CH_2\text{-}CH_2\text{-}S\text{-}CH_2\text{-}CH_2\text{-}SH_2\text{-}CH_2\text{-}CH_2\text{-}S\text{-}CH_3$

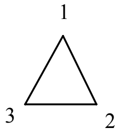
2,5λ^4,8,11-tetrathiadodecane (PIN)

P-22 Monocyclic parent hydrides

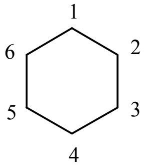
P-22.1 Monocyclic hydrocarbons

P-22.1.1 The names of saturated monocyclic hydrocarbons are formed by attaching the nondetachable prefix ‘cyclo’ to the name of the acyclic saturated unbranched hydrocarbon with the same number of carbon atoms. The generic name of monocyclic hydrocarbons is ‘cycloalkane’. Numbering proceeds sequentially around the ring.

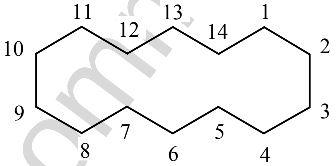
Examples:



cyclopropane (PIN)



cyclohexane (PIN)



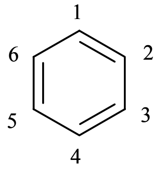
cyclotetradecane (PIN)

P-22.1.2 Unsubstituted monocyclic hydrocarbon polyenes having the maximum number of non-cumulative double bonds and with the general formula of C_nH_n or C_nH_{2n+1}, (with n greater than 6) are called annulenes generically. A specific annulene is named as an [n]annulene, where n is the number of carbon atoms of the ring and is greater than 6. When n is an odd number, i. e., when the annulene has the general formula C_nH_{2n+1}, the extra hydrogen atom is denoted as ‘indicated hydrogen’ (see P-14.6) and is assigned the locant ‘1’. Such annulene names may be used in general nomenclature and are the IUPAC preferred names for parent components in fusion nomenclature. Preferred IUPAC names for fully unsaturated monocyclic hydrocarbons are those of the corresponding cycloalkapolyenes (see P-31.1.3.1).

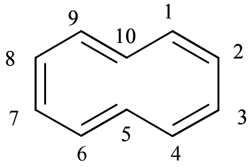
Benzene is the retained name for C_6H_6; the name [6]annulene is not recommended. Annulene names are used as parent components in fusion nomenclature (see P-25.3.2.1.1); but are not used as component prefixes.

In the numbering of annulenes, the locant ‘1’ is placed at any carbon atom in structures having an even number of carbon atoms; in annulenes having an odd number of carbon atoms, the locant ‘1’ is assigned to the carbon atom bearing the indicated hydrogen (see P-14.6). In cycloalkapolyene structures, the locant ‘1’ is always assigned to a carbon atom of a double bond.

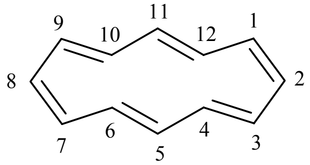
Examples:



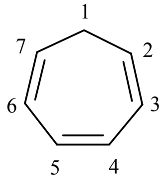
benzene (PIN)
(not [6]annulene)



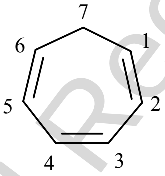
[10]annulene
cyclodeca-1,3,5,7,9-pentaene (PIN)



[12]annulene
cyclododeca-1,3,5,7,9,11-hexaene (PIN)

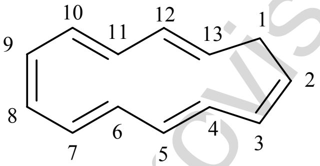


(I)

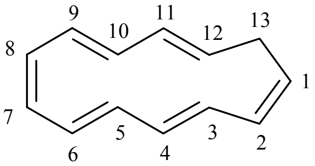


(II)

(I) 1*H*-[7]annulene
(II) cyclohepta-1,3,5-triene (PIN)



(I)

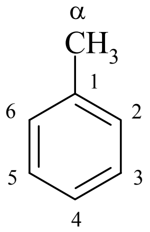


(II)

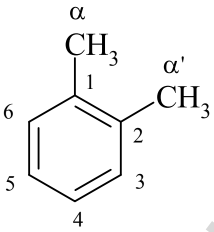
(I) 1*H*-[13]annulene
(II) cyclotrideca-1,3,5,7,9,11-hexaene (PIN)

P-22.1.3 Parent structures having retained names

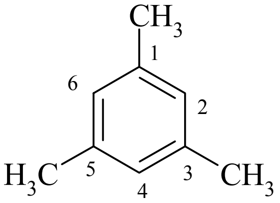
Toluene, xylene and mesitylene are specific parent hydrides that are composed of two components, one cyclic and the other acyclic and saturated. These names are retained due to a long and well established tradition. Toluene and xylene are preferred IUPAC names, but are not substitutable; toluene is substitutable under certain conditions (see P-46.3) for general nomenclature. Mesitylene is a retained name in general nomenclature only and cannot be substituted.



toluene (PIN)
(see P-46.3.1 for substitution rules)



xylene (1,2-,1,3-, and 1,4-isomers, PINs)
(no substitution)
o-, *m*-, and *p*-xylene



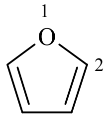
mesitylene
1,3,5-trimethylbenzene (PIN)

P-22.2 Heteromonocyclic parent hydrides

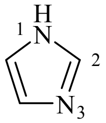
P-22.2.1 Retained names and names of derived chalcogen analogues

The retained names are listed in Table 2.2. The name ‘pyran’ can be modified by functional replacement to generate names for chalcogen analogues.

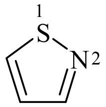
Table 2.2 Retained names of mancude heteromonocyclic parent hydrides



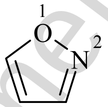
furan (PIN)



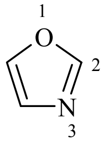
imidazole (PIN)
(1*H* isomer shown)



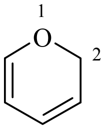
isothiazole
1,2-thiazole (PIN)



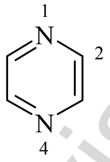
isoxazole
1,2-oxazole (PIN)



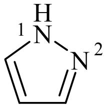
oxazole
1,3-oxazole (PIN)



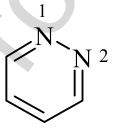
pyran (2*H*-isomer shown) (PIN)
thiopyran (S instead of O) (PIN)
selenopyran (Se instead of O) (PIN)
telluropyran (Te instead of O))PIN)



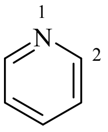
pyrazine (PIN)



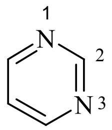
pyrazole (PIN)
(1*H* -isomer shown)



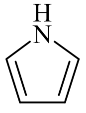
pyridazine (PIN)



pyridine (PIN)

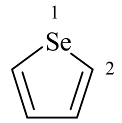


pyrimidine (PIN)

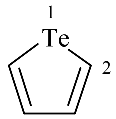


pyrrole (PIN)
(1*H*-isomer shown)

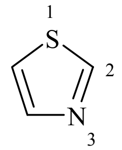
Table 2.2 (cont’d)



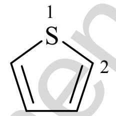
selenophene (PIN)



tellurophene (PIN)

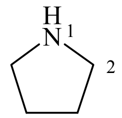


thiazole
1,3-thiazole (PIN)

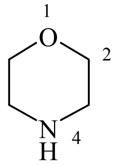


thiophene (PIN)

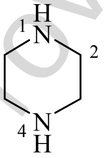
Table 2.3 Retained names of saturated heteromonocyclic parent hydrides used as preferred names and in general nomenclature



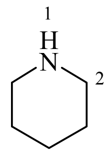
pyrrolidine (PIN)



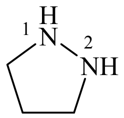
morpholine (PIN)
thiomorpholine (S instead of O) (PIN)
selenomorpholine (Se instead of O) (PIN)
telluromorpholine (Te instead of O) (PIN)



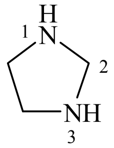
piperazine (PIN)



piperidine (PIN)



pyrazolidine (PIN)



imidazolidine (PIN)

P-22.2.2 Monocycles with 3-10 membered rings (Hantzsch-Widman names)

Monocyclic compounds with no more than ten ring members and containing one or more heteroatoms are named by using the extended Hantzsch-Widman system (ref. 15). Homogeneous heteromonocycles are preselected (see P-12.2).

The elements aluminium, gallium, indium, and thallium are now included in the recommended Hantzsch-Widman system and mercury has been deleted.

P-22.2.2.1 Constructing and numbering Hantzsch-Widman names

P-22.2.2.1.1 Hantzsch-Widman names are formed by combining the ‘a’ prefix(es) for the heteroatom(s) (Table 2.4) with a stem indicating the size of the ring and the degree of hydrogenation (Table 2.5). Vowels between ‘a’ prefixes and between the ‘a’ prefix and the stem are elided. Unsaturated compounds are those having the maximum number of noncumulative double bonds (mancude compounds) and at least one double bond. The presence of a single heteroatom determines the numbering in a monocyclic compound; the heteroatom has the locant ‘1’.

Hantzsch-Widman names are preferred IUPAC names for both the unsaturated and saturated compounds. Hantzsch-Widman names are preselected names for homogeneous heteromonocycles other than hydrocarbons (see P-22.2.5).

Table 2.4 Hantzsch-Widman system prefixes (in decreasing order of seniority)

Element	Bonding number (Valence)	Prefix	Element	Bonding number (Valence)	Prefix
fluorine	1	fluora	antimony	3	stiba
chlorine	1	chlora	bismuth	3	bisma
bromine	1	broma	silicon	4	sila
iodine	1	ioda	germanium	4	germa
oxygen	2	oxa	tin	4	stanna
sulfur	2	thia	lead	4	plumba
selenium	2	selena	boron	3	bora
tellurium	2	tellura	aluminium	3	aluma[1] (not alumina)
nitrogen	3	aza	gallium	3	galla
phosphorus	3	phospha	indium	3	indiga[1] (not inda)

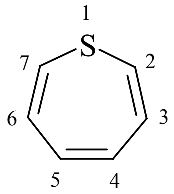
arsenic	3	arsa	thallium	3	thalla

[1] Compare with Table 1.5

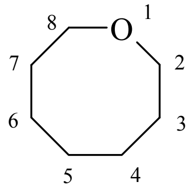
Table 2.5 Hantzsch-Widman system stems

Ring Size	Unsaturated	Saturated	Ring Size	Unsaturated	Saturated
3	irene/irine	irane/iridine	7	epine	epane
4	ete	etane/etidine	8	ocine	ocane
5	ole	olane/olidine	9	onine	onane
6A	ine	ane	10	ecine	ecane
6B (N, Si, Ge, Sn, Pb	ine	inane			
6C (F, Cl, Br, I, N, P, As Sb, Al, Ga, In, Tl)	inine	inane			

Examples:



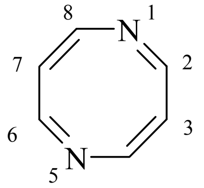
thiepine (PIN)



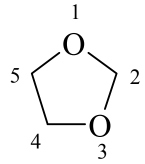
oxocane (PIN)

P-22.2.2.1.2 A multiplicity of the same heteroatom is indicated by a multiplying prefix ‘di’, ‘tri’, ‘tetra’, etc., placed before the appropriate ‘a’ term. The final letter of a multiplying prefix is not elided before a vowel. Lowest possible locants are assigned to heteroatoms, locant ‘1’ being assigned to one of the heteroatoms. Locants are cited at the front of the name, i.e., before the ‘a’ term and any preceding numerical prefixes.

Examples:



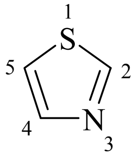
1,5-diazocine (PIN)



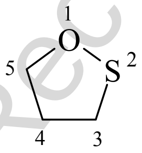
1,3-dioxolane (PIN)

P-22.2.2.1.3 If two or more kinds of heteroatoms occur in the same name, their order of citation follows the sequence: F, Cl, Br, I, O, S, Se, Te, N, P, As, Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, Tl, Hg. The locant '1' is given to a heteroatom that occurs first in the seniority sequence used for citation of the 'a' prefixes. The numbering is then chosen to give lowest locants to heteroatoms considered as a set in ascending numerical order. Locants are cited at the front of the name, in the order of citation of the 'a' prefixes.

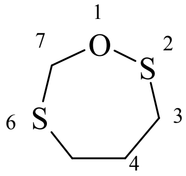
Examples:



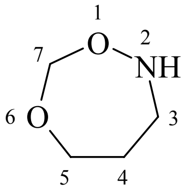
1,3-thiazole (PIN)



1,2-oxathiolane (PIN)



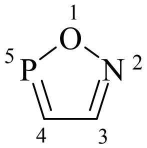
1,2,6-oxadithiepane (PIN)
(not 1,3,7-oxadithiepane;
the locant set '1,2,6 ' is
lower than '1,3,7')



1,6,2-dioxazepane (PIN)
(not 1,3,4-dioxazepane; not
1,3,7-dioxazepane; not 1,6,5-
dioxazepane; the locant set
'1,2,6 'is lower than '1,3,4';
'1,3,7'; or '1,5,6')

If there is a further choice, lowest locants are assigned to heteroatoms in the order that they appear in the seniority sequence (see Table 2.3).

Example:

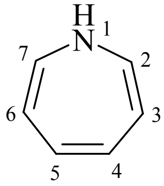


1,2,5-oxazaphosphole (PIN)
(not 1,5,2-oxazaphosphole; N has priority over P for lowest locant)

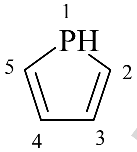
P-22.2.2.1.4 Indicated hydrogen

After the maximum number of noncumulative double bonds has been assigned, any ring atom with a bonding order of three or higher connected to adjacent ring atoms by single bonds only, and carrying one or more hydrogen atoms, is designated by the indicated hydrogen symbol *H*. If there is a choice, such ring atoms are selected for low locants.

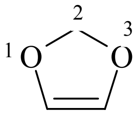
Examples:



1*H*-azepine(PIN)



1*H*-phosphole (PIN)



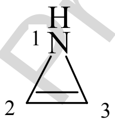
2*H*-1,3-dioxole (PIN)

P-22.2.2.1.5 Selecting Hantzsch-Widman names for 3-, 4-, or 5-membered rings

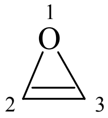
As shown in Table 2.4, for mancude three-membered rings and saturated three-, four-, and five-membered rings two stems are recommended. They are used as follows:

(a) The stem ‘irine’ is used in place of ‘irene’ for rings containing only nitrogen; otherwise the stem ‘irene’ is used.

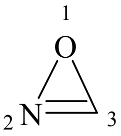
Examples:



1*H*-azirine (PIN)



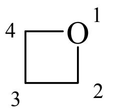
oxirene (PIN)

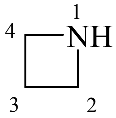


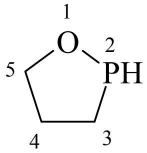
oxazirene (PIN)

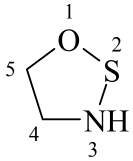
(b) The stems ‘iridine’, ‘etidine’ and ‘olidine’ are used when nitrogen atoms are present in the ring; otherwise the ‘ane’ stems are used.

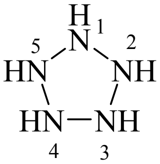
Examples:


oxetane (PIN)


azetidine (PIN)


1,2-oxaphospholane (PIN)

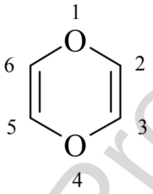

1,2,3-oxathiazolidine (PIN)

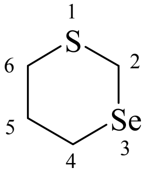

pentaazolidine (preselected name; see P-12.2)

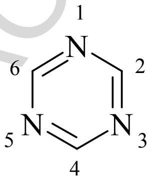
P-22.2.2.1.6 Selecting Hantzsch-Widman names for six-membered rings

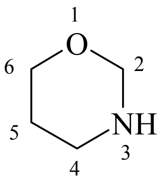
The stem for six-membered rings depends on the least senior heteroatom in the ring, i.e., the heteroatom whose name directly precedes the ending. Heteroatoms are divided into three groups, A, B, and C, each corresponding to a stem for the unsaturated and for the saturated compound (Table 2.5). The stem is selected in accordance with the group to which the **least** senior heteroatom belongs.

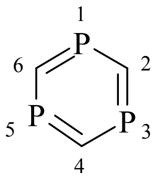
Examples:


1,4-dioxine (PIN)

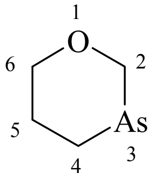

1,3-thiaselenane (PIN)


1,3,5-triazine (PIN)

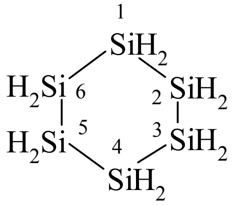

1,3-oxazinane (PIN)



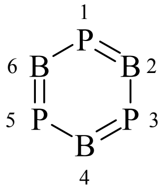
1,3,5-triphosphinine (PIN)



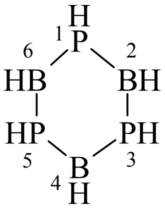
1,3-oxarsinane (PIN)



hexasilinane (preselected name; see P-12.2)



1,3,5,2,4,6-triphosphatriborinine
(preselected name; see P-12.2)



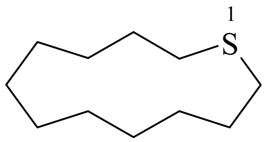
1,3,5,2,4,6-triphosphatriborinane
(preselected name; see P-12.2)

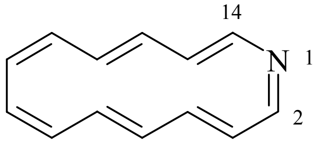
P-22.2.3 Heteromonocyclic hydrides named by skeletal replacement ('a') nomenclature

Mancude and saturated heteromonocyclic compounds with up to and including ten ring members are named by the extended Hantzsch-Widman system. For monocyclic rings with eleven and more ring members, skeletal replacement ('a') nomenclature is used for the fully saturated or fully unsaturated compounds ([*n*]annulenes).

P-22.2.3.1 Skeletal replacement names are formed by placing 'a' prefixes in front of the name of the corresponding cycloalkane or annulene, and, when more than one heteroatom is present, in the following decreasing seniority order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl. For numbering, see P-22.2.3.2.

Examples:



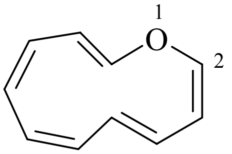


thiacyclododecane (PIN) 1-azacyclotetradeca-1,3,5,7,9,11,13-heptaene (PIN)
aza[14]annulene

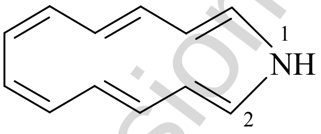
P-22.2.3.2 Numbering

P-22.2.3.2.1 When a single heteroatom is present in the ring, it is assigned the locant ‘1’, which is omitted in the name, unless a locant for an indicated hydrogen atom is present. Low locants are assigned first to the heteroatom and then to unsaturated sites (see P-31.1.3.2). When required, locants for indicated hydrogen atoms are assigned in accordance with P-14.6.

Examples:



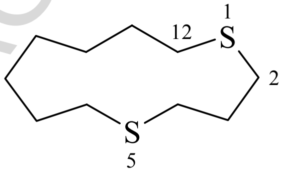
1-oxacycloundeca-2,4,6,8,10-pentaene (PIN)
oxa[11]annulene

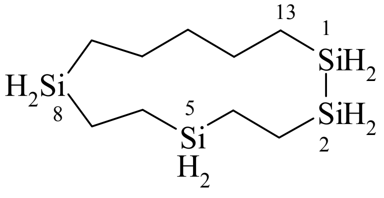


1*H*-1-azacyclotrideca-2,4,6,8,10,12-hexaene (PIN)
1*H*-1-aza[13]annulene

P-22.2.3.2.2 When the same kind of heteroatom occurs more than once, the direction of numbering is chosen to give the lower locants to the heteroatoms as a set.

Examples:

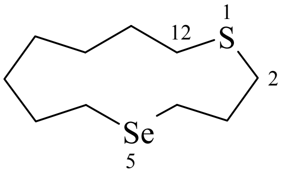




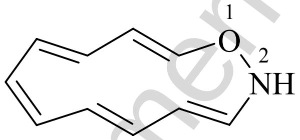
1,5-dithiacyclododecane (PIN) 1,2,5,8-tetrasilacyclotridecane (PIN)

P-22.2.3.2.3 When heteroatoms of different kinds are present, the locant ‘1’ is given to the heteroatom first cited in the order of seniority given above (see P-22.2.3.1). The direction of numbering is then chosen to give lower locants to the heteroatoms as a set without regard to the kind of heteroatom, and then, if necessary, according to the order of seniority above (see P-22.2.3.1). Low locants are assigned first to the heteroatoms and then to the unsaturated sites (see P-31.1.3.2).When required, locants for indicated hydrogen atoms are assigned in accordance with P-14.6.

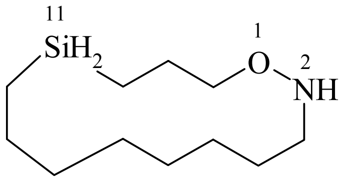
Examples:



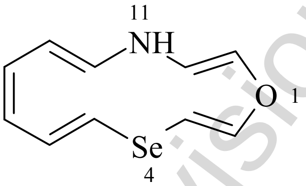
1-thia-5-selenacyclododecane (PIN)



1-oxa-2-azadodeca-3,5,7,9,11-pentanene (PIN)
2*H*-1-oxa-2-aza[12]annulene



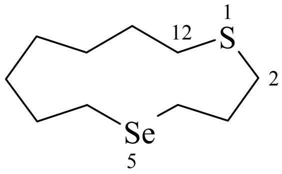
1-oxa-2-aza-11silacyclotetradecane (PIN)



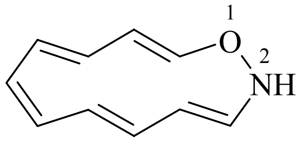
1-oxa-4-selena-11-azatrideca-2,5,7,9,12-pentaene (PIN)
1*H*-1-oxa-4-selena-11-aza[13]annulene

P-22.2.3.2.3 When heteroatoms of different kinds are present, the locant ‘1’ is given to the heteroatom first cited in the order of seniority given above (see P-22.2.3.1). The direction of numbering is then chosen to give lower locants to the heteroatoms as a set without regard to the kind of heteroatom, and then, if necessary, according to the order of seniority above (see P-22.2.3.1). Low locants are assigned first to the heteroatoms and then to the unsaturated sites (see P-31.1.3.2). When required, locants for indicated hydrogen atoms are assigned in accordance with P-14.6.

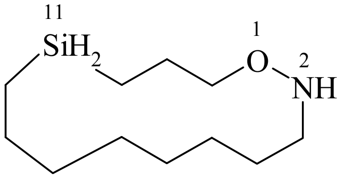
Examples:



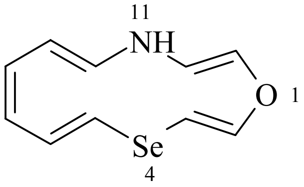
1-thia-5-selenacyclododecane (PIN)



1-oxa-2-aza-cyclododeca-3,5,7,9,11-pentaene (PIN)
2*H*-1-oxa-2-aza[12]annulene



1-oxa-2-aza-11-silacyclotetradecane (PIN)



1-oxa-4-selena-11-azacyclotrideca-2,5,7,9,12-pentaene (PIN)
11*H*-1-oxa-4-selena-11-aza[13]annulene

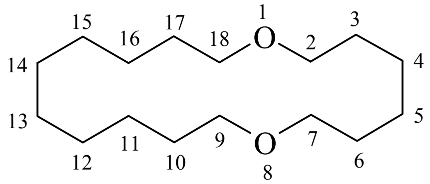
P-22.2.4 Heteromonocycles with eleven or more members having the maximum number of noncumulative double bonds (for generating component names in fusion nomenclature).

Names of heteromonocyclic parent components with more than ten ring members for use in fusion nomenclature are discussed in this subsection. They are used to generate names of components for preferred IUPAC names of fused ring systems; they have also been used as names for the heteromonocycle in general nomenclature as an alternative to the cycloalkapolyene names that are preferred IUPAC names for the heteromonocycles.

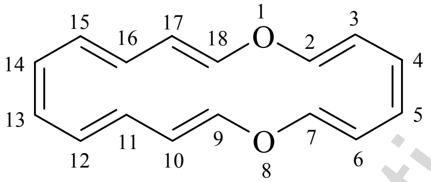
A heteromonocyclic parent component having more than ten members and the maximum number of noncumulative double bonds (mancude) is named by changing the ending ‘ane’ of the name corresponding to the saturated heteromonocycle (see P- 22.2.3) to ‘ine’. Indicated hydrogen atoms are designated as required.

For examples of fusion compounds including this type of heteromonocyclic component, see P-25.2.2.4, P-25.3.6.1 and P-25.3.7.1.

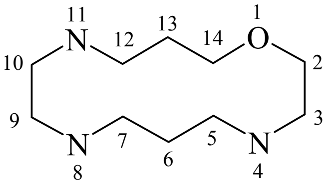
Examples:



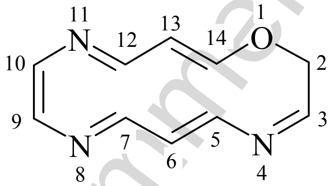
1,8-dioxacyclooctadecane (PIN)



1,8-dioxacyclooctadecine
1,8-dioxacyclooctadeca-2,4,6,9,11,13,15,17-octaene (PIN)



1-oxa-4,8,11-triazacyclotetradecane (PIN)

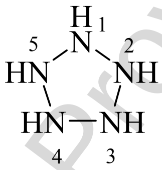


2*H*-1-oxa-4,8,11-triazacyclotetradecine
1-oxa-4,8,11-triazacyclotetradeca-3,5,7,9,11,13-hexaene (PIN)

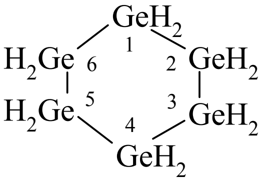
P-22.2.5 Homogeneous monocyclic hydrides other than hydrocarbons and boron hydrides

A saturated heteromonocycle consisting of identical heteroatoms can be named by adding the prefix ‘cyclo’ to the name of the saturated rectilinear chain that has the same number of identical atoms. For alternative methods, see the Hantzsch-Widman extended system described in P-22.2.2 for 3 to 10 membered rings and skeletal replacement (‘a’) nomenclature described in P-22.2.3. The names used to generate preferred IUPAC names for organic derivatives of these heteromonocyclic hydrides are preselected (see P-12.2).

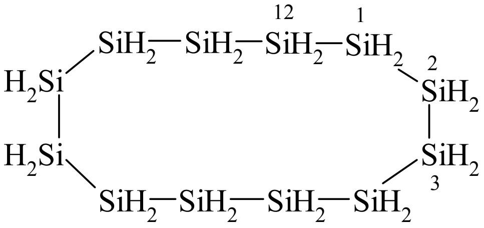
Examples:



cyclopentaazane
pentazolane
(preselected name; see P-12.2)



cyclohexagermane
hexagerminane
(preselected name; see P-12.2)

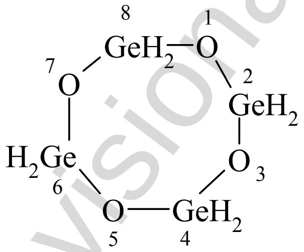


cyclododecasilane
dodecasilacyclododecane (preselected name; see P-12.2)

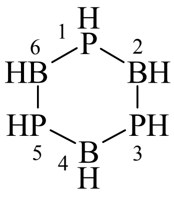
P-22.2.6 Heteromonocyclic hydrides composed of repeating units [(ab)$_n$ cyclic hydrides]

Names may be constructed by citing successively the prefix ‘cyclo’, a multiplying affix (‘di’, ‘tri’, ‘tetra’, etc.) indicating the number of each element in the ring, the ‘a’ terms for the atoms of the repeated unit first cited in the order Tl > In > Ga > Al > Pb > Sn > Ge > Si > Bi > Sb > As > P > N > Te > Se > S > O, and the ending ‘ane’. The terminal letter of an ‘a’ term is elided when followed by a vowel; the terminal letter of a multiplying affix is not elided even when the ‘a’ term begins with a vowel. Numbering starts at one of the skeletal atoms of the element cited last in the name and proceeds continuously around the ring. For alternative methods, see P-22.2.2 for Hantzsch-Widman names and P-22.2.3 for naming monocycles with more than ten members. The names used to generate preferred IUPAC names for organic derivatives of these heteromonocyclic hydrides are preselected (see P-12.2).

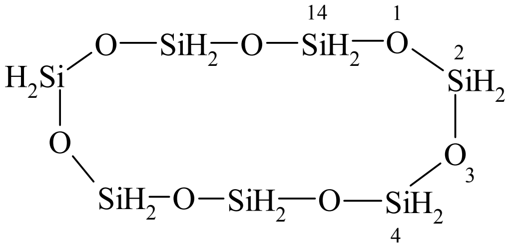
Examples:



cyclotetragermoxane
1,3,5,7,2,4,6,8-tetraoxatetragermocane (preselected name, see P-12.2)



cyclotriboraphosphane
1,3,5,2,4,6-triphosphatriborinane (preselected name, see P-12.2)

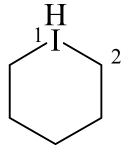


cycloheptasiloxane (see P-22.2.5)
1,3,5,7,9,11,13-heptaoxa-2,4,6,8,10,12,14-heptasilacyclotetradecane
(preselected name, see P-12.2)

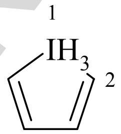
P-22.27 Heteromonocyclic hydrides having heteroatoms with nonstandard bonding numbers.

P-22.2.7.1 The λ-convention is used to denote heteroatoms with nonstandard bonding numbers in heteromonocycles (see P-14.1). The symbol λ^n, where *n* is the bonding number, is cited immediately after the locant denoting the heteroatom with the nonstandard bonding number. The symbol *H*, if required to denote saturated skeletal atoms, is cited at the front of the complete name with the appropriate locant(s).

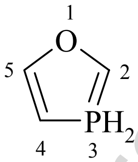
Examples:



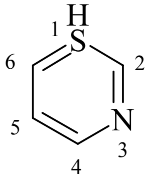
1λ^3-iodinane (PIN)



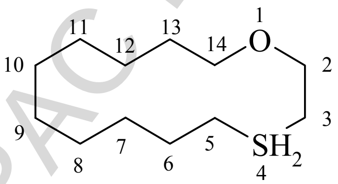
1*H*-1λ^5-iodole (PIN)



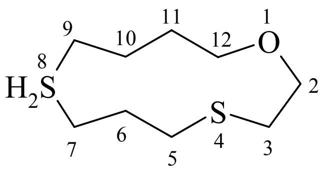
1,3λ^5-oxaphosphole (PIN)



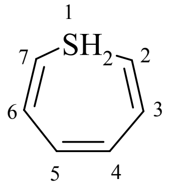
1λ^4,3-thiazine (PIN)



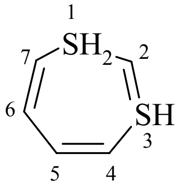
1-oxa-4λ^4-thiacyclotetradecane (PIN)



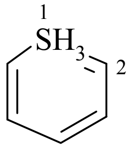
1-oxa-4,8λ^4-dithiacyclododecane (PIN)



1*H*-1λ^4-thiepine (PIN)



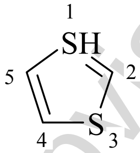
1*H*-1λ^4,3λ^4-dithiepine (PIN)
[the (−SH_2−) group, which includes an indicated hydrogen, is preferred for the low locant]



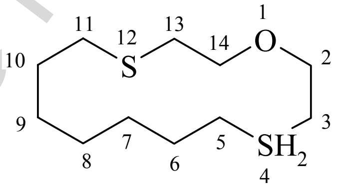
1λ^6-thiopyran (PIN)
(this heteromonocycle has the maximum number of double bonds and one double bond at every position; hence, no indicated hydrogen is cited for the sulfur atom)

P-22.2.7.2 If a further choice is needed between two or more of the same skeletal atom with different bonding numbers, the lower locant is assigned in order of the decreasing value of the bonding number, i.e., λ^6 is selected over λ^4 (see also P-21.2.4).

Examples:



1λ^4,3-dithiole (PIN)



1-oxa-4λ^4,12-dithiacyclotetradecane (PIN)

P-23 Extended von Baeyer system for polyalicyclic compounds

P-23.0 Introduction

This section is based on the recent publication ‘Extension and Revision of the von Baeyer system for naming polycyclic compounds (including bicyclic compounds) (IUPAC Recommendations 1999) (ref. 7). It supersedes Rules A-31, A-32 and B-14 in the 1979 Recommendations (ref. 1) and Rule R-2.4.2 in the 1993 Recommendations (ref. 2). No modifications to the 1999 publication have been made in this Section.

This Section deals only with saturated polyalicyclic ring systems named by the von Baeyer system; for unsaturated systems, see Section P-31.1.4. For naming substituent groups derived from saturated polyalicyclic ring systems, see Section P-29.

P-23.1 Definitions and terminology

P-23.1.1 A ‘bridgehead’ is any skeletal atom of the ring system that is bonded to three or more skeletal atoms (excluding hydrogen).

P-23.1.2 A ‘bridge’ is an unbranched chain of atoms or an atom or a valence bond connecting two bridgeheads.

P-23.1.3 The ‘main ring’ is the ring system that includes as many skeletal atoms of the polycyclic system as possible.

P-23.1.4 The ‘main bridge’ is the bridge included in a bicyclic system and the first selected bridge in a polycyclic system.

P-23.1.5 Two bridgeheads are selected as ‘main bridgeheads’. These two bridgeheads are included in the main ring and connected by the main bridge.

P-23.1.6 A ‘secondary bridge’ is any bridge not included in the main ring or the main bridge.

P-23.1.7 An ‘independent secondary bridge’ links bridgeheads which are part of the main ring or main bridge.

P-23.1.8 A ‘dependent secondary bridge’ links at least one bridgehead that is part of a secondary bridge.

P-23.1.9 A ‘polycyclic system’ contains a number of rings equal to the minimum number of scissions required to convert the system into an acyclic skeleton. The number of rings is indicated by the non-detachable prefix, ‘bicyclo’ (not dicyclo), ‘tricyclo’, ‘tetracyclo’, etc.

P-23.2 Naming and numbering von Baeyer hydrocarbons

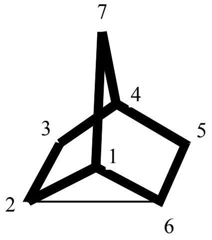
Bi- and polycyclic hydrocarbons that are treated by the von Baeyer system are named by the following rules applied in order until a decision is reached.

- P-23.2.1 Selection of the main ring
- P-23.2.2 Naming of bicyclic alicyclic hydrocarbons
- P-23.2.3 Numbering of bicyclic alicyclic hydrocarbons
- P-23.2.4 Selection of the main bridge
- P-23.2.5 Naming and numbering of tricyclic alicyclic hydrocarbons
- P-23.2.6 Naming and numbering of polyalicyclic hydrocarbons

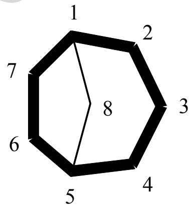
P-23.2.1 Selection of the main ring

The main ring of a polycyclic hydrocarbon ring system is selected so as to include as many skeletal atoms of the structure as possible. The main ring is shown in bold in subsections P-23.2.1 through P-23.2.6.

Examples:



a six membered main ring

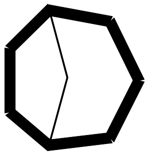


a seven membered main ring

P-23.2.2 Naming bicyclic alicyclic hydrocarbons

Saturated homogeneous bicyclic hydrocarbons having two or more atoms in common are named by prefixing ‘bicyclo’ to the name of the acyclic hydrocarbon having the same total number of skeletal atoms. The numbers of skeletal atoms in each of the two segments connecting the main bridgeheads and in the main bridge are given by arabic numbers cited in descending numerical order separated by full stops and enclosed in square brackets.

Example:

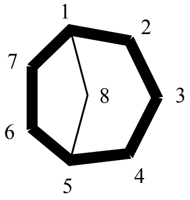


bicyclo[3.2.1]octane (PIN)

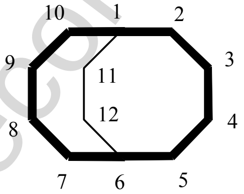
P-23.2.3 Numbering bicyclic alicyclic hydrocarbons

The bicyclic ring system is numbered starting with one of the bridgeheads and proceeding first along the longer segment of the main ring to the second bridgehead, then back to the first bridgehead along the unnumbered segment of the main ring. Numbering is completed by numbering the main bridge beginning with the atom next to the first bridgehead.

Examples:



bicyclo[3.2.1]octane (PIN)

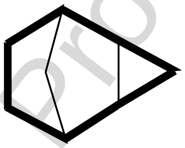


bicyclo[4.4.2]dodecane (PIN)

P-23.2.4 Selection of the main bridge

In a polycyclic ring system there is more than one bridge connecting atoms of the main ring and/or the main bridge. The main bridge (like the main ring hown herein in bold) is the one that includes as many of the atoms not included in the main ring as possible. Bridges other than the main bridge are called 'secondary bridges'.

Example:



P-23.2.5 Naming and numbering tricyclic alicyclic hydrocarbons

P-23.2.5.1 Tricyclic hydrocarbons having an independent secondary bridge are named on the basis of a bicyclic system described in P-23.2.2. Rings not described by the bicyclic system are defined by citing the number of atoms in the independent secondary bridge as an arabic number. The locants of the two attachment points of the independent secondary bridge to the main ring are cited as a pair of superscript arabic numbers (lower first) separated by a comma.

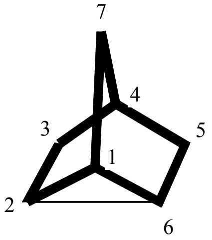
The name of the tricyclic system is then constructed by citing:

(a) the prefix 'tricyclo', in place of 'bicyclo', indicating the presence of three rings in the polyalicyclic system;

(b) numbers indicating the bridge lengths (with the appropriate superscript locants for the secondary bridge) separated by full stops and placed in brackets (e.g. [2.2.1.$0^{2,5}$]);

(c) the name of the acyclic hydrocarbon having the same total number of skeletal atoms.

Examples:



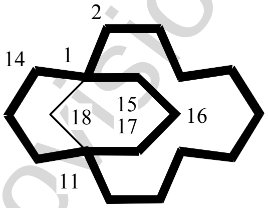
tricyclo[2.2.1.$0^{2,6}$]heptane (PIN)

P-23.2.5.2 Numbering the secondary bridge

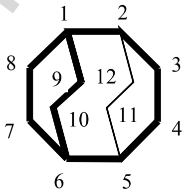
After the main ring and main bridge have been numbered, the independent secondary bridge is numbered continuing from the higher numbered bridgehead of the main ring.

This Rule and Rule P-23.2.6.3 replace Rule A-32.23 in the 1979 Recommendations (ref. 1) and Rule R-2.4.2.2 in the 1993 Recommendations (ref. 2).

Examples:



tricyclo[9.3.3.$1^{1,11}$]octadecane (PIN)



tricyclo[4.2.2.$2^{2,5}$]dodecane (PIN)
(the secondary bridge is numbered
starting from bridgehead 5)

P-23.2.6 Naming and numbering polycyclic alicyclic hydrocarbons

Polycyclic analogues of saturated bi- and tricyclic ring systems (P-23.2.3 and P-23.2.5) are named as described in the following subsections. Independent and dependent secondary bridges are considered here. Rules for numbering all secondary bridges and for naming all polyalicyclic systems are described; their application follows those described for naming and numbering bicyclic systems as described in P-23.2.1 to P-23.2.4 above. An additional rule is necessary to select the main bridge and the secondary bridges.

P-23.2.6.1 Naming polycyclic alicyclic hydrocarbons

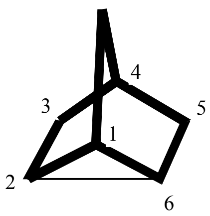
Rings not designated by the bicyclic system described above (P-23.2.2) are defined by citing the number of atoms in each secondary bridge as an arabic number. The locants of the two attachment points of each secondary bridge to the main ring are cited as a pair of superscript arabic numbers (lower first) separated by a comma. The numbers indicating independent secondary bridges (bridges that connect atoms of the bicyclic system) are cited in decreasing order. The procedure for construction of names is given in the following subsections.

P-23.2.6.1.1 The prefixes ‘tricyclo’, ‘tetracyclo’, etc. , in place of ‘bicyclo’, indicate the number of rings in the polyalicyclic system. The number of rings is equal to the number of bond cuts necessary to transform the polycyclic system into an acyclic unbranched or branched skeleton.

P-23.2.6.1.2 The number of atoms in each bridge additional to the main bridge, i.e., the secondary bridges, is indicated by arabic numbers separated by full stops and cited in decreasing numerical order following those describing the bicyclic system, except as provided by P-23.6.1.3. The location of each secondary bridge is indicated by the arabic number locants of the bicyclic structure already numbered; these locants are cited as superscripts to the arabic number denoting its length (number of atoms) and separated by a comma. The assemblage of arabic numbers denoting the length of bridges with superscript numbers, if necessary, is commonly called the ‘von Baeyer descriptor’; it is enclosed in brackets.

P-23.2.6.1.3 Independent secondary bridges are cited before dependent secondary bridges. The numbers indicating dependent secondary bridges are cited in decreasing order (the third example in P-23.2.6.3 illustrates this order of citation).

P-23.2.6.1.4 The name is terminated by the name of the alkane representing the total number of ring atoms; this number corresponds to the sum of the arabic numbers in the numerical descriptor enclosed by brackets plus two (for the two main bridgehead atoms); for example, in the name for the following structure, bicyclo[2.2.1.$0^{2,6}$]heptane, the total number of ring atoms, 7, equals the sum [2 + 2 + 1+ 0] + 2



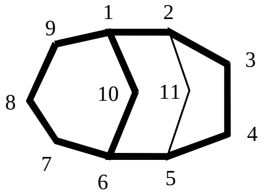
P-23.2.6.2 Selection of the main bridge and secondary bridges

There is often a number of choices to be made in the selection of the main bridge and the secondary bridges. To make such choices, the following criteria are applied in order until a decision can be made.

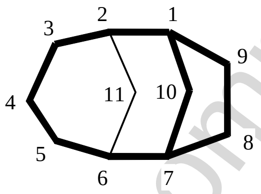
(Note: Numberings shown in the examples below follow the rules given in P-23.2.6.3)

P-23.2.6.2.1 The main ring must be divided as symmetrically as possible by the main bridge, which, as directed in P-23.2.4, includes as many of the atoms not included in the main ring as possible.

Example:



not



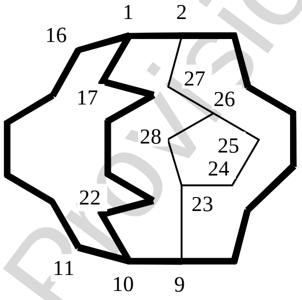
tricyclo[4.3.1.1^{2,5}]undecane (PIN) tricyclo[5.2.1.1^{2,6}]undecane

correct incorrect

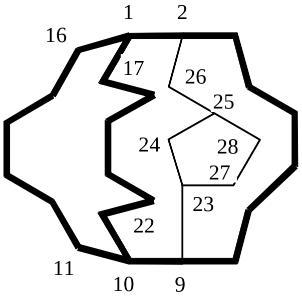
(two bridges of 4 and 3 atoms are more symmetric than two bridges of 5 and 2 atoms)

P-23.2.6.2.2 If there is a choice of independent secondary bridges, the first cited must be as long as possible. Then, if relevant, the second independent secondary bridge must be as long as possible, etc.

Example:



not



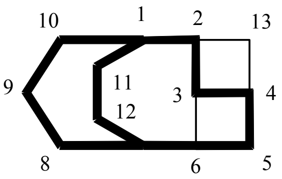
pentacyclo[8.6.6.5^{2,9}.1^{23,26}]octacosane (PIN) pentacyclo[8.6.6.4^{2,9}.2^{23,26}]octacosane

correct incorrect

(the five atom independent bridge between positions 2 and 9 of the main ring is longer than the four membered independent bridge between positions 2 and 9)

P-23.2.6.2.3 The number of dependent secondary bridges is to be kept to a minimum.

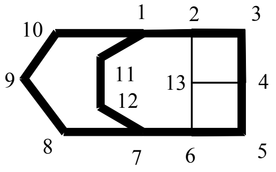
Example:



tetracyclo[5.3.2.1^{2,4}.0^{3,6}]tridecane (PIN)

correct

not



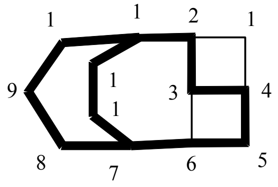
tetracyclo[5.3.2.1^{2,4}.0$^{6.13}$]tridecane

incorrect

(there are no dependent bridges in the correct structure; there is one dependent bridge in the incorrect structure, between 6 and 13)

P-23.2.6.2.4 The superscript locants for the secondary bridges must be as low as possible when considered as a set in ascending numerical order, the decision being made at the first point of difference.

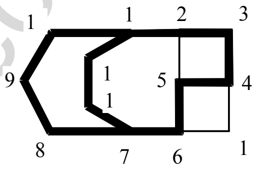
Examples:



tetracyclo[5.3.2.1^{2,4}.0^{3,6}]tridecane (PIN)

correct

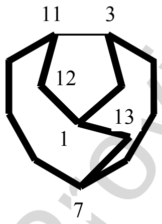
not



tetracyclo[5.3.2.1^{4,6}.0^{2,5}]tridecane

incorrect

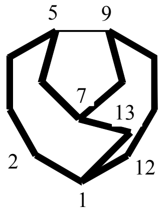
(the locant set '2,3,4,6' is lower than '2,4,5,6')



tricyclo[5.5.1.0^{3,11}]tridecane (PIN)

correct

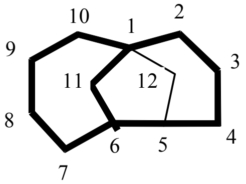
not



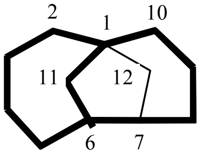
tricyclo[5.5.1.0^{5,9}]tridecane

incorrect

(the locant set '3,11' is lower than '5,9')



not



tricyclo[4.4.1.1^{1,5}]dodecane (PIN)

correct

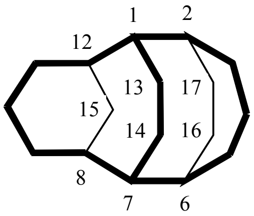
[tricyclo[4.4.1.1^{1,7}]dodecane

incorrect

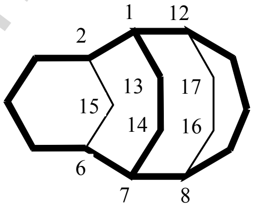
(the locant set ‘1,5’ is lower than ‘1,7’)

P-23.2.6.2.5 The superscript locants shall be as low as possible when considered in their order of citation in the name.

Example:



not



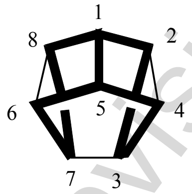
tetracyclo[5.5.2.2^{2,6}.1^{8,12}]heptadecane (PIN)

correct

tetracyclo[5.5.2.2^{8,12}.1^{2,6}]heptadecane

incorrect

[the locant set ‘2,6,8,12’ is lower than ‘8,12,2,6’]



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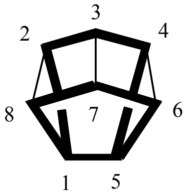


pentacyclo[3.3.0.0^{2,4}.0^{3,7}.0^{6,8}]octane (PIN)

correct

pentacyclo[3.3.0.0^{2,8}.0^{3,7}.0^{4,6}]octane

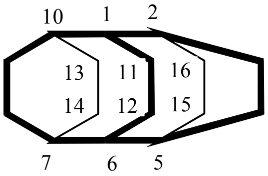
incorrect

(the locant set ‘2,4,3,7,6,8’ is lower than ‘2,8,3,7,4,6’)

P-23.2.6.3 Numbering of secondary bridges

After numbering the main ring and main bridge, independent secondary bridges are numbered before dependent secondary bridges; the numbering continues from the highest number of the main ring and main bridge. Each secondary bridge is numbered in turn starting with the independent secondary bridge linked to the highest numbered bridgehead atom, then the independent secondary bridge linked to the next highest bridgehead atom, and so on. Each atom of a secondary bridge is numbered starting with the atom next to the higher numbered bridgehead.

Examples:



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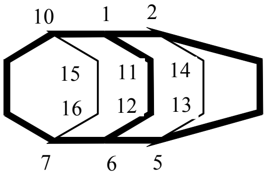
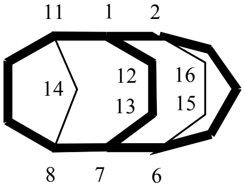
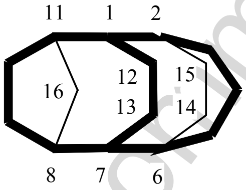


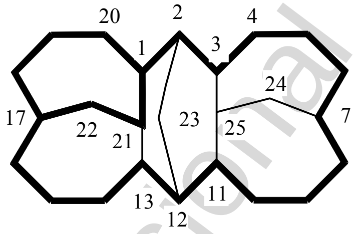
tetracyclo[4.4.2.2^{2,5}.2^{7,10}]hexadecane (PIN)
(the first secondary bridge to be numbered
is linked to bridgehead 10)



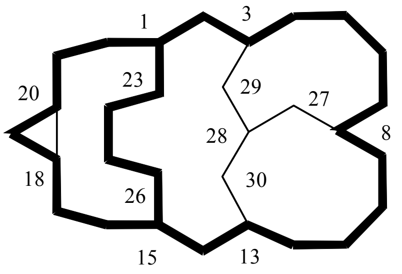
not



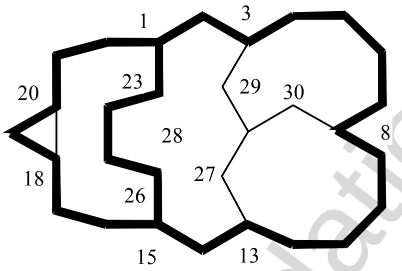
tetracyclo[5.4.2.2^{2,6}.1^{8,11}]hexadecane (PIN)
(the first secondary bridged to be numbered
is linked to bridgehead 11)



hexacyclo[15.3.2.2^{3,7}.1^{2,12}.0^{13,21}.0^{11,25}]pentacosane (PIN)
(the dependent secondary bridge between atoms numbered 11 and 25 is cited last; in the numeric descriptor, the numbers '15, 3, and 2' describe the basic bicyclic system; the numbers '2^{3,7} , 1^{2,12},and 0^{13,21} ' correspond to the three independent secondary bridges; the number '0^{11,25} ' corresponds to the dependent secondary bridge)



not



pentacyclo[13.7.4.$3^{3,8}$.$0^{18,20}$.$1^{13,28}$]triacontane (PIN)
pentacyclo[13.7.4.$3^{3,13}$.$0^{18,20}$.$1^{8,28}$]triacontane

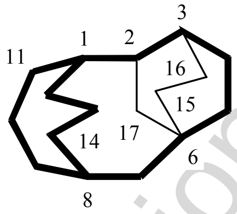
correct incorrect

(the independent bridge is numbered before the dependent bridge; the locant set ‘3,8,18,20,13,28’ is lower than ‘3,13,18,20,8,28’)

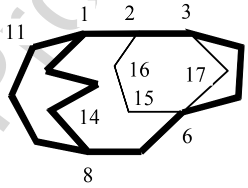
P-23.2.6.4 If there is a further choice for numbering the secondary bridges, the following criteria are considered in order until a decision can be made.

P-23.2.6.4.1 Lower locants are used for the atoms of the bridge linked to the higher numbered bridgehead.

Examples:



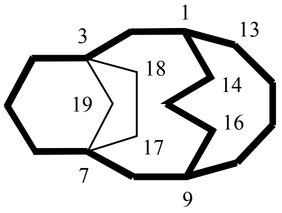
tetracyclo[6.3.3.$2^{3,6}$.$1^{2,6}$]heptadecane (PIN)
(locants 15 and 16 are assigned to the bridge linked to bridgehead atom 3 not 2)



tetracyclo[6.3.3.$2^{2,6}$.$1^{3,6}$]heptadecane (PIN)
(the locant 15 is assigned to the bridge linked to bridgehead atom 3 not 2)

P-23.2.6.4.2 Longer bridges are numbered before shorter bridges.

Example:

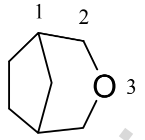


tetracyclo[7.4.3.2^{3,7}.1^{3,7}]nonadecane (PIN)
(the two atom bridge between bridgehead atoms 3 and 7 is numbered before the one atom bridge between the same two bridgehead atoms.)

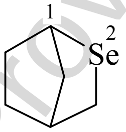
P-23.3 Heterogeneous heterocyclic von Baeyer parent hydrides

P-23.3.1 The only general method to name heterogeneous heterocyclic von Baeyer systems is skeletal replacement (‘a’) nomenclature. The ‘a’ prefixes denoting the heteroatoms are placed in front of the name of the corresponding hydrocarbon named according to P-23.2, cited in the order F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl. Numbering is determined first by the fixed numbering of the hydrocarbon system.

Examples:



3-oxabicyclo[3.2.1]octane (PIN)

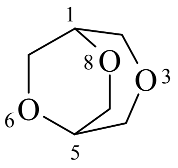


2-selenabicyclo[2.2.1]heptane (PIN)

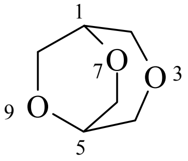
P-23.3.2 When there is a choice for numbering, the following criteria are applied in order until a decision can be made.

P-23.3.2.1 Low locants are assigned to the heteroatoms considered together as a set compared in increasing numerical order. The preferred numbering is the lowest set at the first point of difference.

Example:



not

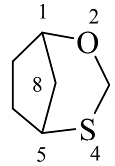


3,6,8-trioxabicyclo[3.2.2]nonane (PIN) [3,7,9-trioxabicyclo[3.2.2]nonane

[the locant set ‘3,6,8’ is lower than ‘3,7,9’]

P-23.3.2.2 If there is still a choice, low locants are assigned in accord with the decreasing seniority order of heteroatoms: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Example:



2-oxa-4-thiabicyclo[3.2.1]octane (PIN)

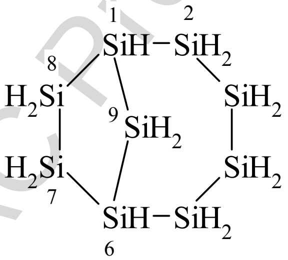
P-23.4 Homogeneous heterocyclic von Baeyer parent hydrides

Heterocyclic von Baeyer systems composed entirely of the same heteroatom are named:

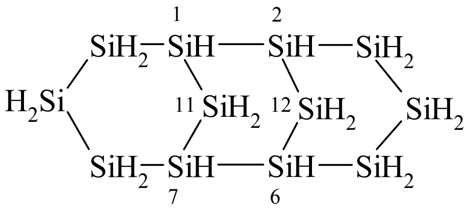
(a) as described for bi- and polycyclic hydrocarbons in P-23.2 and P-24 using the name of the acyclic parent hydride that has the same total number of skeletal atoms; or

(b) by skeletal replacement nomenclature using the ‘a’ prefixes described in P-23.2, in which the total number of heteroatoms is indicated by a numerical term. In either method it is not necessary to give the location of the heteroatoms because all positions are modified by the same heteroatom. Method (a) gives preselected names.

Examples:



(a) bicyclo[4.2.1]nonasilane
(preselected name; see P-12.2)
(b) nonasilabicyclo[4.2.1]nonane



(a) tricyclo[5.3.1.1^{2,6}]dodecasilane
(preselected name; see P-12.2)
(b) dodecasilatricyclo[5.3.1.1^{2,6}]dodecane

P-23.5 Heterogeneous heterocyclic systems composed of alternating hetero atoms

P-23.5.1 Heterogeneous von Baeyer systems composed of alternating skeletal heteroatoms may be named in two ways:

(a) by citing a nondetachable prefix 'bicyclo', 'tricyclo', etc. before a von Baeyer descriptor (see P-23.2.6.1.2) enclosed in square brackets and then, successively:

(i) a multiplying prefix, 'di', 'tri', etc., denoting the number of heteroatoms that are first cited as 'a' terms;

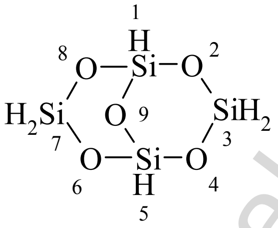
(ii) the 'a' terms denoting the heteroatoms of the system in the reverse order of the recommended seniority for 'a' prefixes (for example, Si before O; see P-23.3.1);

(iii) the ending 'ane'.

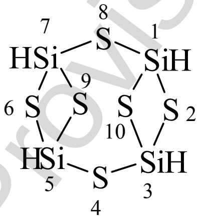
Numbering is the same as for the corresponding hydrocarbon (see P-23.1.3 and 23.1.6);

(b) by applying normal skeletal replacement ('a') nomenclature to the corresponding hydrocarbon.

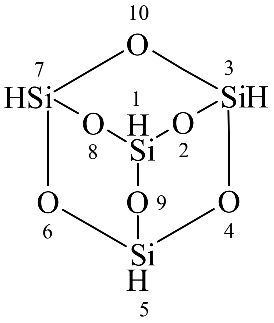
Examples:



(a) bicyclo[3.3.1]tetrasiloxane
(b) 2,4,6,8,9-pentaoxa-1,3,5,7-tetrasilabicyclo[3.3.1]nonane
(preselected name; see P-12.2)



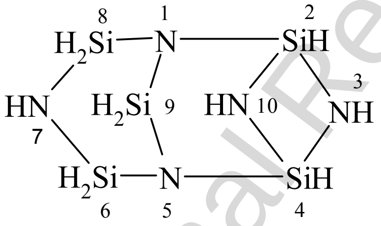
(a) tricyclo[5.1.1.1^{3,5}]tetrasilathiane
(b) 2,4,6,8,9,10-hexathia-1,3,5,7-tetrasilabicyclo[5.1.1.1^{3,5}]decane
(preselected name; see P-12.2)



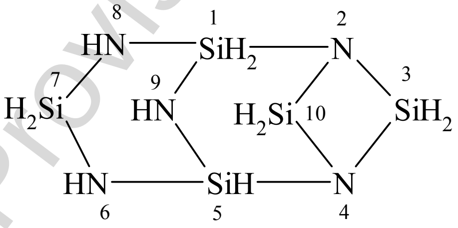
(a) tricyclo[3.3.1.1^{3,7}]tetrasiloxane
(b) 2,4,6,8,9,10-hexaoxa-1,3,5,7-tetrasilabicyclo[3.3.1.1^{3,7}]decane
(preselected name; see P-12.2)

P-23.5.2 Prefixes such as '*1Si*-' or '*1N*-' are used when it is necessary to indicate the atom at the bridgehead that is to have the locant '1 '. Names are identified as (a) and (b) according to the two methods described in P-23.5.1.

Example:



(a) *1N*-tricyclo[3.3.1.1^{2,4}]pentasilazane
(b) 1,3,5,7,10-pentaaza-2,4,6,8,9-pentasilatricyclo[3.3.1.1^{2,4}]decane
(preselected name; see P-12.2)

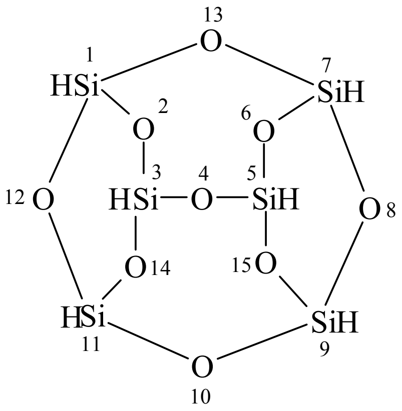


(a) 1*Si*-tricyclo[3.3.1.1^{2,4}]pentasilazane
(b) 2,4,6,8,9-pentaaza-1,3,5,7,10-pentasilatricyclo[3.1.1.1^{2,4}]decane
(preselected name; see P-12.2)

P-23.5.3 Silasesquioxanes, silasesquithianes, etc.

Compounds in which each silicon atom is linked to three oxygen atoms and in which every atom of oxygen is linked to two silicon atoms are named generically silasesquioxanes. Similarly, when the oxygen atoms are replaced by S, Se, Te, or N atoms, the compounds are generically called silasesquithianes, silasesquiazanes, and so forth. They are named by the method described in P-23.5.1(a). The silasesquioxanes have the general formula $Si_{2n}H_{2n}O_{3n}$. The names tetrasilasesquioxanes (n = 2), hexasilasesquioxanes (n = 3), etc., are class names indicating $Si_{2n}H_{2n}E_{3n}$ where E = O, S, Se, Te or N. The silasesquiazanes have the general formula $Si_{2n}H_{3n}N_{3n}$.

Example:

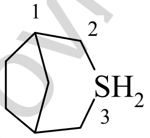


tetracyclo[5.5.1.1^{3,11}.1^{5,9}]hexasiloxane (a hexasilasesquioxane)
2,4,6,8,10,12,13,14,15-nonaoxa-1,3,5,7,9,11-hexasilatetracyclo[5.5.1.1^{3,11}.1^{5,9}]-pentadecane (preselected name; see P-12.2)

P-23.6 Heterocyclic polyalicyclic parent hydrides having heteroatoms with nonstandard bonding numbers

P-23.6.1 The λ-convention, characterized by the symbol λ^n, where 'n' is the bonding number of the heteroatom, is used to identify heteroatoms with nonstandard bonding numbers (see P-14.1). The symbol is placed before the appropriate 'a' prefix.

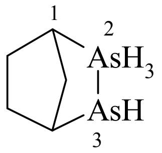
Example:



3λ^4-thiabicyclo[3.2.1]octane (PIN)

P-23.6.2 When there is a choice for numbering, low locants are assigned to heteroatoms with nonstandard bonding numbers expressed by the λ^n symbol in order of decreasing numerical value of the bonding number; for example, in the case of phosphorus, the lower locant is given to a λ^5 phosphorus atom.

Example:

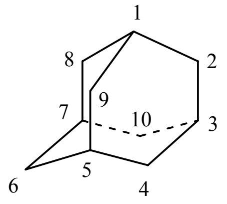


$2\lambda^5$,3-diarsabicyclo[2.2.1]heptane (PIN)

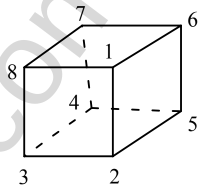
P-23.7 Retained names

The retained names adamantane and cubane are used in general nomenclature and as preferred IUPAC names. The name quinuclidine is retained for general nomenclature only (see Table 2.6).

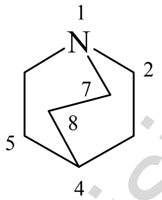
Table 2.6 Retained names for von Baeyer parent hydrides



adamantane (PIN)
tricyclo[3.3.1.$1^{3,7}$]decane



cubane(PIN)
pentacyclo[4.2.0.$0^{2,5}$.$0^{3,8}$.$0^{4,7}$]octane



quinuclidine
1-azabicyclo[2.2.2]octane (PIN)

P-24 Spiro compounds

P-24.0 Introduction

This Section is based on the recent publication ‘Extension and Revision of the Nomenclature for Spiro Compounds, IUPAC Recommendations1999’ (ref. 8). It supersedes Rules A-41, A-43, B-10 and B-12 in the 1979 Recommendations (ref. 1) and Rule R-2.4.3 in the 1993 Recommendations (ref. 2). The alternative methods given by Rules A-42 and B-11 in the 1979 recommendations (ref. 1) have been abandoned.

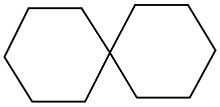
Section P-24.5.2 takes into account appropriate modifications to Section SP-4.1 of the 1999 publication (ref. 8). No other modifications have been made to the 1999 publication.

The spiro ring systems consisting only of monocyclic rings in this Section are saturated systems; for unsaturated systems, see Section P-31.1.5.1.

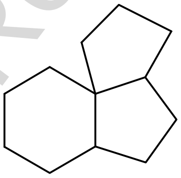
For naming substituent groups see Sections P-29 and P-32.1.2.

P-24.1 Definitions

A ‘spiro union’ is a linkage between two rings that consists of a single atom common to both rings. A ‘free spiro union’ is a linkage that constitutes the only direct union between the two rings.



a free spiro union



a non-free spiro union

The common atom is designated as the ‘spiro atom’. According to the number of spiro atoms present, compounds are distinguished as monospiro, dispiro, trispiro, etc., ring systems. The following recommendations apply only to the naming of parent hydrides containing free spiro unions. For naming spiro compounds with non-free spiro unions, see nomenclature of fused systems (see P-25 and ref. 4).

Spirofusion is the creation of one, and only one, common atom between two rings or ring systems, each ring or ring system contributing one, and only one, atom. It is analogous to the *ortho*- or *ortho*- and *peri*-fusion that creates common bonds between mancude rings or ring systems. Traditionally, *ortho*- or *ortho*- and *peri*-fusion has been called ‘fusion’, with no reference to its specific type of fusion. To avoid any ambiguity, the term ‘spiro’ must always be specified when added to the term ‘fusion’.

P-24.2 Spiro compounds with only monocyclic ring components

P-24.2.4 Heterocyclic spiro compounds with only monocyclic ring components

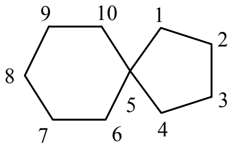
P-24.2.0 Introduction

This Section is concerned only with saturated spiro compounds that consist only of monocyclic rings. For unsaturated systems, see Section P-31.1.5.

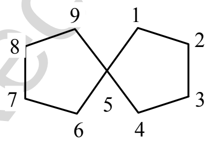
P-24.2.1 Monospiro alicyclic hydrocarbons

Monospiro parent hydrides consisting of two saturated cycloalkane rings are named by placing the nondetachable prefix 'spiro' before the name of the unbranched acyclic hydrocarbon with the same total number of skeletal atoms. The number of skeletal atoms linked to the spiro atom in each ring is indicated by arabic numbers separated by a full stop, cited in ascending order and enclosed in square brackets; this descriptor (called in these recommendations the 'von Baeyer spiro descriptor') is placed between the spiro prefix and the name of the acyclic alkane. Numbering starts in the smaller ring, if one is smaller, with a ring atom next to the spiro atom and proceeds first around that ring and then through the spiro atom and around the second ring.

Examples:



spiro[4.5]decane (PIN)

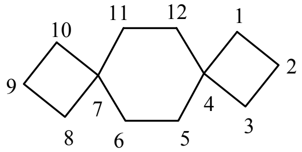


spiro[4.4]nonane (PIN)

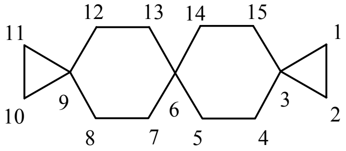
P-24.2.2 Linear polyspiro alicyclic hydrocarbons

Polyspiro parent hydrides consisting of unbranched assemblies of three or more saturated cycloalkane rings are named using the nondetachable prefixes 'dispiro', 'trispiro', etc., according to the number of spiro atoms present, cited in front of the name of the acyclic hydrocarbon that has the same number of skeletal atoms. The von Baeyer spiro descriptor indicates the number of carbon atoms linking the spiro atoms by arabic numbers that are cited in order starting at the smaller terminal ring, if one is smaller, and proceeding consecutively to the other terminal ring through each spiro atom always by the shortest path, and then back to the first spiro atom; the numbers are separated by full stops and enclosed in square brackets. The compound is numbered in the order in which the numbers of the von Baeyer spiro descriptor are cited, including spiro atoms when encountered for the first time. Each time a spiro atom is reached for the second time its locant is cited as a superscript number to the number of the preceding linking atoms.

Examples:



dispiro[3.2.3^7.2^4]dodecane (PIN)

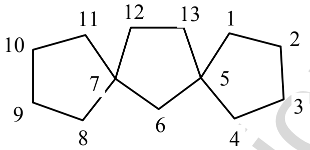


trispiro[2.2.2.2^9.2^6.2^3]pentadecane (PIN)

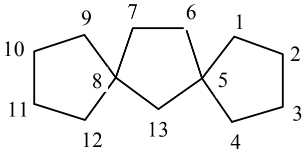
The use of superscript numbers was introduced in the publication ‘Extension and Revision of the Nomenclature for Spiro Compounds and IUPAC Recommendations 1999’ (ref. 8). Even though they are not needed in di- or trispiro compounds their use in branched spiro systems is essential for deriving unambiguous names; therefore, it is recommended that they be used to name all polyspiro compounds, especially when IUPAC preferred names are required.

P-24.2.2.1 If there is a choice of numbers for the spiro descriptor, the smaller numbers are selected because low locants must be allocated to spiro atoms.

Examples:



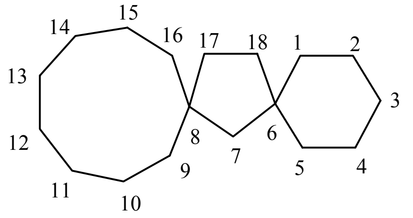
not



dispiro[4.1.4^7.2^5]tridecane (PIN)
correct

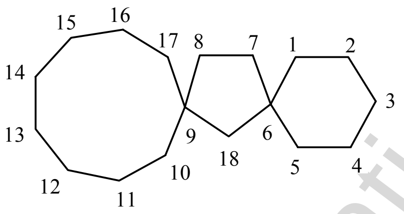
dispiro[4.2.4^8.1^5]tridecane
incorrect

(in the correct name, the number set ‘4,1’ is lower than ‘4,2’ and/or the spiro atom locant set 5,7 is smaller than 5,8)



dispiro[5.1.8^{8}.2^{6}]octadecane (PIN)

correct



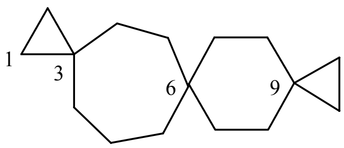
dispiro[5.2.8^{9}.1^{6}]octadecane

incorrect

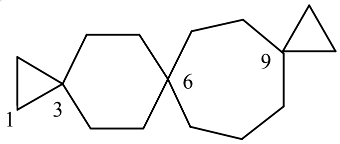
(in the correct name, the number set ‘5,1’ is lower than ‘5,2’ and/or the spiro atom locant set 6,8 is smaller than 6,9)

P-24.2.2.2 If there is still a choice of numbering, the numbers of the von Baeyer descriptors are considered in their order of citation. The name is selected with lower numbers at the first point of difference.

Example:



not



trispiro[2.2.2.2^{9}.2^{6}.3^{3}]hexadecane (PIN)

correct

trispiro[2.2.2.2^{9}.3^{6}.2^{3}]hexadecane

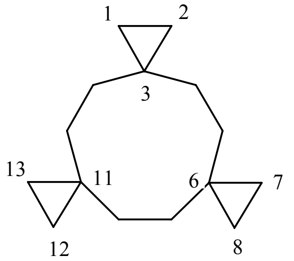
incorrect

(in the correct name, the number set ‘2,2,2,2^{9},2^{6},3^{3} ’ is lower than ‘2,2,2,2^{9},3^{6},2^{3} ’)

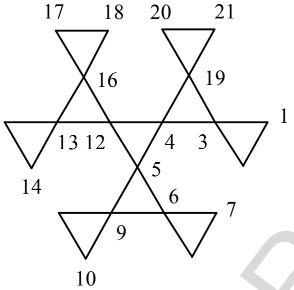
P-24.2.3 Branched polyspiro alicyclic hydrocarbons

Branched polyspiro hydrocarbons composed only of cycloalkane rings are named using ‘dispiro’, ‘trispiro’, etc. before the name of the acyclic hydrocarbon corresponding to the total number of carbon atoms present. The von Baeyer spiro descriptor indicates the number of carbon atoms linking the spiro atoms by lower case arabic numbers that are cited in order starting at the smallest terminal ring, if one is smallest, proceeding consecutively to succeeding terminal rings through each spiro atom always by the shortest path, and then back to the first spiro atom; the numbers are separated by full stops and enclosed in square brackets. The compound is numbered in the order in which the numbers of the spiro von Baeyer descriptor are cited, including spiro atoms when encountered for the first time. Each time a spiro atom is reached for the second time its locant is cited as a superscript number to the preceding number of linking atoms.

Examples:



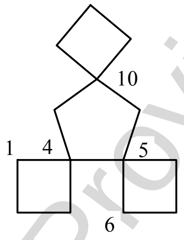
trispiro[2.2.2^{6}.2.2^{11}.2^{3}]pentadecane (PIN)
(the importance of superscripts is illustrated by this example and the second example in P-24.2.2; without the superscripts these different compounds would have identical names)



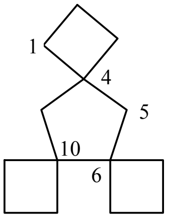
nonaspiro[2.0.0.0.2^{6}.0.2^{9}.0^{5}.0.0.2^{13}.0.2^{16}.0^{12}.0^{4}.0.2^{19}.0^{3}]henicosane (PIN)

P-24.2.3.1 If there is a choice for numbering, lowest locants are assigned to the spiro atoms.

Example:

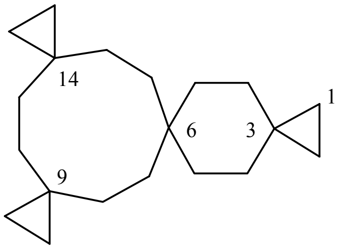


trispiro[3.0.3^{5}.1.3^{10}.1^{4}]tetradecane (PIN)
correct



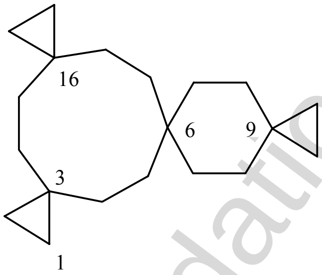
trispiro[3.1.3^{6}.0.3^{10}.1^{4}]tetradecane
incorrect

(in the correct name, the number set of the descriptor ‘3,0’ is lower than ‘3,1’ and/or the spiro atom locant set ‘4,5,10’ is lower than ‘4,6,10’)



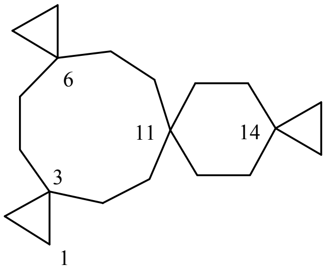
tetraspiro[2.2.2.2^{9}.2.2^{14}.2^{6}.2^{3}]icosane (PIN)

correct



tetraspiro[2.2.2.2^{9}.2^{6}.2.2^{16}.2^{3}]icosane

incorrect



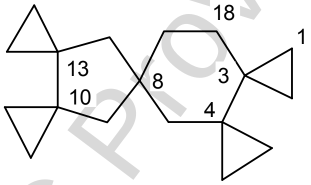
tetraspiro[2.2.2^{6}.2.2.2^{14}.2^{11}.2^{3}]icosane (PIN)

incorrect

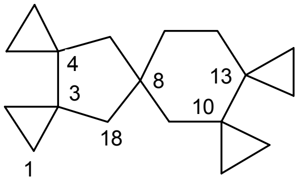
(in the correct name, the spiro locant set '3,6,9,14' is lower than '3,6,9,16' or '3,6,11,14')

P-24.2.3.2 If there is still a choice of numbering, the numbers of the von Baeyer descriptor are considered in their order of citation. The correct name has the lower numbers at first point of difference.

Example:



not



pentaspiro[2.0.2^{4}.1.1.2^{10}.0.2^{13}.1^{8}.2^{3}]octadecane (PIN) pentaspiro[2.0.2^{4}.1.1.2^{10}.0.2^{13}.2^{8}.1^{3}]octadecane

correct incorrect

(in the correct name, the number set of the descriptor '2,0,2,1,1,2,0,2,1,2' is lower than the number set '2,0,2,1,1,2,0,2,2,1', the number '1' being lower than '2' at the ninth position)

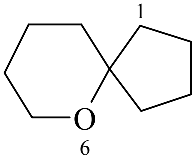
P-24.2.4 Heterocyclic spiro compounds

P-24.2.4.1 Heterocyclic spiro compounds named by skeletal replacement (‘a’) nomenclature
P-24.2.4.2 Homogeneous heterocyclic spiro compounds with only monocyclic components
P-24.2.4.3 Heterocyclic spiro compounds with only monocyclic components composed of alternating heteroatoms

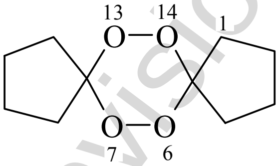
P-24.2.4.1 Heterocyclic spiro compounds named by skeletal replacement (‘a’) nomenclature

P-24.2.4.1.1 When heteroatoms are present in a spiro system composed of only monocyclic rings, skeletal replacement (‘a’) nomenclature is used to name the heterocyclic system. The name of the corresponding hydrocarbon is first constructed as described above (P-24.2). Heteroatoms are then introduced by using the general principles of skeletal replacement (‘a’) nomenclature. The numbering of the spiro hydrocarbon is never modified by the introduction of heteroatoms, but low locants must be attributed to heteroatoms if there is a choice.

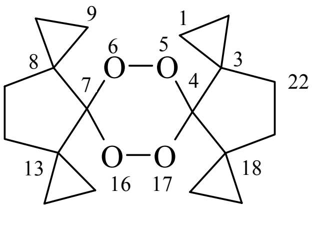
Examples:



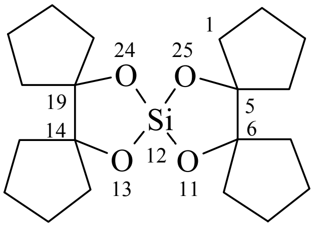
6-oxaspiro[4.5]decane (PIN)
(not 10-oxaspiro[4.5]decane)



6,7,13,14-tetraoxadispiro[4.2.4^{8}.2^{5}]tetradecane (PIN)



5,6,16,17-tetraoxahexaspiro[2.0.2.0.2^{8}.2.2^{13}.0^{7}.2^{4}.0.2^{18}.2^{3}]docosane (PIN)

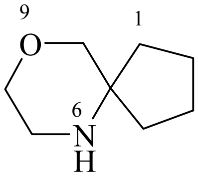


11,13,24,25-tetraoxa-12-silapentaspiro[4.0.4^{6}.1.1.4^{14}.0.4^{19}.1^{12}.1^{5}]pentacosane (PIN)

P-24.2.4.1.2 If there is a choice of name or numbering due to heteroatoms, the following criteria are considered in order until a decision is reached.

(a) Low locants are allocated to heteroatoms as a set regardless of the kind of heteroatom.

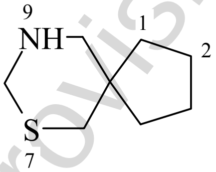
Example:



9-oxa-6-azaspiro[4.5]decane (PIN)

(b) If there is still a choice, low locants are assigned in accord with the following decreasing seniority order of heteroatoms: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Example:

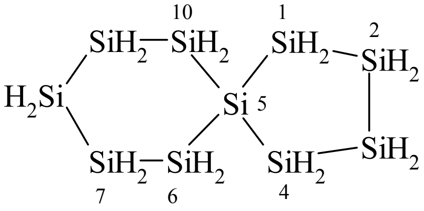


7-thia-9-azaspiro[4.5]decane (PIN)

P-24.2.4.2 Homogeneous heterocyclic spiro compounds with only monocyclic components

Heterocyclic spiro compounds with only monocyclic components and composed entirely of the same heteroatom are named as described in P-24.2 using the name of the homogeneous heteroacyclic parent hydride that has the same total number of skeletal heteroatoms. This method is preferred to skeletal replacement (‘a’) nomenclature described in P-24.2.4.1, in which the total number of heteroatoms is indicated by a numerical term. In either method it is not necessary to give the location of the heteroatoms because all positions are modified by the same heteroatom. The former method produces preselected parent hydride names.

Example:



spiro[4.5]decasilane (preselected name; see P-12.2)
decasilaspiro[4.5]decane

P-24.2.4.3 Heterocyclic spiro compounds consisting only of monocyclic rings and having alternating skeletal heteroatoms are named by two methods.

(a) By citing a prefix such as 'spiro', 'dispiro', etc., before a von Baeyer descriptor (indicating the numbers of heteroatoms linked to each spiro atom in each ring cited in increasing order and separated by a full stop) enclosed in square brackets followed successively by:

(i) a multiplying prefix ('di', 'tri', etc) denoting the number of heteroatoms of the first cited 'a' term that follows;

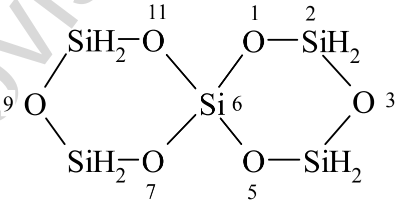
(ii) the 'a' terms of the hetero atoms, cited in the reverse seniority order for 'a' prefixes (see P-21.2.3.1), for example, Si before O);

(iii) the ending 'ane'. The hetero spiro system is numbered as is the corresponding hydrocarbon.

(b) By skeletal replacement ('a') nomenclature as described in P-24.2.4.1.

Method (b) generates preselected names.

Example:

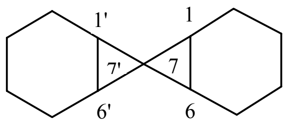


spiro[5.5]pentasiloxane
1,3,5,7,9,11-hexaoxa-2,4,6,8,10-pentasilaspiro[5.5]undecane
(preselected name; see P-12.2)

P-24.3 Monospiro compounds containing two identical polycyclic components

P-24.3.1 Monospiro compounds consisting of two identical polycyclic components are named by placing the nondetachable prefix 'spirobi' before the name of the component ring system enclosed in square brackets. The established numbering system of the polycyclic component system is retained with one system having primed locants. The location of the spiro atom is indicated in the name by the appropriate locants (unprimed first) placed at the front of the name.

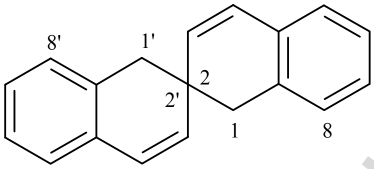
Example:



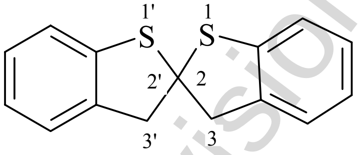
7,7′-spirobi[bicyclo[4.1.0]heptane] (PIN)

P-24.3.2 Where appropriate the maximum number of noncumulative double bonds is added (i.e., the system is made mancude) after construction of the whole skeleton. No indicated hydrogen is cited when none is present in the spiro system. If indicated hydrogen is needed, it is cited in front of the spiro atom locants.

Examples:

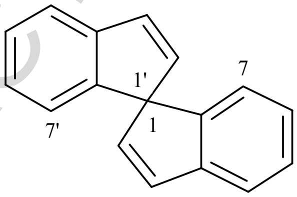


1*H*,1′*H*-2,2′-spirobi[naphthalene] (PIN)

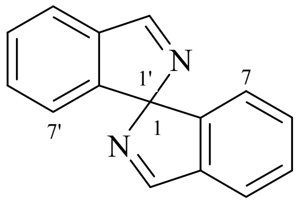


3*H*,3′*H*-2,2′-spirobi[[1]benzothiophene] (PIN)

Note: The double set of brackets in this name occurs because the spiro name requires them and brackets are used to enclose locants belonging to component names (see P-16.4.2.2).



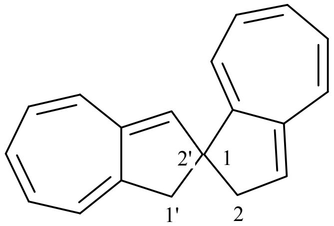
1,1′-spirobi[indene] (PIN)



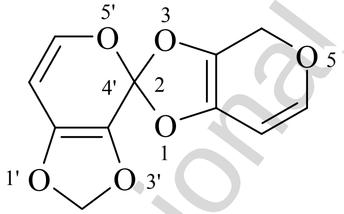
1,1′-spirobi[isoindole] (PIN)

P-24.3.3 If there is a choice for assigning primed locants, the lower number at the spiro atom is unprimed.

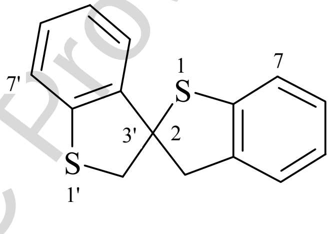
Examples:



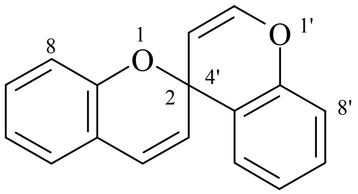
1′*H*,2*H*-1,2′-spirobi[azulene] (PIN)



4*H*-2,4′-spirobi[[1,3]dioxolo[4,5-*c*]pyran] (PIN)



2′*H*,3*H*-2,3′-spirobi[[1]benzothiophene] (PIN)
(the indicated hydrogen at position 2′ may be omitted in general nomenclature, but it must be cited in the preferred IUPAC name)

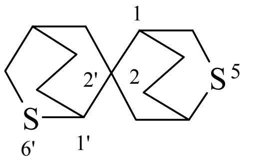


2,4′-spirobi[chromene] (PIN)

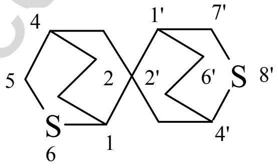
P-24.3.4 Heterocyclic ‘spirobi’ compounds named by skeletal replacement (‘a’) nomenclature

When components of ‘spirobi’ compounds are named by von Baeyer nomenclature, heteroatoms are indicated by skeletal replacement (‘a’) nomenclature. The spirobi- system is named as the saturated bi- or polycyclic alicyclic hydrocarbon and the heteroatoms are denoted by ‘a’ prefixes cited at the front of the completed ‘spirobi’ hydrocarbon name. If there is a choice, low locants are given to the spiro atom, then to the heteroatoms as described in Section P-24.2.4.1.

Examples:



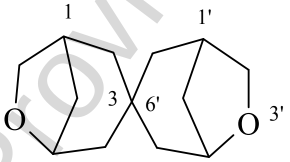
not



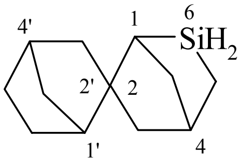
(I) correct

(II) incorrect

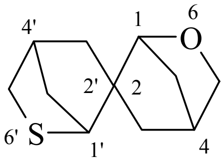
5,6′-dithia-2,2′-spirobi[bicyclo[2.2.2]octane] (**I**) (PIN)
[not 6,8′-dithia-2,2′-spirobi[bicyclo[2.2.2]octane] (**II**); the set of locants ‘5,6′ ’ in (**I**) is lower than ‘6,8′ ’ in (**II**)]



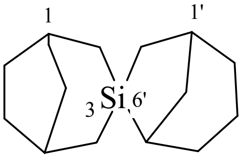
3′,6-dioxa-3,6′-spirobi[bicyclo[3.2.1]octane] (PIN)



6-sila-2,2′-spirobi[bicyclo[2.2.1]heptane] (PIN)



6-oxa-6′-thia-2,2′-spirobi[bicyclo[2.2.1]heptane] (PIN)

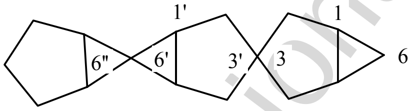


3-sila-3,6′-spirobi[bicyclo[3.2.1]octane] (PIN)

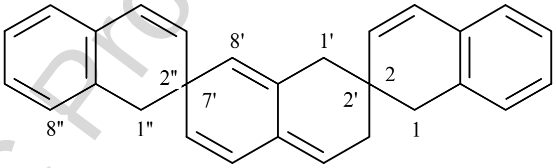
P-24.4 Three identical polycyclic components spirofused together

P-24.4.1 Dispiro compounds with three identical polycyclic components are named by placing the nondetachable prefix ‘dispiroter’ before the name of the component ring system enclosed in square brackets. The Latin multiplicative prefix ‘ter’ (see P-14.2.4) is used to indicate the repetition of identical components. Locants for the middle component are primed and for the third component double primed. The spiro atoms are indicated in front of the name by two pairs of locants separated by a colon. Indicated hydrogen is cited in front of these locants, if needed.

Examples:



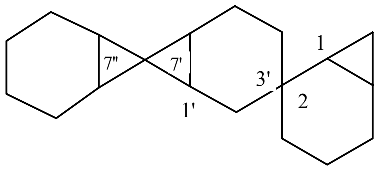
3,3′:6′,6′′-dispiroter[bicyclo[3.1.0]hexane] (PIN)



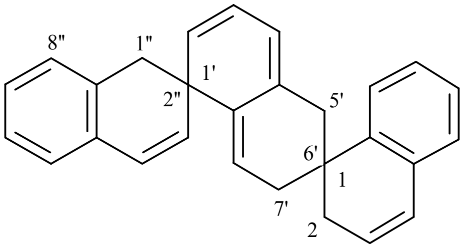
1*H*,1′*H*,1′′*H*,3′*H*-2,2′:7′,2′′-dispiroter[naphthalene] (PIN)

P-24.4.2 If there is a choice for locants, the lowest set of locants for all spiro atoms is selected when compared as a set in increasing order and, if there is a further choice, in order of citation in the name.

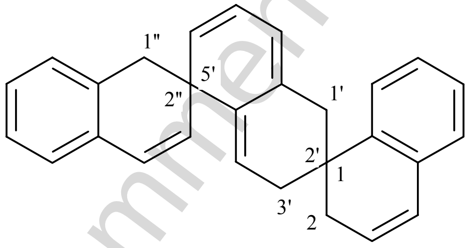
Examples:



2,3′:7′,7″-dispiroter[bicyclo[4.1.0]heptane] (PIN)



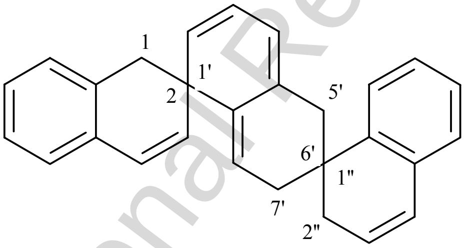
not



(I)
correct

(II)
incorrect

nor



(III)
incorrect

1″*H*,2*H*,5′*H*,7′*H*-1,6′:1′,2″-dispiroter[naphthalene] (**I**) (PIN)
[not 1′*H*,1″*H*,2*H*,3′*H*-1,2′:5′,2″-dispiroter[naphthalene] (**II**),
nor 1*H*,2″*H*,5′*H*,7′*H*-2,1′:6′,1″-dispiroter[naphthalene] (**III**);
the locant set ‘1,1′,2″,6′ ’ in (**I**) is lower than ‘1,2′,2″,5′ ’
in (**II**) or ‘1′,1″,2,6′ ’ in (**III**)]

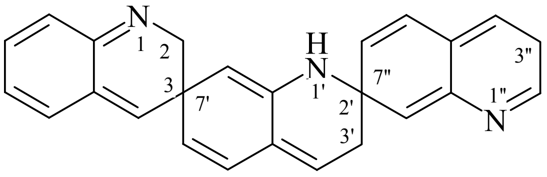
P-24.4.3 Three identical heterocyclic components spiro fused together

Dispiro compounds with three identical heterocyclic components may be named:

(a) by using heterocyclic monocyclic or polycyclic mancude components in the same way as for ‘spiroter’ hydrocarbons (see P-24.4.1). The numbering depends on the fixed numbering of the heterocyclic components;

(b) by skeletal replacement (‘a’) nomenclature when the components are polycyclic von Baeyer compounds; the numbering of the ‘spiroter’ von Baeyer hydrocarbon remains unchanged.

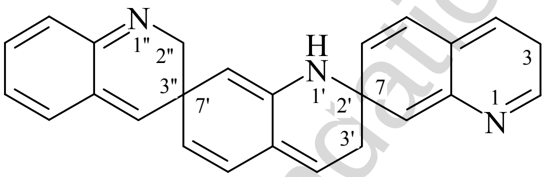
Examples:



(I)

correct

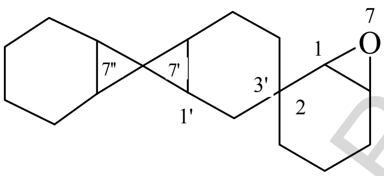
not



(II)

incorrect

1′*H*,2*H*,3′*H*,3″*H*-3,7′:2′,7″-dispiroter[quinoline](**I**) (PIN)
[not 1′*H*, 2″*H*,3*H*,3′*H*-7,2′:7′,3″-dispiroter[quinoline] (**II**);
the locant set ‘ 2′,3,7′,7″ ’ in (**I**) is lower than ‘ 2′,3″,7,7′ ’ in (**II**)]



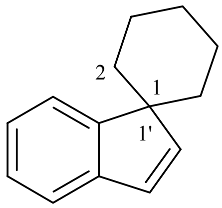
7-oxa-2,3′:7′,7″-dispiroter[bicyclo[4.1.0]heptane] (PIN)

P-24.5 Monospiro compounds with different components at least one of which is polycyclic

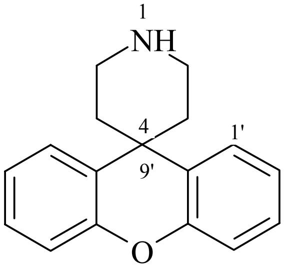
P-24.5.1 Monospiro compounds with different components at least one being a polycyclic ring system to which skeletal replacement (‘a’) nomenclature does not apply, are named by placing the component names in alphanumerical order within square brackets. The position of the spiro atom is denoted by appropriate locants separated by a comma and placed between the names of the two components. Locants of the second components are primed and thus any locants needed to name it are placed in square brackets. Indicated hydrogen is used if necessary.

> After due consideration, the Commission on Nomenclature of Organic Chemistry decided to maintain alphabetical order for naming spiro compounds composed of different components instead of using the seniority order of rings and ring systems. This exceptional case cannot be invoked as a precedent to use alphabetical order as the first criterion when other criteria are senior to it.

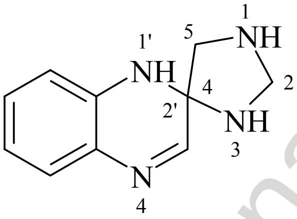
Examples:



spiro[cyclohexane-1,1′-indene] (PIN)



spiro[piperidine-4,9′-xanthene] (PIN)

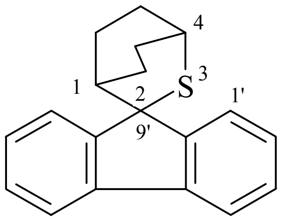


1′*H*-spiro[imidazoline-4,2′-quinoxaline] (PIN)

P-24.5.2 Monospiro compounds with different components at least one being polycyclic and at least one requiring the use of skeletal replacement (‘a’) nomenclature are named as in P-24.5.1; then, the ‘a’ prefixes are introduced and cited before the ‘spiro’ term.

> This is a change from the publication given in ref. 8 (see SP-4.1) in which the ‘a’ prefixes were kept with the component ring system.

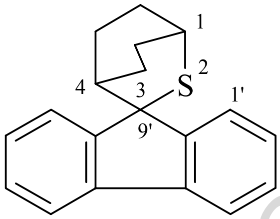
Examples:



(I)

correct

not

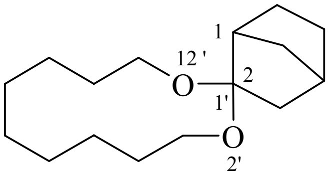


(II)

incorrect

3-thiaspiro[bicyclo[2.2.2]octane-2,9′-fluorene] (**I**) (PIN)
[not 2-thiaspiro[bicyclo[2.2.2]octane-3,9′- fluorene] (**II**);
the locant set ‘2,9′ ’ in (**I**) is lower than ‘3,9′ ’ in (**II**)]

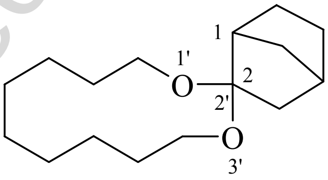
(the format of the ‘correct’ name as given in SP-4.1 in ref. 8,
spiro[fluorene-9,2′-[3]thiabicyclo[2.2.2]octane], is no longer
recommended)



(I)

correct

not



(II)

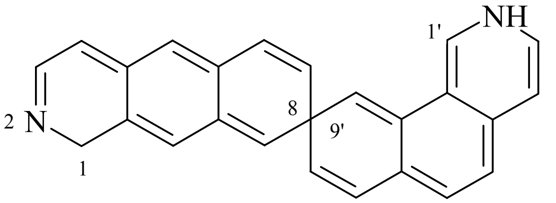
incorrect

2′,12′-dioxaspiro[bicyclo[2.2.1]heptane-2,1′-[cyclododecane] (**I**) (PIN)
[not 1′,3′-dioxaspiro[bicyclo[2.2.1]heptane-2,2′-cyclododecane] (**II**);
the spiro atom of the monocyclic hydrocarbon component is given preference
for low locant]

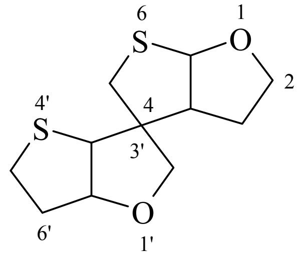
(the format of the ‘correct’ name as given in SP-4.1, ref. 8),
spiro[bicyclo[2.2.1]heptane-2,1′-[2,12]dioxacyclododecane]
is no longer recommended]

P-24.5.3 Alphanumerical order, as described in Section P-14.5, is used when necessary. When Roman letters are inadequate to distinguish alphabetically between two components, criteria based on lower italic fusion letters and numbers, heteroatom locants, and von Baeyer descriptor numbers are used, as appropriate. Locants present in bicyclic fused benzo compounds are directly cited at the front of the spiro name when they correspond to the numbering of the spiro compound; when they do not correspond to those of the spiro compound, they are placed in brackets (see third and fourth examples below).

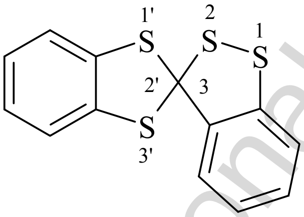
Examples:



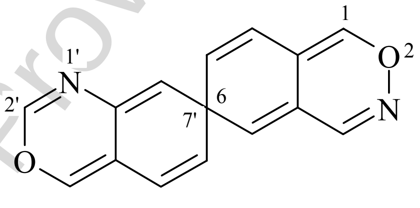
1*H*,2′*H*-spiro[benzo[*g*]isoquinoline-8,9′-benzo[*h*]isoquinoline] (PIN)
(benzo[*g*]…. before benzo[*h*]….)



2′*H*,5*H*-spiro[thieno[2,3-*b*]furan-4,3′-thieno[3,2-*b*]furan] (PIN)
(…[2,3-*b*]… before …[3,2-*b*]…)



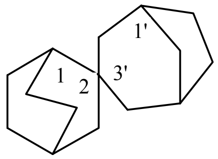
spiro[[1,2]-benzodithiole-3,2′-[1,3]benzodithiole] (PIN)
(1,2-benzo… before 1,3-benzo…)



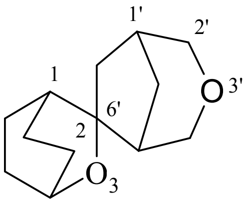
spiro[[2,3]-benzoxazine-6,7′-[3,1]benzoxazine] (PIN)
(2,3-benzoxazine before 3,1-benzoxazine)

P-24.5.4 In the case of components modified by skeletal replacement (‘a’) nomenclature, Rules P-24.5.2 and P-24.5.3 are applied to name the compound before skeletal replacement (‘a’) nomenclature is applied as described in P-24.5.2. The names of components modified by skeletal replacement (‘a’) nomenclature must not be used; thus Rule P-24.5.3 must be applied when required.

Examples:



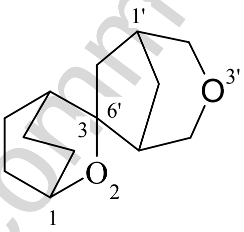
spiro[bicyclo[2.2.2]octane-2′,3-bicyclo[3.2.1]octane] (PIN)
[bicyclo[2.2.2]octane before bicyclo[3.2.1]octane; the descriptor
set ‘2.2.2’ is lower than ‘3.2.1’ (see P-14.5.4)]



(I)

correct

not



(II)

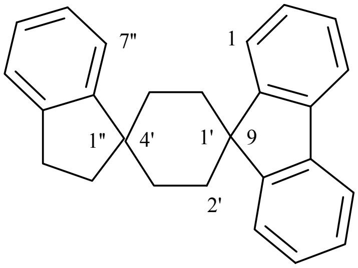
incorrect

3,3′-dioxaspiro[bicyclo[2.2.2]octane-2,6′-bicyclo[3.2.1]octane] (**I**) (PIN)
[not 2,3'-dioxaspiro[bicyclo[2.2.2]octane-3,6'-bicyclo[3.2.1]octane] (**II**);
spiro fusion is preferred to 'a' prefixes for low locants and the locant
set ‘2,6′ ’ in (**I**) is lower than ‘3,6′ ’ in (**II**)]

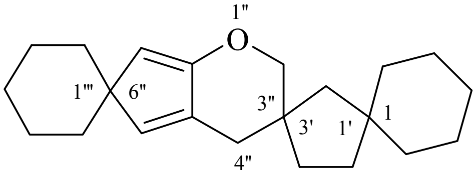
P-24.6 Unbranched polyspiro compounds with different components, one being polycyclic

Unbranched polyspiro compounds with at least two different components and at least one of which is polycyclic are named by placing the component names in order of their occurrence in the structure beginning with the terminal component lower in alphabetical order and enclosing with square brackets. A nondetachable prefix indicating the number of spiro atoms (‘dispiro’, ‘trispiro’, etc.) is placed in front of the enclosed component names. Locants of the first cited component are unprimed, the next one is primed, and so on; accordingly, locants required by the names of the second and later components are enclosed in square brackets. The positions of the spiro atoms are indicated by the appropriate pair of locants separated by a comma and placed between each pair of component ring system names. Indicated hydrogen is used as needed and cited in front of the ‘dispiro’, ‘trispiro’, etc., prefix. If both terminal ring systems are the same, the order for citation of components is determined by comparing the pair of second components from the end of the structure, and so on (See section SP-5 in ref. 8 for further discussion).

Examples:



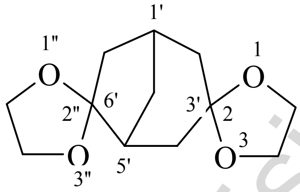
dispiro[fluorene-9,1′-cyclohexane-4′,1″-indene] (PIN)



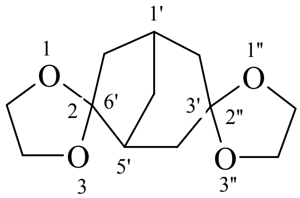
2″*H*,4″*H*-trispiro[cyclohexane-1,1′-cyclopentane-3′,3″-cyclopenta[*b*]pyran-6″,1‴-cyclohexane] (PIN)

P-24.6.1 If there is a choice of locants, the lowest set of locants for all spiro atoms is selected when compared in increasing order and, if there is still a choice, in order of their citation in the name (see P-24.2.4.1).

Example:



not



(I)

correct

(II)

incorrect

dispiro[1,3-dioxolane-2,3′-bicyclo[3.2.1]octane-6′,2″-[1,3]dioxolane] (**I**) (PIN)
[not dispiro[1,3-dioxolane-2,6′-bicyclo[3.2.1]octane-3′-2″-[1,3]dioxolane](**II**);
the locant sets ‘ 2,2″,3′,6′ ’ are identical, but in the name the order of citation
‘ 2,3′,6′,2″ ’ in (**I**) is lower than ‘2,6′,3′,2″’ in (**II**)]

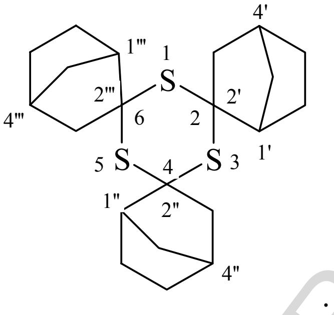
Note: The 'correct' name above is constructed in accordance with the traditional method, and is preferred. An alternative name, dispiro[bicyclo[3.2.1]octane-2,3′:6′,2″-bis([1,3]dioxolane),could be considered as an adaptation of multiplicative nomenclature (see also P-24.7).

P-24.7 Branched polyspiro compounds

When three or more components are spirofused to another single component, the system is described as a branched spirofused system. Terminal components have only one spiro atom.

P-24.7.1 When a central component is spirofused to three or more identical terminal components, the central component is cited first and its locants are unprimed. The terminal components are cited with the appropriate multiplicative prefix (‘tris’, ‘tetrakis’, etc.) and locants primed, double primed, etc. in accordance with the lowest possible locants of the spiro atoms of the central component. The spiro atoms are indicated by pairs of locants separated by a colon. Indicated hydrogen is cited as necessary in front of the appropriate spiro prefix.

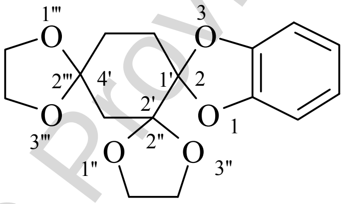
Example:



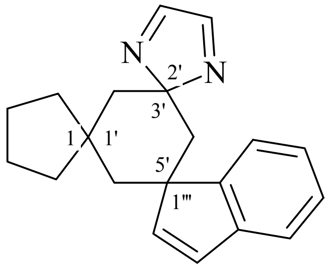
trispiro[1,3,5-trithiane-2,2′:4,2″:6,2‴-tris(bicyclo[2.2.1]heptane)] (PIN)

P-24.7.2 When two or more different terminal components are spirofused to a central component, the alphabetically earliest is cited first with a multiplicative prefix, if appropriate, followed by the central component and then the remaining terminal component(s) in alphabetical order, the first cited being spirofused to the lowest numbered spiro position of the central component.

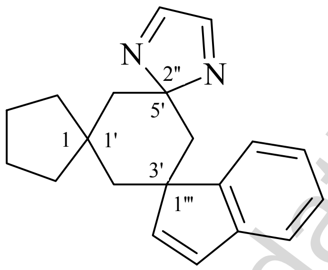
Examples:



trispiro[1,3-benzodioxole-2,1′-cyclohexane-2′,2″:4′,2‴-bis([1,3]dioxolane)] (PIN)



not



(I)

correct

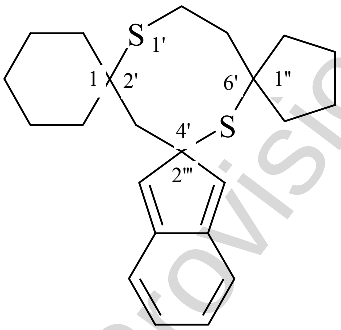
(II)

incorrect

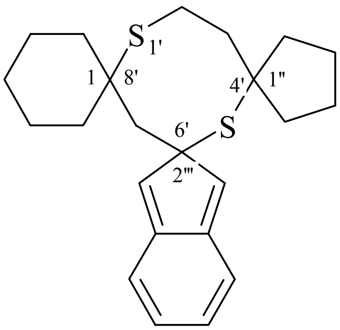
trispiro[cyclopentane-1,1′-cyclohexane-3′-2″- imidazole-5′,1‴-indene] (**I**) (PIN)
[not trispiro[cyclopentane-1,1′-cyclohexane-5′,2″-imidazole-3′,1‴-indene] (**II**);
the locant sets ‘1,1′,1‴,2″,3′,5′’ in both (**I**) and (**II**) are the same, but in the name
the order of citation, ‘1,1′,3′,2″,5′,1‴ ’ in (**I**) is lower than ‘1,1′,5′,2″,3′,1‴ ’
in (**II**) (see P-24.7.3)]

P-24.7.3 If there is a choice of locants, the lowest set of locants for all spiro atoms is selected when compared as a set in increasing order, and, if still undecided, in their order of citation in the name. If a choice still remains, criteria about heteroatoms and indicated hydrogen are taken into consideration (see Section SP-3.2 in ref 8).

Example:



not



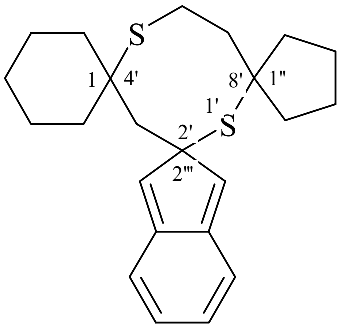
(I)

correct

(II)

incorrect

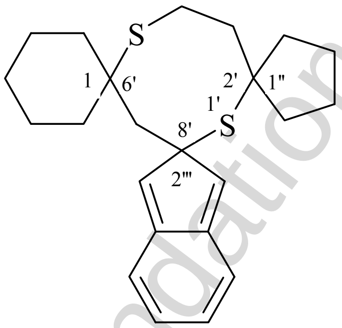
nor



(III)

incorrect

nor



(IV)

incorrect

trispiro[cyclohexane-1,2′-[1,5]dithiocane-6′,1″-cyclopentane-4′,2‴-indene] (**I**) (PIN)
[not trispiro[cyclohexane-1,8′-[1,5]dithiocane-4′,1″-cyclopentane-6′,2‴-indene] (**II**);
nor trispiro[cyclohexane-1,4′-[1,5]dithiocane-8′,1″-cyclopentane-2′,2‴-indene] (**III**);
nor trispiro[cyclohexane-1,6′-[1,5]dithiocane-2′,1″-cyclopentane-8′,2‴-indene] (**IV**);
the locant set ‘1,1″,2′,2‴,4′,6′ ’ in (**I**) is lower than ‘1,1″,2‴,4′,6′,8′ ’ in (**II**).
‘1,1″,2′,2‴,4′,8′ ’ in (**III**), or ‘1,1″,2′,2‴,6′,8′ ’ in (**IV**)]

P-24.8 Spiro systems containing atoms with nonstandard bonding numbers

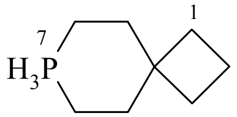
The λ-convention, characterized by the symbol λ^n, is used to identify heteroatoms with nonstandard bonding numbers (see P-14.1). The symbol is placed at the front of the complete name or before the ‘a’ prefix for the atom to which it refers.

P-24.8.1 Spiro compounds with only monocyclic ring components
P-24.8.2 Monospiro compounds containing two identical polycyclic components
P-24.8.3 Three identical components with one nonstandard spiro atom
P-24.8.4 Monospiro compounds with different components at least one of which is polycyclic and a nonstandard spiro atom
P-24.8.5 Unbranched polyspiro compounds with different components at least one of which is polycyclic and at least one nonstandard spiro atom
P-24.8.6 Branched spiro compounds with at least one polycyclic component

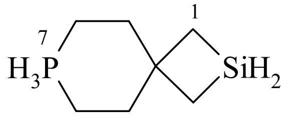
P-24.8.1 Spiro compounds with only monocyclic ring components

P-24.8.1.1 Heteroatoms having nonstandard bonding numbers receive locants in accordance with the numbering of the corresponding spiro hydrocarbon.

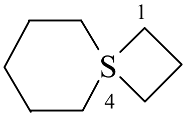
Examples:



7λ^5-phosphaspiro[3.5]nonane (PIN)



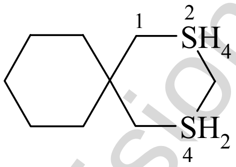
7λ^5-phospha-2-silaspiro[3.5]nonane (PIN)



4λ^4-thiaspiro[5.3]nonane (PIN)

P-24.8.1.2 If there is a choice, lower locants are assigned to heteroatoms with the higher bonding numbers, for example, the lower number is assigned to a λ^6 heteroatom rather than to a λ^4 heteroatom.

Example:

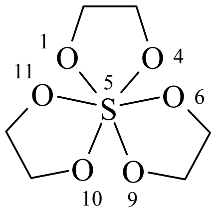


2λ^6-thia-4λ^4-thiaspiro[5.5]undecane (PIN)

P-24.8.1.3 Spiro ring systems composed only of three monocyclic rings and a nonstandard spiro atom.

P-24.8.1.3.1 Ring systems consisting of three monocyclic rings and one nonstandard spiro atom (e.g., a λ^6 spiro atom) are named by placing the prefix 'spiro' before the name corresponding to an acyclic hydrocarbon with the same total number of atoms in the spiro ring system. Heteroatoms are indicated by 'a' prefixes and the nonstandard bonding number by the lambda symbol (see P-14.1). In the von Baeyer spiro descriptor, the locant of the spiro atom is used as a superscript number to indicate each time the spiro atom is revisited.

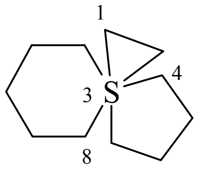
Example:



1,4,6,9,10,13-hexaoxa-5λ^6-thiaspiro[4.4^5.4^5]tridecane (PIN)

P-24.8.1.3.2 If there is a choice for numbering, a small ring is numbered before a larger ring.

Example:

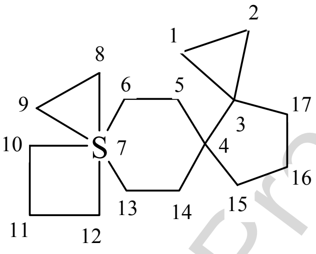


3λ^6-thiaspiro[2.4^3.5^3]dodecane (PIN)

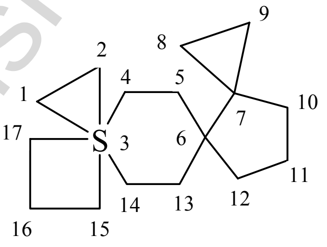
P-24.8.1.4 Polyspiro systems which include three monoalicyclic rings with one nonstandard hetero spiro atom as well as other spiro fusions are named using a combination of methods for naming the polyspiro hydrocarbons and for indicating heteroatoms with nonstandard bonding numbers. If there is a choice for numbering, the following criteria are considered in order until a decision is made.

(a) Low numbers are selected for spiro atoms.

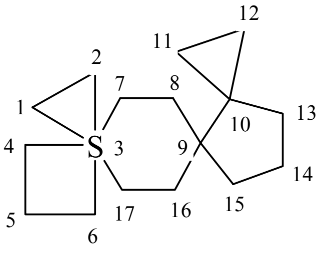
Example:



not



nor



(I)
correct

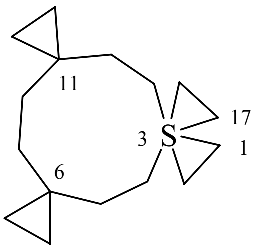
(II)
incorrect

(III)
incorrect

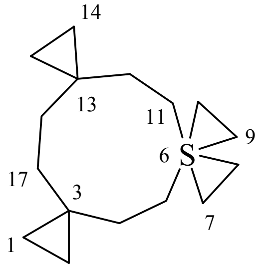
7λ^6-thiatrispiro[2.0.2.2^7.3^7.2^4.3^3]heptadecane (**I**) (PIN)
[not 3λ^6-thiatrispiro[2.4^3.2.0.2^{10}.3^9.2^3.3^3]heptadecane (**II**);
nor 3λ^6-thiatrispiro[2.4^3.2.0.2^{10}.3^9.2^3.3^3]heptadecane (**III**);
the locant set for the spiro atoms in (**I**), '3,4,7', is lower than
'3,6,7' in (**II**) or '3,9,10' in (**III**)]

(b) Low numbers are selected for spiro atoms connecting three rings.

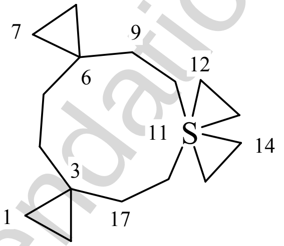
Example:



not



nor



(I) correct

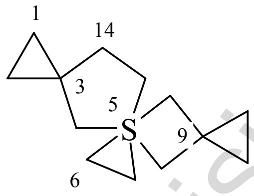
(II) incorrect

(III) incorrect

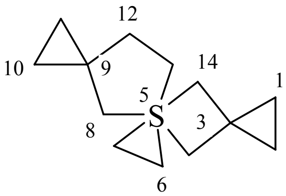
$3\lambda^{6}$-thiatrispiro[2.2.2^{6}.2.2^{11}.2^{3}.2^{3}]heptadecane (**I**) (PIN)
[not $6\lambda^{6}$-thiatrispiro[2.2.2^{6}.2^{6}.2.2^{13}.2^{3}]heptadecane (**II**);
nor $11\lambda^{6}$-thiatrispiro[2.2.2^{6}.2.2^{11}.2^{11}.2^{3}]heptadecane (**III**);
the locant '3' for the spiro atom connecting three rings in (**I**) is lower than '6' in (**II**) or '11' in (**III**)]

(c) Low numbers are selected for the von Baeyer spiro descriptor in order of citation.

Example:



not



(I) correct

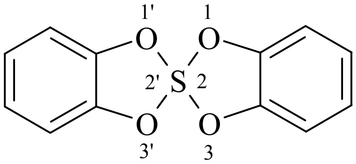
(II) incorrect

$5\lambda^{6}$-thiatrispiro[2.1.2^{5}.1.2^{9}.1^{5}.2^{3}]tetradecane (**I**) (PIN)
[not $5\lambda^{6}$-thiatrispiro[2.1.2^{5}.1.2^{9}.2^{5}.1^{3}]tetradecane (**II**);
the spirodescriptor set '2,1,2,1,2,1,2' in (**I**), is lower than '2,1,2,1,2,2,1' in (**II**)]

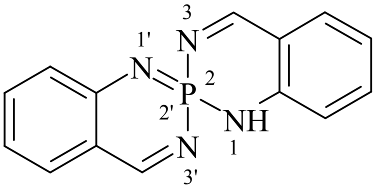
P-24.8.2 Monospiro compounds containing two identical polycyclic systems

The λ^{n} symbol is placed at the front of the complete name formed from the names of two identical components including the heteroatoms in their name. If indicated hydrogen atoms are required, they are placed before the λ symbol. When there is a choice, the locant of the first cited component is used for indicated hydrogen.

Examples:



2λ^4-2,2′-spirobi[[1,3,2]benzodioxathiole] (PIN)

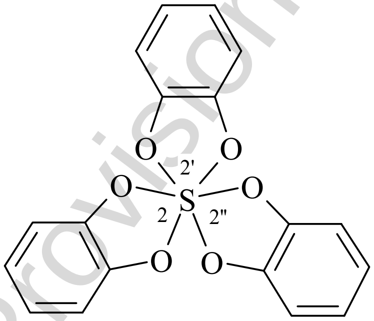


1*H*-2λ^5-2,2′-spirobi[1,3,2-benzodiazaphosphinine] (PIN)

P-24.8.3 Three identical polycyclic components with one nonstandard spiro atom

Ring systems composed of three identical polycyclic components and only one spiro atom are named by placing the prefix spiroter- before the name of the polycyclic component enclosed in square brackets. The three spiro locants are cited at the front of the name preceded by the λ-symbol with its locant.

Example:

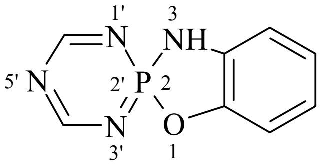


2λ^6-2,2′,2″-spiroter[[1,3,2]benzodioxathiole] (PIN)

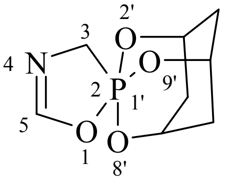
P-24.8.4 Monospiro compounds containing a nonstandard spiro atom and different components at least one of which is polycyclic.

P-24.8.4.1 Monospiro ring systems composed of two different ring systems and a spiro heteroatom with a nonstandard bonding number are named by placing the prefix spiro in front of the names of the components in alphabetical order and with appropriate spiro locants. The lowest locant (unprimed) is used to denote the spiro-fusion and the appropriate λ symbol is placed at the front of the name. Indicated hydrogen, if necessary, is added in front of the λ symbol. Any additional atom with a nonstandard bonding number is treated as a part of the name of the heterocycle; the λ symbol is cited with the appropriate locant.

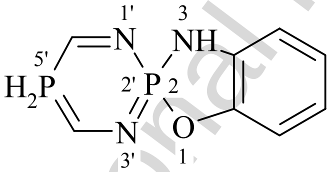
Examples:



3*H*-2λ^5-spiro[1,3,2-benzoxazaphosphole-2,2′-[1,3,5,2]triazaphosphinine] (PIN)



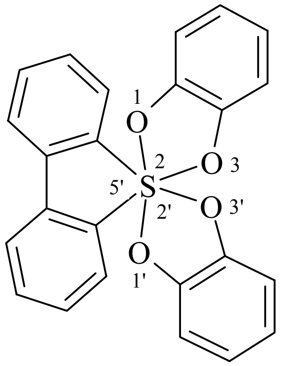
3*H*-λ^5-spiro[1,4,2-oxazaphosphole-2,1′-[2,8,9]trioxa[1]phosphaadamantane] (PIN)
3*H*-λ^5-spiro[1,4,2-oxazaphosphole-2,1′-[2,8,9]trioxa[1]phosphatricyclo[3.3.1.1^{3,7}]decane]
(adamantane, a retained name, is preferred to its systematic von Baeyer name)



3*H*-2λ^5-spiro[1,3,2-benzoxazaphosphole-2,2′-[1,3,2,5λ^5]diazadiphosphinine] (PIN)

P-24.8.4.2 When three components, represented by two different individual compounds, are present, the name of the component that is cited second is placed in parentheses to highlight this unusual situation.

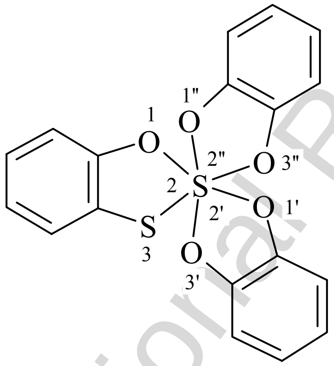
Example:



$2\lambda^{6}$-spiro[1,3,2-benzodioxathiole-2,2′-([1,2,3]benzoxadithiole)-2,5″-dibenzo[*b*,*d*]thiophene] (PIN)

P-24.8.4.3 Two identical components are denoted by the prefix ‘bis’.

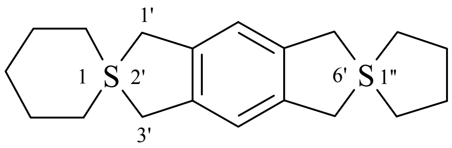
Example:



$2\lambda^{6}$-spiro[bis([1.3.2]benzodioxathiazole)-2,2′:2,2″-[1,2,3]benzoxadithiole] (PIN)

P-24.8.5 Unbranched polyspiro compounds with different components at least one of which is polycyclic and with at least one nonstandard spiro atom are named using the method described in P-24.6. The λ-symbol denoting a spiro junction is associated with the least primed locants and placed in front of the name; it is preceded by indicated hydrogen(s), as needed.

Example:

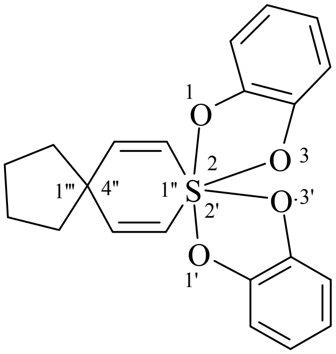


1′*H*,3′*H* -$1\lambda^{4}$,$6'\lambda^{4}$-dispiro[thiane-1,2′-benzo[1,2-*c*:4,5-*c*′]dithiophene-6′,1″-thiolane] (PIN)

P-24.8.6 Branched spiro compounds with at least one polycyclic component

If two or more different terminal components are spirofused to a central component, the alphabetically earliest is cited first with multiplicative prefixes, if appropriate, followed by the central component and the remaining terminal components in alphabetical order. The λ symbol is placed at the front of the complete name and is denoted by the lowest spiro locant.

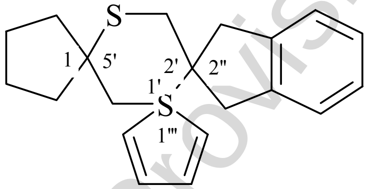
Example:



$2\lambda^6$-dispiro[bis(1,3,2-benzodioxathiole)-2,1″:2′,1″-thiopyran-4″,1‴-cyclopentane] (PIN)

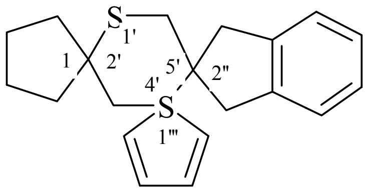
When there is a choice for locants, the lowest set of locants for all spiro atoms is selected, first by comparing them as a set in increasing numerical order, and, if still undecided, in the order of citation in the name. If a choice still remains, criteria involving the heteroatoms and indicated hydrogen atoms are taken into consideration (see Section P-3.2 in ref. 8)

Examples:



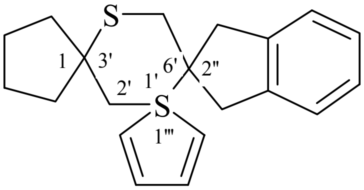
(I)
correct

not



(II)
incorrect

nor



(III)

incorrect

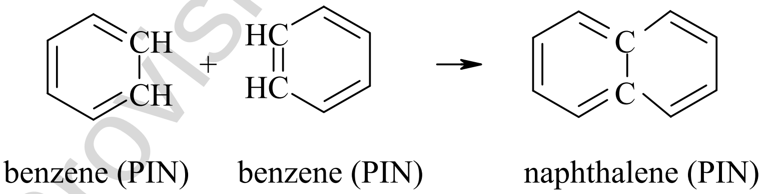
1′λ^4-trispiro[cyclopentane-1,5′-[1,4]dithane-2′,2″-indane-1′,1‴-thiophene] (**I**) (PIN)
[not 4′λ^4-trispiro[cyclopentane-1,2′-[1,4]dithane-5′,2″-indane-4′,1‴-thiophene] (**II**);
nor 1′λ^4-trispiro[cyclopentane-1,3′-[1,4]dithane-6′,2″-indane-1′,1‴-thiophene] (**III**);
the locant set ‘1,1′,1‴,2′,2″,5′ ’ in (**I**) is lower than ‘1,1‴,2′,2″,4′,5′ ’ in (**II**), or ‘1,1′,1‴,2″,3′,6′ ’ in (**III**)]

P-25 Fused and bridged fused systems

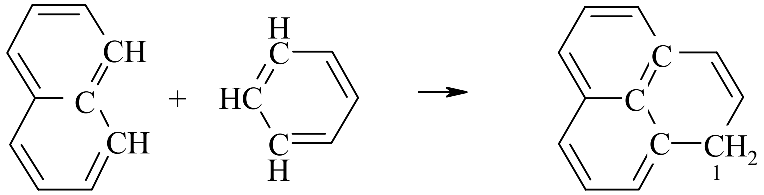
P-25.0 Introduction

This section is based on the document entitled ‘Nomenclature of Fused and Bridged Fused Ring System, IUPAC Recommendations 1998’ (ref. 4).

In nomenclature, fusion is the operation that creates a common bond between two rings, each ring contributing one bond and the two atoms directly attached to the bond. This type of fusion is called *ortho*- or *ortho*- and *peri*-fusion if two adjacent bonds are involved. The term fusion is also used todesc ribe the operation creating a common atom between two ring systems, each contributing one atom. This type of fusion is called spirofusion (see P-24.1). Traditionally, ortho- and ortho- and peri-fusion were simply called fusion and the resulting polycyclic systems were referred to as fused ring systems or fused ring compounds. The term 'spirofusion' is new in nomenclature, and to avoid ambiguity 'fusion' should not be used without the prefix 'spiro' when 'spirofusion' is intended."

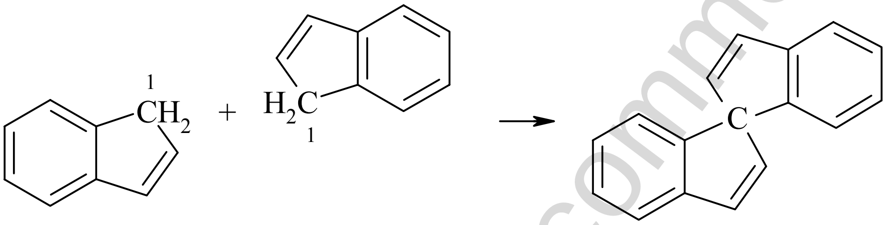


[naphthalene results from the fusion (*ortho*-fusion) of two benzene rings (one bond and two atoms in common)]



naphthalene (PIN) benzene (PIN) 1*H*-phenalene (PIN)

[1*H*-phenalene results from the fusion (*ortho*- and *peri*-fusion) of a naphthalene ring system and a benzene ring (two bonds and three atoms in common]



indene (PIN) indene (PIN) 1,1′-spirobi[indene] (PIN)

[spiro[biindene] results from the spirofusion of two indene ring systems (one atom in common)]

This section deals with fused (*ortho*- and *ortho*- and *peri*-fused) ring systems and bridged fused (*ortho*- and *ortho*- and *peri*-fused) ring systems. Spirofusion is described in Section P-24. This section is intended only as an introduction to the vast field of fusion nomenclature discussed in the document entitled 'Nomenclature of Fused and Bridge Fused Ring Systems' (ref. 4). The principles presented herein use rather simple examples; for more complex ring systems the publication noted above or the '*Ring Systems Handbook*', published by the Chemical Abstracts Service (ref. 16), should be consulted. Changes from previous rules are highlighted.

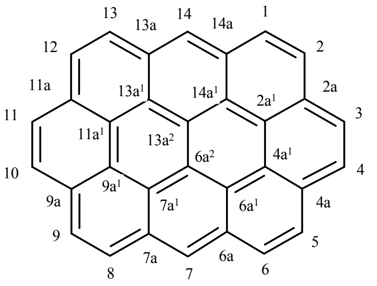
P-25.1 Names of hydrocarbon parent compounds are divided into two categories.

P-25.1.1 Retained names used for parent components and as attached components
P-25.1.2 Names formed systematically using endings and prefixes used for parent components and as attached components

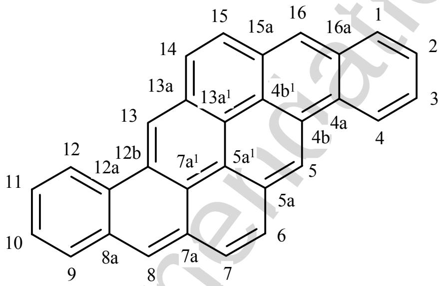
P-25.1.1 Retained names for hydrocarbons (also called trivial names) used for parent components and for attached components

Retained names for polycyclic hydrocarbons are listed in Table 2.7, in decreasing order of seniority for being chosen as parent components in fusion nomenclature. Their numbering is indicated as the result of the application of the specific criteria used to number fused ring systems described in Section P-25.3.3.

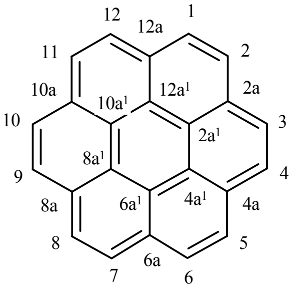
Table 2.7 Retained names of hydrocarbon parent components in descending order of seniority (the senority order is indicated by the number preceding the name; the lower the number the higher the senority)



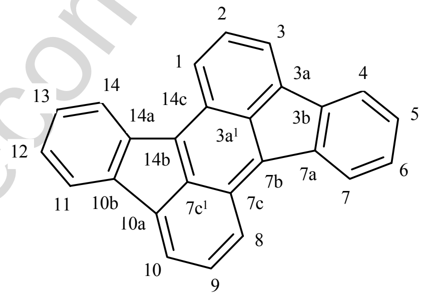
(1) ovalene (PIN)



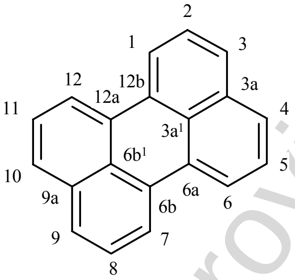
(2) pyranthrene (PIN)



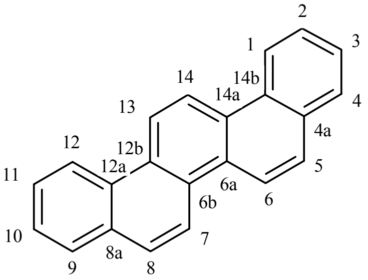
(3) coronene (PIN)



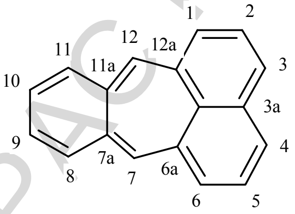
(4) rubicene (PIN)



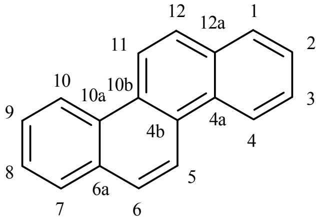
(5) perylene (PIN)



(6) picene (PIN)

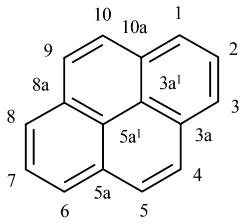


(7) pleiadene (PIN)

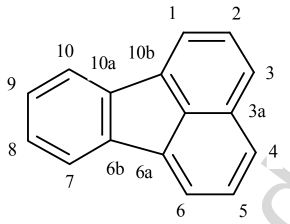


(8) chrysene (PIN)

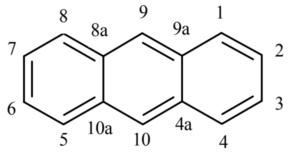
Table 2.5 (cont'd.)



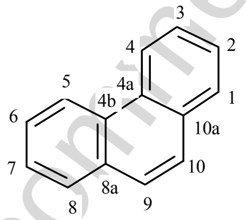
(9) pyrene (PIN)



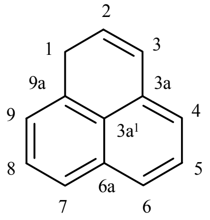
(10) fluoranthene (PIN)



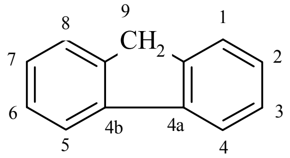
(11) anthracene (PIN)
(special numbering)



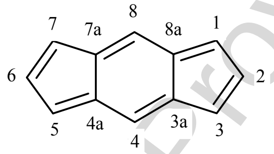
(12) phenanthrene (PIN)
(special numbering)



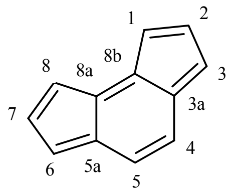
(13) phenalene (PIN)
(1*H*-isomer shown)



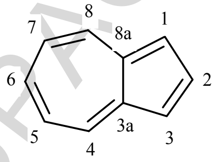
(14) fluorene (PIN)
(9*H*-isomer shown)



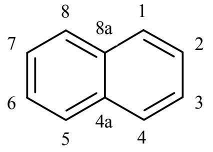
(15) *s*-indacene (PIN)



(16) *as*-indacene (PIN)

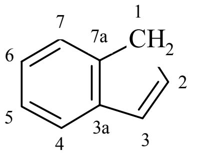


(17) azulene (PIN)



(18) naphthalene (PIN)

Table 2.5 (cont'd.)



(19) indene (PIN)
(1*H*-isomer shown)

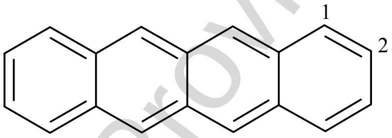
P-25.1.2 Systematically named hydrocarbon parent components

Names for some hydrocarbon parent components, having the maximum number of noncumulated double bonds and having at least two rings of five or more ring members are systematically formed using a prefix and an ending or term representing the nature and arrangement of the component rings. Rules for numbering are described in Section P-25.3.3.

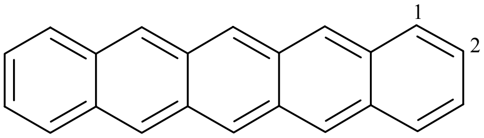
P-25.1.2.1	Polyacenes
P-25.1.2.2	Polyaphenes
P-25.1.2.3	Polyalenes
P-25.1.2.4	Polyphenylenes
P-25.1.2.5	Polynaphthylenes
P-25.1.2.6	Polyhelicenes
P-25.1.2.7	Ace...ylenes

P-25.1.2.1 Polyacenes. A hydrocarbon parent component consisting of four or more *ortho*-fused benzene rings in a straight linear arrangement is named by citing a numerical prefix (‘tetra’, ‘penta’, etc.) denoting the number of rings followed by the ending ‘acene’ (derived from the retained name anthracene) with elision of a letter ‘a’.

Examples:



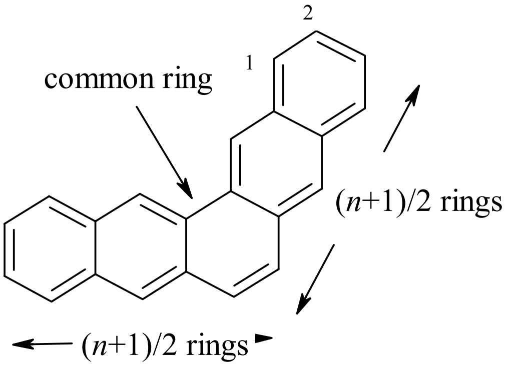
tetracene (PIN)
(formerly naphthacene)



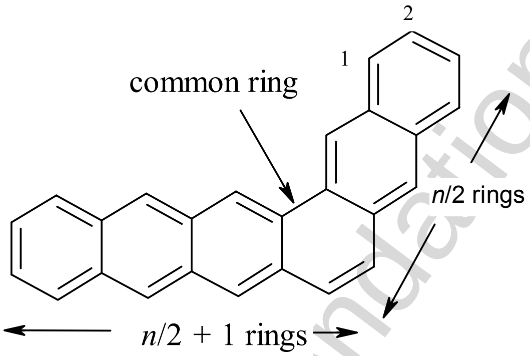
pentacene (PIN)

P-25.1.2.2 Polyaphenes. A hydrocarbon parent component consisting of *n* *ortho*-fused benzene rings ($n > 3$) forming two straight linear arrangements of $(n + 1)/2$ rings (if *n* is odd) or $n/2$ and $(n/2) + 1$ rings (if *n* is even) with a common benzene ring and that make a formal angle of 120° with each other is named by citing the numerical prefix (‘tetra’, ‘penta’, etc.) denoting the total number of benzene rings followed by the ending ‘phene’ (derived from **phen**anthrene).

Example:



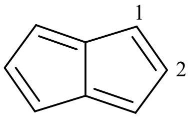
pentaphene (n = 5) (PIN)



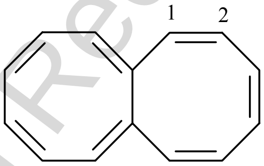
hexaphene (n = 6) (PIN)

P-25.1.2.3 Polyalenes. A hydrocarbon parent component consisting of two identical *ortho*-fused monocyclic hydrocarbon rings is named by citing the numerical prefix ('penta', 'hepta', etc.) that denotes the number of carbon atoms in each ring followed by the ending 'alene' (derived from naphthalene) with elision of a letter 'a'. The name naphthalene is retained.

Examples:



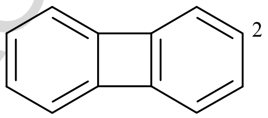
pentalene (PIN)



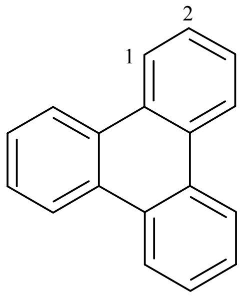
octalene (PIN)

P-25.1.2.4 Polyphenylenes. A hydrocarbon parent component consisting of a monocyclic hydrocarbon with an even number of carbon atoms and benzene rings *ortho*-fused to alternate sides is named by citing a numerical prefix ('tri', 'tetra', etc.) denoting the number of benzene rings followed by the term 'phenylene'. The traditional name biphenylene is retained.

Examples:



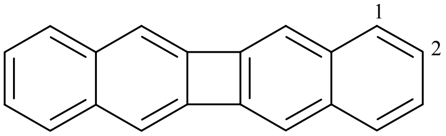
biphenylene (PIN)
(not diphenylene)



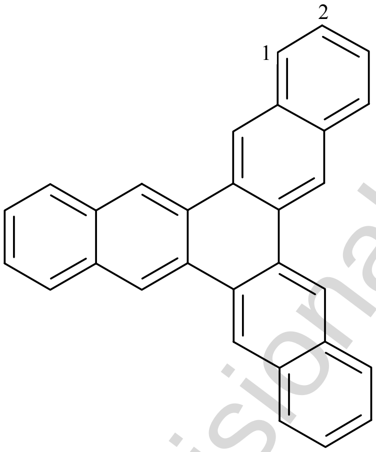
triphenylene (PIN)

P-25.1.2.5 Polynaphthylenes. A hydrocarbon parent component that consists of a monocyclic hydrocarbon with an even number of carbon atoms *ortho*-fused on alternate sides to the 2,3-positions of naphthalene rings is named by citing a numerical prefix ('tri', 'tetra', etc.) denoting the number of naphthalene rings followed by the term 'naphthylene'. The series begins with three naphthalene rings, trinaphthylene. The first member of the series, which would be dinaphthylene, is named as a fused hydrocarbon, i.e., dibenzo[*b*,*h*]biphenylene, and thus is not considered as a parent component.

Examples:



dibenzo[*b*,*h*]biphenylene (PIN)
(not dinaphthylene)

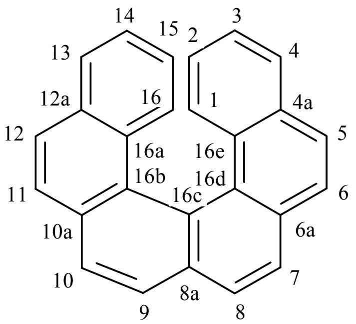


trinaphthylene (PIN)

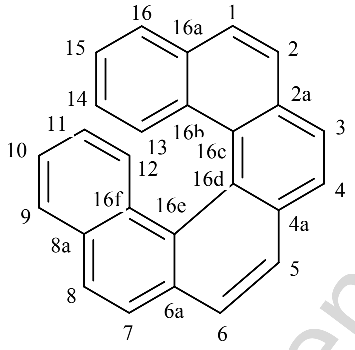
P-25.1.2.6 Polyhelicenes. A hydrocarbon parent component of six or more rings that consists of a benzene ring *ortho*-fused to the 3,4-position of phenanthrene and further benzene rings fused in a similar way is named by citing a numerical prefix ('hexa', 'hepta', etc.) denoting the total number of benzene rings forming a helical arrangement followed by the term 'helicene'.

Note that the definition of polyhelicenes has been changed. The series begins with six rings and not five rings as indicated in the 1993 Guide (R-2.4.1.3.6 in ref. 2) and in the Glossary of Class Names (ref. 17). A further change related to the orientation and numbering has been recommended in the comprehensive fused ring nomenclature document 'Nomenclature of Fused and Bridged Fused Systems' (ref. 4). This new orientation and numbering are presented in Section P-25.3.3.

Example:



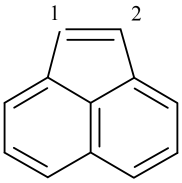
hexahelicene (PIN)
(new orientation
and numbering)



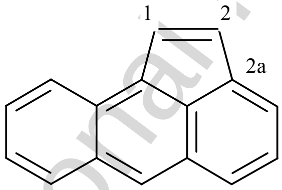
(orientation and numbering
no longer recommended; but
still in use by CAS, ref 16)

P-25.1.2.7 Ace...ylenes. A hydrocarbon parent component that consists of a five membered ring *ortho*- and *peri*-fused to naphthalene, anthracene, or phenanthrene is named by adding the prefix ‘ace’ to the retained name and changing the ending ‘alene’, ‘acene’, or ‘ene’, respectively, to ‘ylene’.

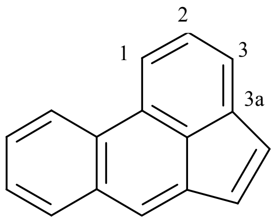
Examples:



acenaphthylene (PIN)



aceanthrylene (PIN)



acephenanthrylene (PIN)

P-25.2 Names of heterocyclic parent components are divided into two categories.

P-25.2.1	Retained names used for parent components and as attached components
P-25.2.2	Names formed systematically using endings and prefixes used for parent components and attached components

P-25.2.1 Retained names for heterocycles (also called trivial names) with the maximum number of noncumulative double bonds (mancude systems) used for parent components and as attached components are given in Table 2.8.

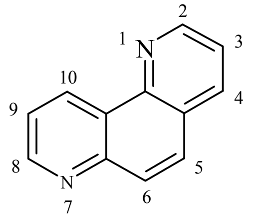
Ring systems are arranged in decreasing order of seniority for parent compounds in accordance with the seniority order described in Section P-25.4.2.2 and exemplified in Section P-25.9.1.

Functional replacement, as described in Section P-35 is used to replace O by S, Se, and Te to generate names of chalcogen analogues of chromene, isochromene and xanthene (see Table

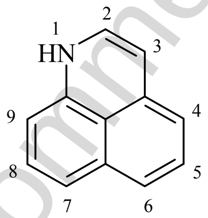
2.8). Some names listed in Table 2.8 can be modified by a system of replacement specific to some nitrogen-containing compounds, in which N is replaced by As or P. The modified names are listed in Table 2.9; the modifiable compounds are marked by the symbol ◊ in Table 2.8.

Rules for numbering are described in Section 25.3.3.

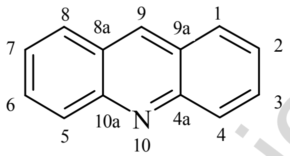
Table 2.8 Retained names of heterocyclic parent components in descending order of seniority (the senority order is indicated by the number preceding the name; the lower the number, the higher the seniority; names denoted by the symbol ◊ are further modified as shown in Table 2.9)



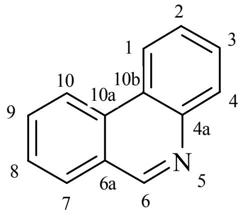
(1) phenanthroline (PIN)
(1,7-isomer shown; other isomers are: 1,8-; 1,9-; 1,10-; 2,7-; 2,8-; 2,9-; 3,7-; 3,8-; 4,7-)



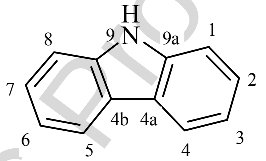
(2) perimidine (PIN)
(1*H*-isomer shown)



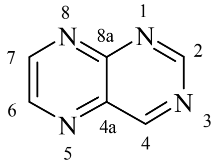
(3) acridine ◊ (PIN)
(special numbering)



(4) phenanthridine ◊ (PIN)
(special numbering)

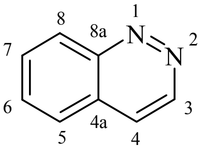


(5) carbazole (PIN)
(9*H*-isomer shown; special numbering)

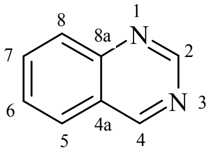


(6) pteridine (PIN)

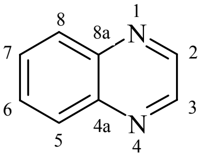
Table 2.7 (cont'd.)



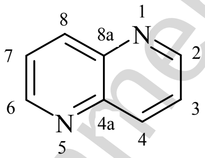
(7) cinnoline (PIN)



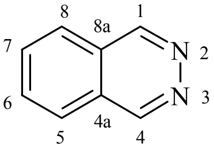
(8) quinazoline (PIN)



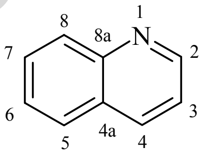
(9) quinoxaline (PIN)



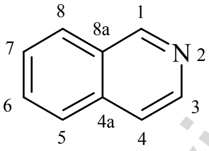
(10) naphthyridine (PIN)
(1,5-isomer; other isomers
are 1,6-; 1,7-; 1,8-; 2,6-; 2,7-)



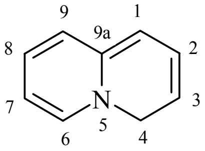
(11) phthalazine (PIN)



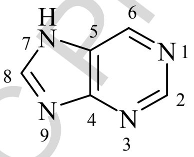
(12) quinoline ◊ (PIN)



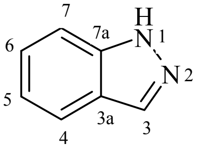
(13) isoquinoline ◊ (PIN)



(14) quinolizine ◊ (PIN)
(4*H*-isomer shown)

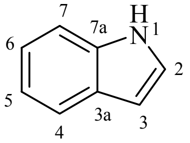


(15) purine (PIN)
(special numbering)

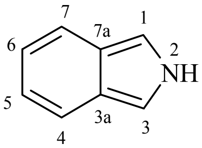


(16) indazole (PIN)
(1*H*-isomer shown)

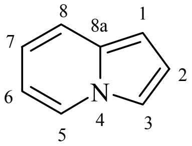
Table 2.7 (cont'd)



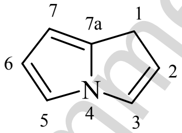
(17) indole ◊ (PIN)
(1*H*-isomer shown)



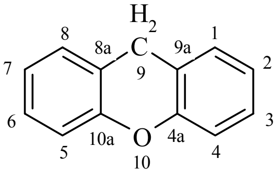
(18) isoindole ◊ (PIN)
(2*H*-isomer shown)



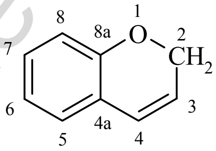
(19) indolizine ◊ (PIN)



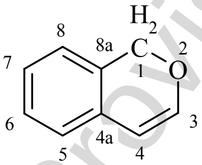
(20) pyrrolizine (PIN)
(1*H*-isomer shown)



(21) xanthene (PIN)
(9*H*-isomer shown)
thioxanthene (S instead of O) (PIN)_
selenoxanthene (Se instead of O) (PIN)
telluroxanthene (Te instead of O) (PIN)



(22) chromene (PIN)
(2*H*-isomer shown)
thiochromene (S instead of O) (PIN)
selenochromene (Se instead of O) (PIN)
tellurochromene (Te instead of O) (PIN)



(23) isochromene (PIN)
(1*H*-isomer shown)
isothiochromene (S instead of O) (PIN)
isoselenochromene (Se instead of O) (PIN)
isotellurochromene (Te instead of O) (PIN)

Table 2.9 Names for nitrogenous parent components modified by P and As replacement
(For the seniority of P ans As containing ring systems see P-25.3.2.4 and P-25.8.1)

In the following names, arsenic or phosphorus atoms replace nitrogen atoms

Nitrogen ring system	Arsenic ring system	Phosphorus ring system
acridine (PIN)	acridarsine (PIN)	acridophosphine (PIN)
indole (PIN)	arsindole (PIN)	phosphindole (PIN)
indolizine (PIN)	arsindolizine (PIN)	phospindolizine (PIN)
isoindole (PIN)	isoarsindole (PIN)	isophosphindole (PIN)
isoquinoline (PIN)	isoarsinoline (PIN)	isophosphinoline (PIN)
phenathridine (PIN)	arsanthridine (PIN)	phosphanthridine (PIN)
quinoline (PIN)	arsinoline (PIN)	phosphinoline (PIN)
quinolizine (PIN)	arsinolizine (PIN)	phosphinolizine (PIN)

P-25.2.2 Systematically named heterocyclic components

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P-25.2.2.1 Heteromonocyclic parent components
P-25.2.2.2 Heteranthrene components
P-25.2.2.3 Pheno...ine components
P-25.2.2.4 Heteromonocyclic components fused to a benzene ring

P-25.2.2.1 Heteromonocyclic parent components

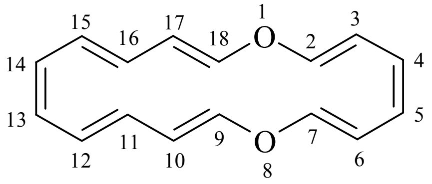
P-25.2.2.1.1 Heteromonocyclic rings with three through ten ring members having the maximum number of noncumulative double bonds are used as parent components as well as attached components. Retained names are given in Tables 2.2 and 2.3. Hantzsch-Widman names are discussed in P-22.2.2.

P-25.2.2.1.2 Names of heteromonocyclic parent components with more than ten ring members used in fusion nomenclature are discussed in this subsection; they are used only in fusion nomenclature.

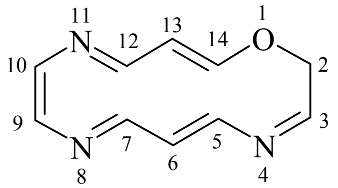
A heteromonocyclic parent component having more than ten members and the maximum number of noncumulative double bonds (mancude) is named by changing the ending 'ane' of the corresponding saturated heteromonocycle (see P- 22.2.3) to 'ine'.

For examples of fusion compounds including this type of heteromonocyclic components, see P-25.2.2.4.

Examples:



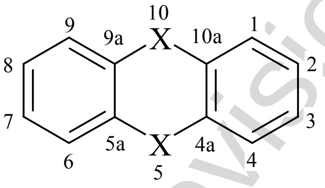
1,8-dioxacyclooctadecine
1,8-dioxacyclooctadeca-2,4,6,9,11,13,15,17-octaene (PIN)

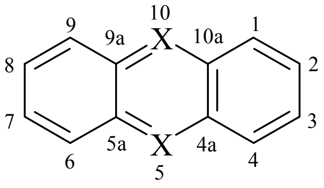


2*H*-1-oxa-4,8,11-triazacyclotetradecine
1-oxa-4,8,11-triazacyclotetradeca-3,5,7,9,11,13-hexaene (PIN)

P-25.2.2.2 Heteranthrene components

A heterotricyclic parent component consisting of two benzene rings fused to a 1,4-diheterabenzene in which the heteroatoms are the same is named by attaching the appropriate 'a' prefix to the ending 'anthrene' (from anthracene), with elision of a letter 'a'. The allowed heteroatoms are O, S, Se, Te, P, As, Si, and B. When the heteroatoms are nitrogen atoms, the component is named 'phenazine' (a retained name). The numbering is standard, as shown. Rules for numbering are described in Section P-25.3.3.





X = O oxanthrene (PIN)
(formerly dibenzo[1,4]dioxine)
X = S thianthrene (PIN)
X = Se selenanthrene (PIN)
X = Te telluranthrene (PIN)

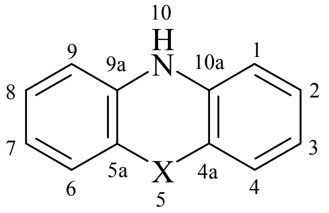
X = P phosphanthrene (PIN)
X = As arsanthrene (PIN)
X = SiH silanthrene (PIN)
X = B boranthrene (PIN)

P-25.2.2.3 Pheno...ine components

A heterotricyclic parent component consisting of two benzene rings fused to a 1,4-diheterabenzene in which the heteroatoms are different is named by adding the prefix 'pheno' to the appropriate Hantzsch-Widman name (see P-22.2.2), eliding the 'o' before a following vowel.

Numbering is standard and depends on the nature of the heteroatoms. Rules for numbering are described in Section 25.3.3.

Examples:

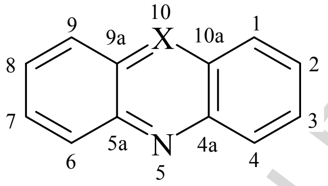


X = O phenoxazine (PIN, 10*H*-isomer shown)

X = S phenothiazine (PIN, 10*H*-isomer shown)

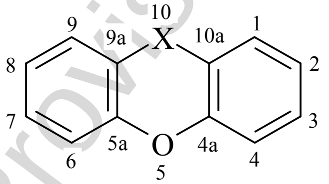
X = Se phenoselenazine (PIN, 10*H*-isomer shown)

X = Te phenotellurazine (PIN, 10*H*-isomer shown)



X = P phenophosphazinine (PIN)
(formerly called phenophosphazine)

X = As phenarsazinine (PIN)
(formerly called phenoarsazine)



X = S phenoxathiine (PIN)_

X = Se phenoxaselenine (PIN)

X = Te phenoxatellurine (PIN)

X = PH phenoxaphosphinine (PIN, 10*H*-isomer shown)
(formerly called phenoxaphosphine)

X = AsH phenoxarsinine (PIN, 10*H*-isomer shown)
(formerly called phenoxarsine)

X = SbH phenoxastibinine (PIN, 10*H*-isomer shown)
(formerly called phenoxantimonine)

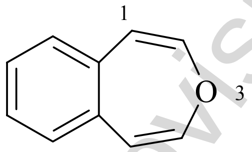
X = AsH; and S instead of O: phenothiarsinine (PIN, 10*H*-isomer shown)
(formerly called phenothiarsine)

P-25.2.2.4 Heteromonocyclic components fused to a benzene ring

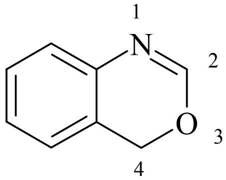
Unless listed as a retained name in Table 2.7, such as quinoline and cinnoline, a benzene ring fused to a heteromonocycle of five or more members (a benzoheterocycle) is named by placing the locant(s) indicating the position(s) of the heteroatom(s) at the front of the name consisting of the fusion prefix 'benzo' followed by a retained name, a Hantzsch-Widman systematic name, or a name formed by skeletal replacement ('a') nomenclature as described in P-25.2.2.1.2. The locants cited correspond to the full bicyclic structure. As in Hantzsch-Widman names, locants are placed in the order corresponding to the order of citation of the heteroatoms in the heterocyclic component. The locant '1' is always assigned to the atom of the heterocyclic component next to a fusion atom. Heteroatoms are allocated lowest locants as a set, without regard to kind; if there is a choice, lowest locants are assigned in accordance with the seniority of the 'a' prefixes (see Table 2.3). Locants may be omitted when the name is unambiguous. The letter 'o' of the 'benzo' prefix is elided when followed by a vowel. Indicated hydrogen is placed at the front of the name, when required.

"Benzo names" offer several advantages. They are simpler in the sense that they do not require fusion descriptors. However, their primary advantage is in their use as components of fusion names; they provide a larger portion of structure and remove one full level in the construction of names for larger heterocyclic fused ring systems.

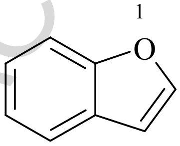
Examples:



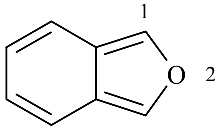
3-benzoxepine (PIN)
(not benzo[*d*]oxepine)
(not 3-benzooxepine)



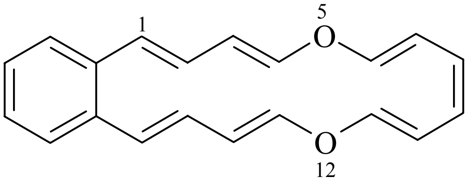
4*H*-3,1-benzoxazine (PIN)
(not 4*H*-benzo[*d*][1,3]oxazine)
(not 4*H*-3,1-benzooxazine)



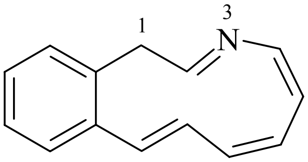
1-benzofuran (PIN)
(not benzofuran)
(not benzo[*b*]furan)



2-benzofuran (PIN)
(not isobenzofuran)
(not benzo[*c*]furan)



5,12-benzodioxacyclooctadecine (PIN)
(not benzo[*m*][1,8]dioxacyclooctadecine)



1*H*-3-benzazacycloundecine (PIN)
(not 1*H*-benzo[*h*][1]azacycloundecine)
(not 1*H*-3-benzoazacycloundecine)

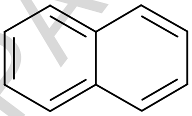
P-25.3 Constructing fusion names

P-25.3.1 Definitions, terminology and general principles

P-25.3.1.1 Definitions

P-25.3.1.1.1 *ortho*-Fused. Two rings that have only two atoms and one bond in common are said to be *ortho*-fused.

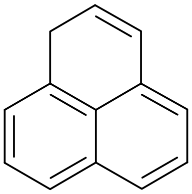
Example:



The two benzene rings of naphthalene are *ortho*-fused.

P-25.3.1.1.2 *ortho*- and *peri*-Fused. In a polycyclic compound a ring *ortho*-fused to different sides of two other rings that are themselves *ortho*-fused together (i.e. there are three common atoms between the first ring and the other two) is said to be *ortho*- and *peri*-fused to the other two rings.

Example:



phenalene is considered as being composed of three benzene rings, each of which is *ortho*- and *peri*-fused to the other two.

P-25.3.1.1.3 Fusion atom. Any atom of a fused ring system that is common to two or more rings.

P-25.3.1.1.4 Peripheral atom. Any atom that forms part of the outer perimeter of a fused ring system

P-25.3.1.1.5 Interior atom. Any fusion atom that is not peripheral.

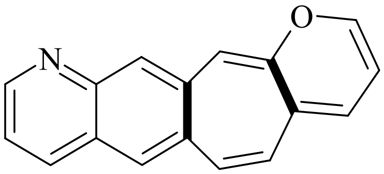
P-25.3.1.2 Terminology

P-25.3.1.2.1 Components of a fused ring system. Fusion components are mancude rings or ring systems that can be named without the application of any fusion nomenclature principles. Fused ring systems that do not have such a name are named by joining together the names of appropriately selected fusion components.

P-25.3.1.2.2 Parent component. The parent component according to the terminology of the 1998 recommendations (ref. 4) (referred to as base component in the 1979 publication, 1; and principal component in the 1993 Recommendations, ref. 2) is the one with highest seniority according to the criteria given in P-25.3.2.4. A parent component may be mono- or polycyclic, but it must be a mancude ring or ring system. Its name is never modified and is cited last in the name of the fused system.

P-25.3.1.2.3 Attached component. The components of a fused system not included in the parent component are called attached components. The attached components are called first-order, second-order, etc. attached components when they correspond to the first, second, etc. attached component reached when moving away from the parent component across fusion sites. An attached component may be mono- or polycyclic, but it must be a mancude ring or ring system. Fusion sites are bold lines in the following examples.

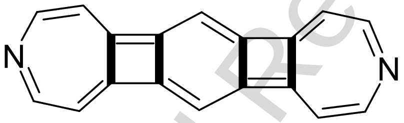
Example:



The bicyclic component at the left end of the above structure is the parent component, the seven-membered ring fused to the parent component is the first-order attached component; the six-membered ring fused to the first-order attached component is the second-order attached component. ☐

P-25.3.1.2.4 Interparent component. In a system that consists of two (or more) parent components *ortho*- or *ortho*- and *peri*-fused to the same attached component, the latter is called interparent component. Likewise, if two (or more) parent components are fused to three or more appropriately attached components, there will be two first-order interparent components and a second-order interparent component. Fourth-, fifth, etc. order components may be present in more complex systems.

Example:



The two seven-membered rings are the parent components; the two four-membered rings are the first order interparent components; the six-membered ring is the second-order interparent component.

P-25.3.1.3 General principles

'*ortho*-Fused' or '*ortho*- and *peri*-fused' polycyclic systems with the maximum number of noncumulative double bonds (mancude) containing at least two rings of five or more members, and that have no accepted retained or systematic name described in sections P-25.1 and P-25.2 are named by prefixing to the name of a component ring or ring system (the parent component) designations of the other component(s) (attached components).

> In the 1998 Recommendations (ref 4), the requirement that for application of fusion nomenclature at least two rings of five or members must be present, contained in the 1979 Recommendations (ref 1), was removed. For selection of Preferred IUPAC Names, this requirement is reinstated here. However, in general nomenclature, the fusion system can be applied equally to smaller rings, as in cyclobutabenzene.

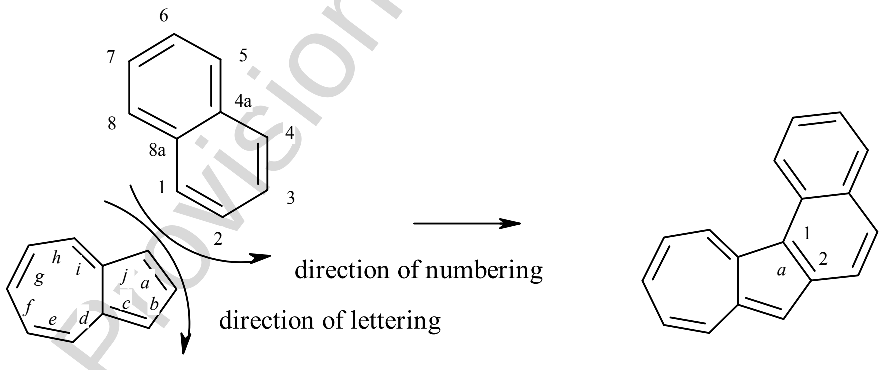
The parent component is selected by applying criteria of seniority as described in P-25.3.2.4 below. In a fusion name, the name of the parent component is that of the component itself. The names of attached components are formed by replacing the last letter 'e' by 'o' in the name of the component, i.e., indeno from indene (or by adding the letter 'o' when no final letter 'e' is present, i.e., pyrano from pyran) or by other means described in P-25.3.2.2 below. There is no elision of the final letter 'o' or 'a' before a vowel (see Rule FR-4.7, ref. 4).

Locants that describe structural features of components, such as positions of heteroatoms, are kept with the name of the component and are enclosed within square brackets.

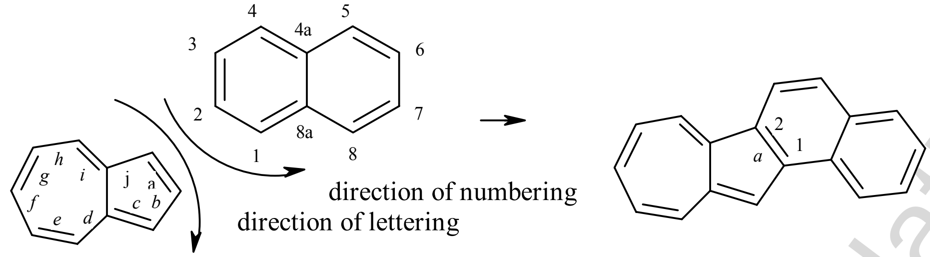
> In previous rules (Rule A-21.4, ref. 1), the elision of the final letter 'o' of acenaphtho, benzo, naphtho and perylo and the final letter 'a' of the monocyclic prefixes cyclopropa, cyclobuta, etc. was recommended. This practice is still used in Chemical Abstracts index nomenclature for acenaphtho, benzo, naphtho and the cycloalka prefixes. Names such as benzo[*g*]isoquinoline and cyclohepta[*cd*]-*s*-indacene are now recommended in place of benz[*g*]isoquinoline and cyclohept[*cd*]-*s*-indacene, respectively.

Isomers are distinguished by lettering, continuously, each peripheral side of the parent component (including sides whose locants are distinguished by letters, for example, 2a,3a) using the italic letters *a, b, c,* etc., beginning with *a* for the side numbered 1,2; *b* for 2,3; etc.. To the letter as early in the alphabet as possible that denotes the side where the fusion occurs are prefixed, if necessary, the numbers of the positions of attachment of the other component. These numbers are chosen to be as low as is consistent with the numbering of the compound and their order conforms to the direction of lettering of the parent component. In this document these letters and numbers are placed within the structure of the ring or ring system.

Examples:



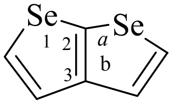
azulene (PIN) + naphthalene (PIN) ⟶ naphtho[1,2-*a*]azulene (PIN)
(parent component) (attached component)



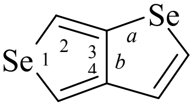
azulene (PIN) + naphthalene (PIN) ⟶ naphtho[2,1-*a*]azulene (PIN)
(parent component) (attached component)

The numbers and letters, separated by commas when required, are enclosed in square brackets and placed immediately after the designation of the attached component; there is no space or hyphen either preceding or following the brackets. Hyphens separate the two parts of a fusion descriptor, i.e., numbers and italicized letters. This expression merely defines the manner of fusion of the components. Indicated hydrogen atoms are added to the names, as required, using locants characterizing the fused system.

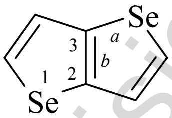
Examples:



selenopheno[2,3-*b*]selenophene (PIN)



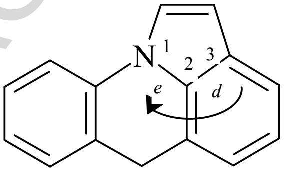
selenopheno[3,4-*b*]selenophene (PIN)



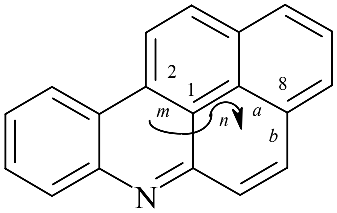
selenopheno[3,2-*b*]selenophene (PIN)

ortho- and *peri*-Fused systems require a fusion descriptor that indicates all fused bonds. All letters referring to the parent component are cited, but only locants of the nonfused atoms of the attached component are indicated. Letters are not separated by commas in the fusion descriptor.

Examples:



6*H*-pyrrolo[3,2,1-*de*]acridine



naphtho[2,1,8-*mna*]acridine

P-25.3.2 Constructing two component fusion names

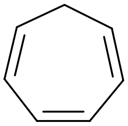
A component may be monocyclic or polycyclic. Systematic construction proceeds stepwise, as follows.

P-25.3.2.1 Selecting and naming parent components for fusion nomenclature

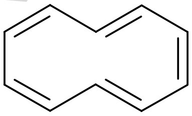
P-25.3.2.1.1 Monocyclic hydrocarbons (Annulenes).

Monocyclic parent components are named as [*n*]annulenes where *n* represent the number of carbon atoms. The series starts at $n = 7$, because the retained name ‘benzene’ is preferred for $n = 6$. The use of the name ‘annulene’ in fusion nomenclature was recommended in 1993 (see R-2.4.1.1, ref. 2) to obviate the potential ambiguity of using contracted traditional names, such as cycloheptene to denote 1,3,5-cycloheptatriene.

Examples:



1*H*-[7]annulene
(no longer cycloheptene as)
fusion component)
cyclohepta-1,3,5-triene (PIN)



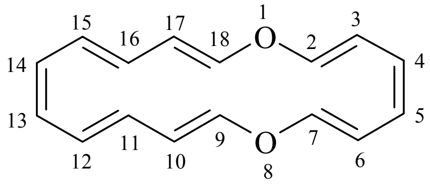
[10]annulene
(no longer cyclodecene as)
fusion component)
cyclodeca-1,3,5,7,9-pentaene (PIN)

P-25.3.2.1.2 Heteromonoycles

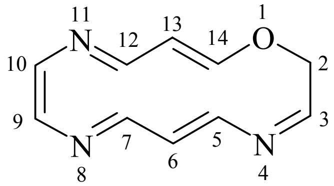
The retained names given in Table 2.2, except for ‘isothiazole’, ‘isoxazole’, ‘thiazole’ and ‘oxazole’, and Hantzsch-Widman names for unsaturated heteromonocycles (see P-) are used as parent components in fusion nomenclature. The names ‘isothiazole’, ‘isoxazole’, ‘thiazole’ and ‘oxazole’, although permitted in general nomenclature, are not recommended for the names of components in preferred IUPAC fusion names. The Hantzsch-Widman names 1,2-thiazole, 1,2-oxazole, 1,3-thiazole and 1,3-oxazole, respectively, must be used; the locants are enclosed in square brackets in the completed fusion name.

Heteromonocycles having more than ten members and the maximum number of noncumulative double bonds whose names are denoted by the 'ine' ending described in P-22.2.4 are used as parent components in preferred IUPAC fusion names.

Examples:



1,8-dioxacyclooctadecine
1,8-dioxacyclooctadeca-2,4,6,9,11,13,15,17-octaene (PIN)



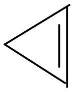
2*H*-1-oxa-4,8,11-triazacyclotetradecine
1-oxa-4,8,11-triazacyclotetradeca-3,5,7,9,11,13-hexaene (PIN)

P-25.3.2.1.3 Names of the hydrocarbons and heterocycles described in Sections P-25.1.2 and P-25.2.2 and retained names listed in Tables 2.2, 2.6 (see P-25.3.2.1.3 and P-25.3.2.1.4), 2.7, and 2.8 are used as parent components for preferred IUPAC fusion names.

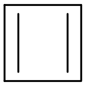
P-25.3.2.2 Names of prefixes to denote attached components.

P-25.3.2.2.1 Monocyclic hydrocarbon prefixes for attached components other than 'benzo', are formed by dropping 'ne' from the name of the appropriate saturated monocyclic hydrocarbon. These names represent the form with the maximum number of noncumulative double bonds. There is no upper limit to this rule.

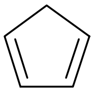
Examples:



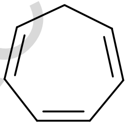
cyclopropa (PIN)
(from cyclopropane, PIN)



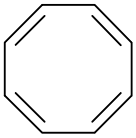
cyclobuta (PIN)
(from cyclobutane, PIN)



cyclopenta (PIN)
(from cyclopentane, (PIN)



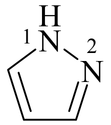
cyclohepta (PIN)
(from cycloheptane, (PIN)
(not [7]annuleno)



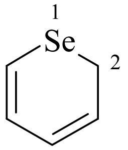
cycloocta (PIN)
(from cyclooctane, PIN)
(not [8]annuleno)

P-25.3.2.2.2 Prefixes for attached components derived from the name of a parent component described in P-25.3.2.1.2 and P-25.3.2.1.2 are named by changing the final letter "e" in to the letter 'o' or by adding the letter 'o' when no final letter 'e' is present.

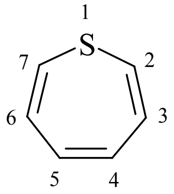
Examples:



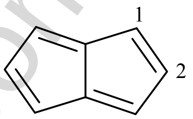
pyrazolo (PIN)
(derived from 1*H*-pyrazole, PIN)



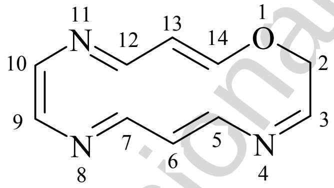
selenopyrano (PIN)
(derived from 2*H*-selenopyran, PIN)



thiepino (PIN)
(derived from thiepine, (PIN)



pentaleno (PIN)
(derived from pentalene, PIN)



1-oxa-4,8,11-triazacyclotetradecino (PIN)
(derived from 2*H*-1-oxa-4,8,11-triazacyclotetradecine, PIN)

P-25.3.2.2.3 Retained names

Only the following contracted names are retained for preferred IUPAC fusion names:

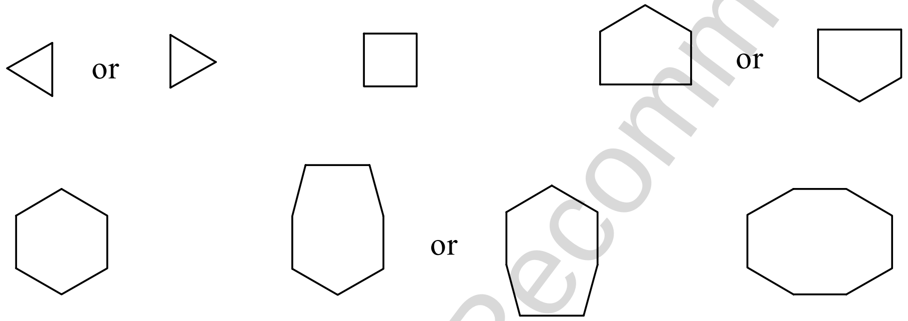
anthra (PIN)	from	anthracene (PIN)	naphtho (PIN)	from	naphthalene (PIN)
benzo (PIN)	from	benzene (PIN)	phenanthro (PIN)	from	phenanthrene (PIN)
furo (PIN)	from	furan (PIN)	imidazo (PIN)	from	imidazole (PIN)
pyrido (PIN)	from	pyridine (PIN)	pyrimido (PIN)	from	pyrimidine (PIN)
thieno (PIN)	from	thiophene (PIN)			

P-25.3.2.3 Orientation of fused ring systems

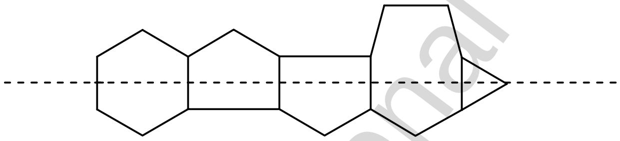
P-25.3.2.3.1 Drawing of ring structures

For the purpose of selecting parent components and for numbering of fused ring systems, the structures of fused ring compounds must be drawn in a specific manner according to a set of criteria that must be applied in order until a decision is reached.

Individual rings of a polycyclic '*ortho*-fused' or '*ortho*- and *peri*-fused' hydrocarbon ring system are drawn in such a way so that as many as possible of the various individual rings are arranged in horizontal rows. Such rows are characterized by a horizontal axis that divides each individual ring into two approximate halves. Permitted shapes for three to eight membered rings are as follows:



Example:



a horizontal row and its horizontal axis

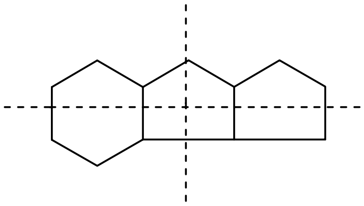
P-25.3.2.3.2 Criteria for the selection of the preferred orientation

Polycyclic fused ring systems are oriented in accordance with the following criteria, that are considered in order until a decision is reached.

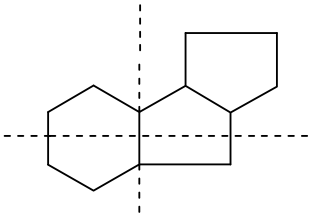
(a) Maximum number of rings in a horizontal row.

Fused ring systems are drawn in order to achieve the maximum number of *ortho*-fused rings, with vertical common bonds, in a horizontal row. The relevant vertical bonds are always those furthest apart. If the correct orientation is not immediately apparent the horizontal row is bisected by a horizontal axis and a vertical axis to form four quadrants. Rings which are not bisected by the horizontal axis do not belong to the main row and are not considered in the counting of rings in the main row.

Example:



3 rings in horizontal row



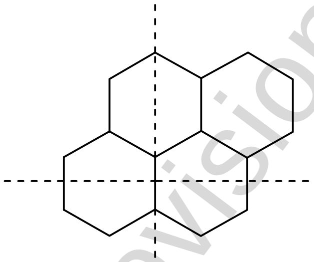
2 rings in horizontal row

Accordingly, polyacenes are senior to polyaphenes for an equal number of rings, and anthracene is senior to phenanthrene

(b) Maximum number of rings in upper right quadrant

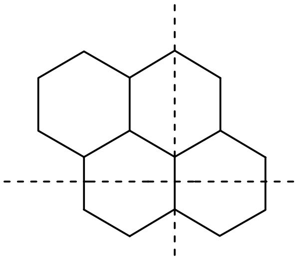
In the preferred orientation, the maximum number of rings must appear above and to the right of the horizontal row (upper right quadrant). For this purpose, the center of the horizontal row is defined as the central common bond if there is an even number of rings in the row, and the center of the central ring if there is an odd number of rings. In counting rings in a quadrant those rings that are divided by an axis are considered as two halves, and a ring bisected by both axes, counts as four quarters (one in each quadrant). Rings that are bisected by the horizontal axis but are not directly *ortho*-fused to the main row are not considered when counting how many rings are in the horizontal row.

Examples:

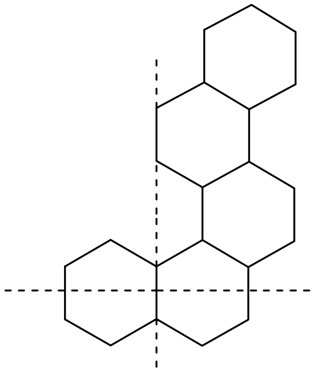


2 rings in horizontal row
2 rings in upper right quadrant
(correct orientation)

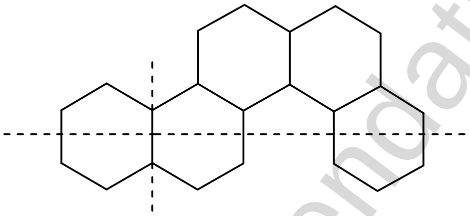
not



2 rings in horizontal row
1 ring in upper right quadrant
(incorrect orientation)



not



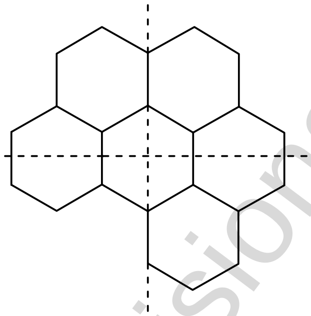
2 rings in the horizontal row
3½ rings in upper right quadrant
(correct orientation)

2 (not 3) rings in the horizontal row
3 rings in upper right quadrant
(incorrect orientation)

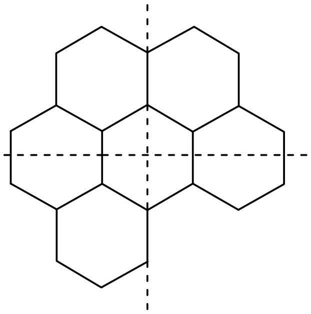
Accordingly, phenanthrene (1½ rings in the upper right quadrant) is senior to phenalene, [1 ring (two ½ rings) in the upper right]quadrant.

(c) Minimum number of rings in the lower left quadrant.

Example:



not

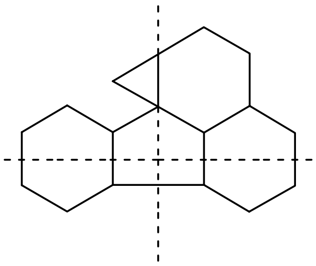


3 rings in horizontal row
1¾ rings in upper right quadrant
¾ ring in lower left quadrant

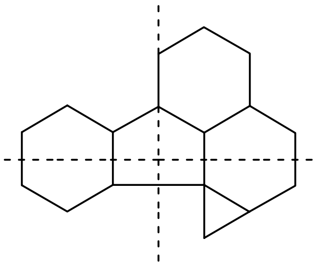
3 rings in horizontal row
1¾ rings in upper right quadrant
1¾ rings in lower left quadrant

(d) Maximum number of rings above the horizontal row

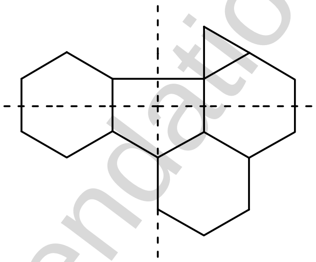
Example:



not



nor



3 rings in horizontal row	3 rings in horizontal row	3 rings in horizontal row
1¾ rings in upper right quadrant	1¾ rings in upper right quadrant	1¾ rings in upper right quadrant
¾ ring in lower left quadrant	¾ ring in lower left quadrant	¾ ring in lower left quadrant
3½ rings above horizontal row	2½ rings above horizontal row	2½ rings above horizontal row

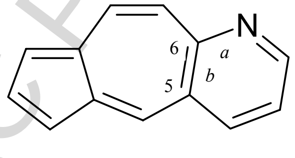
P-25.3.2.4 Seniority criteria for selecting the parent component

The components of the fused ring system are selected and named according to P-25.3.2.1 and P-25.3.2.2. When it is necessary to locate nomenclatural features, such as indicated hydrogen or atoms with nonstandard bonding numbers, another system of locants must be used, i.e., the locants that are used to number the completed fused ring system. In this document, these locants are placed outside the structure, as shown for retained names in Tables 2.2, 2.7, and 2.8. This system is fully explained and exemplified in P-25.3.3.

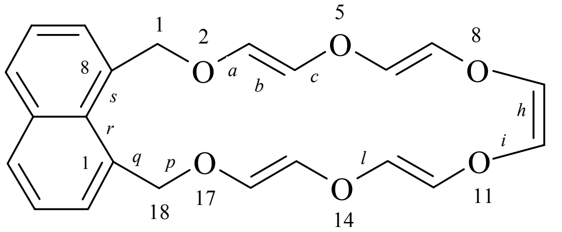
If there is a choice for selecting the parent component, the following criteria are considered, in order, until a decision can be made.

(a) A component containing at least one of the heteroatoms occuring earlier in the following order: N > F > Cl > Br > I > O > S > Se > Te > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

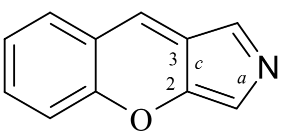
Examples:



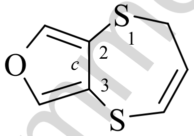
azuleno[6,5-*b*]pyridine (PIN)
[pyridine (heterocycle) is senior to azulene (carbocycle)]



1*H*,18*H*-naphtho[1,8-*rs*][1,4,7,10,13,16]hexaoxacyclohenicosine (PIN)
[1,4,7,10,13,16-hexaoxacyclohenicosine (heterocycle) is senior to naphthalene (carbocycle)]



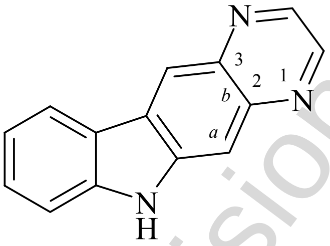
chromeno[2,3-*c*]pyrrole (PIN)
(pyrrole is senior to chromene; N > O)



thiepino[2,3-*c*]furan (PIN)
(furan is senior to thiepine; O > S)

(b) A component containing the greater number of rings.

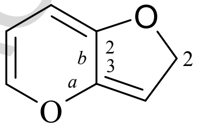
Example:



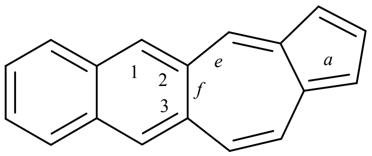
6*H*-pyrazino[2,3-*b*]carbazole (PIN)
[carbazole (3 rings) is senior to quinoxaline (2 rings)]

(c) A component containing the larger ring at the first point of difference when comparing rings in order of decreasing size

Examples:



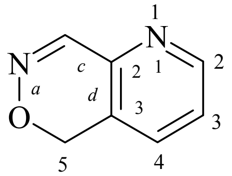
2*H*-furo[3,2-*b*]pyran (PIN)
[pyran (6 ring) preferred to furan (5 ring)]



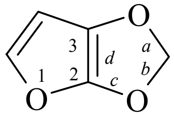
naphtho[2,3-*f*]azulene (PIN)
[azulene (7,5 rings) preferred to to naphthalene (6,6 rings)]

(d) A component containing the greater number of heteroatoms of any kind.

Examples:



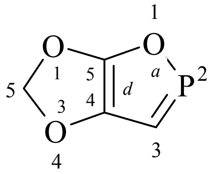
5*H*-pyrido[2,3-*d*][1,2]oxazine(PIN)
[oxazine (2 heteroatoms) preferred
to pyridine (1 heteroatom)]



2*H*-furo[2,3-*d*][1,3]dioxole (PIN)
[dioxole (2 heteroatoms) preferred
to furan (1 heteroatom)]

(e) A component containing the greater variety of heteroatoms

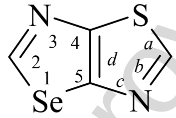
Examples:



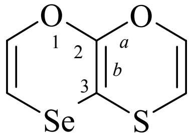
5*H*-[1,3]dioxolo[5,4-*d*][1,2]oxaphosphole (PIN)
[1,3]dioxolo[*d*][1,2]oxaphosphole
(an O and a P atom preferred to two O atoms)

(f) A component containing the greater number of heteroatoms most senior when considered in the order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Examples:



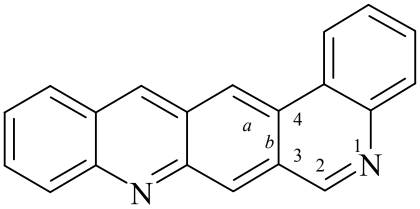
[1,3]selenazolo[5,4-*d*][1,3]thiazole (PIN)
(S,N senior to Se,N)



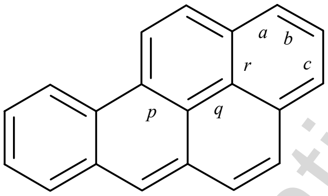
[1,4]oxaselenino[2,3-*b*]oxathiine (PIN)
(O,S senior to O,Se)

(g) A component containing the greatest number of rings in a horizontal row when it is drawn in the preferred orientation according to P-25.3.2.3.

Examples:



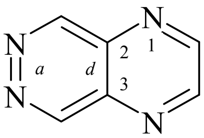
quinolino[4,3-*b*]acridine (PIN)
[acridine (3 rings in horizontal row) preferred to phenanthridine (2 rings in horizontal row)]



benzo[*pqr*]tetraphene (PIN)
[tetraphene (3 rings in horizontal row) preferred to chrysene or pyrene (2 rings inhorizontal row)]

(h) A component with the lower locants for heteroatoms

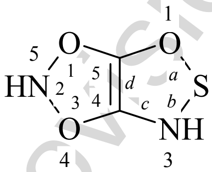
Example:



pyrazino[2,3-*d*]pyridazine (PIN)
(locants ‘1,2’ of pyridazine preferred to locants ‘1,4’ of pyrazine)

(i) A component with the lower locants for the heteroatoms when considered in the order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

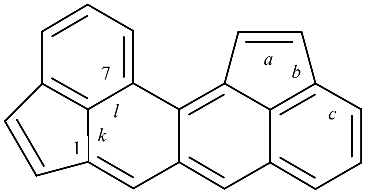
Example:



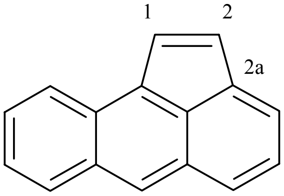
3*H*,5*H*-[1,3,2]oxathiazolo[4,5-*d*][1,2,3]oxathiazole (PIN)
(locants ‘1,2,3’ are senior to ‘1,3,2’)

(j) A component with the lower locants for the peripheral fusion carbon atoms (see P-25.3.3.1 for numbering of fusion carbon atoms).

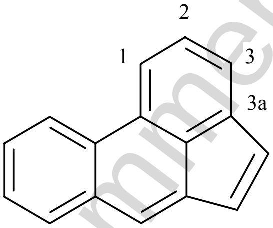
Example:



indeno[1,7-*kl*]aceanthrylene (PIN)
(the locant 2a in aceanthrylene is lower than 3a in acephenanthrylene; see below)



aceanthrylene (PIN)

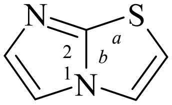


acephenanthrylene (PIN)

P-25.3.2.5 Assembling components and naming fused systems. The following are considered when assembling components and naming fused systems.

P-25.3.2.5.1 A heteroatom common to two components must be indicated in the name of each component.

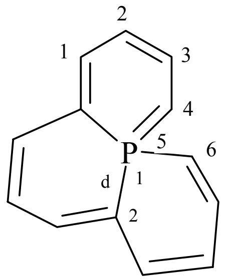
Example:



imidazo[2,1-*b*][1,3]thiazole (PIN)

P-25.3.2.5.2 An atom with a nonstandard bonding number is indicated by the lambda convention (see P-14.1) The nonstandard bonding number *n* is indicated as a superscript to the symbol λ, for example λ^5; this symbol follows the locant of the atom with the nonstandard bonding number in accordance with the numbering of the fused system and is cited at the beginning of the name of the fused ring system.

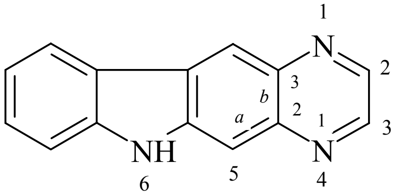
Example:



5λ^5-phosphinino[2,1-*d*]phosphinolizine (PIN)

P-25.3.2.5.3 Indicated hydrogen is cited at the beginning of the name preceded by an appropriate locant of the fused ring system.

Example:



6*H*-pyrazino[2,3-*b*]carbazole (PIN)

P-25.3.3 Numbering fused ring systems

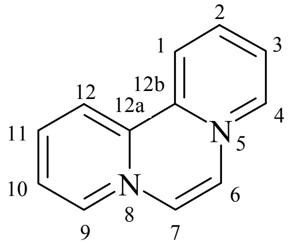
Fused systems with retained names, systematic names, or fused names are systematically numbered in the same manner. Anthracene, phenanthrene, acridine and carbazole are exceptions; their traditional numberings are retained. Two types of numbering are to be considered.

P-25.3.3.1 Peripheral numbering
P-25.3.3.2 Interior numbering

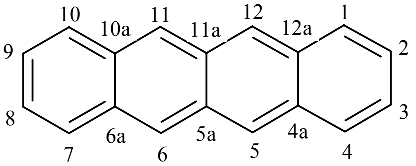
P-25.3.3.1 Peripheral numbering

P-25.3.3.1.1 The numbering of peripheral atoms in the preferred orientation starts from the uppermost ring in the upper right quadrant. If there is more than one uppermost ring the ring furthest to the right is chosen. Numbering starts from the nonfused atom most counterclockwise in the ring selected and proceeds in a clockwise direction around the system, including fusion heteroatoms but not fusion carbon atoms. Each fusion carbon atom is given the same number as the immediately preceding nonfusion skeletal atom, modified by a Roman letter ‘a’, ‘b’, ‘c’, ‘d’, etc.

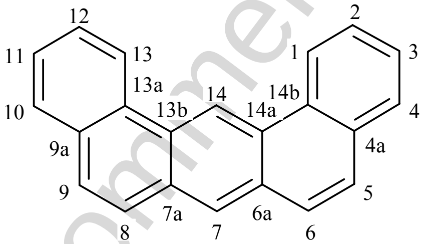
Examples:



dipyrido[1,2-*a*:2′,1′-*c*]pyrazine (PIN)



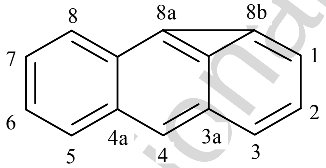
tetracene (PIN)



dibenzo[*a*,*j*]anthracene (PIN)

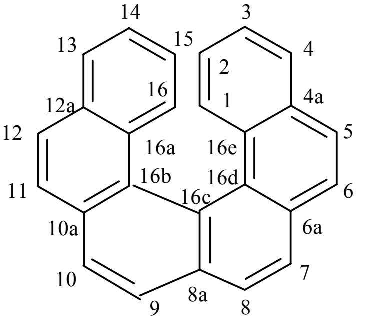
If a ring system does not have a nonfusion atom, then numbering starts in the next ring encountered when proceeding round the system in a clockwise direction.

Example:



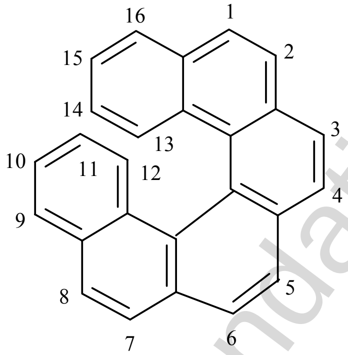
cyclopropa[*de*]anthracene (PIN)

Sections FR-5.3, FR-5.4 and FR-5.4 in ref. 4 describe numbering for more complex structures. In particular, the orientation and numbering of helicenes has been changed. The recommended numbering and former numbering for hexahelicene are shown below. Higher helicenes follow the same pattern. A helicene is oriented so that a terminal ring is located in the upper right quadrant; numbering always begins in this terminal ring.



hexahelicene (PIN)
(correct IUPAC orientation
and numbering)

not

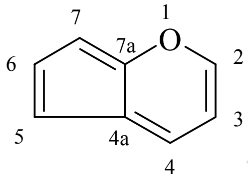


(former orientation and numbering;
still used by CAS)

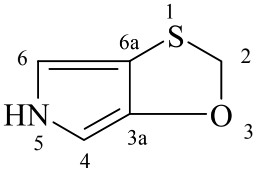
P-25.3.3.1.2 If alternative numbering for a ring system remains after the application of P-25.3.3.1.1 (including alternative locations for heteroatoms), the following criteria are applied in order until a decision is reached.

(a) Low locants are assigned to heteroatoms, considered as a set without regard to kind

Examples:



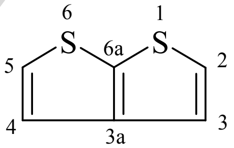
cyclopenta[*b*]pyran (PIN)



2*H*,5*H*-[1,3]oxathiolo[4,5-*c*]pyrrole (PIN)

(b) Low locants are assigned to heteroatoms in the order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

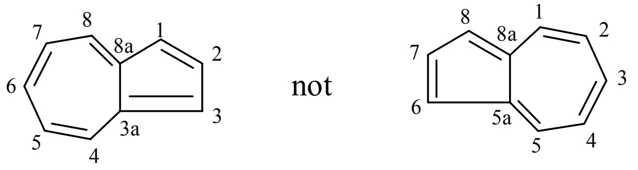
Example:



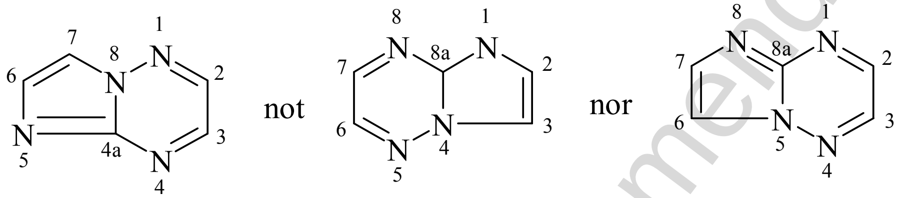
thieno[2,3-*b*]furan (PIN)

(c) Low locants are assigned to fusion carbon atoms

Examples:



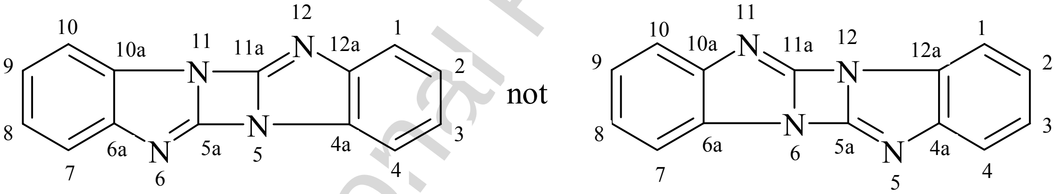
azulene (PIN)
(locants 3a,8a are lower than 5a,8a)



imidazo[1,2-*b*][1,2,4]triazine (PIN)
(locant 4a is lower than 8a)

(d) Low locants are assigned to fusion rather than nonfusion heteroatoms of the same element.

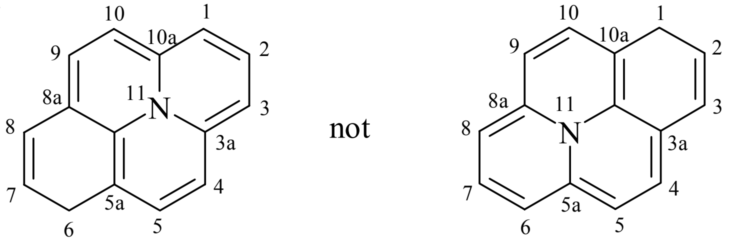
Example:



[1,3]diazeto[1,2-*a*:3,4-*a*′]dibenzimidazole (PIN)
(5 is lower than 6)

(e) Low locants are assigned so that an interior heteroatom is nearer (i.e., fewer bonds in the pathway) to the lowest numbered fusion peripheral atom (see P-25.3.3.2 for interior numbering).

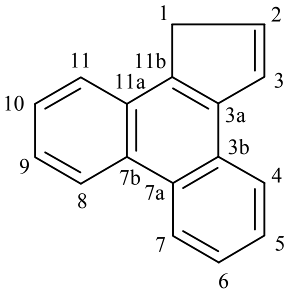
Example:



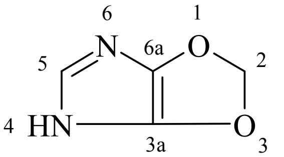
6*H*-quinolizino[3,4,5,6-*ija*]quinoline (PIN)
(3a is lower than 5a for the lowest locant next to the nitrogen atom)

(f) Low locants are assigned to indicated hydrogen atoms (expressed or implied)

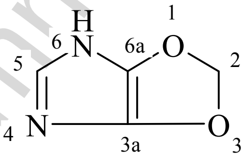
Examples:



1*H*-cyclopenta[*l*]phenanthrene (PIN)



not



2*H*,4*H*-[1,3]dioxolo[4,5-*d*]imidazole (PIN) 2*H*,6*H*-[1,3]dioxolo[4,5-*d*]imidazole

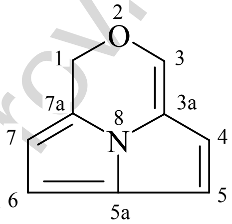
correct incorrect

(The locant set 2,4 for indicated hydrogen atoms is lower than 2,6)

P-25.3.3.2 Interior numbering of heteroatoms

P-25.3.3.2.1 Interior heteroatoms that are not identified by skeletal replacement (‘a’) nomenclature are numbered after the peripheral atoms continuing the established number sequence [see also P-25.3.3.1.2(e)]. Compare the numbering of interior carbon atoms (see P-25.3.3.3).

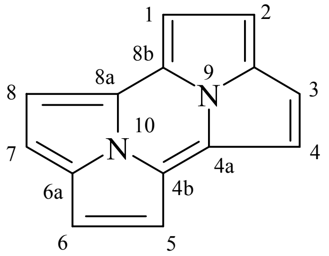
Example:



1*H*-[1,4]oxazino[3,4,5-*cd*)pyrrolizine (PIN)

P-25.3.3.2.2 If there is a choice, the shortest pathway in terms of the number of bonds from each heteroatom to the periphery is determined. The lower number is given to the heteroatom whose shortest pathway connects to the lowest numbered peripheral atom.

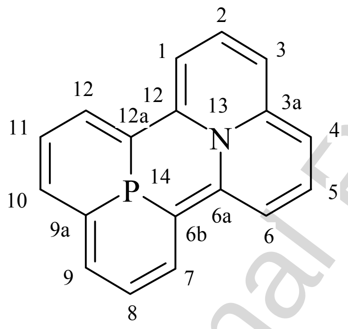
Example:



pyrazino[2,1,6-*cd*:3,4,5-*c′,d′*]dipyrrolizine (PIN)
(the heteroatom numbered 9 is one bond
away from 2a, which is lower than 4b)

P-25.3.3.2.3 If there is a choice between heteroatoms of different elements, the lower locant is assigned in accordance with the order F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Example:

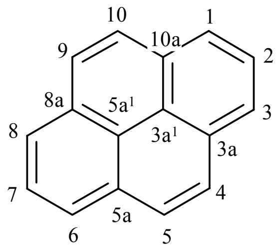


phosphinolizino[4′,5′,6′:3,4,5][1,4]azaphosphinino[2,1,6-*de*]quinolizine (PIN)
(the nitrogen atom has a lower locant than the phosphorus atom)

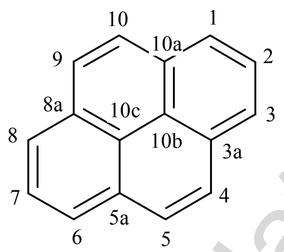
P-25.3.3.3 Numbering of interior carbon atoms

A major change to the rule for interior numbering of carbon atoms is now recommended (see FR-5.5.2 in ref. 4). Interior atoms are numbered by identifying the minimum number of bonds linking them to a peripheral atom. The locant for the interior atom is that of the peripheral atom with a superscript number corresponding to the number of bonds between the two atoms. The previous rule (Rule A-22.2 in ref. 1) recommended that interior atoms follow the highest numbered peripheral atom adding Roman letters in sequence to the appropriate peripheral number.

Examples:

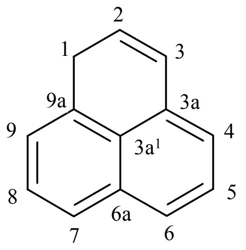


not

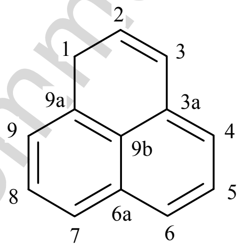


pyrene (PIN)
(recommended numbering)

(former numbering, no longer recommended
but still used by CAS)

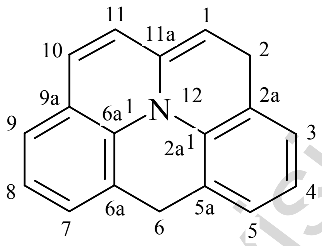


not

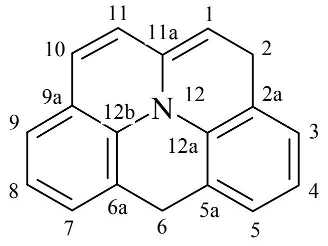


1*H*-phenalene (PIN)
(recommended numbering)

(former numbering, no longer recommended
but still used by CAS)



not

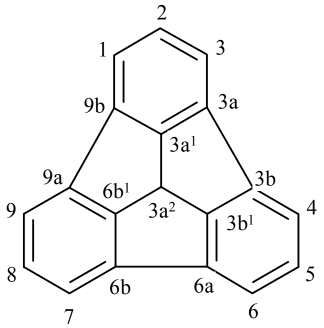


2*H*,6*H*-quinolizino[3,4,5,6,7-*defg*]acridine (PIN)
(recommended numbering)

(former numbering, not recommended
but still used by CAS)

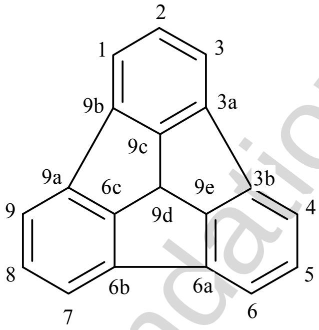
If there is a choice of interior atom locants lower locants are selected.

Example:



$3a^2H$-benzo[3,4]pentaleno[2,1,6,5-*jklm*]fluorine (PIN)
(recommended numbering)

not



(former numbering, no longer recommended but still used by CAS)

P-25.3.4 Constructing polycomponent fused systems

When several components must be considered, one, and only one, can be the parent component. All other components are attached components. A component attached directly to the parent component is called a 'first-order component'. A component attached to a first-order component is called a 'second-order' component, and so on. The parent and the attached first order components are named as indicated for two component systems (see P-25.3.2).

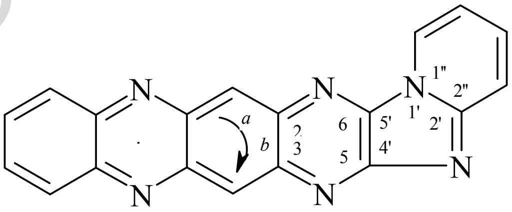
P-25.3.4.1 Three types of fusion names are considered in these recommendations.

P-25.3.4.1.1 Fusion names composed of first- and higher attached components
P-25.3.4.1.2 Identical attached components
P-25.3.4.1.3 Multiparent names

P-25.3.4.1.1 Fusion names composed of attached first- and higher-order components

The procedure for indicating common bond(s) between an attached first order component and a higher order attached component follows that for the attachment of the parent compound to the first order attached component except that numerical locants are used instead of letters and the two sets of locants are separated by a colon. The locants of second order attached component are primed to contrast with those of first-order attached components. The locants of third order attached components are doubly primed, and so on.

Example:

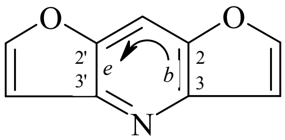


pyrido[1″,2″:1′,2′]imidazo[4′,5′:5,6]pyrazino[2,3-*b*]phenazine (PIN)

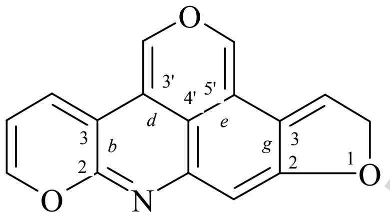
P-25.3.4.1.2 Identical attached components

Multiplicity of components that are identical and are all fused to a parent component or an attached component is indicated by the use of the prefix ‘di-’, ‘tri-’, etc. (or ‘bis-’, ‘tris-’, etc). The multiplying prefix is not considered in deciding alphabetical order. A colon separates the sets of locants, and a comma is used when letters only are present.

Example:



difuro[3,2-*b*:2′,3′-*e*]pyridine (PIN)

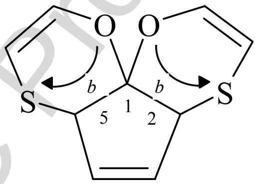


5H-furo[2,3-*g*]dipyrano[2,3-*b*:3′,4′,5′-*b*′]quinoline (PIN)
(furo before dipyrano)

P-25.3.4.1.3 Multiparent names

Multiple occurrences of the parent component in a multiparent system is indicated by the use of multiplying prefixes, ‘di’, ‘tri’, etc, or ‘bis’, ‘tris’, etc. To distinguish between the parent components, the second has primed locants, the third double primed, etc.

Example:



cyclopenta[1,2-*b*:5,1-*b*′]bis[1,4]oxathiazine (PIN)

P-25.3.4.2 Constructing polycomponent fusion names

Polycomponent fusion names are constructed by using specific orders of seniority and rules. They are elaborated as follows.

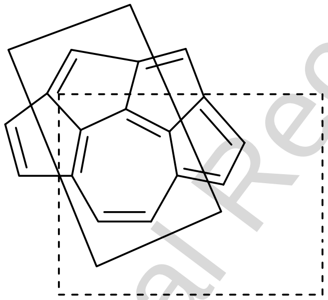
P-25.3.4.2.1 Order of seniority for selecting parent components

When there are two or more locations for a parent component in a fused ring structure, the following criteria are applied sequentially until a complete distinction is obtained. In the examples below, the senior location is identified by a solid box and other locations with a dashed box. Second order components in names are in bold, for didactic purposes only.

The senior location is:

(a) The location that enables the whole ring system to be named by fusion nomenclature, thus excluding names of bridge fused systems.

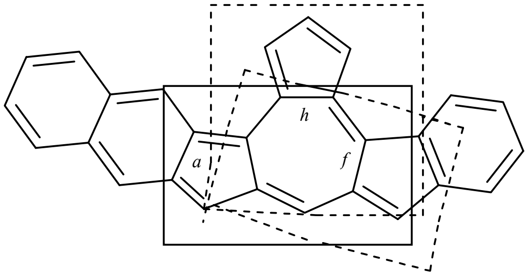
Example:



cyclopenta[*ij*]pentaleno[2,1,6-*cde*]azulene (PIN)
(not 1,9-methenopentaleno[1,6-*ef*]azulene)
(not 1,9-methenodicyclopenta[*cd,f*]azulene)
(names including the prefix ‘metheno’ are bridged fused names)

(b) The location that results in a name that does not require attached components higher than first-order. For didactic purposes only, names of attached components of higher order than first-order are written in bold type.

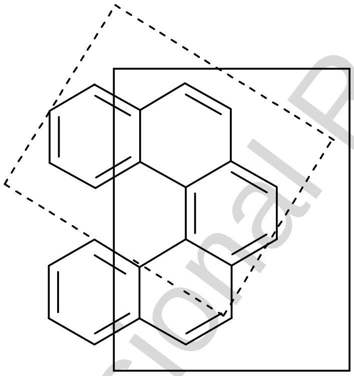
Example:



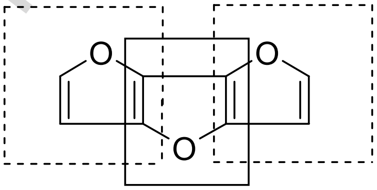
cyclopenta[*h*]indeno[2,1-*f*]naphtho[2,3-*a*]azulene (PIN)
(not benzo[*a*]**benzo**[5,6]indeno[2,1-*f*]cyclopenta[*h*]azulene
nor **benzo**[5,6]indeno[1,2-*e*]indeno[2,1-*h*]azulene; there is
no second-order component in the recommended name)

(c) The location that results in the maximum number of first-order attached components, second-order components, etc. This criterion results in the minimum number of higher-order attached components, hence, fewer primed fusion descriptors.

Examples:



dibenzo[*c,g*]phenanthrene (PIN)
(not naphtho[2,1-*c*]phenanthrene; two
attached components preferred to one)

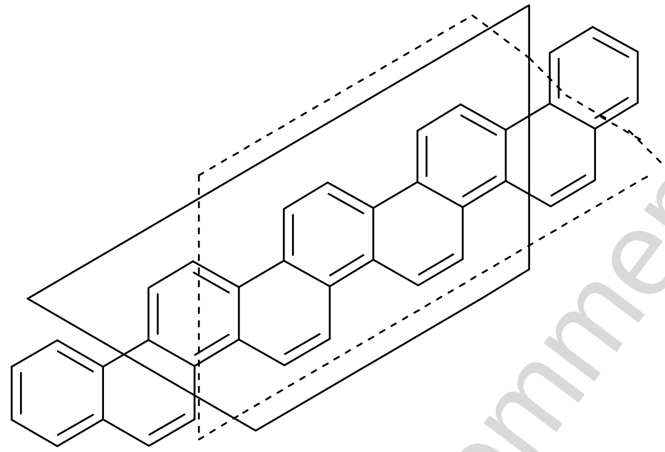


difuro[3,2-*b*:2′,3′-*d*]furan (PIN, a multiplicative prefix name)
(not furo[3,2-*b*:4′,5,-*b*′]difuran (a multiparent name)

(two attached components preferred to one)

(d) A location that permits the expression of the maximum number of identical attached components with multiplicative prefixes.

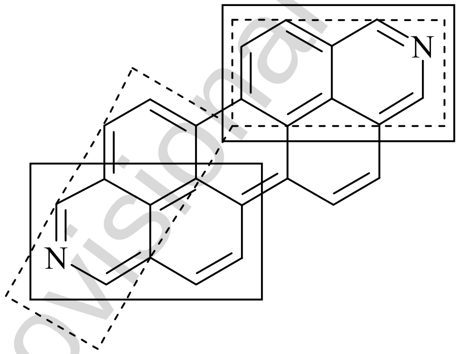
Example:



dinaphtho[1,2-*c* :2,1-*m*]picene (PIN)
(not benzo[*c*]phenanthreno[2,1-*m*]picene

(e) A location that uses a senior interparent component.

Example:



anthra[2,1,9-*def*:6,5,10-*d′e′f′*]diisoquinoline (PIN)
(not phenanthro[2,1,10-*def*:7,8,9-*d′e′f′*]diisoquinoline;
anthracene is senior to phenanthrene)

(f) A location that results in preferred attached components, first-order, then second-order, etc. This criterion is embellished and illustrated in the original publication (see FR-3.1.1 in ref. 4).

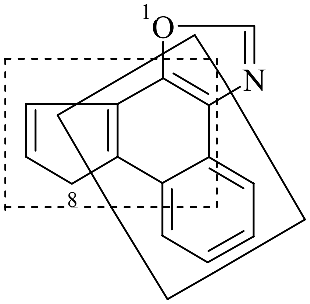
P-25.3.4.2.2 Selection of attached components

After selection of the parent component (see P-25.3.2.4) [or parent components and interparent component(s) if a multiparent name is chosen], other rings are identified as far as possible as attached components. If there is a choice, first-order attached components are considered first, then second-order components, etc. The following criteria are applied in order only until a complete decision is made.

In the examples below, the preferred attached component is marked with a solid box and the alternatives with dashed boxes.

(a) If there are alternative first order attached components, the senior ring or ring system is selected. The same procedure is applied to second-order attached components, and so on.

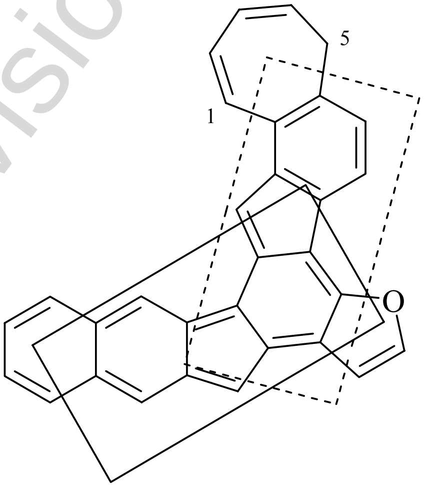
Example:



8*H*-cyclopenta[3,4]napththo[1,2-*d*][1,3]oxazole (PIN)
(not 8*H*-benzo[6,7]indeno[5,4-*d*][1,3]oxazole;
naphthalene is senior to indene)

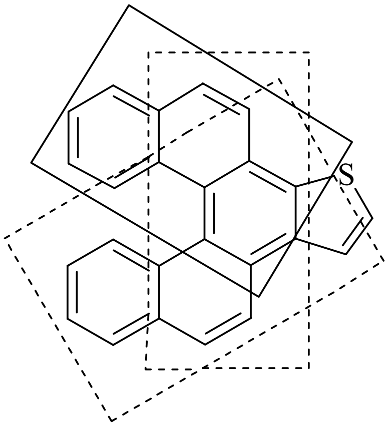
(b) The location that has lowest locants as a set for fusion to the parent component

Example:



5*H*-benzo[6,7]cyclohepta[4′,5′]indeno[1′,2′:3,4]fluoreno[2,1-*b*]furan (PIN)
(not 5*H*-benzo[5′,6′]indeno[1′,2′:1,2]cyclohepta[7,8]fluoreno[4,3-*b*]furan;
locants 1,2 are lower than 3,4 for the ‘fluoreno’ attached component)

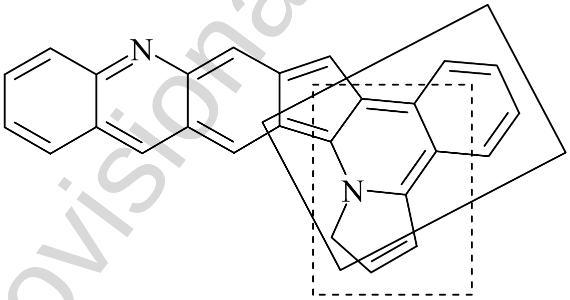
(c) The location that has lowest locants for fusion to the parent component in order of citation.
Example:



naphtho[2′,1′:3,4]phenanthro[1,2-*b*]thiophene (PIN)
(not naphtho[2′,1′:3,4]phenanthro[2,1-*b*]thiophene,
nor dibenzo[3,4:5,6]phenanthro[9,10-*b*]thiophene;
the locants ‘1,2’ for the ‘phenanthro’ attached component,
in order of citation, are lower than ‘2,1’ or ‘9,10’)

This procedure is continued exploring outwards to the senior second-order attached components.

Example:

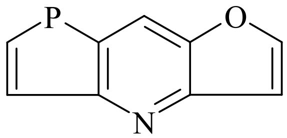


7*H*-pyrrolo[2″,1″:1′,2′]isoquinolino[4′,3′:4,5]cyclopenta[1,2-*b*]acridine (PIN)
(not 7*H*-benzo[7′,8′]indolizino[6′,5′:4,5]cyclopenta[1,2-*b*]acridine;
isoquinoline is senior to indolizine)

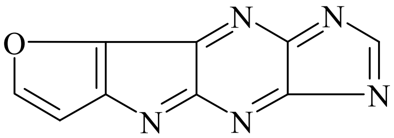
P-25.3.4.2.3 Order of citation of fusion prefixes

(a) Fusion between two components is indicated by the method described in P-25.3.1. All attached components are cited in front of the parent component. Each second order attached component is cited at the front of the first order attached component to which it is fused, and so on to higher order attached components. If there are two or more different components, or sets of components, attached to a lower order component, they are cited in alphabetical order.

Examples:



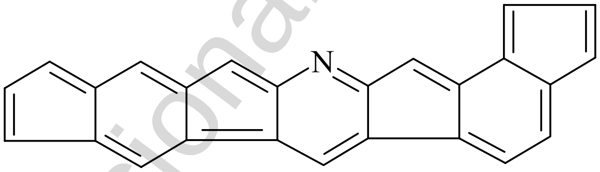
furo[3,2-*b*]thieno[2,3-*a*]pyridine (PIN)
(furo is cited before thieno)



furo[2′,3′:4,5]pyrrolo[2,3-*b*]imidazo[4,5-*e*]pyrazine (PIN)
(furo…pyrrolo is cited before imidazo)

In the case of indacene, if the only distinction is between *as*-indacene and *s*-indacene, then the italic characters are considered. Otherwise, they are treated as indacene for consideration of alphabetical order. It should be noted that *s*-indacene is senior to *as*-indacene in the order of seniority of components.

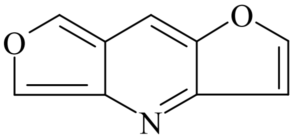
Example:



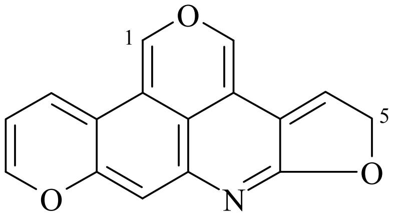
as-indaceno[2,3-*b*]-*s*-indaceno[1,2-*e*]pyridine (PIN)

(b) If two or more identical components are fused to a third component, they are cited together using multiplying prefixes (‘di’, ‘tri’, etc.; or ‘bis’, ‘tris’, etc.). The citation of different components is in alphabetical order of the names of the components, just as for simple multiplicative prefixes in substitutive nomenclature. The multiplicative prefix is considered only when it is an integral part of a multipart fusion prefix.

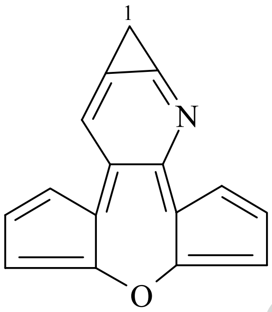
Examples:



difuro[3,2-*b*:3′,4′-*e*]pyridine (PIN)



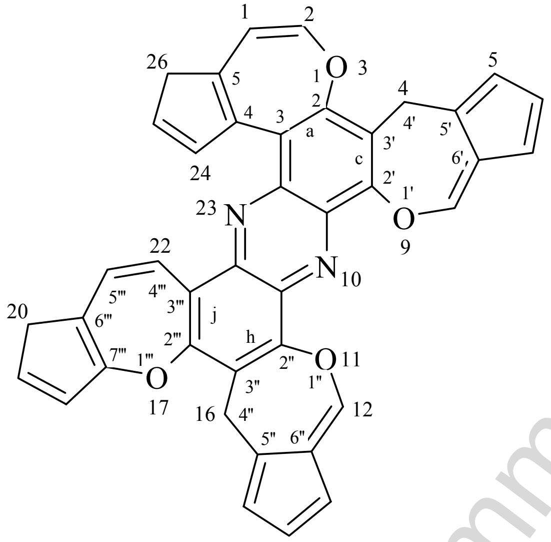
5*H*-furo[3,2-*g*]dipyrano[2,3-*b*;3′,4′,5′-*de*]quinoline (PIN)
(furo is cited before pyrano)



1*H*-cyclopropa[*b*]dicyclopenta[2,3:6,7]oxepino[4,5-*e*]pyridine (PIN)
(not 1*H*-dicyclopenta[2,3:6,7]oxepino[4,5-*b*]cyclopropa[*e*]pyridine; cyclopropa is cited before dicyclopentaoxepino, which is treated as one component)

(c) If two or more groups of components differ only by virtue of the fusion locants within the group, these locants are used to determine the order of citation of prefixes; lower locant sets are cited earlier.

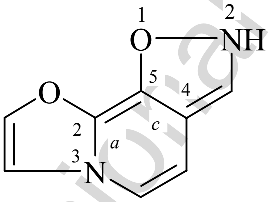
Example:



4*H*,16*H*,20*H*,26*H*-cyclopenta[4,5]oxepino[3,2-*a*]bis(cyclopenta[5,6]oxepino)[3′,2′-*c*:2″,3″-*h*]cyclopenta[6‴,7‴]oxepino[2‴,3‴-*j*]phenazine (PIN)

(d) If two or more groups of components only differ by virtue of heteroatom locants, these locants are used to determine the order; lower locant sets are cited earlier.

Example:



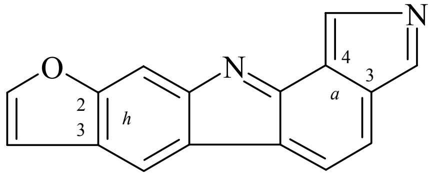
2*H*-[1,2]oxazolo[5,4-*c*][1,3]oxazolo[3,2-*a*]pyridine (PIN)

P-25.3.4.2.4 Choice of locants

If there is a choice of locants, letters, or numerals (consistent with the numbering of the component), the lower letters or numbers are selected in accordance with the following criteria, which are considered in order until a complete decision can be made.

(a) Parent component letters as a set.

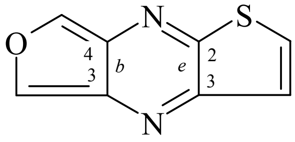
Example:



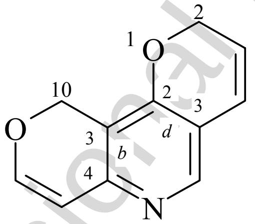
furo[3,2-*h*]pyrrolo[3,4-*a*]carbazole (PIN)
(not furo[2,3-*b*]pyrrolo[3,4-*i*]carbazole;
a,*h* is lower than *b*,*i*)

(b) Parent component letters in order of citation.

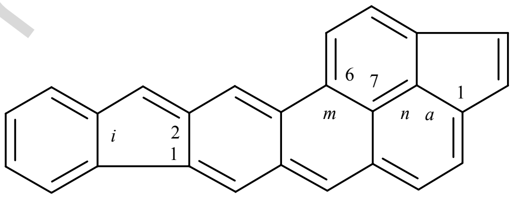
Examples:



furo[3,4-*b*]thieno[2,3-*e*]pyrazine (PIN)
(not furo[3.4-*e*]thieno[2,3-*b*]pyrazine;
b...*e* is lower than *e*...*b*)



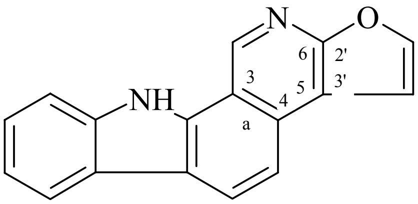
2*H*,10*H*-dipyrano[4,3-*b*:2′,3′-*d*]pyridine (PIN)
(not 2*H*,10*H*-dipyrano[2,3-*d*:4′,3′-*b*]pyridine;
b...*d* is lower than *d*...*b*)



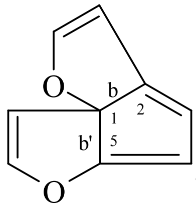
diindeno[1,2-*i*:6′,7′,1′-*mna*]anthracene (PIN)
(not diindeno[6,7,1-*mna*:1′,2′-*i*]anthracene;
i...*mna* is lower than *mna*...*i*)

(c) Set of locants of the first-order attached components for fusion to the parent component.

Example:



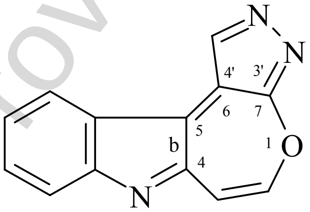
10*H*-furo[3′,2′:5,6]pyrido[3,4-*a*]carbazole (PIN)
(not 10*H*-furo[2′,3′:2,3]pyrido[5,4-*a*]carbazole;
the locant set ‘3,4’ is lower than ‘4,5’ for attaching
pyrido to carbazole)



cyclopenta[1,2-*b*:5,1-*b*′]difuran (PIN, a multiparent name)
(not cyclopenta[1,2-*b*:2,3-*b*′]difuran;
the locant set ‘1,1,2,5’ is lower than ‘1,2,2,3’)

(d) First-order attached component locants for fusion to the parent component in order of citation.

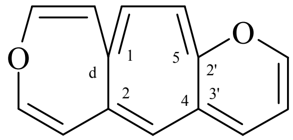
Example:



pyrazolo[4′,3′:6,7]oxepino[4,5-*b*]indole (PIN)
(not pyrazolo[3′,4′:2,3]oxepino[5,4-*b*]indole;
the locant set ‘4,5’ is lower than ‘5,4’)

(e) Locants for lower-order attached components as a set for fusion to higher-order attached component.

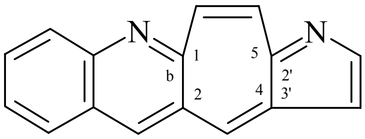
Example:



pyrano[3′,2′:4,5]cyclohepta[1,2-*d*]oxepine (PIN)
(not pyrano[2′,3′:5,6]cyclohepta[1,2-*d*]oxepine;
the locant set ‘4,5’ is lower than ‘5,6’)

(f) Locants for lower-order attached components for fusion to higher-order attached components in order of citation.

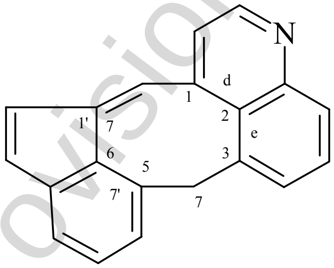
Example:



pyrrolo[3′,2′:4,5]cyclohepta[1,2-*b*]quinoline (PIN)
(not pyrrolo[2′,3′:5,4]cyclohepta[1,2-*b*]quinoline;
the locant set ‘4,5’ is lower than ‘5,4’)

(g) Locants for higher-order attached components as a set for fusion to the lower-order attached component.

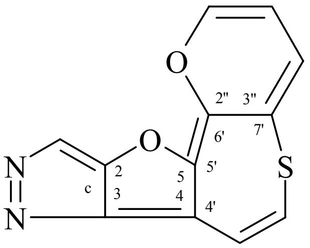
Example:



7*H*-indeno[7′,1′:5,6,7]cycloocta[1,2,3-*de*]quinoline (PIN)
(not 7*H*-indeno[3′,4′:5,6,7]cycloocta[1,2,3-*de*]quinoline;
the locant set ‘1′,7′ ’ is lower than ‘3′,4′ ’)

(h) Locants for higher-order components in fusion to lower order components in order of citation.

Example:



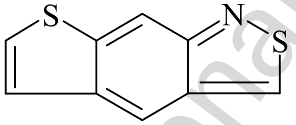
pyrano[2″,3″:6′,7′]thiepino[4′,5′:4,5]furo[3,2-*c*]pyrazole (PIN)
(not pyrano[3″,2″:2′,3′]thiepino[5′,4′:4,5]furo[3,2-*c*]pyrazole;
the locant set ‘4′,5′ ’ is lower than ‘5′,4′ ’)

P-25.3.5 Heteromonocyclic rings fused to a benzene ring as components

Heterobicyclic compounds consisting of a heteromonocycle fused to a benzene ring in which the benzene ring is not part of a system having a retained name such as quinoline or naphthalene are treated as a single component unit (a ‘benzoheterocycle, see P-25.2.2.4). They may be treated as a parent component or an attached component depending on the order of seniority described in P-25.3.2.4. However, this approach is not be used if it disrupts a multiparent system (see P-25.3.5.3, below) or the use of multiplicative prefixes (see P-25.3.6.1, below).

P-25.3.5.1 A benzoheterocycle as a parent component

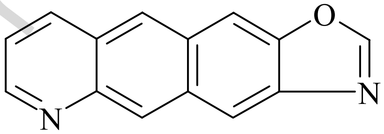
Example:



thieno[3,2-*f*][2,1]benzothiazole (PIN)
(2,1-benzothiazole is senior to 1-benzothiophene)

P-25.3.5.2 A more senior component as parent component

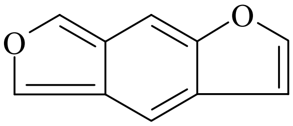
Example:



[1,3]benzoxazolo[6,5-*g*]quinoline (PIN)
(quinoline is senior to 1,3-benzoxazole)

P-25.3.5.3 A multiparent name is preferred to a fused system, when there is a choice.

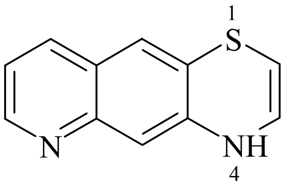
Example:



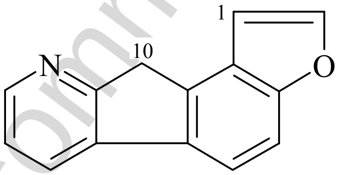
benzo[1,2-*b*:4,5-*c*′]difuran (PIN)
(not furo[3,4-*f*][1]benzofuran;
a multiparent name is preferred to a
two component fused name)

P-25.3.5.4 Retained names are senior to names of benzoheterocycles

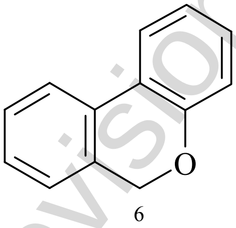
Examples:



4*H*-[1,4]thiazino[2,3-*g*]quinoline (PIN)
(the retained name quinoline
must be used)



10*H*-furo[3′,2′-4,5]indeno[2,1-*b*]pyridine (PIN)
(not [1]benzofuro[5′,4′:3,4]cyclopenta-
[1,2-*b*]pyridine; pyridine is senior to
furan; indene, as a retained name, must
be used)

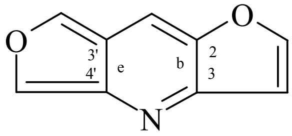


6*H*-benzo[*c*]chromene (PIN)
(not 6*H*-benzo[*c*][1]benzopyran; the retained name
chromene must be used; not 6*H*-benzo[*b*,*d*]pyran;
chromene is the larger parent component]

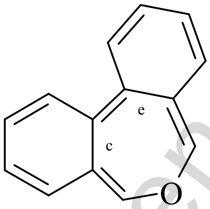
P-25.3.6 Treatment of identical attached components

P-25.3.6.1 Two or more components that are identical and both fused to a parent component are indicated by the use of multiplying prefixes (di-, tri-, etc. or bis-, tris-, etc.). If a complete set of locants is used for first order attached components fused to the parent component, they are cited together separated by a colon. If abbreviated sets of locants are used, the letters are separated by a comma. If complete sets of locants are used for second order attached components fused to a first order attached component, or for higher order cases, the locants are cited together separated by a semicolon. If abbreviated sets are used, they are separated by a colon. To distinguish between two or more components of the same order, the locants of the second component are primed (or double primed if the first is primed, etc.), the third double primed, and so on.

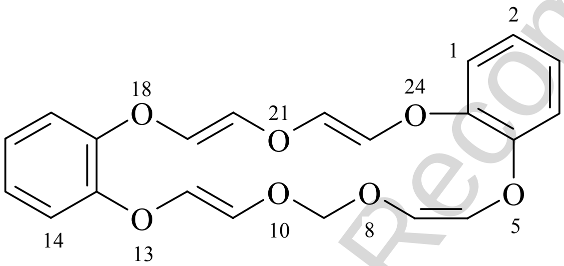
Examples:



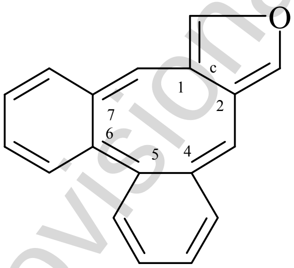
difuro[3,2-*b*:3′,4′-*e*]pyridine (PIN)



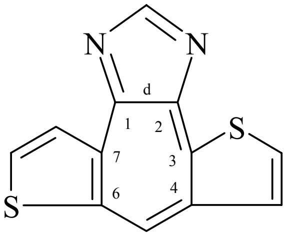
dibenzo[*c*,*e*]oxepine (PIN)



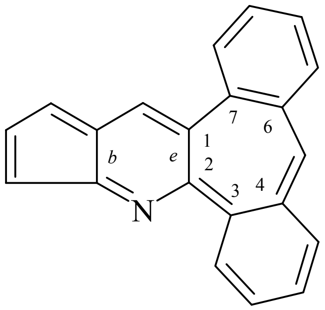
dibenzo[*g*,*p*][1,3,6,9,12,15,18]heptaoxacycloicosine (PIN)



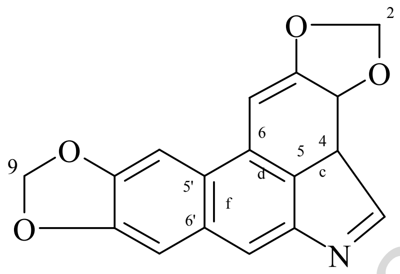
dibenzo[4,5:6,7]cycloocta[1,2-*c*]furan (PIN)



dithieno[2′,3′:3,4;2″,3″:6,7]cyclohepta[1,2-*d*]imidazole (PIN)



cyclopenta[*b*]dibenzo[3,4:6,7]cyclohepta[1,2-*e*]pyridine (PIN)

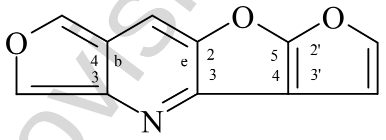


2*H*,9*H*-bis[1,3]benzodioxolo[4,5,6-*cd*:5′,6′-*f*]indole (PIN)

P-25.3.6.2 Additional components attached to a system with a multiplicative prefix.

Fusion of a higher order attached component to a system named with a multiplicative prefix requires each set of attached components to be specified separately.

Example:

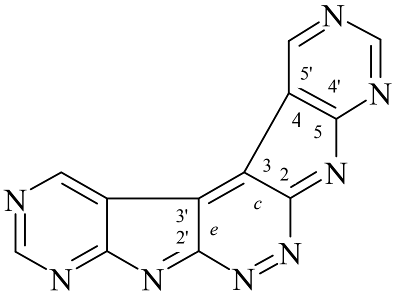


furo[3,4-*b*]furo[3′,2′:4,5]furo[2,3-*e*]pyridine (PIN)

P-25.3.6.3 Groups of identical components with identical fusion locants.

Two or more groups of identical components (including identical fusion locants between these components) fused to another component, are indicated by the use of the multiplying prefixes bis-, tris-, etc., and the group of components is cited within parentheses.

Example:



bis(pyrimido[5′,4′:4,5]pyrrolo)[2,3-*c*:3′,2′-*e*]pyridazine (PIN)

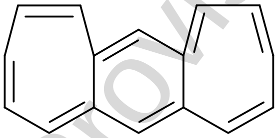
P-25.3.7 Multiparent systems

Two or more nonoverlapping locations for parent components that are *ortho-* or *ortho*- and *peri*-fused to the same first-order interparent component are treated as a multiparent system and given a multiparent name. Similarly a system with three, five, seven, etc. interparent components is treated as an extended multiparent system. Each pair of second or higher order interparent components must be identical.

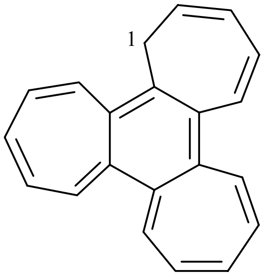
P-25.3.7.1 Multiparent systems with one interparent component

Multiple occurrences of the parent component in a multiparent system are indicated by the use of a multiplying prefix (‘di’, ‘tri’, etc. or ‘bis’, ‘tris’, etc.). To distinguish between the parent components the second parent component, has primed letters, the third double primed, etc.; the sets of locants are separated by a colon.

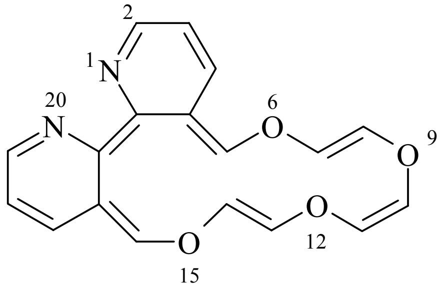
Examples:



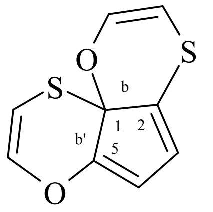
benzo[1,2:4,5]di[7]annulene (PIN)



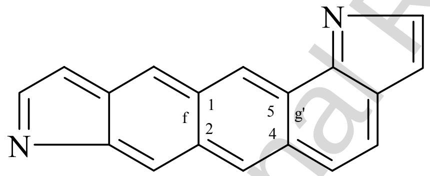
1*H*-benzo[1,2:3,4:5,6]tri[7]annulene (PIN)



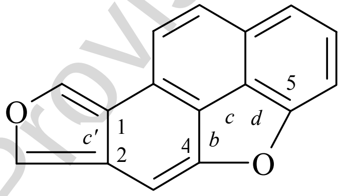
[1,4,7,10]tetraoxacyclohexadecino[13,12-*b*:14,15-*b*′]dipyridine (PIN)



cyclopenta[1,2-*b*:5,1-*b*′]bis[1,4]oxathiazine (PIN)



benzo[1,2-*f*:4,5-*g*′]diindole (PIN)

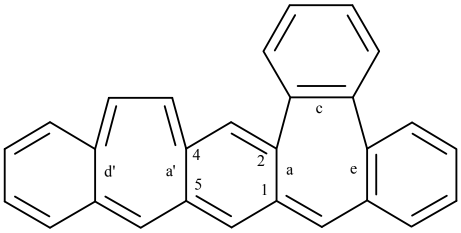


phenanthro[4,5-*bcd*:1,2-*c*′]difuran (PIN)

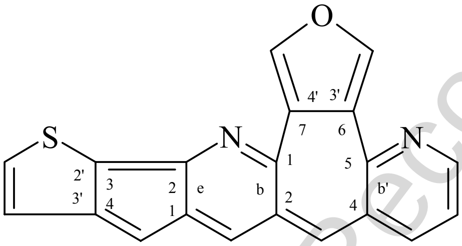
P-25.3.7.2 Additional attached components

Additional attached components may be fused to any of the components of a multiparent system. If the choice of locants described in P-24.4.5.2.4 does not permit a final choice, seniority is given to the unprimed component and the fusion letters are assigned with the lower letter used for fusion to the connecting component. Great care is needed with the use of primes, double primes, etc. to ensure that there is no ambiguity. Thus additional components fused to the interparent component(s) are cited next to the prefix for the interparent component.

Examples:



tribenzo[*c*,*d*′,*e*]benzo[1,2-*a*:4,5-*a*′]di[7]annulene (PIN)



thieno[2′,3′:3,4]cyclopenta[1,2-*e*]furo[3′,4′:6,7]cyclohepta[1,2-*b*:5,4-*b*′]dipyridine (PIN)
(the furan ring is fused to the interparent component; thus, alphabetical order does not apply)

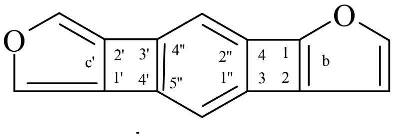
P-25.3.7.3 Multiparent systems with three or more interparent components

When two (or more) possible parent components are separated by an odd number of interparent components and these are ordered symmetrically with respect to their component rings (but not necessarily with their fusion locants), the whole system is treated as a multiparent system. Second and higher-order interparent components are named using the multipying prefixes ‘di’, ‘tri’, etc. or ‘bis’, ‘tris’, etc. Two methods are to be considered. Method (a) generates IUPAC preferred names.

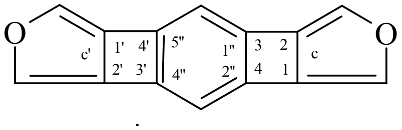
(a) This method is extended to all compounds, with appropriate locants assigned to interparent components, unprimed and primed for first-order interparent components, double primed for second-order interparent components, tripled primed for third-order interparent components, and so on.

(b) When symmetry permits grouping of interparent components and parent components, such groups can be formed and cited as such using the multiplying prefixes ‘bis’, ‘tris’, etc. to denote groups that are enclosed within parentheses . Unprimed locants only are used within such groupings.

Examples:



(a) benzo[1″,2″:3,4;4″,5″:3′,4′]dicyclobuta[1,2-*b*:1′,2′-*c*′]difuran (PIN)

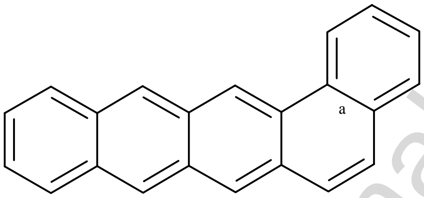


(a) benzo[1″,2″:3,4;4″,5″:3′,4′]dicyclobuta[1,2-*c*:1′,2′-*c*′]difuran (PIN)
(b) benzo[1″,2″:3,4;4″,5″:3′,4′]bis(cyclobuta[1,2-*c*]furan)

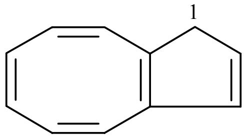
P-25.3.8 Omission of locants

P-25.3.8.1 When there is no ambiguity, numerical and/or letter locants may be omitted in a system with only first order attached components.

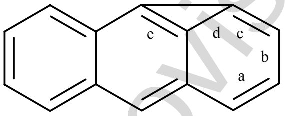
Examples:



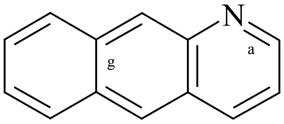
benzo[*a*]tetracene (PIN)



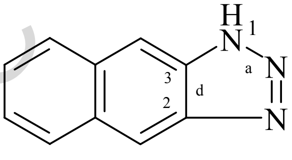
1*H*-cyclopenta[8]annulene (PIN)



cyclopropa[*de*]anthracene (PIN)

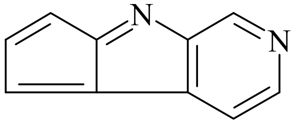


benzo[*g*]quinoline (PIN)



1*H*-naphtho[2,3][1,2,3]triazole (PIN)

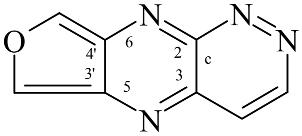
P-25.3.8.2 Locants are also omitted when there is no ambiguity for the fusion of a terminal attached component.
Example:



cyclopenta[4,5]pyrrolo[2,3-*c*]pyridine (PIN)

P-25.3.8.3 When locants are required for the fusion of a higher-order component then all locants for linking components must be cited.

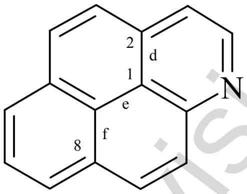
Example:



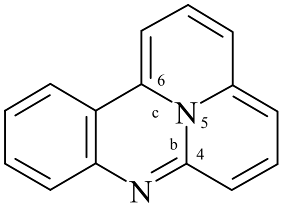
furo[3′,4′;5,6]pyrazino[2,3-*c*]pyridazine (PIN)

P-25.3.8.4 The numerical locants of peripheral fusion carbon atoms of a component are omitted with an *ortho*- and *ortho*- and *peri*-fused system.

Examples:



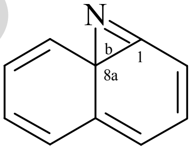
naphtho[2,1,8-*def*]quinoline (PIN)



quinolizino[4,5,6-*bc*]quinazoline (PIN)

Both terminal fusion atom locants for *ortho*-fusion must be cited even if one is a fusion atom.

Example:



naphtho[1,8a]azirine (PIN)

P-25.4 Bridged fused systems

This Section is based on the publication ‘Nomenclature of Fused and Bridged Fused Ring Systems’ (ref. 4). It deals mainly with naming bridged fused ring systems having only independent bridges. For naming bridged fused ring systems having dependent bridges, consult the full publication (ref. 4).

P-25.4.1 Definitions and terminology

P-25.4.1.1 Bridged fused ring system. A ring system in which some of the rings constitute a fused ring system (see P-25.0 - P-25.3) and the remaining rings are created by one or more bridges.

P-25.4.1.2 Bridge. An atom or group of atoms is named as a bridge by means of a prefix if it fulfills one or more of the following:

(a) if it connects two or more non-adjacent positions of the same ring in a fused ring system;

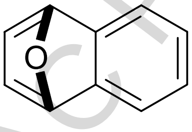
(b) if it connects two or more positions of different rings of a fused ring system and does not thereby form a new *ortho*- and *peri*-fused ring;

(c) if it connects positions of a ring of a fused ring system to a previously described bridge but cannot be included as part of that bridge;

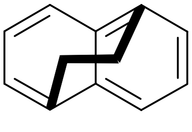
(d) if it connects the atoms at the end of a bond common to two rings of a fused ring system;

(e) if it is used to describe a system with only *ortho*- or *ortho*- and *peri*-fusions that cannot be named entirely by fusion principles.

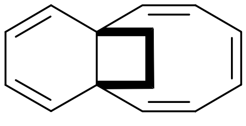
Examples (bridges are indicated in bold):



criterion (a)



criterion (b)



criterion (d)

P-25.4.1.3 Bridgehead atom. An atom of a fused ring system to which a bridge is attached.

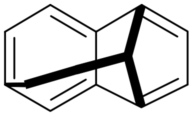
P-25.4.1.4 Simple bridge prefix. A bridge that describes an atom, or groups of atoms, that may be described as a single unit, *e.g.*, ‘epoxy’, ‘butano’, ‘benzeno’.

P-25.4.1.5 Composite bridge. A group of atoms that can only be considered as a contiguous sequence of simple bridges, e. g., (epoxymethano) = epoxy + methano = −O-CH_2−.

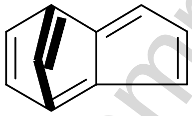
P-25.4.1.6 Bivalent bridge. A bridge that is connected by single bonds to two different positions of a fused ring system or bridged fused ring system. All bridges described in P-25.4.2.1 are simple bridges.

P-25.4.1.7 Polyvalent bridge. A bridge that is connected to a fused ring system by three or more single bonds or their multiple bond equivalent. Polyvalent bridges may often be described by a combination of two simple bivalent bridges. Polyvalent bridges may be further classified as bipodal, tripodal, etc., when the bridge is attached to two, three, or more positions of the fused ring system.

Examples:



a tripodal bridge

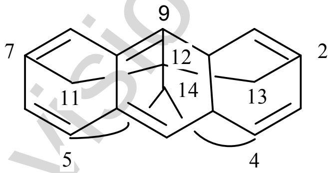


a bipodal bridge

P-25.4.1.8 Independent bridge. A bridge that only connects two or more positions of a fused ring system (see dependent bridge).

P-25.4.1.9 Dependent bridge. A bridge that connects one or more positions of a fused ring system to one or more positions of a simple or composite independent bridge, and cannot be expressed as part of a larger composite bridge.

Example:



4,5,12-epimethanetriyl-2,9,7-epipropane[1,2,3]triylanthracene (PIN)
(the epimethanetriyl bridge C-14 is a dependent bridge;
the epipropane[1,2,3]triyl bridge at C-11 to C-13 is an
independent bridge)

P-25.4.2 Names of bridges

The extensive list of bridge names given in the publication on fused ring and bridged fused ring nomenclature (ref. 4) has been carefully reviewed and updated in the context of the recommendations given herein. Most of the changes occurred in the names of acyclic heteroatom bridge names (see P-25.4.2.1.4)

P-25.4.2.1 Bivalent bridges.

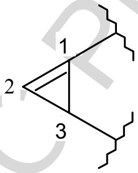
P-25.4.2.1.1 A bivalent acyclic hydrocarbon bridge is named as a prefix derived from the corresponding rectilinear hydrocarbon name by changing the final letter ‘e’ to ‘o’. The locant for a double bond, if present, is indicated in square brackets between the hydrocarbon prefix and the ending ‘eno’; this locant is not the locant used in the final numbering of the bridged fused ring system (see P-25.4.4). If there is a choice low numbers are preferred (e.g., prop[1]eno rather than prop[2]eno).

Examples:

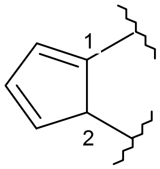
methano (PIN)	$–CH_2–$
ethano (PIN)	$–CH_2\text{-}CH_2–$
propano (PIN)	$–CH_2\text{-}CH_2\text{-}CH_2–$
etheno (PIN)	$–CH{=}CH–$
prop[1]eno (PIN)	$–CH{=}CH\text{-}CH_2–$
but[1]eno (PIN)	$–CH{=}CH\text{-}CH_2\text{-}CH_2–$
but[2]eno (PIN)	$–CH_2\text{-}CH{=}CH\text{-}CH_2–$
buta[1,3]dieno (PIN)_	$–CH{=}CH\text{-}CH{=}CH–$

P-25.4.2.1.2 A bivalent monocyclic hydrocarbon bridge other than benzene is named by the same prefix as that used as a fusion prefix (P-25.3.2.2). To distinguish between these two, ‘epi’ is added in front of the name when used as a bridge prefix; the letter ‘i’ in the prefix ‘epi’ is elided before the letters ‘i’ and ‘o’ of the following term. The bridge is assumed to have the maximum number of noncumulative double bonds consistent with its attachments to the fused ring system or to other bridges. The positions of the free valences of the bridge are indicated by locants in square brackets cited directly in front of the bridge name; these locants are not those used for bridge atoms in the final structure. Locants for indicated hydrogen atoms, if present, are those for the final structure and are cited in front of the completed name.

Examples:



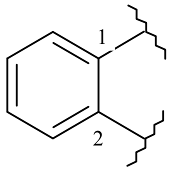
[1,3]epicyclopropa (PIN)



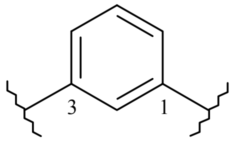
[1,2]epicyclopenta (PIN)

P-25.4.2.1.3 Bivalent cyclic hydrocarbon bridges not named in P-25.4.2.1.2 are named as a prefix derived from the corresponding hydrocarbon name by replacing the terminal letter ‘e’ by ‘o’. If the name of the bridge is the same as the name of the fusion prefix, the bridge prefix is distinguished by the prefix ‘epi-’. The letter ‘i’ is elided if followed by a vowel. Locants are used in the same way as described in section P-25.4.2.1.2.

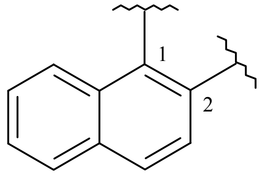
Examples:



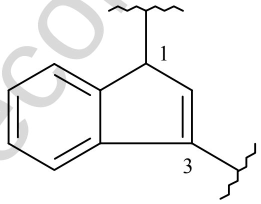
[1,2]benzeno (PIN)
(not [1,2]benzo)



[1,3]benzeno (PIN)
(not [1,3]benzo)



[1,2]naphthaleno (PIN)
(not epi[1,2]naphtho; naphtho is the name of a fusion prefix)



[1,3]epindeno (PIN)

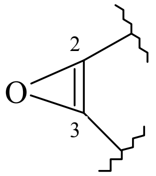
P-25.4.2.1.4 A bivalent acyclic homogeneous heteroatom bridge is named by an appropriate prefix based either on a substitutive prefix name or the name of the corresponding parent hydride. Bridge prefixes based on a substitutive prefix, in use today or formerly recommended, are distinguished by the prefix ‘epi’ (or ‘ep’ before the letter ‘i’ or ‘o’ of the following term). Bridge prefixes based on the name of a parent hydride are named in the same way as for acyclic hydrocarbon bridge prefixes (see P-25.4.2.1.1). Heteroatoms with nonstandard bonding numbers are described by the λ-convention (see P-14.1).

Examples:

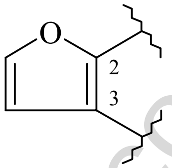
epoxy (PIN)	–O–	azano (not epimino)	–NH–
epidioxy (PIN)	–OO–	epidiazano (PIN)	–NHNH–
epitrioxy (PIN)	–OOO–	epidiazeno (PIN)	–N=N–
sulfano (PIN)	–S–	epitriazano (PIN)	–NHNHNH–
λ^4-sulfano (PIN)	$-SH_2-$	(epitriaz[1]eno) (PIN)	$-\overset{3}{N}H-\overset{2}{N}=\overset{1}{N}-$

disulfano (PIN)	–SS–	phosphano (PIN)	–PH–
selano (PIN) (not episeleno)	–Se–	silano(PIN)	$-SiH_2-$
tellano (PIN)	–Te–	borano (PIN)	–BH–

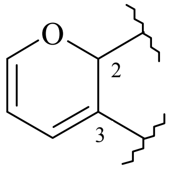
P-25.4.2.1.5 A bivalent heterocyclic bridge is named as a prefix derived from the corresponding heterocyclic compound by adding a letter ‘o’ with elision of a final letter ‘e’ if present. If the heterocyclic system requires the citation of locants, these are given in square brackets in front of the name of the prefix. If the name of the bridge is the same as the fusion prefix, the bridge prefix is distinguished by the prefix ‘epi’ (or ‘ep’ before the letter ‘i’ or ‘o’ of the following term.
Examples:



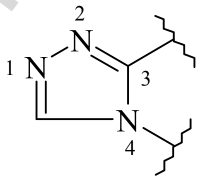
epoxireno (PIN)



[2,3]furano (PIN)
(not epi[2,3]furano)



[2,3]epipyrano (PIN)



[3,4]epi[1,2,4]triazolo (PIN)

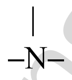
P-25.4.2.2 Polyvalent bridges

P-25.4.2.2.1 A polyvalent bridge consisting of one atom (other than hydrogen) is named by an appropriate prefix based either on a substitutive prefix name or the name of the corresponding parent hydride. Polyvalent bridges are enclosed by parentheses in names of bridged fused systems; as a reminder, parentheses are placed around the names of the bridges themselves in the examples below). For ‘epi’, see P-25.4.2.1.4.

Examples:

(metheno) (PIN)	–CH=	(epimethanetriyl) (PIN)	$-\overset{|}{C}H-$
(epimethanediylylidene) (PIN)	$-\overset{|}{C}=$	(epiazanediyl) (PIN) (not epimino)	–NH–

(azeno) (PIN) $-N=$ (epinitrilo) (PIN)


$-\overset{|}{N}-$

P-25.4.2.2.2 A polyvalent polyatomic bridge is named as the appropriate polyvalent substituent group and enclosed in parentheses in names (as a reminder, parentheses are placed around the names of the bridges themselves in the examples below). If necessary, the positions of the free valences are indicated by appropriate locants cited directly in front of the associated ending. The suffix ‘ylidene’ is restricted to those cases in which there is a double bond between the bridge and the fused system. When there is a choice of numbering the bridge, preference is given to (a) the suffix ‘yl’, (b) the suffix ‘ylidene’, (c) double bonds. For ‘epi’, see P-25.4.2.1.4.

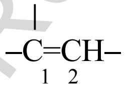
Examples:

(epiethanylylidene) (PIN) $-CH_2-CH=$

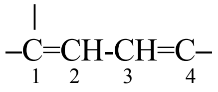
(epiethane[1,1,2]triyl) (PIN)


$-\underset{1}{\overset{|}{C}H}-\underset{2}{CH_2}-$

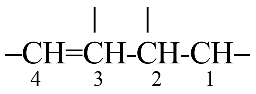
(epiethene[1,1,2]triyl) (PIN)


$-\underset{1}{\overset{|}{C}}=\underset{2}{CH}-$

(epibuta[1,3]diene[1,1,4]triyl (PIN)

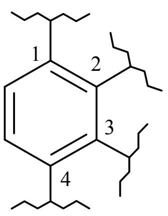

$-\underset{1}{\overset{|}{C}}=\underset{2}{CH}-\underset{3}{CH}=\underset{4}{C}-$

(epibut[3]ene[1,1,2,4]tetrayl) (PIN)


$-\underset{4}{CH}=\underset{3}{\overset{|}{C}H}-\underset{2}{\overset{|}{C}H}-\underset{1}{CH}-$

(epidiazenediylidene) (PIN) $=N-N=$

(epibenzene[1,2,3,4]tetrayl) (PIN)

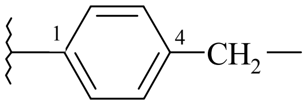


P-25.4.2.3 Composite bridges

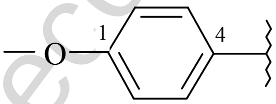
Composite bridge names are formed by combining the names of two or more simple bridges. Unless cited first, the prefix 'epi' (or 'ep' before the letter 'i' or 'o' of the following term.) is omitted. The prefixes are cited in order starting from the terminal prefix with a heteroatom appearing first in the list: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl. Then alphabetical order is used. Composite bridges are enclosed within parentheses in names of bridged fused compounds; as a reminder, parentheses are placed around the names of bridges themselves.

Examples:

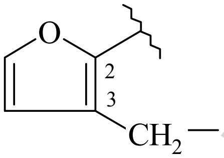
(epoxymethano) (PIN)	$–O\text{-}CH_2–$
(azanoethano) (PIN)	$–NH\text{-}CH_2\text{-}CH_2–$
(epoxysulfanooxy) (PIN)	–O-S-O–



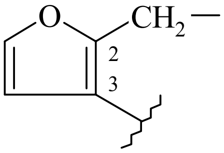
([1,4]benzenomethano) (PIN)



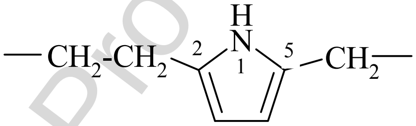
(epoxy[1,4]benzeno) (PIN)



([2,3]furanomethano) (PIN)



([3,2]furanomethano) (PIN)



(ethano[2,5]pyrrolomethano) (PIN)

P-25.4.3 Procedure for naming bridged fused ring systems

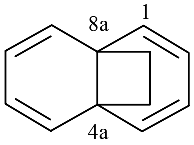
P-25.4.3.1 Selection of bridge

When a polycyclic ring system cannot be named completely as a fused ring system, possible ways for naming it as a bridged fused system are considered. Bridges are selected so that a recommended fused ring system as described in P-25.4.2.3 is obtained.

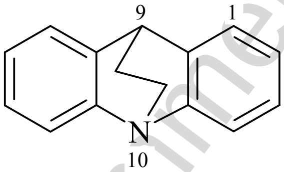
P-25.4.3.2 Naming of *ortho*- or *ortho*- and *peri*-fused systems

The ring system that remains after removal of the bridge(s) is named following P-25.1 through P-25.3. The maximum number of noncumulative double bonds is assigned after the insertion of the bridge. Hence, in order to allow for the necessary free valences to the bridge, the fused ring system may differ from the isolated ring system in the number of noncumulative double bonds and/or the need for indicated hydrogen. If needed, indicated hydrogen is used to identify the required isomer and is cited in front of the completed bridged fused ring name.

Examples:



4a,8a-ethanonaphthalene (PIN)



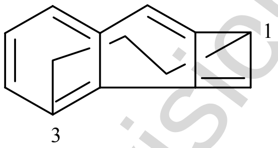
9*H*-9,10-ethanoacridine (PIN)

P-25.4.3.3 Selection of fused ring system to be bridged

If there is a choice for selecting the fused ring system to be bridged, the criteria in the following list are applied in order until a complete decision is reached. The fused ring system, before bridging must:

(a) contain the maximum number of rings.

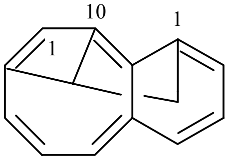
Examples:



1*H*-1,3-propanocyclobuta[*a*]indene (PIN)

correct

not



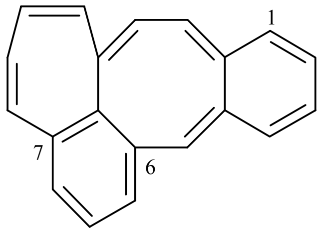
8,10,1-epiethane[1,1,2]triylbenzo[8]annulene

incorrect

(the correct name has three rings in the fused system; the incorrect name has only two rings in the fused system)

(b) include the maximum number of skeletal atoms

Example:

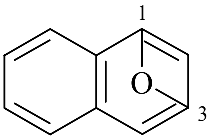


6,7-epiprop[1]en[1]yl[3]ylidenebenzo[*a*]cyclohepta[*e*][8]annulene (PIN)
(not 4,5-buta[1,3]dienodibenzo[*a,d*][8]annulene)

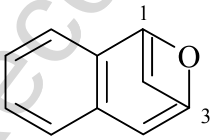
(the fused ring system benzo[*a*]cyclohepta[*e*][8]annulene has 17 atoms whereas the fused ring system dibenzo[*a,d*][8]annulene has only 16 atoms)

(c) contain the minimum number of heteroatoms in the fused ring system.

Example:



not



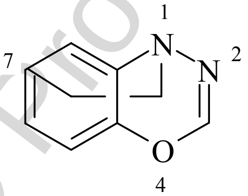
1,3-epoxynaphthalene (PIN)
correct

1,3-methenoisochromene
incorrect

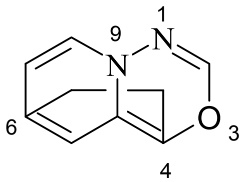
(the correct name has no heteroatoms in the fused system; the incorrect one has one hetero atom in its fused system)

(d) consist of the most senior ring system, when the seniority order is applied to the whole fused ring system (see P-44.2):

Example:



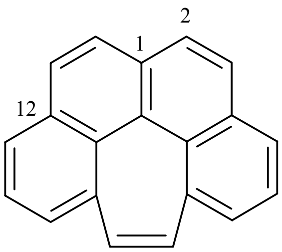
not



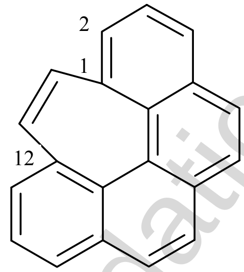
1,7-ethano[4,1,2]benzoxadiazine (PIN)
correct

4,6-ethanopyrido[1,2-*d*][1,3,4]oxadiazine
incorrect

(in the correct two-ring system, the locant set 1,2,4 for heteroatoms is lower than 1,3,9)



not



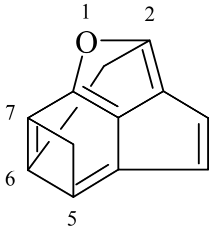
1,12-ethenobenzo[4,5]cyclohepta[1,2,3-*de*]naphthalene (PIN)
correct

1,12-ethenobenzo[*c*]phenanthrene
incorrect

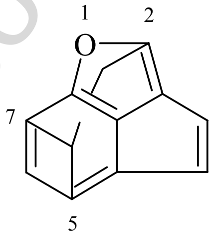
(in the correct name the ring size set 7,6,6,6 is preferred to 6,6,6,6)

(e) have the minimum number of composite bridges:

Examples:



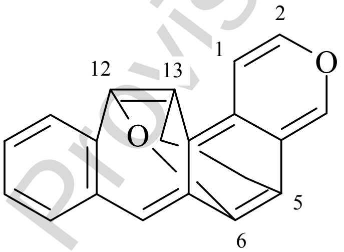
not



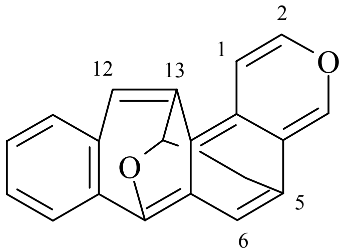
2,6:5,7-dimethanoindeno[7,1-*bc*]furan (PIN)
correct

5,7,2-epiethane[1,1,2]triylindeno[7,1-*bc*]furan
incorrect

(the correct name has no composite bridges; the incorrect name has one composite bridge)



not



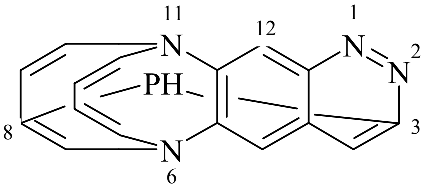
6,12-epoxy-5,13-methanobenzo[4,5]cyclo-[1,2-*f*]isochromene (PIN)
correct

7,5,13-(epoxyepimethanetriyl)benzo-[4,5]cyclohepta[1,2-*f*]isochromene
incorrect

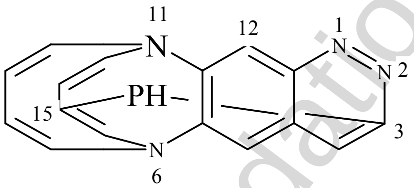
(the correct name has no composite bridges; the incorrect name has one)

(f) have the minimum number of dependent bridges:

Example:



not



6,11-buta[1,3]dieno-3,8-phosphano[1,4]-diazocino[2,3-*g*]cinnoline (PIN)

correct

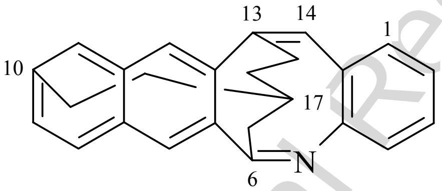
3,14-phosphano-6,11-buta[1,3]dieno[1,4]-diazocino[2,3-*g*]cinnoline

incorrect

(the correct name has no dependent bridges; the incorrect name has one dependent bridge)

(g) have the minimum number of atoms in dependent bridges:

Example:

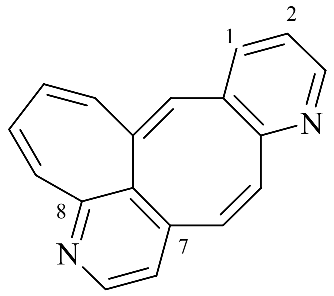


6,17-methano-10,13-pentanonaphtho[2,3-*c*][1]benzazocine (PIN)
(not 13,17-ethano-6,10-butanonaphtho[2,3-*c*][1]benzazocine)
(not 10,17-ethano-6,13-butanonaphtho[2,3-*c*][1]benzazocine)

(the correct name has only one atom in a dependent bridge)

(h) have the maximum number of bivalent bridges; thus ‘diyl’ is senior to ‘ylylidene’, ‘triyl’, diylidene’, ‘diylylidene’, or ‘tetrayl’, etc. Similarly ‘ylylidene’ is senior to ‘triyl’, etc..

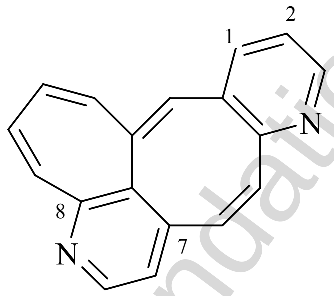
Examples:



8,7-(azenoetheno)cyclohepta[4,5]cycloocta[1,2-*b*]pyridine (PIN)

correct

not



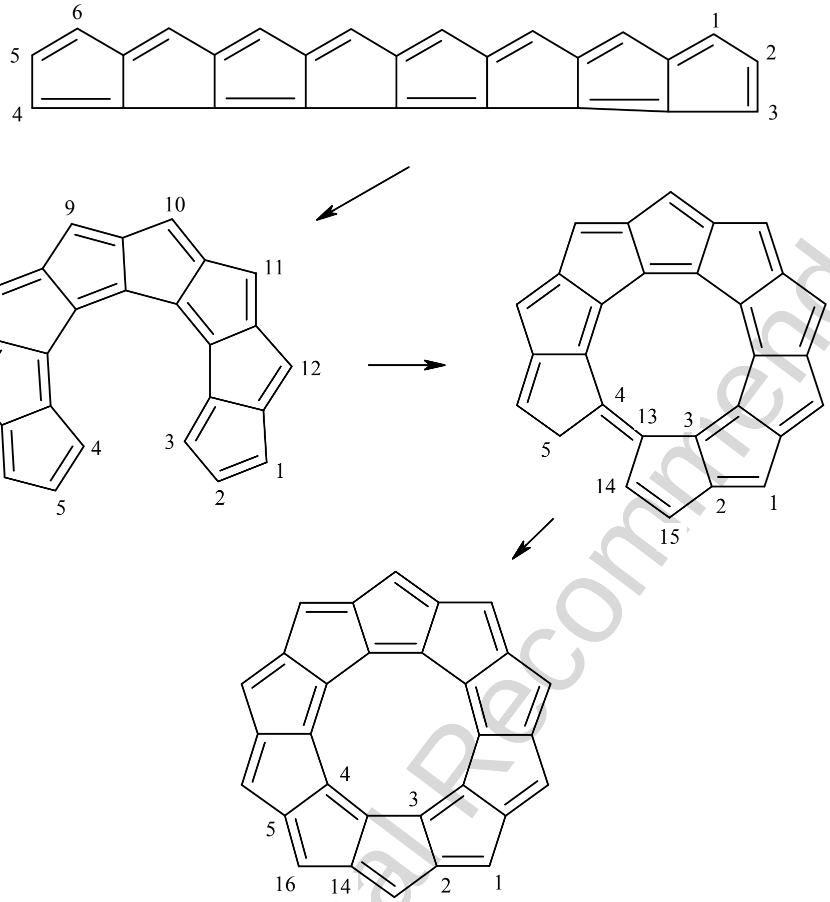
8,7-(azenoethanediylidene)cyclohepta[4,5]cycloocta[1,2-*b*]pyridine

incorrect

(the correct name has a composite bridge consisting of a trivalent bridge and a divalent bridge name whereas the composite bridge in the incorrect name consists of a trivalent bridge name and a tetravalent bridge name

(i) have the lowest locants at the location of bridges, first for independent bridges then dependent bridges.

Example:



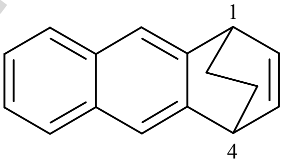
5,14-(metheno)-2,3,4-epiprop[2]ene[1,3]diyl[1]ylidenedicyclopenta[*f*,*f* ′]-pentaleno[1,2-*a*:6,5-*a* ′]dipentalene (PIN)

[not 5,14-(metheno)-2,4,3-epiprop[2]ene[1,3]diyl-[1]ylidenedicyclo-penta[*f*,*f* ′]pentaleno[1,2-*a*:6,5-*a* ′]dipentalene)

(the locants ‘2,3,4’ for the independent bridge are lower than ‘2,3,4’)

(j) have the maximum number of noncumulative double bonds in the parent ring system.

Example:



1,4-dihydro-1,4-ethanoanthracene (PIN)
(not 1,2,3,4-tetrahydro-1,4-ethenoanthracene)

P-25.4.4 Naming bridged fused ring systems

P-25.4.4.1 Order of citation of first order bridges

If there is more than one bridge, they are cited in alphabetical order, unless one is dependent on another. In this case, the dependent bridge is cited in front of all independent bridges.

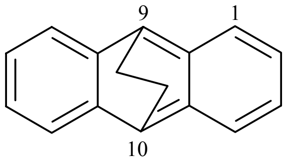
P-25.4.4.2 Attachment locants

The fused ring system is numbered in the usual way.

P-25.4.4.2.1 Symmetric bridges

The locants of the positions on the fused ring system to which the bridge(s) is (are) attached are cited in numerical order in front of the bridge name:

Example:

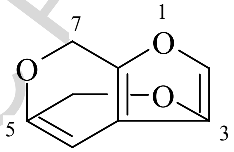


9,10-methanoanthracene (PIN)

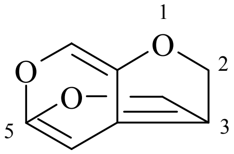
P-25.4.4.2.2 Asymmetric bridges

The locants of the positions on the fused ring system to which the bridge is attached are cited in the order implied by the name of the asymmetric bridge (locant order for the free valences of the bridge is given in section P-25.4.1). If there is a choice, locants are cited in numerical order. Indicated hydrogen atoms are cited at the front of the name.

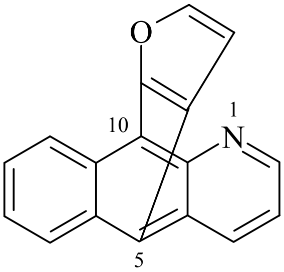
Examples:



7*H*-3,5-(epoxymethano)furo[2,3-*c*]pyran (PIN)



2*H*-5,3-(epoxymethano)furo[2,3-*c*]pyran (PIN)



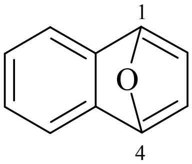
10,5-[2,3]furanobenzo[*g*]quinoline (PIN)

P-25.4.4.3 Choice of attachment locants

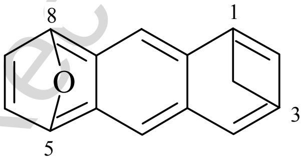
If there is a choice of attachment locants after the application of P-25.4.4.2, seniority is established in the following order:

(a) the lowest set of locants for all the bridge attachment points considered as a set.

Examples:



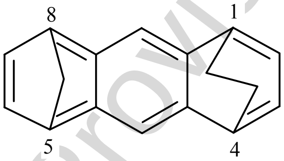
1,4-epoxynaphthalene (PIN)
(not 5,8-epoxynaphthalene)



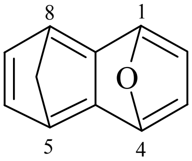
5,8-epoxy-1,3-methanoanthracene (PIN)
(not 1,4-epoxy-5,7-methanoanthracene)
(the set 1,3,5,8 is lower than 1,4,5,7)

(b) lowest locants in the order of citation for the bridges:

Examples:



1,4-ethano-5,8-methanoanthracene (PIN)

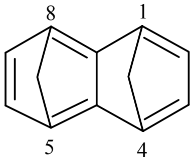


1,4-epoxy-5,8-methanonaphthalene (PIN)

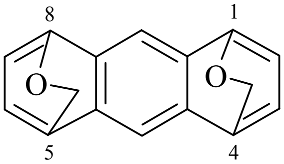
P-25.4.4.4 Identical bridges

Two or more identical bridges are indicated by the numerical prefixes ‘di’, ‘tri’, etc. with single bridges, or ‘bis’, ‘tris’, etc. with composite bridges or if ‘di’, ‘tri’, etc. would be ambiguous. The locant pairs of the bridges are separated by colons.

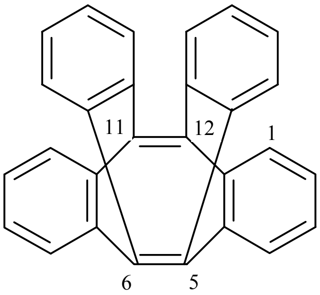
Examples:



1,4:5,8-dimethanonaphthalene (PIN)



1,4:8,5-bis(epoxymethano)anthracene (PIN)

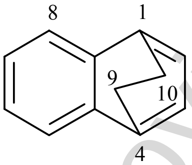


5,12:6,11-di[1,2]benzenodibenzo[*a*,*e*][8]annulene (PIN)

P-25.4.5 Numbering of bridge atoms

Bridge atoms are numbered continuing from the highest locant of the fused ring system. If there is more than one bridge atom (excluding hydrogen) the numbering starts at the end of the chain or ring atom connected to the bridgehead of the fused ring system having the highest locant. With composite bridges, each component is completely numbered before the next component. Fusion atoms in fused ring bridges are numbered in accordance with P-25.3.3.1.1.

Example:



1,4-ethanonaphthalene (PIN)

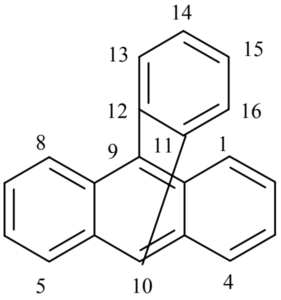
P-25.4.5.1 When there is a choice of locants, lowest locants are assigned according to the following criteria, in order, until a definitive decision is reached.

(a) low locants for heteroatoms;

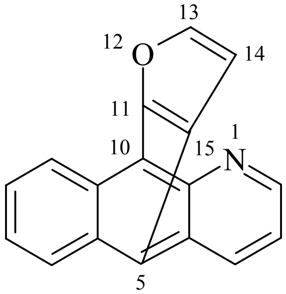
(b) low locants for bridgehead atoms within a bridge;

(c) number the remaining atoms (excluding hydrogen) consecutively.

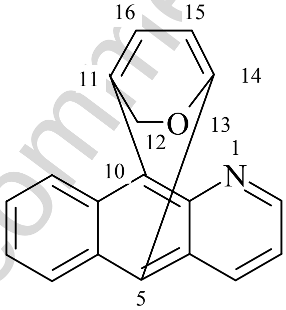
Examples:



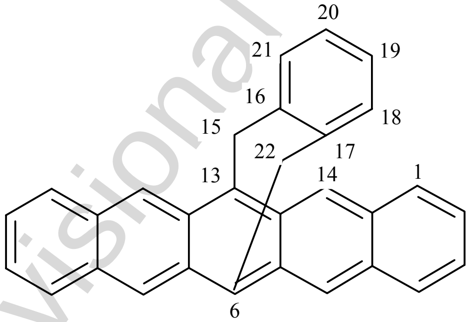
9,10-[1,2]benzenoanthracene (PIN)



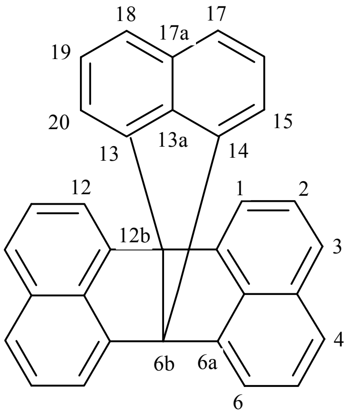
10,5-[2,3]furanobenzo[*g*]quinoline (PIN)



12*H*-2,10-[2,5]epipyranobenzo[*g*]quinoline (PIN)



6,13-(methano[1,2]benzenomethano)pentacene (PIN)

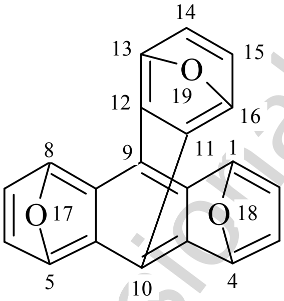


6b,12b-[1,8]naphthalenoacenaphthyleno[1,2-*a*]acenaphthylene (PIN)
(locants 13a and 17a are generated in conformity with P-25.3.3.1.1)

P-25.4.6 Order for numbering bridges

P-25.4.6.1 Independent bridges are numbered before dependent bridges.

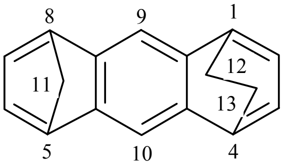
Example:



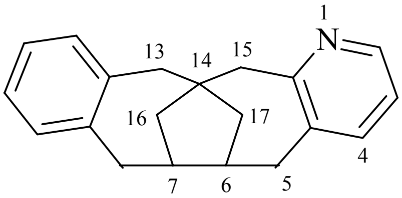
13,16-epoxy-1,4:5,8-diepoxy-9,10-[1,2]benzenoanthracene (PIN)
(dependent bridges are cited before independent bridges but are numbered after them)

P-25.4.6.2 If there is more than one bridge of the same type (dependent or independent), seniority is given to the bridge attached to the bridgehead with the higher locant at the first point of difference.

Examples:



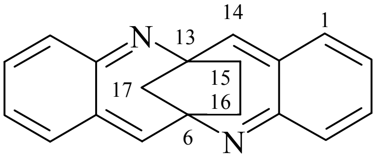
1,4-ethano-5,8-methanoanthracene (PIN)



6,14:7,14-dimethanobenzo[7,8]cycloundeca[1,2-b]pyridine (PIN)

P-25.4.6.3 If two bridges are attached to the same bridgehead atoms, they are numbered in accordance with their order of citation.

Example:

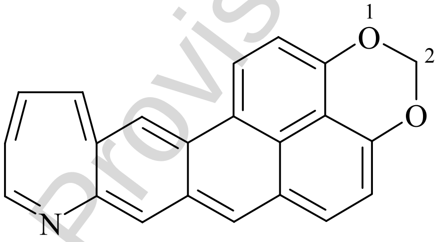


6,13-ethano-6,13-methanodibenzo[*b*,*g*][1,6]diazecine (PIN)

P-25.5 Limitations of fusion nomenclature

The fusion principles described in P-25.1 through P-25.3 apply only between pairs of components. It is not possible by these principles to name a system in which a third component is *ortho*- and *peri*-fused to two components that are themselves *ortho*- or *ortho*- and *peri*-fused together. It is important to recall that benzoheterocycles are considered as one component, thus permitting the construction of names that would not otherwise be possible.

Example:



2*H*-[1,3]benzodioxino[6′,5′,4′:10,5,6]anthra[2,3-*b*]azepine (PIN)

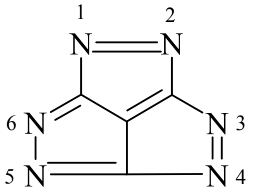
(a normal fusion name is not possible when the four components azepine, anthracene, 1,3-dioxine and benzene are treated individually; the use of a benzo name component is necessary; 1-benzazepine cannot be the parent ring because this would require breaking of the attached component having a retained name, anthra, which is not allowed, see P-25.3.5)

When a third component is *ortho*- and *peri*-fused to two components that are themselves *ortho*- or *ortho*- and *peri*-fused together, the following procedures are applied in order until a name can be formed.

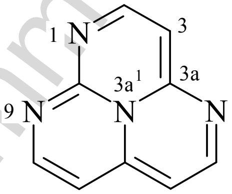
P-25.5.1 Skeletal replacement (‘a’) nomenclature

If the corresponding hydrocarbon fused ring system can be named by fusion principles or has a retained name, then heteroatoms are identified by skeletal replacement (‘a’) nomenclature using the appropriate ‘a’ prefixes (see P-22.2.3). The numbering of the fused hydrocarbon system is not altered by the ‘a’ prefixes.

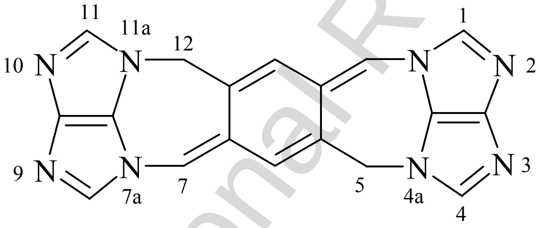
Examples:



1,2,3,4,5,6-hexaazacyclopenta[*c,d*]pentalene (PIN)



1,3a^{1},4,9-tetraazaphenalene (PIN)

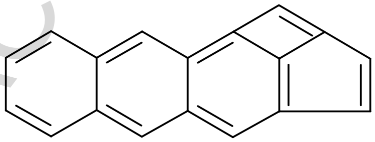


5*H*,12*H*-2,3,4a,7a,9,10,11a,14a-octaazadicyclopenta[*i,j*:*i′,j′*]benzo[1,2-*f*:4,5-*f′*]diazulene (PIN)

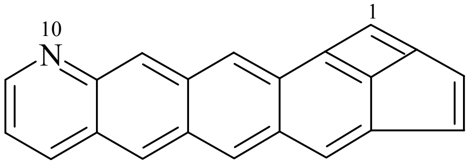
P-25.5.2 Selection of a less senior hydrocarbon parent component

A less preferred hydrocarbon parent component is selected that will permit a fusion name. Second and third choice parent components are chosen according to the seniority order for selecting the senior parent component (see P-25.3.2.4).

Examples:



cyclobuta[1,7]indeno[5,6-*b*]naphthalene (PIN)
(anthracene cannot be selected as senior parent component;
naphthalene, not indene, is next in seniority order for
selection as a parent component)



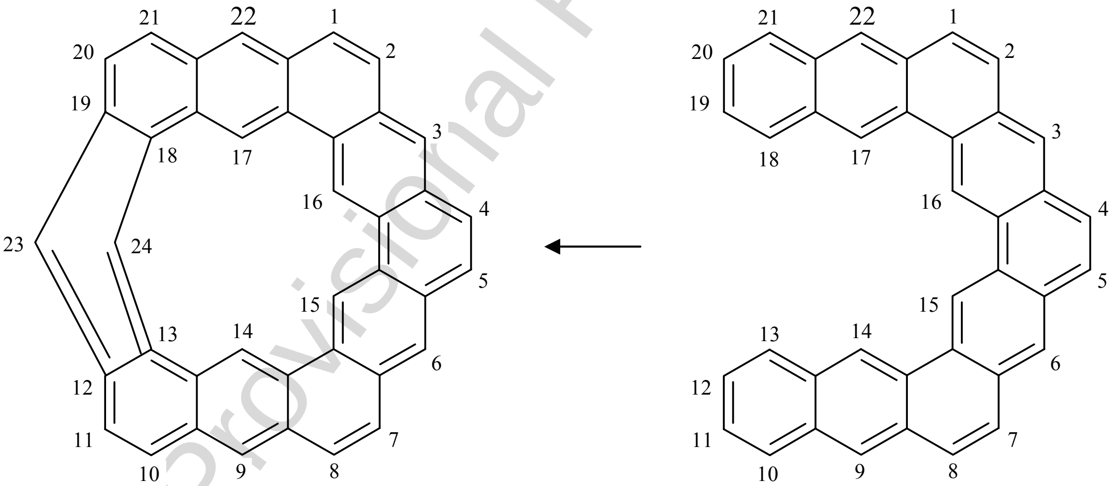
10-azacyclobuta[1,7]indeno[5,6-*b*]anthracene (PIN)

[neither quinoline nor pyridine can be used as the senior parent component because neither naphthalene nor anthracene, respectively, can be used as the senior attached component; therefore ‘a’ nomenclature must be used (see P.25.5.1) and since the preferred hydrocarbon tetracene cannot be used, the next senior component, anthracene, is chosen as the parent component]

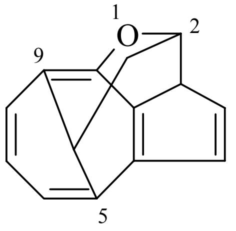
P-25.5.3 Use of bridging nomenclature

A bridged fused system (see Section P-25.4) is used to generate names not possible by using normal fusion nomenclature. A fused system is first envisaged; additional rings are created by using bridges.

Examples:



12,19:13,18-dimethenodinaphtho[2,3-*a*: 2′.3′-*o*]pentaphene (PIN)



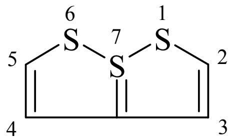
1-oxa-5,9,2-epiethane[1,1,2]triylcycloocta[1,2,3-*cd*]pentalene (PIN)

P-25.6 Fused ring systems with skeletal atoms with nonstandard bonding numbers

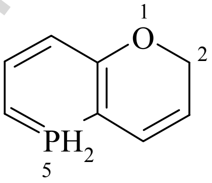
The λ-convention is used to describe atoms with nonstandard bonding numbers (ref. 12) in fused ring systems. The symbol λ^n is used, where '*n*' is the bonding number of the atoms; it is cited immediately after the locant denoting the atom having the nonstandard bonding number. The symbol *H*, denoting indicated hydrogen atom(s) with the appropriate locant(s), if present, is cited at the front of the complete name.

The λ symbol is used with all rings and ring systems described in this section: monocyclic and polycyclic with retained and fusion names, bi- and polyalicyclic as well as heterocycles formed by 'a' nomenclature, as described above in P-25.5.1. Atoms with nonstandard bonding numbers in fused ring systems are indicated only in the complete ring system, not in component rings. Names and numbering are unchanged, unless a choice must be made between two otherwise equivalent atoms; in which case, low locants are attributed to atoms with the higher bonding numbers, i.e., λ^6 before λ^4.

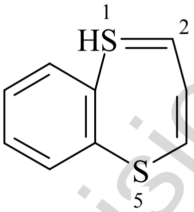
Examples:



7λ^4-[1,2]dithiolo[1,5-*b*][1,2]dithiole (PIN)



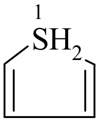
2*H*-5λ^5-phosphinino[3,2-*b*]pyran (PIN)



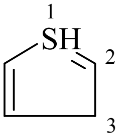
1λ^4,5-benzodithiepine (PIN)

After the maximum number of noncumulative double bonds has been assigned, any ring atom with a bonding order of three or higher connected to adjacent ring atoms by single bonds only, and carrying one or more hydrogen atoms, is designated by the indicated hydrogen symbol *H*. If there is a choice, such ring atoms are selected for low locants.

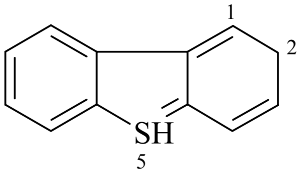
Example:



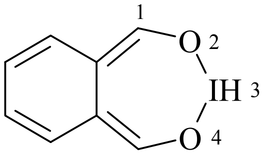
1*H*-1λ^4-thiophene (PIN)



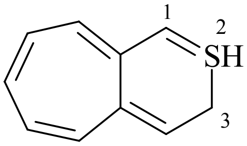
3*H*-1λ^4-thiophene (PIN)



$2H$-5λ^4-dibenzothiophene (PIN)



$3H$-3λ^3,2,4-benziodadioxepine (PIN)



$3H$-2λ^4-cyclohepta[*c*]thiopyran (PIN)

P-25.7 Double bonds, indicated hydrogen, and the δ-convention

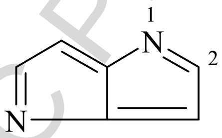
The treatment of double bonds is formalized in fusion nomenclature. A maximum of noncumulative double bonds must be present in fused and bridged fused systems. When hydrogen atoms are in excess at specific positions, they are denoted in names by indicated hydrogen atom(s). To the contrary, the presence of cumulated formal double bonds is also possible. This feature is expressed by the δ-convention (Delta-Convention) (see ref. 18). These two aspects of fused and bridged fused systems are described in this Section.

P-25.7.1 Indicated hydrogen

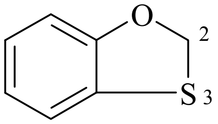
P-25.7.1.1 Maximum number of non-cumulative double bonds

The names of polycyclic fused ring systems are considered to correspond to the structure with the maximum number of noncumulative double bonds consistent with the appropriate bonding number of the skeletal atoms. To achieve this result, components are fused together and noncumulative double bonds are redistributed in the completed fused system. Hydrogen atoms not attached to atoms connected by double bonds are denoted as indicated hydrogen atom(s).

Examples:



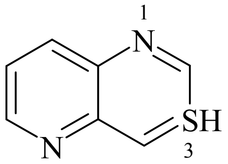
pyrrolo[3,2-*b*]pyrrole (PIN)



$2H$-1,3-benzoxathiole (PIN)

If atoms with nonstandard bonding numbers are present, they must be indicated using the λ-convention (and if necessary the δ-convention). The stated bonding number is used in assigning noncumulative double bonds.

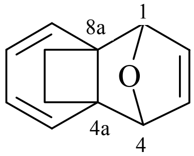
Example:



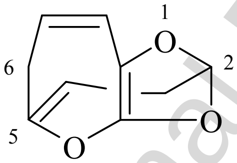
3λ^4-pyrido[3,2-*d*][1,3]thiazine (PIN)

In bridged fused systems, the distribution of noncumulative double bonds in the parent fused ring system is accomplished after allowance has been made for the bonds existing between the bridge(s) and the fused ring system. Rings that are part of a bridge are treated separately, after consideration of the free valences of the bridge.

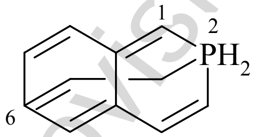
Examples:



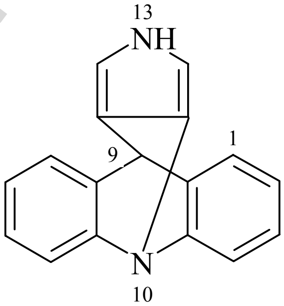
1,4-epoxy-4a,8a-ethanonaphthalene (PIN)



2*H*,6*H*-2,5-(ethanylylidene)[1,3]dioxolo[4,5-*b*]oxepine (PIN)



2*H*-2λ^5-2,6-(ethanylylidene)isophosphinoline (PIN)

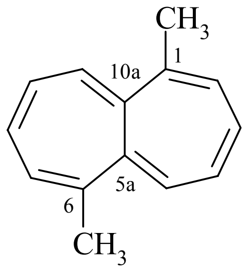


9*H*,13*H*-9,10-[3,4]epipyrroloacridine (PIN)

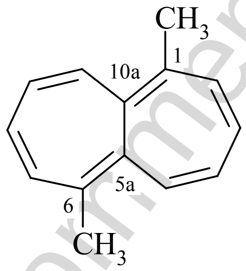
P-25.7.1.2 Localized double bonds

If it is necessary to identify isomers that differ only by virtue of the location of localized double bonds, this differentiation is indicated by the use of the Greek letter Δ. The locant cited corresponds to the lowest numbered atom of the localized double bond.

Examples:



1,6-dimethyl-Δ^{1}-heptalene (PIN)



1,6-dimethyl-$\Delta^{1(10a)}$-heptalene (PIN)

P-25.7.1.3 Citation of indicated hydrogen

When a name applies equally to two or more isomeric systems with the maximum number of non-cumulative double bonds and when the name can be made specific by indicating the position of one or more hydrogen atoms in the structure, this specifically is accomplished by adding to the name the italicized symbol *H* for each of these hydrogen atoms, preceded by the appropriate locant(s).

In general nomenclature, omission of indicated hydrogen atoms is permitted in some parent fused ring systems, when unsubstituted, for example indene rather than 1*H*-indene, but 1*H*-indene-3-carboxylic acid. Omission of indicated hydrogen is permitted in the following ring systems:

fluorene	9*H*
indene	1*H*
phenalene	1*H*
indazole	1*H*
indole	1*H*
isochromene (and chalcogen analogs)	1*H*
isoindole	2*H*
perimidine	1*H*
purine	7*H*
pyrrole	1*H*
xanthene	9*H*

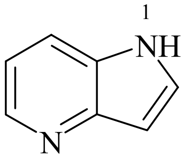
Omission of indicated hydrogen is also permitted in general nomenclature, if no ambiguity would result, for example 1,3-benzodioxole, rather than 2*H*-1,3-benzodioxole.

In IUPAC preferred names, however, all indicated hydrogen atoms must be cited when the names are constructed in accordance with the principles of fusion nomenclature.

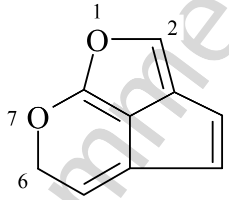
P-25.7.1.3.1 *ortho*- and *ortho*- and *peri*-fused ring systems

Indicated hydrogen is identified by the locant of the relevant position and cited at the front of the names of the whole ring system, including replacement terms, if any.

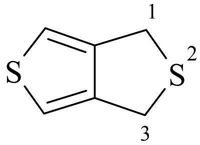
Examples:



1*H*-pyrrolo[3,2-*b*]pyridine (PIN)



6*H*-1,7-dioxacyclopenta[*cd*]indene (PIN)



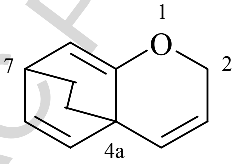
1*H*,3*H*-thieno[3,4-*c*]thiophene (PIN)

P-25.7.1.3.2 Bridged fused ring systems

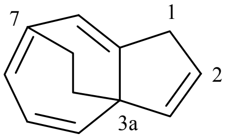
All indicated hydrogen atoms are indicated at the front of the complete name.

> This is a change from the previous rule (see Section A-34.4 in ref. 1), which recommended that indicated hydrogen atoms be separated and placed in front of the part (bridge or fused ring system) they qualify.

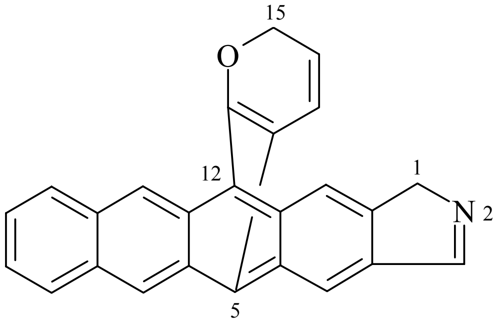
Examples:



2*H*,7*H*-4a,7-ethanochromene (PIN)



1*H*-3a,7-ethanoazulene (PIN)

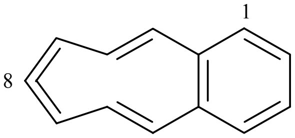


1*H*,15*H*-12,5-[2,3]epipyranoanthra[2,3-*f*]isoindole (PIN)

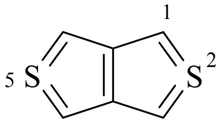
P-25.7.2 The δ-convention

The presence of contiguous formal double bonds at a skeletal atom in a cyclic parent hydride whose name normally implies the maximum number of noncumulative double bonds is described by the symbol δ^c, where '*c*' is the number of double bonds (see ref. 18). The δ^c symbol is cited immediately after an expressed locant for the skeletal atom in the name of the compound and follows the λ^n symbol, if present.

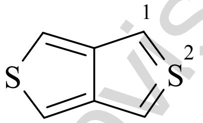
Examples:



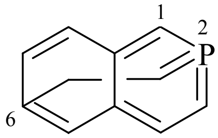
8δ^2-benzo[9]annulene (PIN)



2$\lambda^4\delta^2$,5$\lambda^4\delta^2$-thieno[3,4-*c*]thiophene (PIN)



2$\lambda^4\delta^2$-thieno[3,4-*c*]thiophene (PIN)



2$\lambda^5\delta^2$-6,2-(epiethanylylidene)isophosphinoline (PIN)

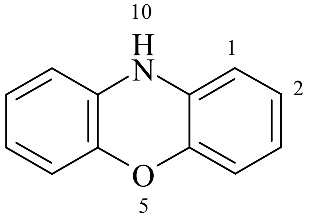
P-25.8 Parent compounds in decreasing order of seniority (partial lists)

In this Section rings and ring systems are listed in decreasing order of seniority for selection as a parent component. The first list contains heterocyclic parent components, the second hydrocarbon parent components.

P-25.8.1 Partial list of heterocyclic parent components in decreasing order of seniority

The following list contains parent heterocycles arranged in decreasing order of seniority for selection as the parent component for fusion names. Ring systems containing Hg as given in ref. 4 are not included in these recommendations.

The parent heterocycles are arranged by ring analysis, i.e., in decreasing order of number of rings, ring size, and in accordance with the priority given to heteroatoms, N, O, S, Se, Te, P, etc. and their number; for example phenoxazine (10*H*-isomer shown) is:



phenoxazine	$C_4NO-C_6-C_6$	
phenothiazine	$C_4NS-C_6-C_6$	
phenoselenazine	$C_4NSe-C_6-C_6$	
phenotellurine	$C_4NTe-C_6-C_6$	
phenophosphazinine	$C_4NP-C_6-C_6$	
phenarazinine	$C_4NAs-C_6-C_6$	
phenazine	$C_4N_2-C_6-C_6$	
phenanthroline	$C_5N-C_5N-C_6$	(in accordance with the positions of nitrogen atoms, in decreasing order of seniority: 1,7; 1,8; 1,9; 1,10; 2,7; 2,8, 2,9; 3,7; 3,8;4,7)
perimidine	$C_4N_2-C_6-C_6$	
acridine	$C_5N-C_6-C_6$	
phenanthridine	$C_5N-C_6-C_6$	
carbazole	$C_4N-C_6-C_6$	
pteridine	$C_4N_2-C_4N_2$	
cinnoline	$C_4N_2-C_6$	
quinazoline	$C_4N_2-C_6$	
quinoxaline	$C_4N_2-C_6$	
1,5-naphthyridine	C_5N-C_5N	
1,6-naphthyridine	C_5N-C_5N	
1,7-naphthyridine	C_5N-C_5N	
1,8-naphthyridine	C_5N-C_5N	
phthalazine	$C_4N_2-C_6$	
2,6,naphthyridine	C_5N-C_5N	
2,7-naphthyridine	C_5N-C_5N	
quinoline	C_5N-C_6	
isoquinoline	C_5N-C_6	
quinolizine	C_5N-C_5N	
purine	$C_3N_2-C_4N_2$	
indazole	$C_3N_2-C_6$	
indole	C_4N-C_6	
isoindole	C_4N-C_6	
indolizine	C_4N-C_5N	
pyrrolizine	C_4N-C_4N	

Seven-membered heterocyclic rings or larger with at least one nitrogen atom, e.g., azepine		
Six-membered heterocyclic rings with at least three heteroatoms including at least one nitrogen atom, e.g., 1,3,5-oxadiazine		
Six-membered heterocyclic rings with at least one nitrogen atom and a different heteroatom, e.g., 1,2-thiazine		
pyridazine	C_4N_2	
pyrimidine	C_4N_2	
pyrazine	C_4N_2	
pyridine	C_5N	
Five-membered heterocyclic rings with at least three heteroatoms , including at least one nitrogen atom, e.g., 1,2,5-oxadiazole (formerly called furazan)		
Five-membered heterocyclic rings with one nitrogen atom and a different heteroatom, e.g., 1,2-oxazole		
pyrazole	C_3N_2	
imidazole	C_3N_2	
pyrrole	C_4N	(the indicated hydrogen may be omitted)
Four- or three-membered heterocyclic rings with at least one nitrogen atom, e.g., azirene		
Heterocyclic ring with halogen atom, but no nitrogen atom, e.g., $1\lambda^5$-1,2-iodoxole		
phenoxathiine	$C_4OS\text{-}C_6\text{-}C_6$	
phenoxaselenine	$C_4OSe\text{-}C_6\text{-}C_6$	
phenoxatellurine	$C_4OTe\text{-}C_6\text{-}C_6$	
phenoxaphosphinine	$C_4OP\text{-}C_6\text{-}C_6$	
phenoxarsinine	$C_4OAs\text{-}C_6\text{-}C_6$	
phenoxastibinine	$C_4OSb\text{-}C_6\text{-}C_6$	
oxanthrene	$C_4O_2\text{-}C_6\text{-}C_6$	(formerly called dibenzo[*b,e*][1,4]dioxine
xanthene	$C_5O\text{-}C_6\text{-}C_6$	
chromene	$C_5O\text{-}C_6$	
isochromene	$C_5O\text{-}C_6$	
Seven-membered heterocyclic ring or larger with at least one oxygen atom (no nitrogen atom), e.g., oxepine		
Six-membered heterocyclic ring with two or more heteroatoms, at least one of which is oxygen, e.g., 1,4-dioxine		
pyran	C_5O	
Five-membered heterocyclic ring with two or more heteroatoms, one of which is oxygen (no nitrogen atom), e.g., 1,3-dioxole		
furan	C_4O	
Four- or three-membered heterocyclic ring with at least one oxygen atom (no nitrogen atom), e.g., oxirene		
phenothiarsinine	$C_4SAs\text{-}C_6\text{-}C_6$	
thianthrene	$C_4S_2\text{-}C_6\text{-}C_6$	
thioxanthene	$C_5S\text{-}C_6\text{-}C_6$	
thiochromene	$C_5S\text{-}C_6$	
isothiochromene	$C_5S\text{-}C_6$	

Heteromonocyclic ring with at least one sulfur atom (no N nor O atoms). For example:	
thiopyran	C_5S
thiophene	C_4S
selanthrene	C_4Se_2-C_6-C_6
selenoxanthene	C_5Se-C_6-C_6
selenochromene	C_5Se-C_6
isoselenochromene	C_5Se-C_6
Heteromonocyclic ring with at least one selenium atom (no N, O nor S atoms), for example:	
selenopyran	C_5Se
selenophene	C_4Se
telluranthrene	C_4Te_2-C_6-C_6
telluroxanthene	C_5Te-C_6-C_6
tellurochormene	C_5Te-C_6
isotellurochromene	C_5Te-C_6
Heteromonocyclic ring with at least one tellurium atom (no N, O, S, nor Se atoms), for example	
telluropyran	C_5Te
tellurophene	C_4Te
phosphanthrene	C_4P_2-C_6-C_6
acridophosphine	C_5P-C_6-C_6
phosphanthridine	C_5P-C_6-C_6
phosphinoline	C_5P-C_6
isophosphinoline	C_5P-C_6
phosphinolizine	C_5P-C_5P
phosphindole	C_4P-C_6
isophosphindole	C_4P-C_6
phosphindolizine	C_4P-C_4P
Heteromonocyclic ring with at least one phosphorus atom (no N, O, S, Se, nor Te atoms)	
arsanthrene	C_4As_2-C_6-C_6
acridarsine	C_5As-C_6-C_6
arsanthridine	C_5As-C_6-C_6
arsinoline	C_5As-C_6
isoarsinoline	C_5As-C_6
arsinolizine	C_5As-C_5As
arsindole	C_4As-C_6
isoarsindole	C_4As-C_6
arsindolizine	C_4As-C_4As
Heteromonocyclic ring with at least one arsenic atom, and Sb, Bi, Si, Ge, Sn, Pb, B, Al, Ga, In, and Tl as possible atoms.	
silanthrene	C_4Si-C_6-C_6
boranthrene	C_4B-C_6-C_6

P-25.8.2 Partial list of hydrocarbon parent components in decreasing order of seniority

Parent components are arranged (1) in decreasing order of number of rings; (2) in decreasing order of ring size; (3) in decreasing order of senior orientation; (4) for aceanthrylene and acephenanthrylene, in increasing order of fusion atom locants.

ovalene	$C_6C_6C_6C_6C_6C_6C_6C_6C_6C_6$
octaphenylene	$C_{16}C_6C_6C_6C_6C_6C_6C_6C_6$
tetranaphthylene	$C_8C_6C_6C_6C_6C_6C_6C_6C_6$
nonacene	$C_6C_6C_6C_6C_6C_6C_6C_6C_6$
nonaphene	$C_6C_6C_6C_6C_6C_6C_6C_6C_6$
nonahelicene	$C_6C_6C_6C_6C_6C_6C_6C_6C_6$
octacene	$C_6C_6C_6C_6C_6C_6C_6C_6$
ocataphene	$C_6C_6C_6C_6C_6C_6C_6C_6$
pyranthrene	$C_6C_6C_6C_6C_6C_6C_6C_6$
octahelicene	$C_6C_6C_6C_6C_6C_6C_6C_6$
hexaphenylene	$C_{12}C_6C_6C_6C_6C_6C_6$
heptacene	$C_6C_6C_6C_6C_6C_6C_6$
heptaphene	$C_6C_6C_6C_6C_6C_6C_6$
trinaphthylene	$C_6C_6C_6C_6C_6C_6C_6$
coronene	$C_6C_6C_6C_6C_6C_6C_6$
heptahelicene	$C_6C_6C_6C_6C_6C_6C_6$
rubicene	$C_6C_6C_6C_6C_6C_5C_5$
hexacene	$C_6C_6C_6C_6C_6C_6$
hexaphene	$C_6C_6C_6C_6C_6C_6$
hexahelicene	$C_6C_6C_6C_6C_6C_6$
tetraphenylene	$C_8C_6C_6C_6C_6$
pentacene	$C_6C_6C_6C_6C_6$
pentaphene	$C_6C_6C_6C_6C_6$
perylene	$C_6C_6C_6C_6C_6$
picene	$C_6C_6C_6C_6C_6$
pleiadene	$C_7C_6C_6C_6$
tetracene	$C_6C_6C_6C_6$
tetraphene	$C_6C_6C_6C_6$
chrysene	$C_6C_6C_6C_6$
pyrene	$C_6C_6C_6C_6$
triphenylene	$C_6C_6C_6C_6$
aceanthrylene	$C_6C_6C_6C_5$
acephenanthrylene	$C_6C_6C_6C_5$
fluoranthene	$C_6C_6C_5C_5$
anthracene	$C_6C_6C_6$
phenanthrene	$C_6C_6C_6$
phenalene	$C_6C_6C_6$
fluorene	$C_6C_6C_5$
acenaphthylene	$C_6C_6C_5$
biphenylene	$C_6C_6C_4$

s-indacene	$C_6C_5C_5$
as-indacene	$C_6C_5C_5$
heptalene	C_7C_7
azulene	C_7C_5
naphthalene	C_6C_6
indene	C_6C_5
pentalene	C_5C_5
Monocyclic hydrocarbons	(in decreasing order of size)

P-26 Phane nomenclature

P-26.0 Introduction

Phane Nomenclature is specific to cyclic or acyclic compounds composed of rings or ring systems directly linked to each other or linked by atoms or chains.

Cyclophanes are recognized as a class of compounds (ref. 17). The term originally applied to compounds having two 1,4-phenylene groups held face to face by $–[CH_2]_n–$ bridges. It now designates compounds having:

(a) saturated and/or mancude rings or ring systems, or assemblies of saturated and/or mancude rings or ring systems and;

(b) atoms and/or saturated or unsaturated chains as alternate components of a large ring.

Phane nomenclature is used to name cyclophanes and has been extended to linear compounds containing a minimum of four rings or ring systems. This section is based on the publication ‘Phane nomenclature, Part I. Phane parent names (ref. 5) and contains no modifications to the recommendations therein.

P-26.1 Concepts and terminology

Definitions of terms that will be encountered in the construction of phane names are given below. These terms refer to types of operations, to the components of phane names, and to details of structures involved in the operations.

P-26.1.1 Simplification and amplification

The fundamental operations of phane nomenclature are illustrated in Fig. 1. The operation proceeding from left to right is called simplification; the reverse operation is called amplification, or phane replacement.

The simplification operation illustrates the initial step in the process of constructing a phane name, i.e., nomenclaturally significant segments of a complex cyclic structure are replaced by single atom symbols, called superatoms, thus producing a simplified skeleton that can more easily be named. The phane parent hydride name is then formed from the name of the simplified skeleton and of those of the cyclic components (called amplificants) that were simplified to superatoms. In contrast to other bonds associated with the amplificant, the bonds marked by arrows in Fig. 1 do not disappear in the simplification or amplification operations.

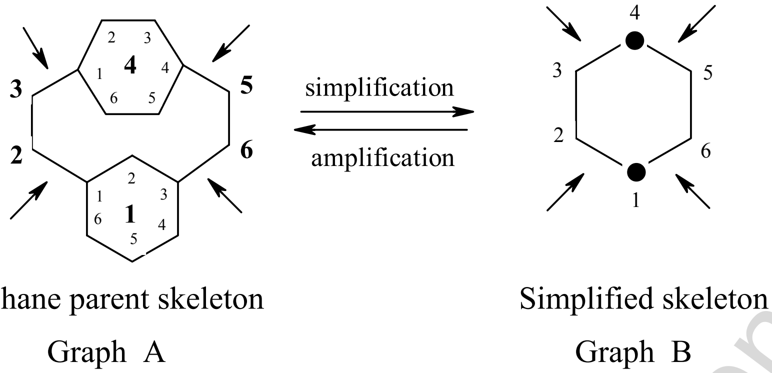


Fig. 1. Phane nomenclature conversion diagram

P-26.1.2 Simplified skeleton of the phane parent hydride, simplified phane parent graph, simplified skeletal name, and skeletal locants.

Graph B in Fig. 1 at which simplication ends and amplification starts is called the simplified skeleton of the phane parent hydride, or simply the simplified skeleton, and is represented by a simplified phane parent graph. Its name is the simplified skeletal name. A simplified skeletal name implies a specific skeletal numbering; its locants are the skeletal locants, which become the primary locants for the phane parent hydride. In Fig. 1, the skeletal locants are denoted by large numbers; they are the same in the simplified skeleton and in the phane parent skeleton.

P-26.1.3 Superatom and superatom locants

The 'atoms' of the simplified skeleton shown by the symbol ● in positions '1' and '4' in Graph B in Fig. 1 that appear on simplification and disappear in amplification are called superatoms. Their locants are called superatom locants.

P-26.1.4 Amplificant, amplification prefix, and amplificant locants.

A multiatomic unit (a ring or a ring system) of structure replacing a superatom in the amplification operation is called an amplificant; the six-membered rings in Graph A are amplificants. They are expressed in a phane parent name by amplification prefixes. Each such prefix implies a specific numbering of the amplificant; the respective locants are called amplificant locants and are shown as the smaller numbers in Graph A.

P-26.1.5 Attachment atoms and attachment locants.

The atoms of an amplificant to which the bonds marked by arrows in Fig. 1 are attached are called attachment atoms and their locants are attachment locants. In Graph A in Fig. 1, amplificant locants '1' and '4' are the attachment locants of the upper ring and amplificant locants '1' and '3' are the attachment locants of the lower ring.

P-26.1.6 Phane parent skeleton, phane parent name, and phane parent hydrides

The skeletal graph at the start of the simplification operation or resulting from an amplification operation is called a phane parent skeleton. Correspondingly, the combination of the simplified skeletal name, amplification prefixes, and the appropriate superatom and attachment locants, is called a phane parent name. The term parent implies that it can be combined with names for other components derived from the operations of systematic nomenclature of organic chemistry, such as substituent prefixes, hydrogenation prefixes and endings, and characteristic group suffixes. In the absence of such other components, the compound is a phane parent hydride, which means that the name implies the order (valence) of all bonds of the skeletal parent and thus the number of hydrogen atoms attached to each of the skeletal atoms.

P-26.2 Components of phane parent names

P-26.2.1 Simplified skeletal names

A simplified skeletal name consists of the term ‘phane’ preceded by a prefix denoting the structure of the simplified skeleton; this name is a parent for amplification but for no other operation. The simplification operation must be done in such a way that the amplificants can be expressed by amplification prefixes (see P-26.2.2).

A bond order of one is assumed for all bonds expressed by a simplified skeletal name. Atoms not identified by superatoms represent, by convention, carbon atoms with a bonding number (valence) of four in accordance with the principles of nomenclature of organic compounds.

Superatoms of a simplified skeletal name are assigned the lowest locants or the lowest set of locants, consistent with the numbering of the skeletal class to which it belongs. The lowest set of locants is the one that has the locant with the lowest numerical value at the first point of difference, when the sets are compared term by term in order of increasing value (see P-14.3.4).

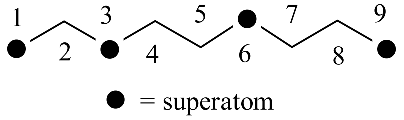
Four types of simplified skeletal structures are described below.

Names of simplified skeletons consists of, in order, of a prefix (‘cyclo’, ‘bicyclo’, ‘spiro’, etc.) indicating the type of structure, a numerical term ‘di’, ‘tri’, ‘tetra’, etc. indicating the number of nodes (including those designating superatoms), and the term phane. No prefix is used to name linear phanes.

The nodes are numbered in accordance with the recommended numbering for each type of structure, as indicated in Chapter 2. Superatoms are given the lowest possible locants.

P-26.2.1.1 Unbranched acyclic skeletal structure

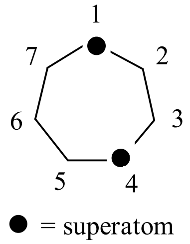
Example:



nonaphane
(see first example, P-26.4.1.2 and first example, P-26.5.1)

P-26.2.1.2 Monocyclic skeletal structure

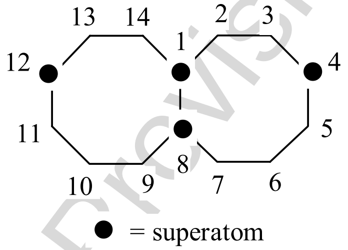
Example:



cycloheptaphane
(see first example, P-26.4.1.4; second example, P-26.4.2.2; and first example, P-26.4.3.3)

P-26.2.1.3 Polyalicyclic (von Baeyer) skeletal structure

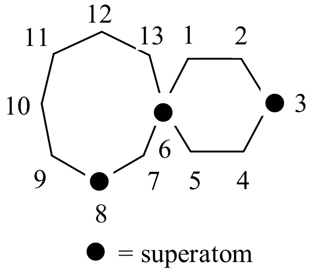
Example:



bicyclo[6.6.0]tetradecaphane
(see third example, P-26.4.2.2)

P-26.2.1.4 Spiro skeletal structure

Example:



spiro[5.7]tridecaphane
(see second example, P-26.4.2.4)

P-26.2.2 Amplification prefixes

P-26.2.2.1 Naming amplification prefixes

Names of amplificant prefixes are those of allowed rings or ring systems (see P-26.2.2.2.1) modified by changing the final letter ‘e’ to ‘a’, or adding the letter ‘a’ when no final letter ‘e’ is present.

Examples:

pyrrole(PIN)	pyrrola (PIN)
furan (PIN)	furana (PIN)
naphthalene (PIN)	naphthalena (PIN)
anthracene (PIN)	anthracena (PIN)

P-26.2.2.2 Parent hydride names for deriving amplification prefixes

P-26.2.2.2.1 Allowed parent hydrides

An amplification prefix can be derived from mancude monocycles and polycycles (having the maximum number of noncumulative double bonds), bridged fused ring systems, saturated monocycles, saturated bicycloalkanes and polycycloalkanes (von Baeyer hydrocarbons), and spiro alkanes. In addition stereoparents are allowed, such as ‘gonane’ or ‘morphinane’ (see Chapter 10). Numbering of the parent is retained.

P-26-2.2.2.2 Disallowed names of parent hydrides

(a) the following parent hydride names are not allowed:

(1) spirobi names such as ‘1,1′-spirobi[indene] (PIN);

(2) spiro ring systems with at least one fused ring system or polycycloalkane, such as ‘spiro[1,3-dioxolane-2,1′-indene] (PIN) or spiro[bicyclo[2.2.2]octane-2,1′-cyclohexane] (PIN)

(3) ring assembly names, such as ‘1,1′-biphenyl’ (PIN).

(b) modified parent hydride names; the corresponding modifications are made once the phane parent hydride has been fully constructed:

(1) by ‘hydro’ prefixes, such as ‘9,10-dihydroanthracene’ (PIN);

(2) by ‘-ene’ or ‘-yne’ endings, such as ‘cyclohexene’ (PIN);

(3) by ‘a’ replacement terms, such as ‘1-azabicyclo[3.2.1]octane’ (PIN);

(4) by suffixes, such as ‘cyclohexanecarboxylic acid’ (PIN) and ‘cyclohexanone’(PIN);

(5) by substitutive prefixes, such as ‘ethylbenzene’ (PIN).

(c) functional parent hydrides having retained names, such as ‘benzoic acid’ (PIN), ‘aniline’ (PIN).

(d) names of cyclic compounds formed by functional class nomenclature, such as ‘benzyl chloride’.

(e) partially hydrogenated parent hydride names having retained names, such as ‘indane’, ‘chromane’.

P-26.2.2.3 Order of citation of amplification prefixes

Amplification prefixes are cited in a name in decreasing order of their ring seniority (see P-44.2).

P-26.2.3 Multiple identical amplificants

Amplificants occurring more than once in a parent phane skeleton are expressed by use of an appropriate multiplicative term, either ‘di’, ‘tri’, etc. or ‘bis’, ‘tris’, etc. It is not necessary that the identical amplification prefixes have also identical locants.

P-26.2.3.1 The multiplying prefixes ‘di’,’tri’, ‘tetra’, etc. are used in front of simple amplification prefixes, i.e., dibenzena, tripyridina.

P-16.2.4.2 The multiplying prefixes ‘bis’, ‘tris’, ‘tetrakis’, etc. are used before an amplification prefix when it begins with a multiplying prefix as in ‘bicyclo[2.2.1]heptane’ (PIN), ‘1,3-dioxole’ (PIN); or it begins with a name component that could be preceded by a multiplying prefix indicating a multiple occurrence of that name component, as in ‘1,4-oxazine’ (PIN), ‘2-benzoxepine’ (PIN), or ‘1,4-methanonaphthalene’ (PIN).

P-26.3 Superatom locants and amplificant attachment locants

After the simplified skeletal name and the amplification prefix names have been determined, the phane parent hydride name is completed by adding the locants for the superatoms and the attachment locants. These locants are cited before an amplification prefix; the superatom locant is cited first followed by the attachment locants enclosed in parentheses.

P-26.3.1 Superatom locants

Superatom locants are assigned the lowest locants of the simplified skeleton consistent with the numbering of the class to which it belongs. An amplification prefix preceded by a multiplicative term indicating the presence of like amplificants requires the appropriate number of superatom locants, which are cited in ascending numerical order.

When like amplificants also have identical attachment locants, their attachment locants are arranged in ascending numerical order of the first cited superatom locant.

P-26.3.2 Attachment locants

The locants in parentheses in a phane parent hydride name are the attachment locants of the amplificant whose position in the phane parent skeleton is specified by the preceding superatom locant. The specific order of the attachment locants in the set describes precisely how their respective amplificant is attached to the rest of the phane parent skeleton. Amplificants retain the locants of the cyclic parent hydride from which they are derived.

P-26.3.2.1 Identical attachment locant sets for multiple identical amplificants are cited only once in a name; they follow the set of superatom locants corresponding to the identical amplificants.

Example:

1,4(1,4)-dibenzenacycloheptaphane (PIN)
[not 1(1,4),4(1,4)-dibenzenacycloheptaphane;
see second example, P-26.4.1.4]

P-26.3.2.2 The locants in an attachment locant set are arranged so that of any two locants the one cited first is adjacent to the lower locant of the phane parent skeleton.

Example:

1(1,3),4(1,4)-dibenzenacycloheptaphane (PIN)
[not 1(1,3)-benzena-4(1,4)-benzenacycloheptaphane;
see second example, P-26.4.2.2]

P-26.4 Numbering of phane parent hydrides

The following rules are used for numbering phane parent hydrides. These rules are hierarchical, i.e., each particular rule is applied only to alternatives not eliminated by preceding rules.

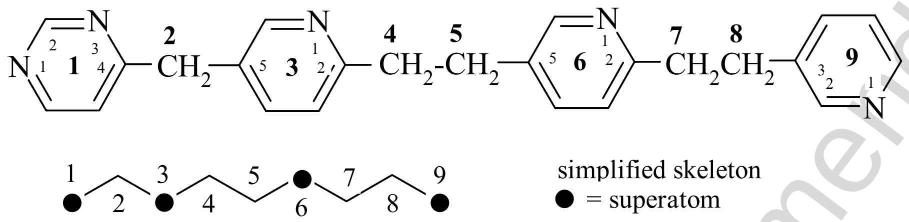
P-26.4.1 Numbering of phane parent skeletons and amplificants

P-26.4.1.1 The numbering of a phane parent skeleton is first determined by the rules governing the appropriate skeletal class to which it belongs. When because of skeletal symmetry, these rules leave alternatives, the numbering that gives the lowest set of locants for the superatoms is selected. The lowest set of locants is the one that has the lowest numerical value at the first point of difference, when the sets are compared term by term in increasing numerical value, as defined in the general rule P-14.3.4.

P-26.4.1.2 Numbering of an amplificant is determined primarily by the numbering rules that apply to the parent name from which the amplification prefix is derived. When there is a choice, the general rule of lowest locants is used, as described in the preceding rule.

These two rules, P-26.4.1.1 and P-26.4.1.2, are exemplified by the following examples.

Examples:



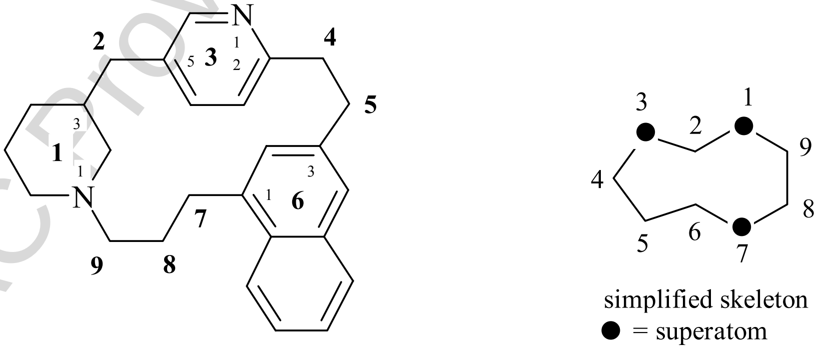
1(4)-pyrimidina-3,6(5,2),9(3)-tripyridinanonaphane (PIN)

[not 9(4)-pyrimidina-1(3),4,7(2,5)-tripyridinanonaphane]
[see P-26.2.1.1 and P-26.4.1.1; the superatom locant set of the correct name, '1,3,6,9', is lower than '1,4,7,9 ')]

[not 1(4)-pyrimidina-3,6(2,5),9(3)-tripyridinanonaphane]
[see P-26.3.2.2; the first locant of the attachment locant set '(2,5)' is not the locant adjacent to the lower locant of the simplified skeleton]

[not 1(4)-pyrimidina-3(5,2),6(5,2),9(3)-tripyridinanonaphane]
[see P-26.3.2.1; the identical attachment locant sets '(5,2)' must be contracted to '3,6(5,2)']

[not 1(4)-pyrimidina-3,6(3,6),9(3)-tripyridinanonaphane]
[see P-26.4.1.2; the attachment locant set '(5,2)' of the pyridine amplificant in the correct name, written in the ascending numerical order '(2,5)' for comparison, is lower than the set '(3,6)']



3(5,2)-pyridina-1(3,1)-piperidina-6(3,1)-naphthalenacyclononaphane (PIN)

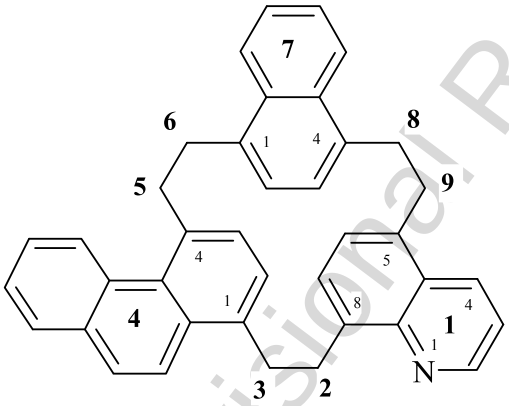
[not 1(5,2)-pyridina-3(3,1)-piperidina-7(3,1)-naphthalenacyclononaphane]
[not 7(5,2)-pyridina-5(1,3)-piperidina-1(3,1)-naphthalenacyclononaphane]

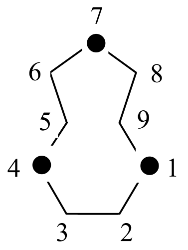
[see P-26.4.2.1; the superatom locant set of the correct name ‘1,3,6’ is lower than the locant set ‘1,5,7’ in either of the above names]

[not 3(2,5)-pyridina-1(1,3)-piperidina-6(1,3)-naphthalenacyclononaphane]
[see P-26.3.2.2; the first locant of each the attachment locant sets ‘(2,5)’, ‘(1,3)’ and ‘(1,3)’ for the pyridine, piperidine, and naphthalene amplificants, respectively, is not the locant adjacent to the lower locant of the parent phane skeleton]

P-26.4.1.3 Amplification of symmetrical simplified phane skeletons with at least two superatoms representing different amplificants results in the loss of symmetry and creates numbering alternatives. In such cases, the lower available superatom locant is assigned to an amplificant that appears earlier in the seniority of rings and ring systems (see P-44.2). The application of this procedure may require a sequence of steps. First, the lowest available superatom locant(s) is (are) assigned to the amplificants appearing first in the seniority order. Then, the same procedure is applied successively to assign remaining superatom locants to the rest of the amplificants.

Example:





simplified skeleton
● = superatom

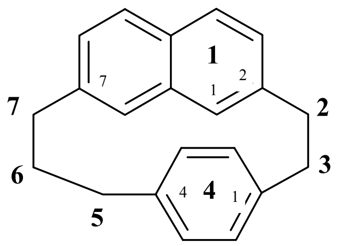
1(8,5)-quinolina-4(1,4)-phenanthrena-7(1,4)-naphthalenacyclononaphane (PIN)

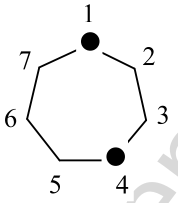
[not 1(8,5)-quinolina-4(1,4)-naphthalena-7(4,1)-phenanthrenacyclononaphane]
[the senior amplificant is quinoline (see P-44.2) and must receive the lowest superatom locant ‘1’; the phenanthrene amplificant is second in seniority (see P-44.2) and therefore must be given the second lowest superatom locant, ‘4’]

[not 1(8,5)-quinolina-4(4,1)-phenanthrena-7(1,4)-naphthalenecyclononaphane]
[see P-26.3.2.2; the attachment locants of phenanthrene amplificant ,‘(4,1)’ are not correctly cited; the first locant of the attachment locant set is not the locant adjacent to the lower locant of the phane parent skeleton, ‘3’]

P-26.4.1.4 When, because of symmetry, these rules leave a choice, an amplificant is numbered in such a way that the lower attachment locant is adjacent to the lower locant of the phane parent skeleton.

Examples:



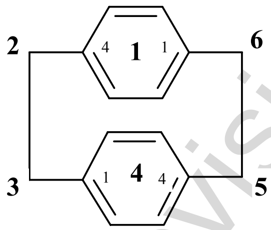


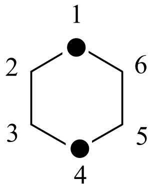
simplified skeleton
● = superatom

1(2,7)-naphthalena-4(1,4)-benzenacycloheptaphane (PIN)
[see P-26.4.1.2 and P-26 4.1.1; the lowest locant set for the superatoms in the phane parent skeleton is ‘1,4’; the senior amplificant, naphthalene (see P-44.2), must be assigned to the superatom locant ‘1’]

[not 1(2,7)-naphthalena-4(4,1)-benzenacycloheptaphane]
[not 1(7,2)-naphthalena-4(4,1)-benzenacycloheptaphane]

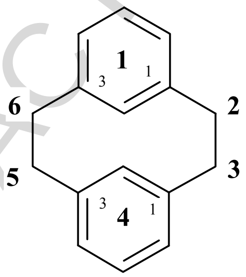
[the correct citation for the attachment locant sets, ‘(1,4)’ for benzene and ‘(2,7)’ for naphthalene, places the lower attachment locant adjacent to the lower locant of the phane skeleton]

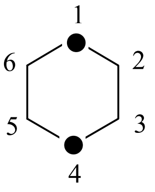




simplified skeleton
● = superatom

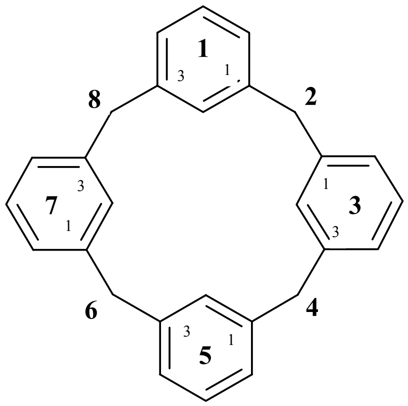
1,4(1,4)-dibenzenacyclohexaphane (PIN)

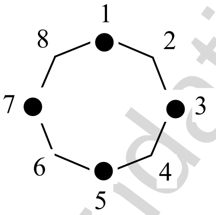




simplified skeleton
● = superatom

1,4(1,3)-dibenzenacyclohexaphane (PIN)





simplified skeleton
● = superatom

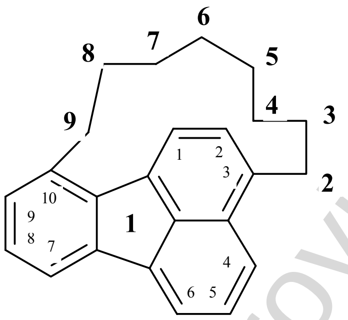
1,3,5,7(1,3)-tetrabenzenacyclooctaphane (PIN)

P-26.4.2 Numbering of simplified phane skeletons with respect to amplificant numbering

Numbering alternatives are found in symmetrical simplified skeletons when amplification by a single unsymmetrical amplificant or by identical amplificants having different attachment locants removes the symmetry. Choice among such alternatives is made according to the following rules.

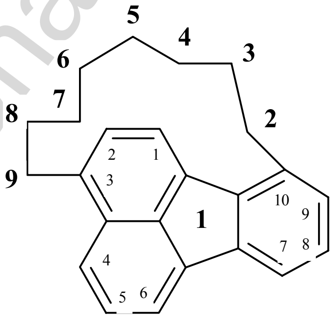
P-26.4.2.1 When a single amplificant is unsymmetrical, the lower locant of the phane parent skeleton must be adjacent to the lower attachment locant of the amplificant.

Example:

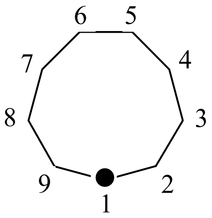


(a)

not



(b)



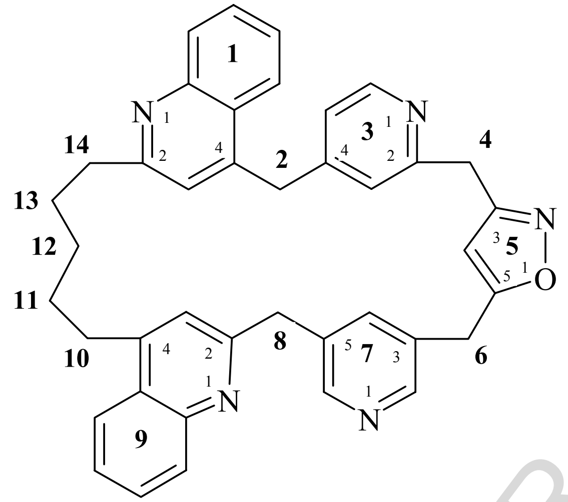
simplified skeleton
● = superatom

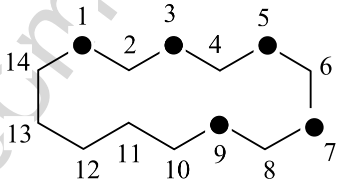
1(3,10)-fluoranthenacyclononaphane **(a)** (PIN)

[not 1(10,3)-fluoranthenacyclononaphane **(b)**]
(the lower amplificant locant ‘3’must be adjacent to the lower skeletal locant ‘2’)

P-26.4.2.2 When two amplificants can be given the lower of two superatom locants, the lower locant is assigned to the superatom representing the amplificant with the lower set of attachment locants. When necessary, this procedure is applied to other amplificants in accordance with their order of seniority until two or more identical amplificants have different attachment locants (see last example).

Examples:

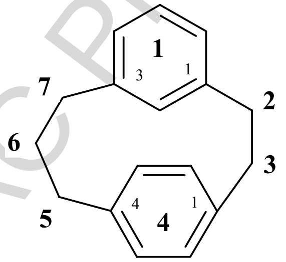


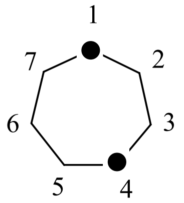


simplified skeleton
● = superatom

1(4,2),9(2,4)-diquinolina-3(4,2),7(3,5)-dipyridina-5(3,5)-[1,2]oxazolacyclotetradecaphane (PIN)

[not 1,9(2,4)-diquinolina-3(5,3),7(2,4)-dipyridina-5(3,5)-[1,2]oxazolacyclotetradecaphane] [the attachment locant set for the senior quinoline amplificants (see P-26.2.2.3), ‘4,2’ and ‘2,4’, respectively, when compared in ascending numerical order are the same, but when the attachment locant sets for the pyridine amplificants, ‘(4,2)’ and ‘(5,3)’, respectively, are compared in ascending numerical order, ‘(2,4)’ and ‘(3,5)’, respectively, the former is lower and therefore the attachment locant set ‘(4,2)’ is associated with the superatom with the lower locant ‘3’]



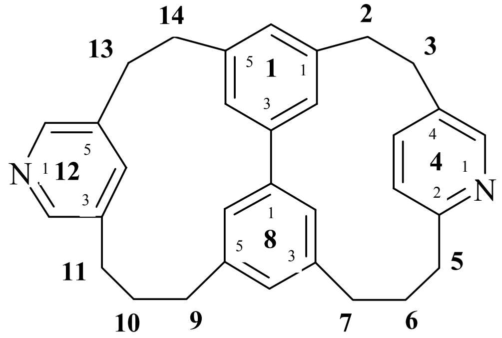


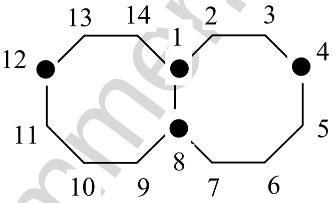
simplified skeleton
● = superatom

1(1,3),4(1,4)-dibenzenacycloheptaphane (PIN)

[not 1(1,4),4(1,3)-dibenzenacycloheptaphane] (the lower attachment locant set ‘(1,3)’ is not associated with the superatom having the lower locant)

[not 1(1,3),4(4,1)-dibenzenacycloheptaphane]
(in the attachment locant set (4,1), the first locant is not the one adjacent to the lower locant of the phane parent skeleton, see P-26.3.2.2)

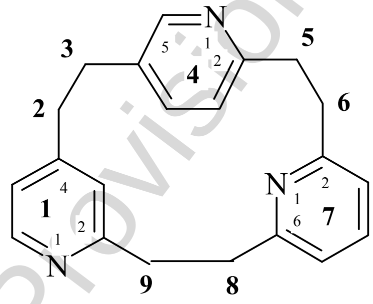


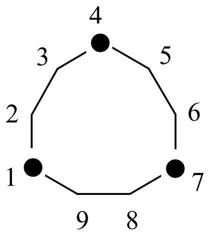


simplified skeleton
● = superatom

4(5,2),12(3,5)-dipyridina-1,8(1,3,5)-dibenzenabicyclo[6.6.0]tetradecaphane (PIN)

[not 4(3,5),12(2,5)-dipyridina-1,8(1,3,5)-dibenzenabicyclo[6.6.0]tetradecaphane]
[for the pyridine amplificants the attachment locant set ‘(5,2)’, when compared in ascending numerical order, i.e., ‘(2,5)’, is lower than ‘(3,5)’; therefore the pyridine amplificant with the locant set ‘(5,2)’ must be associated with the lower superatom locant, ‘4’]



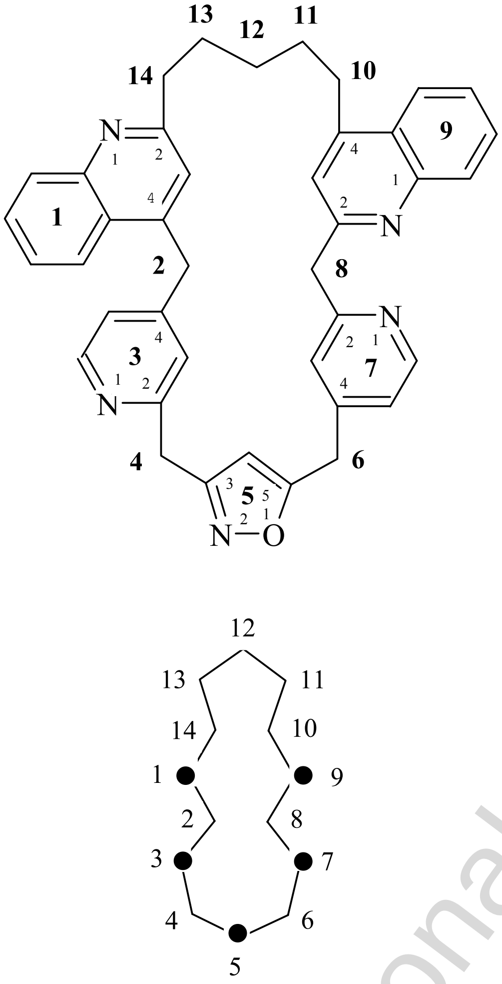


simplified skeleton
● = superatom

1(4,2), 4(5,2),7(2,6)-tripyridinacyclononaphane (PIN)
[the attachment locant sets ‘(2,4)’,’(2,5)’ and ‘(2,6)’ must be assigned to superatoms ‘1’, ‘4’, and ‘7’, respectively; the arrangement of the locants in each set is governed by P-26.3.2.2]

P-26.4.2.3 If, after the application of P-26.4.2.2, a choice is still necessary and a single unsymmetrical amplificant remains, P- 26.4.2.1 is applied to the single unsymmetrical amplificant.

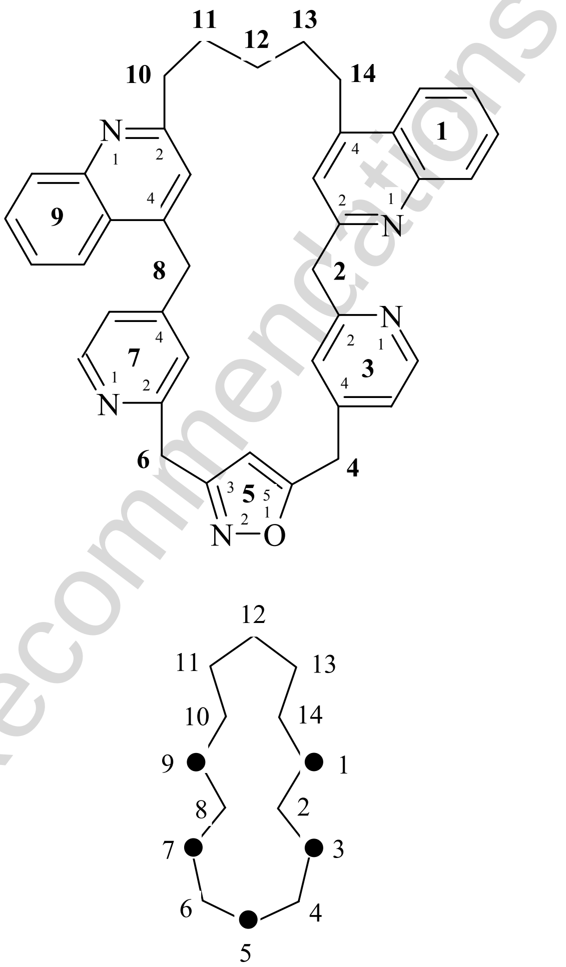
Example:



simplified skeleton
● = superatom

I

not



simplified skeleton
● = superatom

II

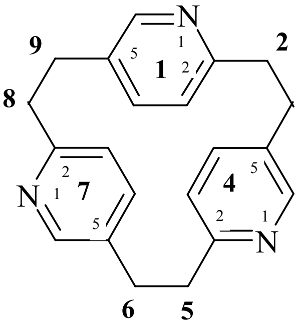
1(4,2),9(2,4)-diquinolina-3,7(4,2)-dipyridina-5(3,5)-[1,2]oxazolacyclotetradecaphane (**I**) (PIN)

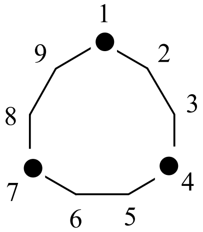
[not 1(2,4),9(4,2)-diquinolina-3,7(2,4)-dipyridina-5(5,3)-[1,2]oxazolacyclotetradecaphane (**II**)]

[each of the identical pairs of amplificants, quinoline and pyridine, have identical attachment locants, '(2,4)' and '(2,4)', respectively; the single unsymmetrical amplificant, 1,2-oxazole, remains to which P-26.4.2.1 applies; its lower attachment locant '3' must be adjacent to the lower locant of the parent phane skeleton, '4']

P-26.4.2.4 When two numberings for a simplified phane skeleton are still possible, the selected numbering is that which gives the lower locant set when attachment locants of all amplificants, as they appear in the name, are compared in the increasing order of their corresponding superatom locants.

Examples:

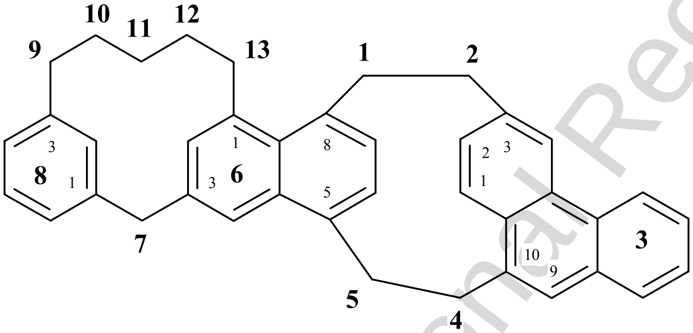


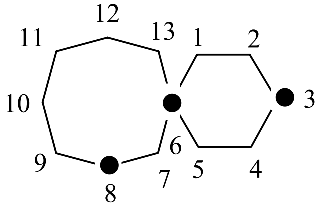


simplified skeleton
● = superatom

1(2,5),4,7(5,2)-tripyridinacyclononaphane (PIN)

[not 1(5,2),4,7(2,5)-tripyridinacyclononaphane]
[when compared in the order of increasing value of the corresponding superatoms, the amplificant locant set ‘(2,5)(5,2)(5,2)’ in the correct name is lower than ‘(5,2)(2,5)(2,5)’]

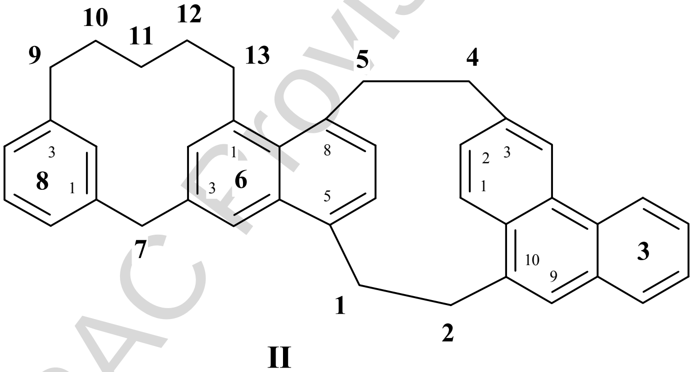


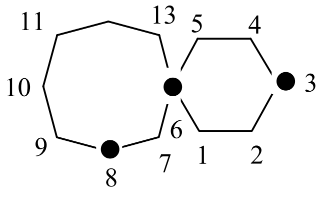


simplified skeleton
● = superatom

I

not





simplified skeleton
● = superatom

II

3(3,10)-phenanthrena-6(8,5,3,1)-naphthalena-8(1,3)-benzenaspiro[5.7]tridecaphane (PIN)

[not 3(10,3)-phenanthrena-6(5,8,3,1)-naphthalena-8(1,3)-benzenaspiro[5.7]tridecane]
[the set of attachment locants ‘(3,10)(8,5,3,1)(1,3)’ in the correct name cited for comparison in the in order of the increasing value of their corresponding superatom

locants, is lower than ‘(10,3)(5,8,3,1)(1,3)’, the corresponding set of attachment in the incorrect name]

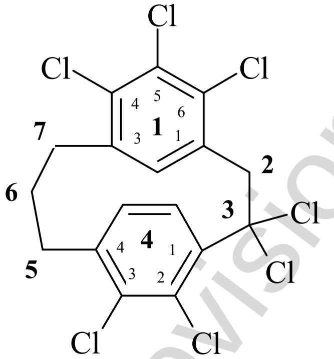
P-26.4.3 Numbering of phane parent hydrides

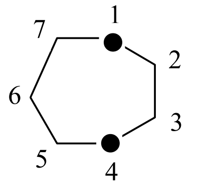
P-26.4.3.1 In a phane parent hydride, the locants for atoms that do not belong to amplificants are the locants of the simplified skeleton. However, locants for the atoms of the amplificants must be distinguished from the arabic number locants of the simplified skeleton. Thus, locants for amplificant atoms are constructed by citing the actual locants of the amplificant as superscripts to the locant of the superatom that represents the amplificant in the simplified skeleton.

P-26.4.3.2 In a substituted phane parent hydride name, a series of composite locants based on the superatom locant must not be contracted. As it is the rule for citing locants in front of detachable prefixes, there must be a number of locants corresponding to the multiplying prefix , ‘di’, ‘tri’, etc. in front of the prefix.

P-26.4.3.3 The seniority of a composite locant is determined first on the basis of its primary locants, i.e., the locants of the phane parent skeleton, and, if these locants are identical, on the basis of the complete composite locant itself, i.e., the primary locant and its superscripts.

Examples:



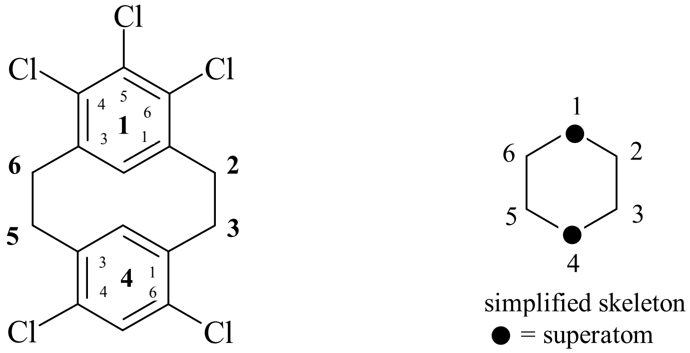


simplified skeleton
● = superatom

1^4,1^5,1^6,3,3,4^2,4^3-heptachloro-1(1,3),4(1,4)-dibenzenacycloheptaphane (PIN)

[not $1^{4,5,6}$,3,3,$4^{2,3}$-heptachloro-1(1,3),4(1,4)-dibenzenacycloheptaphane] [superscript locants denoting positions on amplificants are not contracted (see P-26.4.3.2)]

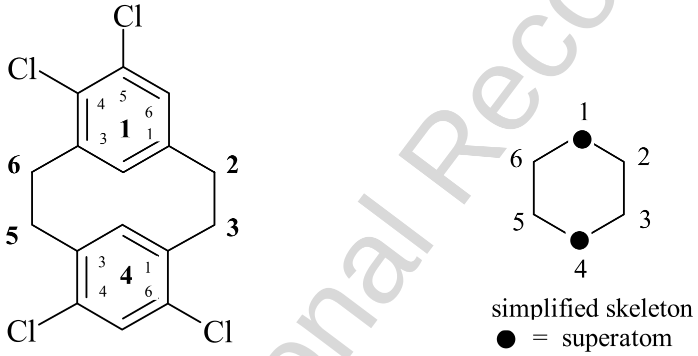
[not 1^2,1^3,2,2,4^4,4^5,4^6-heptachloro-1(1,4),4(1,3)-dibenzenacycloheptaphane] [the amplificant with the lower attachment locant set is not assigned to the superatom with the lowest locant (see P-26-4.3.3)]



$1^4,1^5,1^6,4^4,4^6$-pentachloro-1,4(1,3)-dibenzenacyclohexaphane (PIN)

[not $1^4,1^6,4^4,4^5,4^6$-pentachloro-1,4(1,3)-dibenzenacyclohexaphane]

[the primary locant set ‘1,1,1,4,4’ is lower than the locant set ‘1,1,4,4,4’ (see P-26.4.3.3)]



$1^4,1^5,4^4,4^6$-tetrachloro-1,4(1,3)-dibenzenacyclohexaphane (PIN)

[not $1^4,1^6,4^5,4^6$-tetrachloro-1,4(1,3)-dibenzenacyclohexaphane]

[the primary locant sets ‘1,1,4,4’, are identical but the composite locant set ‘$1^4,1^5,4^4,4^6$’ is lower than ‘$1^4,1^6,4^5,4^6$’ (see P-26.4.3.3)]

P-26.5 Skeletal replacement (‘a’) nomenclature in phane nomenclature

Skeletal replacement (‘a’) nomenclature is applied in two ways in phane nomenclature:

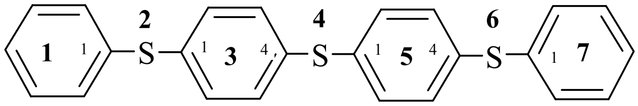
(1) to name phane parent hydrides having heteroatoms located in the simplified parent skeleton, i.e., heteroatoms not in names of amplification prefixes;

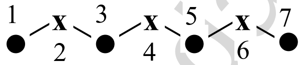
(2) to indicate heteroatoms in heterocyclic amplificants whose names cannot be used as amplification prefixes because they, themselves, are named by skeletal replacement ('a') nomenclature, for example, heteromonocycles having more than ten members and polycyclic von Baeyer systems.

The general principles, conventions and rules described for skeletal replacement ('a') nomenclature in Section P-15.4 are fully applicable to the appropriate phane parent hydrides.

P-26.5.1 Skeletal replacement ('a') nomenclature in simplified phane names is accomplished in two steps. First, the parent phane hydrocarbon is named and then the heteroatoms are denoted by means of nondetachable 'a' prefixes cited in front of the name so created. Locants for the heteroatoms are assigned according to the numbering of the simplified parent skeleton

Examples:

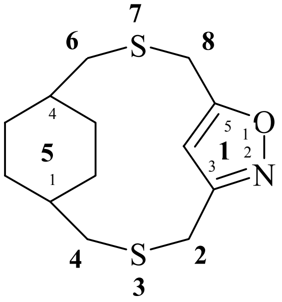


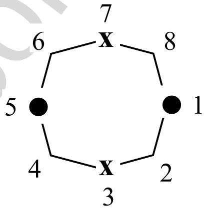


simplified skeleton
● = superatom
x = heteroatom

Step 1: 1,7(1),3,5(1,4)-tetrabenzenaheptaphane

Step 2: 2,4,6-trithia-1,9(1),3,5(1,4)-tetrabenzenaheptaphane (PIN)

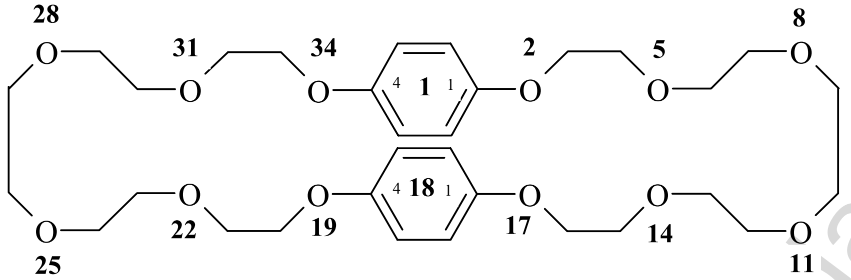


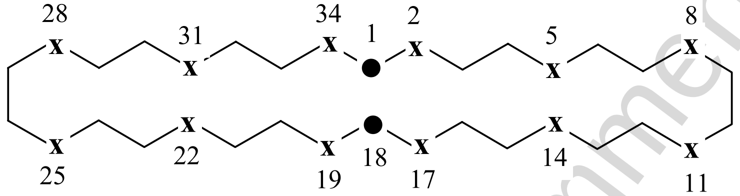


simplified skeleton
● = superatom
x = heteroatom

Step 1: 1(3,5)-[1,2]oxazola-5(1,4)-cyclohexanacyclooctaphane

Step 2: 3,7-dithia-1(3,5)-[1,2]oxazola-5(1,4)-cyclohexanacyclooctaphane (PIN)





simplified skeleton
● = superatom
x = heteroatom

Step 1: 1,18(1,4)-dibenzenacyclotetratriacontaphane

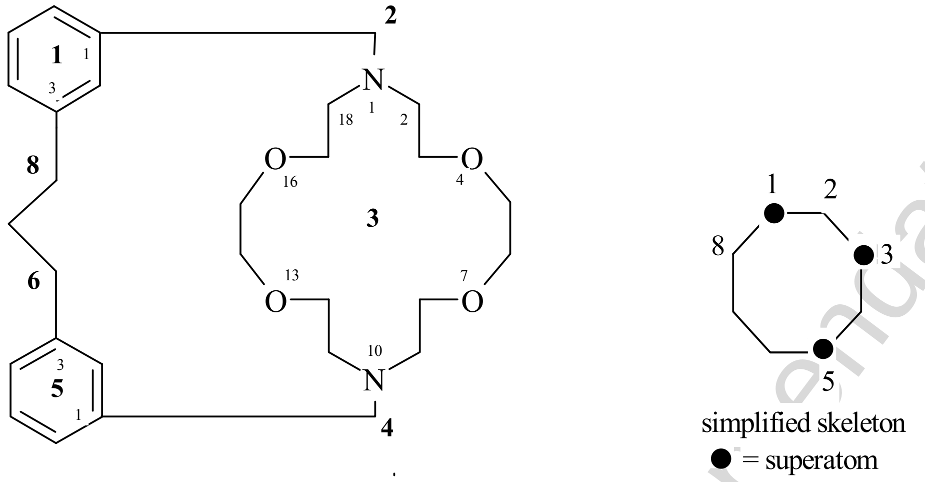
Step 2: 2,5,8,11,14,17,19,22,25,28,31,34-dodecaoxa-1,18(1,4)-dibenzenacyclotetratriacontaphane (PIN)

P-26.5.2 Skeletal replacement ('a') nomenclature in amplificants

Locants for heteroatoms in amplificants are assigned according to the numbering of the simplified skeleton and the position of heteroatoms in the amplificants following the instructions in P-26.4 for substituent locants. Thus, positions of heteroatoms in amplificants are described by composite locants.

> Note: Since the numbering of the heteroamplificant is fixed by the locants of the corresponding hydrocarbon amplificant, the numbering of the heteroatoms may not correspond to the numbering of the heteromonocycle, itself.

Example:



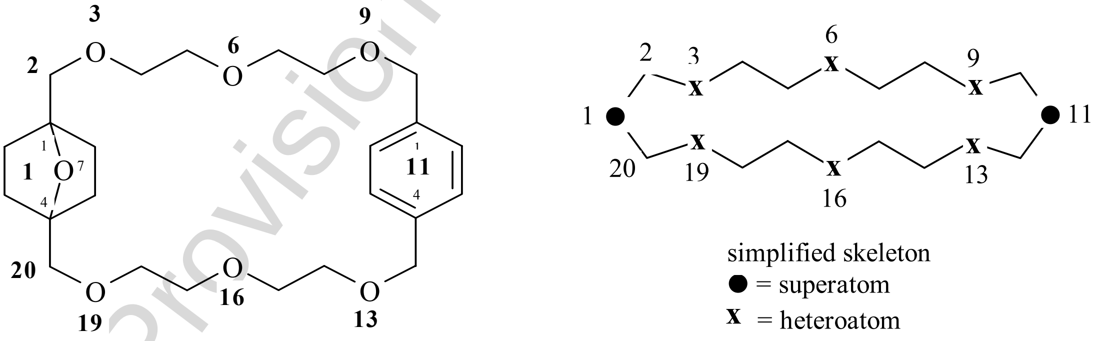
Step 1: 3(1,10)-cyclooctadecana-1,5(1,3)-dibenzenacyclooctaphane

Step 2: $3^4,3^7,3^{13},3^{16}$-tetraoxa-$3^1,3^{10}$-diaza-3(1,10)-cyclooctadecana-1,5(1,3)-dibenzenacyclooctaphane (PIN)

P-26.5.3 Simultaneous skeletal replacement ('a') in simplified skeletal names and amplificants

When skeletal replacement occurs in both simplified skeletons and in amplificants both P-26.5.1 and P-26.5.2 are applied.

Example:



Step 1: 1(1,4)-bicyclo[2.2.1]heptana-11(1,4)-benzenacycloicosaphane

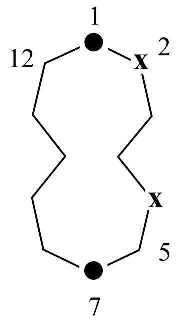
Step 2: 1^7,3,6,9,13,16,19-heptaoxa-1(1,4)-bicyclo[2.2.1]heptana-11(1,4)-benzenacycloicosaphane (PIN)

P-26.5.4 Numbering of heterophane parent hydrides with respect to heteroatoms

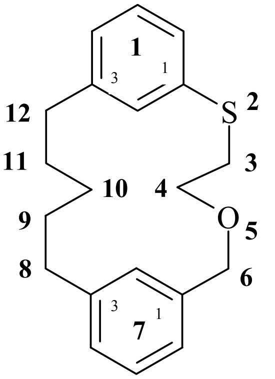
When there is a choice for numbering heterocyclic amplificants named by skeletal replacement ('a') nomenclature or for numbering simplified phane skeletons in which skeletal replacement has taken place, the following criteria are applied, in the order given, until a decision is reached.

P-26.5.4.1 Lowest locants are assigned to heteroatoms considered without regard to the nature of the heteroatom, first for the set of primary locants for the heteroatoms, i.e., the locants of the simplified skeleton (without including any superscript numbers), and then, if these locants are identical, with regard to the set of the complete heteroatom locants, which include the primary and the superscript numbers.

Examples:

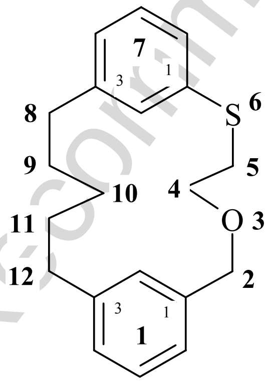


simplified skeleton
● = superatom
x = heteroatom

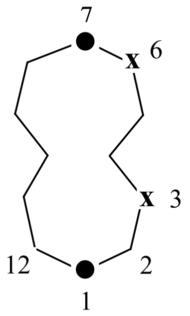


I

not



II

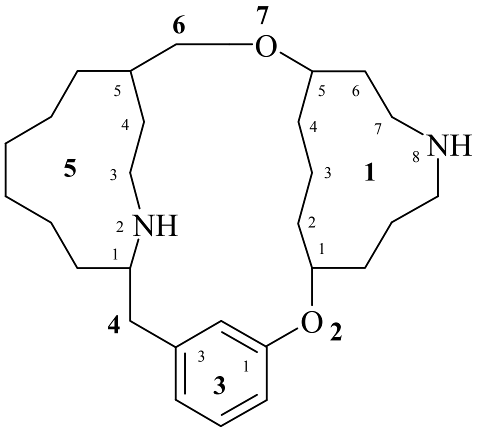


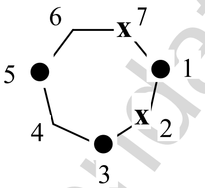
simplified skeleton
● = superatom
x = heteroatom

Step 1 : 1,7(1,3)-dibenzenacyclododecaphane [(**I**) and (**II**)]

Step 2: 5-oxa-2-thia-1,7(1,3)-dibenzenacyclododecaphane (**I**) (PIN)

[not 3-oxa-6-thia-1,7(1,3)-dibenzenacyclododecaphane]
[the locant set of the heteroatoms in **(I)** , ‘2,5’, is lower than the locant set in **(II)**, ‘3,6’]





simplified skeleton
● = superatom
x = heteroatom

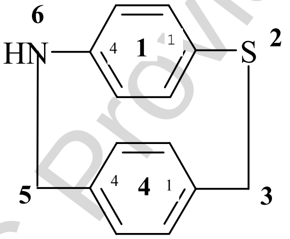
Step 1: 1,5(1,5)-dicycloundecana-3(1,3)-benzenacycloheptaphane

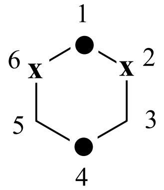
Step 2: 2,7-dioxa-1^8,5^2-diaza-1,5(1,5)-dicycloundecana-3(1,3)-benzenacycloheptaphane (PIN)

[not 4,6-dioxa-1^2,5^8-diaza-1,5(1,5)-dicycloundecana-3(1,3)-benzenacycloheptaphane]
[the primary locant set for the heteroatoms in the correct name, cited for comparison in ascending order '1,2,5,7', is lower than the locant set '1,4,5,6']

P-26.5.4.2 Lowest locants are assigned to heteroatoms considered in the order of their seniority: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl (see P-15.4), first with regard to the set for primary locants for heteroatoms , i.e., the locants of the simplified skeleton (the locants without including any superscript numbers), and then, if these locants are identical, to the set of the complete heteroatom locants, which includes the primary locants and the superscript numbers (see P-26.4.3.3).

Examples:



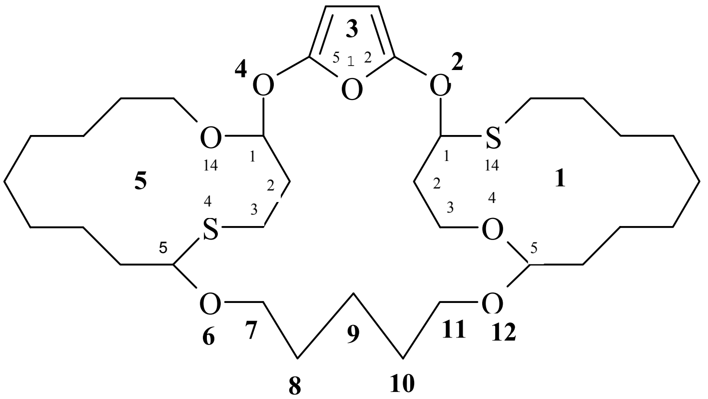


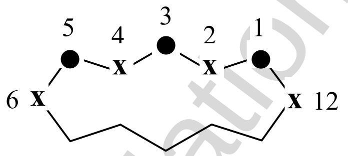
simplified skeleton
● = superatom
x = heteroatom

Step 1: 1,4(1,4)-dibenzenacyclohexaphane

Step 2: 2-thia-6-aza-1,4(1,4)-dibenzenacyclohexaphane (PIN)

[not 6-thia-2-aza-1,4(1,4)-dibenzenacyclohexaphane]
[since the 'a' prefix 'thia' is senior to 'aza' in skeletal replacement ('a') nomenclature (see P-15.4), it must be given the lower locant]

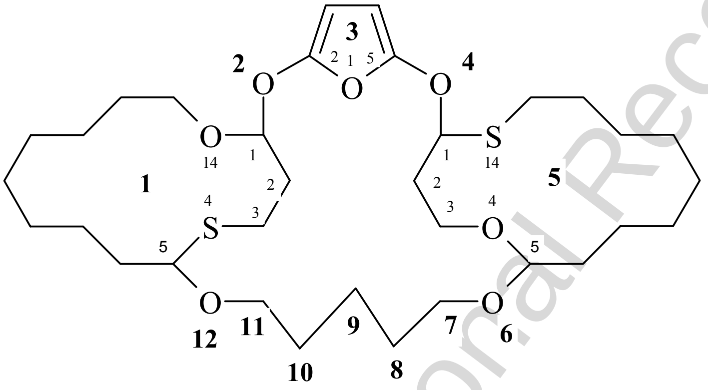


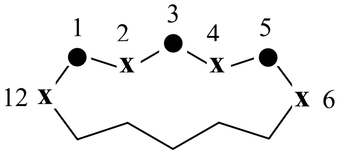


simplified skeleton
● = superatom
x = heteroatom

I

not





simplified skeleton
● = superatom
x = heteroatom

II

Step 1: 3(2,5)-furana-1,5(1,5)-dicyclotetradecanacyclododecaphane

Step 2: 1^{4},2,4,5^{14},6,12-hexaoxa-1^{14},5^{4}-dithia-3(2,5)-furana-1,5(1,5)dicyclotetradecanacyclododecaphane (**I**) (PIN)

[not 1^{14},2,4,5^{4},6,12-hexaaoxa-1^{4},5^{14}-dithia-3(2,5)-furana-1,5(1,5)-dicyclotetradecanacyclododecaphane (**II**)]

[application of P-26.5.4.1 reveals that both the primary locant sets and the primary locant sets including the composite locants for the heteroatoms without regard to the kind of heteroatom are the same for both names, '1,1,2,4,5,5,6,12' and '1^{4},1^{14},2,4,5^{4},5^{14},6,12', respectively. The primary locant sets for the senior prefix 'oxa'

are also the same in both cases, '1,2,4,5,6,12', but for the locant sets including composite locants, the locant set for the prefix 'oxa' in the correct name, 1^{4},2,4,5^{14},6,12, is lower than the locant set for 'oxa' in the incorrect name, '1^{14},2,4,5^{4},6,12']

P-27 Fullerenes

P-27-0 Introduction

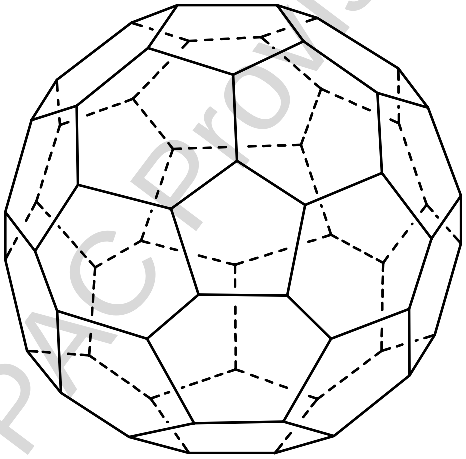
A preliminary survey of the nomenclature and terminology of fullerenes was published in 1997 (ref. 19). This Section is based on the IUPAC Recommendations 2002 (ref. 10), that deal in depth with two fullerenes, i.e. the most commonly known fullerene having 60 carbon atoms and one of its C-70 homologues.

This Section is devoted to parent hydrides only. Derivatives are described in Chapter 6, radicals and ions are discussed in Chapter 7. Chapter 8 includes a brief mention of fullerenes in the discussion on the configurational notation.

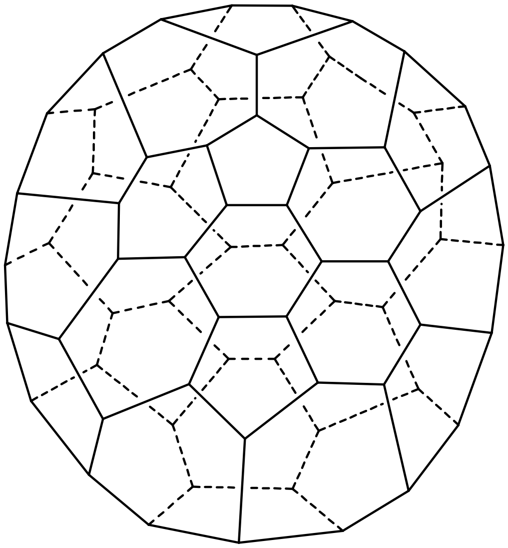
P-27.1 Definitions

P-27.1.1 Fullerenes

Fullerenes are compounds composed solely of an even number of carbon atoms, which form a cage-like fused ring polycyclic system with twelve five-membered rings and the rest six-membered rings (see ref. 17). The archetypal example is [60]fullerene, where the atoms and bonds delineate a truncated icosahedron. The term has been broadened to include any closed cage structure consisting entirely of three-coordinate carbon atoms.



(C_{60}-I_h)[5,6]fullerene



(C_{70}-$D_{5h(6)}$)[5,6]fullerene

P-27.1.2 Fulleranes

Fulleranes are fully saturated fullerenes, for example, $C_{60}H_{60}$.

P-27.1.3 Fulleroids

Heterofullerenes, norfullerenes, homofullerenes, and secofullerenes have been called ‘fulleroids’ (fullerene-like), because they resemble fullerenes in structure but do not conform to the definition of a fullerene as given above. It is convenient to refer to them as fulleroids and name them as modified fullerenes.

P-27.2 Fullerene names

P-27.2.1 Systematic names

The recommended systematic names for fullerenes include the number of carbon atoms, the point group symbol, the size of the rings, the relative arrangement of rings, and the term ‘fullerene’, all combined to give names, such as (C_{60}-I_h)[5,6]fullerene and (C_{70}-$D_{5h(6)}$)[5,6]fullerene for the two fullerenes discussed in this Section. The parenthetical prefix gives the carbon content and the point group symbol and the bracketed numbers indicate the ring sizes in the fullerene. The latter is important in fullerenes with rings other than five- and six-membered. The subscript (6) following the point group symbol D_{5h} in the latter name indicates that the five-membered ring on the five-fold symmetry axis is surrounded by six-membered rings. This differentiates this fullerene from an isomeric fullerene which has five-membered rings surrounding the five-membered ring on the five fold symmetry axis, which would have the name (C_{70}-$D_{5h(5)}$)[5,6]fullerene.

The recommended names have the same information as the corresponding names used by the Chemical Abstracts Service (CAS), but in a different format. The corresponding CAS names are [5,6]fullerene-C_{60}-I_h and [5,6]fullerene-C_{70}-$D_{5h(6)}$, respectively (see ref. 10).

P-27.2.2 Trivial names

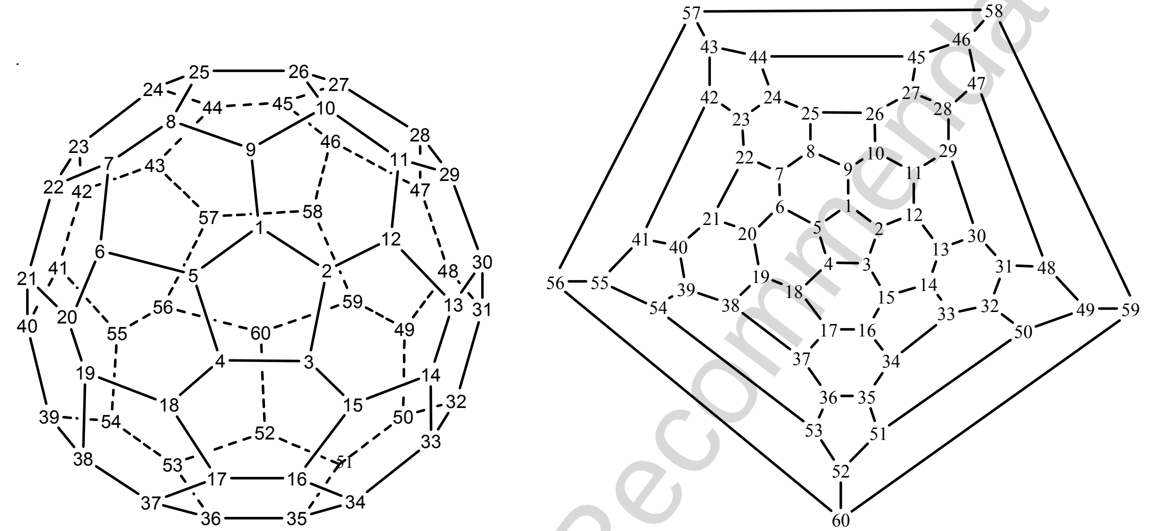
The names [60-I_h]fullerene and [70-D_{5h}]fullerene (shortened to [60]fullerene and [70-D_{5h}]fullerene in usage) given in the IUPAC Preliminary Survey (ref. 19) are names first introduced in the literature for the (C_{60}-I_h)[5,6] and (C_{70}-$D_{5h(6)}$)[5,6] fullerenes. They were based on the limited definition of fullerenes restricted to five and six-membered rings. Since important information is missing from these names, they are considered as trivial names only for these specific compounds.

P-27.2.3 Preferred IUPAC names

IUPAC systematic names are preferred to CAS and trivial names. These names are not fully interchangeable. They each depend on a specific methodology for generating names of derivatives. But, most important, they do correspond to different numbering systems, one for IUPAC systematic and CAS names, another one for trivial names (see P-27.3). Preferred names for fullerenes and fullerene derivatives are those that use preferred components when a choice is possible.

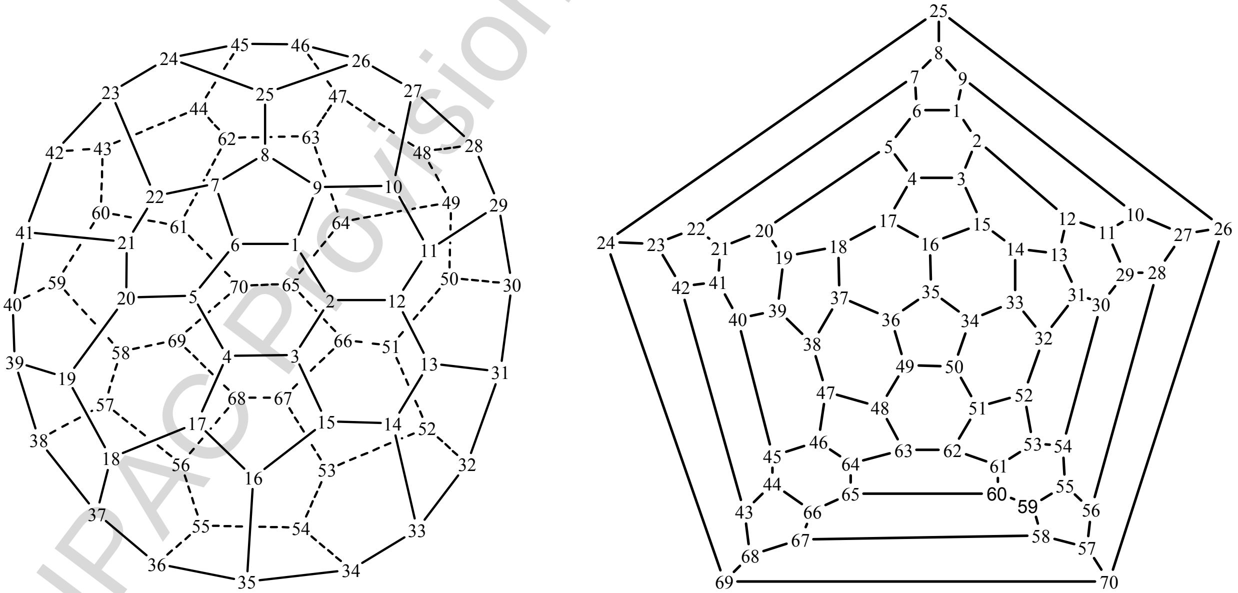
P-27.3 Numbering of fullerenes

Systematic numbering is not yet a fully solved issue in the nomenclature of fullerenes. The objectives are to achieve a continuous numbering and use a well defined starting point for all fullerenes. Studies are still underway. The criteria for numbering the (C_{60}-I_h)[5,6]fullerene and (C_{70}-$D_{5h(6)}$)- [5,6]fullerene are discussed in the IUPAC publication (ref. 10). It is important to note that the systematic numbering used with IUPAC systematic names is derived from the system developed by the Chemical Abstracts Service and that the two systems are identical for these two specific fullerenes. The numbering associated with trivial names is different, as it is based on principles like 'most reactive bond'. The two systems of numbering are shown below for three dimensional structures and Schlegel representations.



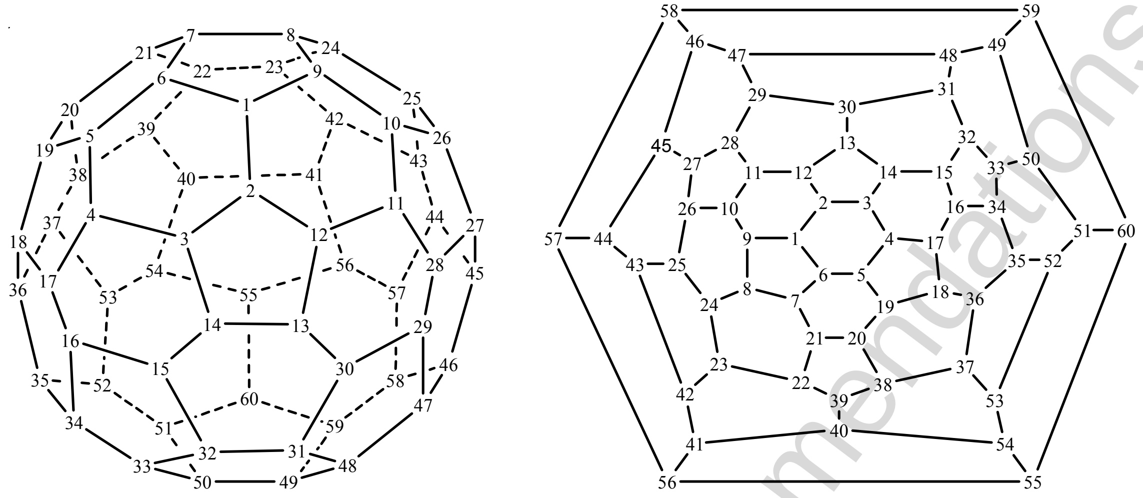
3-D Representation Schlegel representation

(C_{60}-I_h)[5,6]fullerene (systematic numbering) (PIN)



3-D Representation Schlegel representation

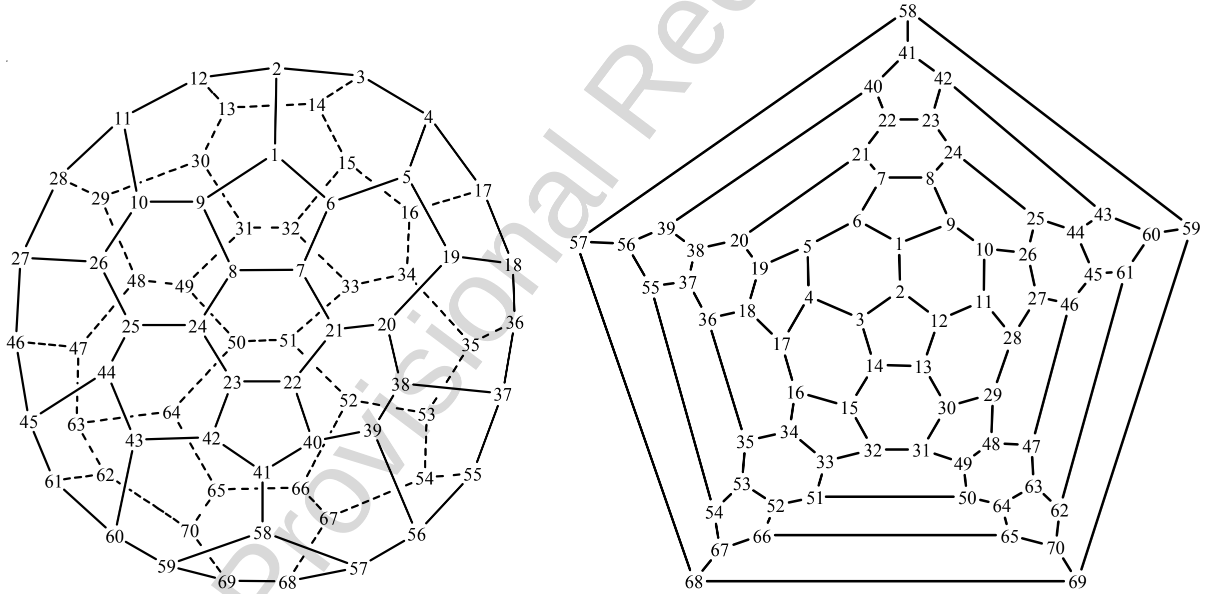
(C_{70}-$D_{5h(6)}$)[5,6]fullerene (systematic numbering) (PIN)



3-D Representation

Schlegel representation

[60]fullerene (trivial numbering)



3-D Representation

Schlegel representation

[70-D_{5h}]fullerene (Trivial Numbering)

P-27.4 Structurally modified fullerenes

P-27.4.0 Introduction
P-27.4.1 Homofullerenes
P-27.4.2 Norfullerenes
P-27.4.3 Secofullerenes

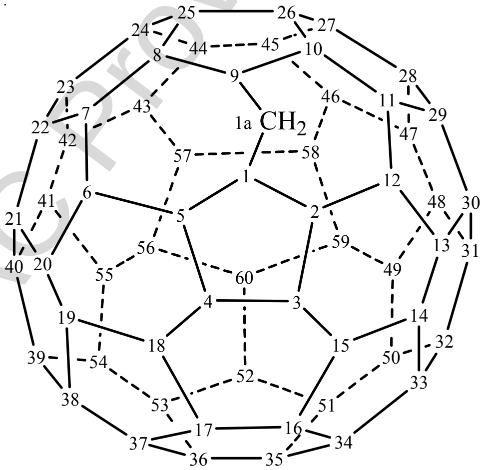
P-27.4.0 Introduction

The addition or removal of carbon atoms in a given fullerene does not create a new fullerene system described by a new number of carbon atoms and point group symbol, but is described by modifying the name of the unmodified fullerene using a nondetachable prefix, ‘homo’ or ‘nor’, respectively. In this way, fullerenes are parent structures analogous to fundamental structures used in the nomenclature of natural products (see Chapter 9). Similarly, the cleavage of a bond or the formation of new bonds in specific situations is expressed by using the nondetachable prefixes ‘seco’ and ‘cyclo’, respectively, which are also used in the nomenclature of natural products.

P-27.4.1 Homofullerenes

The replacement of a carbon-carbon bond of a fullerene by a methylene ($-CH_2-$) group is described by attaching the nondetachable prefix ‘homo’ to the name of the parent fullerene. The original numbering of the parent fullerene is retained. The location of the homo operation is described by a compound locant formed according to the method devised for insertion of a methylene group into a bond connector of a fundamental structure in the nomenclature of natural products (see P-93.2.2.2). The addition of two or more methylene groups is indicated by appropriate multiplying prefixes ‘di’, ‘tri’, etc. placed in front of the prefix ‘homo’. The compound locant is formed by adding the letter ‘a’ (‘b’, ‘c’, etc. if more than one methylene group replaces the bond) to the pair of locants which are the lowest locants consistent with the numbering of the fullerene, and enclosing the higher number in parentheses, for example ‘1(9)a’. Such compound locants must be used as locants for substituents or heteroatoms where there is ambiguity; where there is no ambiguity simple locants formed by adding the letter ‘a’ to the lowest locant, such as ‘1a’ for the case above, may be used. Locants to denote the addition of methylene group(s) are differently used in the nomenclature of natural products (see P-93.2.2). Locants used by CAS are also different and must not be used to describe the replacement by methylene groups in preferred names of fullerenes (see Fu-4.1, ref. 10).

Example:



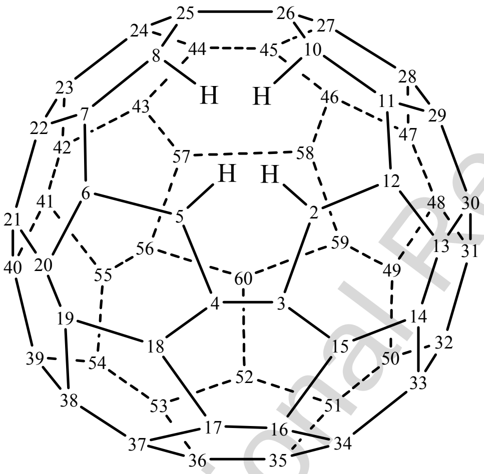
1a*H*-1(9)a-homo(C_{60}-I_h)[5,6]fullerene (PIN)

P-27.4.2 Norfullerenes

The nondetachable prefix ‘nor’ describes the deletion of carbon atoms from a fullerene structure; however, bonds attached to the atom removed are not reconnected as is the case in the nomenclature of natural products (see P-93.1). As a result, the connectivity of remaining atoms may be reduced from three to two, which requires the presence of hydrogen atoms. An even number of hydrogen atoms is implied in the name; if there is an odd number, one is expressed as indicated hydrogen because one carbon atom has changed from sp^2 to sp^3 hybridization. A connectivity of three may be satisfied by a heteroatom, such as nitrogen or boron and a connectivity of two by a heteroatom such as oxygen or sulfur; these heteroatoms are introduced in a separate operation. Locants for the atoms must be as low as possible.

The use of the ‘nor’ prefix in the nomenclature of natural products is not the same and must not be used in, or adapted to, fullerene nomenclature.

Example:

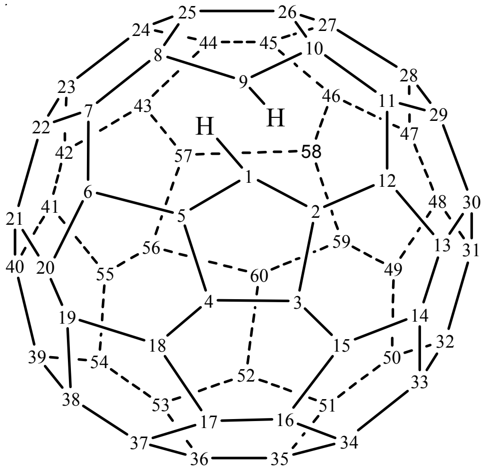


1,9-dinor(C_{60}-I_h)[5,6]fullerene (PIN)

P-27.4.3 Secofullerenes

The nondetachable prefix ‘seco’ indicates the cleavage of fullerene bonds. Numbering of the parent fullerene is retained; where there is a choice, lowest possible locants are used to describe the seco operation. The valence requirements of the resulting carbon atoms with a connectivity of two are satisfied by hydrogen atoms following rearrangement of the double bonds. The hydrogen atoms are implied in the name of the secofullerene.

Example:



1,9-seco(C_{60}-I_h)[5,6]fullerene)PIN)

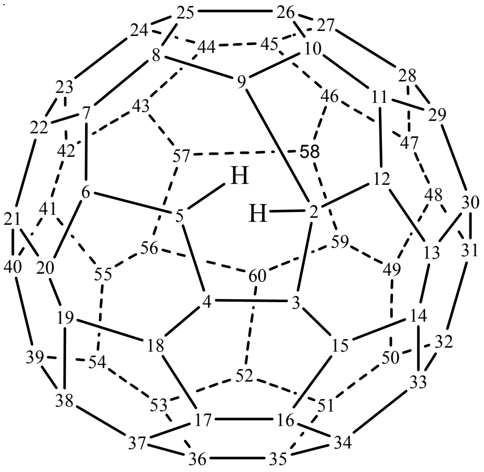
P-27.4.4 Cyclofullerenes

The nondetachable prefix ‘cyclo’ indicates the formation of a bond between two atoms of a modified fullerene or multifullerene structure. It almost always occurs in combination with one or more of the structure modifying prefixes ‘homo’, ‘nor’, and ‘seco’. No single fullerene is yet known that uses only ‘cyclo’. See the example under P-27.4.5.

P-27.4.5 Combination of structure modifying operations

When more than operation has been performed in a fullerene structure, the prefixes designating these operations are cited in names in the order cyclo, seco, homo, and nor in front of the name of the fullerene. This is the reverse order that the operation indicated by the prefix has for assignment of lowest locants. Nor prefixes are considered first for lowest locants and homo prefixes are senior to seco and cyclo for lowest locants since homo locants may be needed for the latter operations. Locants for cyclo and seco prefixes are determined by the lowest set of locants, then by the order of citation of the locants in the name.

Example:

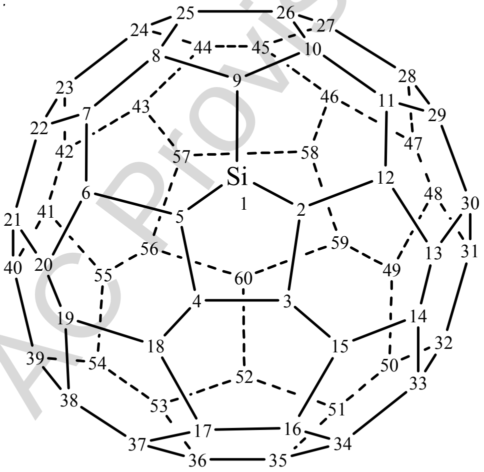


$2H$-2,9-cyclo-1-nor(C_{60}-I_h)[5,6]fullerene (PIN)

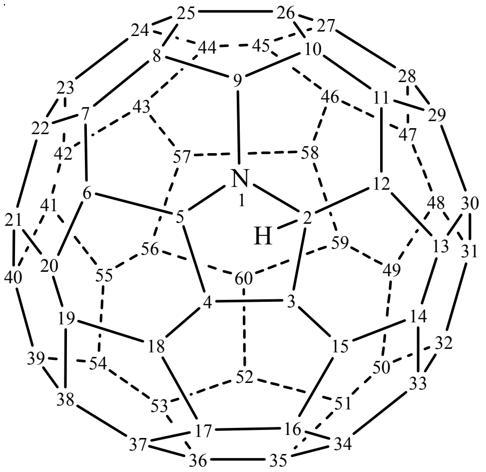
P-27.5 Replacement of skeletal atoms

P-27.5.1 Fullerenes in which carbon atoms have been replaced by one or more heteroatoms are called 'heterofullerenes'. Skeletal replacement ('a') nomenclature is used to name fullerenes in which carbon atoms have been replaced by heteroatoms having standard bonding numbers according to the 'a' prefixes of organic replacement nomenclature (see P-15.4) or bonding numbers indicated by the λ-convention (see P-14.1). The parent name is 'fullerene' if double bonds are present or possible in the parent fullerene; if double bonds are not possible, the parent name is 'fullerane'. The heteroatoms include all elements capable of being tricoordinate, including metals and semimetals. Replacement names for fullerenes in which all carbon atoms have been replaced by the same or different heteroatoms are preselected names (see P-12.2). Replacement of carbon atoms by trivalent heteroatoms may result in the need for indicated hydrogen.

Examples:



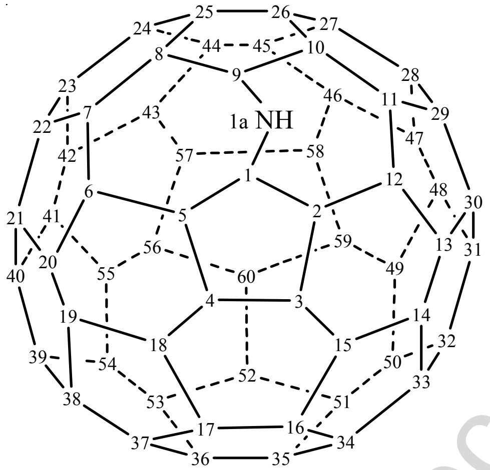
sila(C_{60}-I_h)[5,6]fullerene (PIN)



$2H$-1-aza(C_{60}-I_h)[5,6]fullerene (PIN)

P-27.5.2 When ‘homo’, ‘nor’, ‘seco’ or ‘cyclo’ prefixes co-occur with skeletal replacement terms, such as ‘oxa’ or ‘aza’, the replacement prefixes are cited in names in order of their seniority before structure modifying prefixes. Structure modifying prefixes are assigned low locants over replacement prefixes.

Example:



1a*H*-1a-aza-1(9)a-homo(C_{60}-I_h)[5,6]fullerene (PIN)

P-27.6 Addition of rings and ring systems to fullerenes

Addition of rings or ring systems to a fullerene is expressed as a *ortho* fusion operation, a bridging operation, or as a spirofusion operation as previously described in this Chapter.

P-27.6.1 Fullerenes *ortho* fused to organic rings or ring systems
P-27.6.2 Bridged fullerenes
P-27.6.3 Spirofullerenes

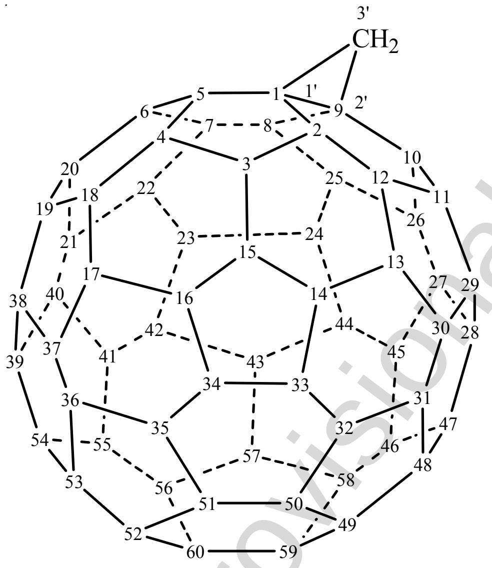
P-27.6.1 Fullerenes and modified fullerenes *ortho* fused to organic rings or ring systems

Fullerenes or modified fullerenes that share an adjacent pair of atoms with an organic ring or ring system are named by adapting the principles of fusion nomenclature described in Section P-25. As in normal organic fused ring systems, the pair of atoms shared by the fullerene or modified fullerene and the organic ring or ring system is regarded as part of both components. However, unlike normal fused systems, each component retains its own bonding pattern and numbering. Because of the nature of bonding in fullerenes, the fusion bond is always a single bond and the fusion atoms cannot accept an ‘exo’ double bond. After fusion, nonfullerene components other than alicyclic bi- and polycyclic ring systems have the maximum number of non cumulated double bonds and indicated hydrogen is cited as needed.

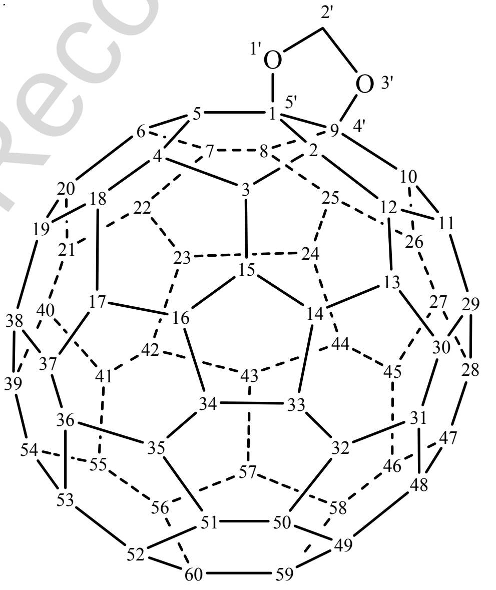
Organic rings and ring systems, including monocyclic rings and all polycyclic ring systems except spiro ring systems, are always cited as prefixes to the name of the fullerene or modified fullerene that is always the parent component. Each system retains its own name and numbering both for indicating fusion sites and for indicating positions of substitution. The fullerene or modified fullerene locants are always unprimed, and primes are added to the the fused organic rings or ring systems in the order described below. The fusion is described by citing the primed locants of the organic ring or ring system component and the unprimed locants of the fullerene or modified fullerene in that order, enclosed in brackets and separated by a colon. Locants for monocyclic hydrocarbons are omitted in preferred IUPAC names.

The methodology used to name fused derivatives of fullerenes is also used for naming fused fundamental structures in the nomenclature of natural products (see P-97). It is important to note that it must be integrally applied as described to generate IUPAC names. CAS names are different and more in line with the normal fusion operation in which the parent component is the senior ring or ring system. When this approach must be used, CAS names of fullerenes and modified fullerenes must be used. Furthermore, it is possible to replace fusion operations by bridging operations, as for example, when the ring component is a cyclopropane or an oxirene ring. In these cases, bridging by using the bridging prefixes ‘methano’ or ‘epoxy’ (see P-25.4) can be an important alternative; it was recommended in the preliminary survey (see ref. 19). In general nomenclature, if this method is used, it must be associated with trivial fullerene names, including their specific numbering, to avoid any confusion with IUPAC names and numbering.

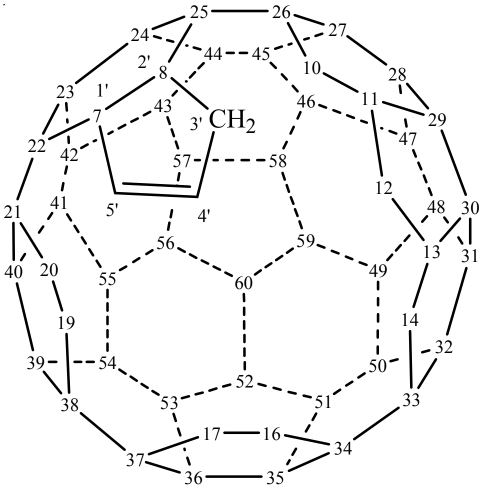
Examples:



3′*H*-cyclopropa[1,9](C_{60}-I_h)[5,6]fullerene (PIN)



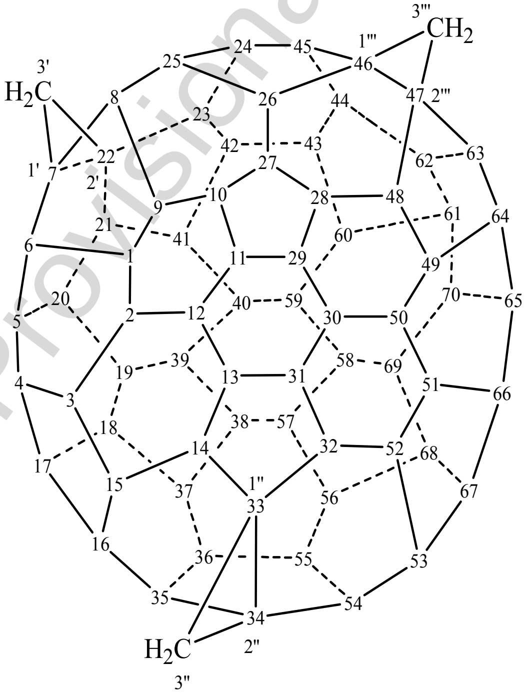
[1,3]dioxolo[4′,5′:1,9](C_{60}-I_h)[5,6]fullerene (PIN)



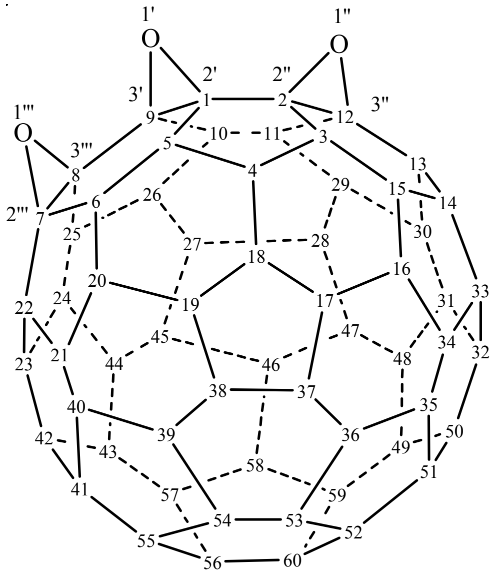
3′*H*-cyclopenta[7,8]-1,2,3,4,5,6,9,12,15,18-decanor(C_{60}-I_h)[5,6]fullerene (PIN)

When two or more of the same nonfullerene component are fused to a fullerene, primes are assigned according to the increasing value of the lower fullerene fusion locant. When different nonfullerene components are attached to a fullerene, primes are assigned in the alphanumerical order of the fusion prefix in the name reading from left to right, respecting the criterion for multiples of the same nonfullerene component just given. This methodology also applies to rings and ring systems fused to modified fullerenes.

Examples:



3′*H*,3″*H*,3‴*H*-tricyclopropa[7,22:33,34:46,47](C_{70}-I_h)[5,6]fullerene (PIN)

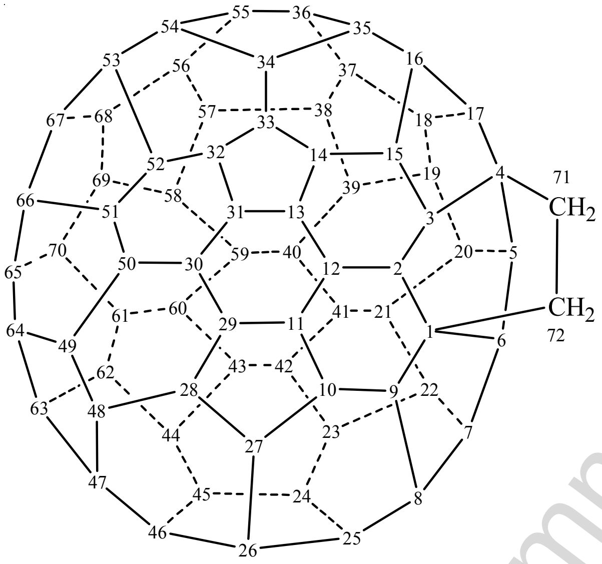


tris(oxireno)[2′,3′:1,9 ;2″,3″:2,12;2‴,3‴:7,8](C_{60}-I_h)[5,6]fullerene (PIN)

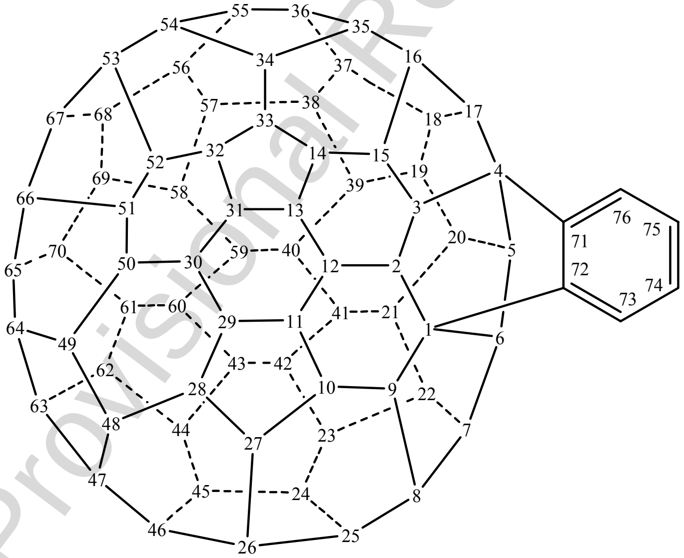
P-27.6.2 Bridged fullerenes

Bridges between nonadjacent atoms of a fullerene or modified fullerene are named and numbered according to established principles and rules for bridged fused ring systems (see P-25.4). Numbering of bridging atoms begins with the number following the highest number of the fullerene and starts with the atom adjacent to the fullerene atom with the higher locant number. Bridges between rings fused to fullerene and a parent fullerene. between two different rings fused to the same fullerene, or between two or more fullerenes joined by fused rings or ring systems are named using established bridge prefix names, but numbering begins with the bridge atom adjacent to the fused component with the least primed numbers and continues from this atom.

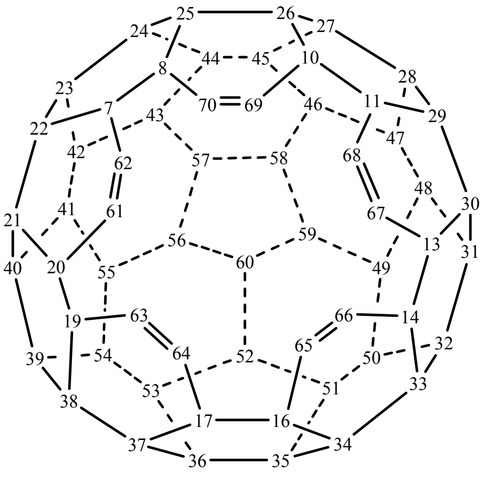
Examples:



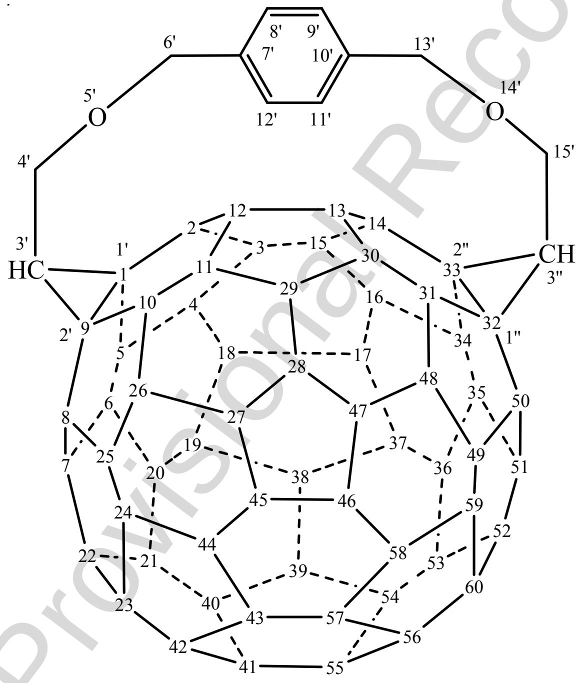
1,4-ethano(C$_{70}$-$D_{5h(6)}$)[5,6]fullerene (PIN)



1,4-[1,2]benzeno(C$_{70}$-$D_{5h(6)}$)[5,6]fullerene (PIN)



7,20:8,10:11,13:14,16:17,19-pentaetheno-1,2,3,4,5,6,9,12,15,18-decanor(C$_{60}$-I_{h})[5,6]fullerene (PIN)



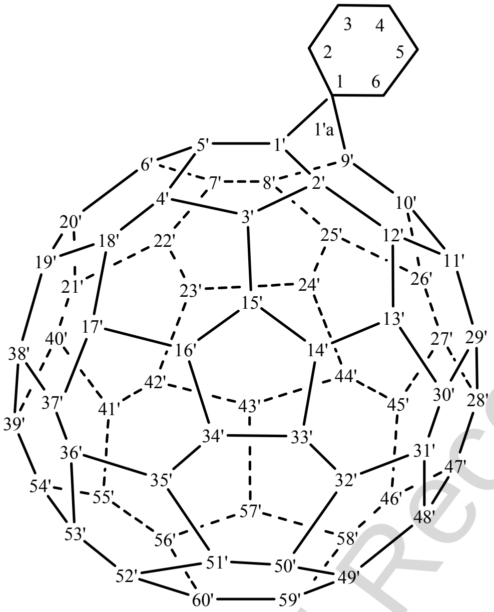
3′,3″-(methanooxymethano[1,4]benzenomethanooxymethano)-
3′H,3″H-dicyclopropa[1,9:32,33] (C$_{60}$-$D_{5h(6)}$)[5,6]fullerene (PIN)

P-27.6.3 Spiro fullerenes

Fullerenes cannot themselves form spiro compounds directly due to their specific connectivity and, as mentioned earlier, spiro ring systems are not fused to fullerenes.

Spiro fullerenes formed from homofullerenes and fullerenes fused to organic ring or ring systems follow the normal procedure for naming organic spiro systems that contain at least one polycyclic ring system, as described in P-24.5. Spiro fullerene parent hydrides will not necessarily have unprimed numbers as locants, as the alphanumerical order is used to name this type of spiro compound.

Example:



spiro[cyclohexane-1,1′a-[1a*H*-1(9)a]-homo(C_{60}-I_h)[5,6]fullerene] (PIN)

P-28 Ring assemblies

P-28.0 Introduction

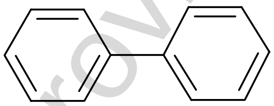
Assemblies of cyclic parent hydrides linked by single or double bonds are described in this Section. They are named by using the so-called ‘Latin multiplying prefixes’, ‘bi’, ‘ter’, ‘quater’, etc. to indicate the number or rings or ring systems in the assembly.

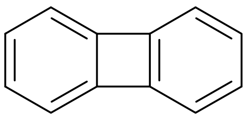
A new numbering system is recommended for ring assemblies composed of more than two rings or ring systems. The elimination of primed locants is intended to improve the perception of the relationship between structures and names.

Names of substituent groups described further in Section 29 are used in this Section.

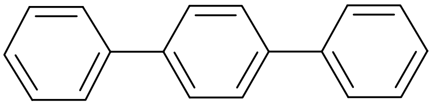
P-28.1 Definitions

Two or more cyclic systems (single rings or fused systems, alicyclic von Baeyer systems, spiro systems, phane systems, fullerenes) that are directly joined to each other by single or double bonds are called ‘ring assemblies’ when the number of such direct ring junctions is one less than the number of cyclic systems involved.

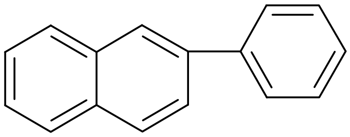

a ring assembly


a fused ring system

Ring assemblies are composed of identical cyclic systems (rings or ring systems); assemblies of nonidentical cyclic systems (rings or ring systems) are not called ring assemblies for the purposes of organic nomenclature, for example:



three identical rings
(a ring assembly)



two different ring systems

P-28.2 Ring assemblies of two identical cyclic systems with no indicated hydrogen atoms

P-28.2.1 Ring assemblies with a single bond junction

Assemblies of two identical cyclic systems joined by a single bond are named by one of two methods:

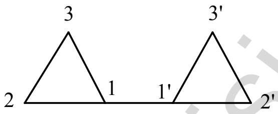
(1) by placing the prefix 'bi' before the name of the corresponding parent hydride enclosed in parentheses, if necessary. Parentheses are used to avoid confusion with von Baeyer names;

(2) by placing the prefix 'bi' before the name of the corresponding substituent group (for names of substituent groups, see P-29), enclosed in parentheses, if necessary.

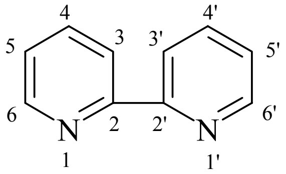
Except for biphenyl, for which method (2) is used, method (1) leads to preferred IUPAC names.

Each cyclic system is numbered in the usual way, one with unprimed locants, the other with primed locants, indicating the positions of attachment. Lowest possible locants must be used to denote the positions of attachment.

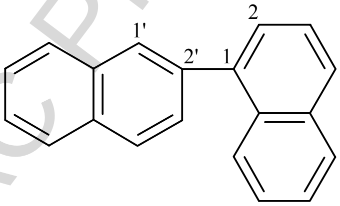
Examples:



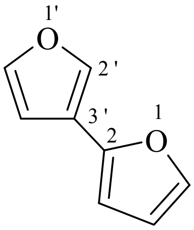
(1) 1,1′-bi(cyclopropane) (PIN)
(2) 1,1′-bi(cyclopropyl)



(1) 2,2′-bipyridine (PIN)
(2) 2,2′-bipyridyl



(1) 1,2′-binaphthalene (PIN)
(2) 1,2′-binaphthyl

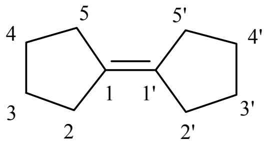


(1) 2,3′-bifuran (PIN)
(2) 2,3′-bifuryl

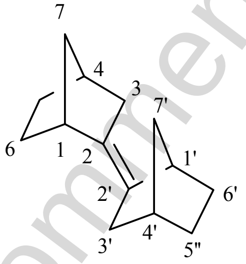
P-28.2.2 Ring assemblies with a double bond junction

When two cyclic systems are linked by a double bond, method (2) described in P-28.2.1 is the sole method recommended. Method (2) has also been used in which the presence of a double bond was indicated by the Greek letter Δ and the point of attachment of the ring was given by superscript locants numbers. This method is not continued in these recommendations; accordingly, ring assemblies of three or more identical cyclic systems interconnected by double bonds must be named by other methods (see P-31).

Examples:

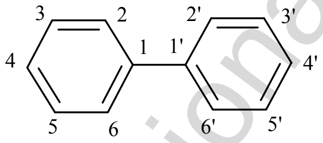


1,1′-bi(cyclopentylidene) (PIN)
(not $\Delta^{1,1'}$-bicyclopentylidene)



2,2′-bi(bicyclo[2.2.1]heptan-2-ylidene) (PIN)
(not $\Delta^{2,2'}$-bicyclo[2.2.1]heptanylidene)

P-28.2.3 A ring assembly composed of two benzene rings is named by method (2) described in P-28.2.1; locants are required for the IUPAC preferred name.



1,1′- biphenyl (PIN)
biphenyl

P-28.3 Unbranched ring assemblies consisting of three or more identical cyclic systems

P-28.3.1 Unbranched ring assemblies consisting of three or more identical cyclic systems are named by placing an appropriate numerical prefix ‘ter-’, ‘quater-’, ‘quinque-’, etc. before the name of the parent hydride corresponding to the repetitive unit. Exceptionally, ring assemblies composed of three or more benzene rings are named by using the term ‘phenyl’. For phane names, where appropriate, see P-26)

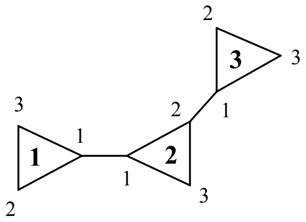
Assemblies of three or more identical cyclic systems may be numbered by one of the two following methods. Method (a) is used for preferred IUPAC names.

(a) Each cyclic system of the assembly is numbered consecutively and each ring or ring system is numbered in its usual way. Composite locants (see P-14.3.1) are formed by citing the locants denoting positions in each ring or ring system as superscripts to the locants indicating the position of a cyclic system in the assembly (ref. 20). Points of attachment are assigned the lowest possible locants. For another possible numbering system, see ref. 21.

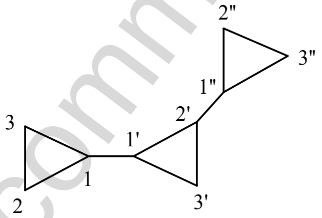
(b) Unprimed locants are assigned to one of the terminal cyclic systems, the other cyclic systems being primed serially. Points of attachment are assigned the lowest locants possible; unprimed numbers are lower than primed.

Locants indicating points of attachment are placed before the name of the assembly, in ascending order; locants denoting junctions are separated by a comma and sets of junction locants are separated by a colon.

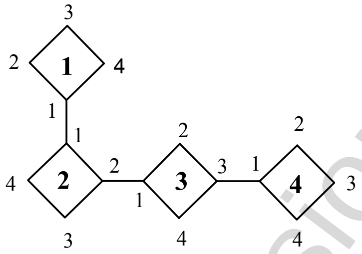
Examples (the number in parentheses reflects the method given in P-28.2.1; the letter reflects the numbering method given in P-28.3.1):

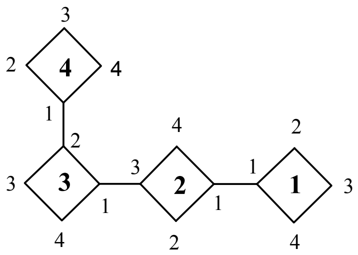


(1a) $1^1,2^1:2^2,3^1$-tercyclopropane (PIN)



(1b) 1,1′:2′,1″-tercyclopropane

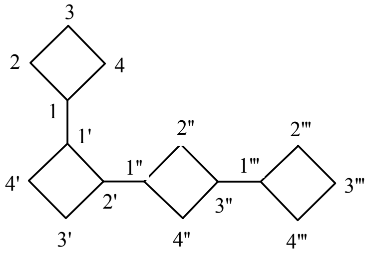




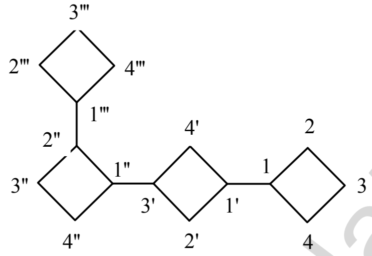
(1a) $1^1,2^1:2^2,3^1:3^3,4^1$-quatercyclopropane (PIN)
correct numbering

(1a) $1^1,2^1:2^3,3^1:3^2,4^1$-quatercyclopropane
incorrect numbering

(the locant set $1^1,2^1:2^2,3^1:3^3,4^1$ in 1a is lower than the locant set $1^1,2^1:2^3,3^1:3^2,4^1$ in 1b)



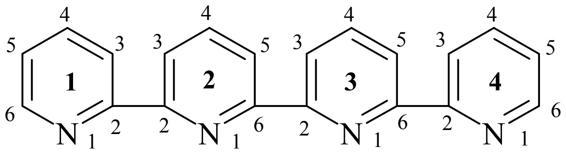
not



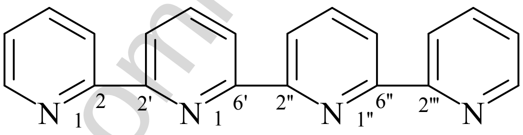
(1b) 1,1′:2′,1″:3″,1‴-quatercyclobutane
correct numbering

(1b) 1,1′:3′,1″:2″,1‴-quatercyclobutane
incorrect numbering

(the locant set 1,1′:2′,1″:3″,1‴ in 2a is lower than 1,1′:3′,1″:2″,1‴ in 2b)



(1) $1^2,2^2:2^6,3^2:3^6,4^2$-quaterpyridine (PIN)

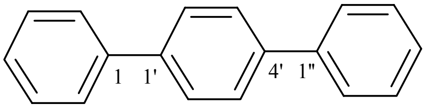


(2) 2,2′:6′,2″:6″,2‴-quaterpyridine

P-28.3.2 As exceptions to the use of parent hydride names, the names terphenyl, quaterphenyl, etc. are used.

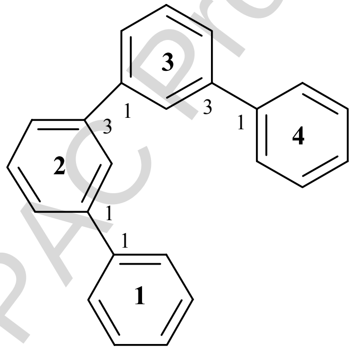
Examples (the numerical number reflects the method given in P-28.2.1; the letter the numbering method given in P-28.3.1):

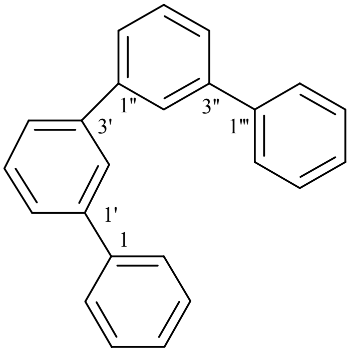
or



(2a) $1^1,2^1:2^4,3^1$-terphenyl (PIN)

(2b) 1,1′:4′,1″-terphenyl
p-terphenyl





(2a) $1^1,2^1:2^3,3^1:3^3,4^1$-quaterphenyl (PIN)

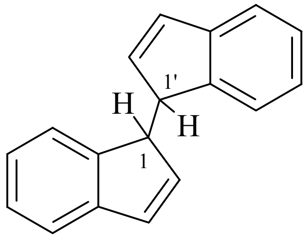
(2b) 1,1′:3′,1″:3″,1‴-quaterphenyl
m-quaterphenyl

P-28.4 Ring assemblies of identical cyclic systems with indicated hydrogen atom(s)

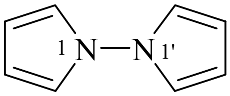
P-28.4.1 Ring assemblies are named and numbered according to P-28.2 and P-28.3 ignoring the indicated hydrogen atoms of the rings or ring systems. The maximum number of double bonds is added taking into account the junction positions. Any remaining saturated ring positions are designated as indicated hydrogen, placed together with the appropriate locant(s) at the front of the name of the assembly.

> The citation of indicated hydrogen, if needed, at the front of the name of the ring assembly is a change from previous practice where indicated hydrogen was kept with the name of the individual ring, for example, 2,2′-bi-2*H*-pyran. This required that the indicated hydrogen had to be able to be at the same position in each ring of the ring assembly, as in 2,3′-bi-1*H*-indole. By citing the indicated hydrogen in front of the name of the ring assembly, which follows the new procedure for naming bridged fused systems (see P-25.7.1.3.2) and spiro ring systems (see P-24.3.2) that utilize indicated hydrogen, more assemblies of rings can be treated as ring assemblies, for example, 1*H*,2′*H*-2,4′-biindene. The advantages of this method become more obvious when naming derivatives such as a ketone or bivalent

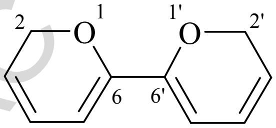
Examples:



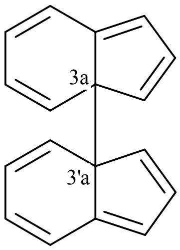
1*H*,1′*H*-1,1′-biindene (PIN)
(not 1,1′-bi-1*H*-indene



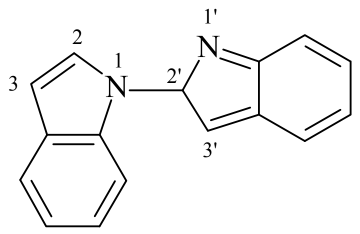
1,1′-bipyrrole (PIN)
(no indicated hydrogen needed)
(not 1,1′-bi-1*H*-pyrrole)



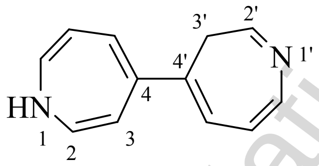
. 2*H*,2′*H*-6,6′-bipyran (PIN)
(not 6,6′-bi-2*H*-pyran)



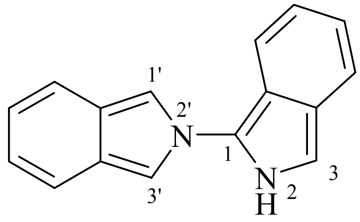
3a,3′a-biindene
(no indicated hydrogen needed)
(not 3a,3′a-bi-3a*H*-indene)



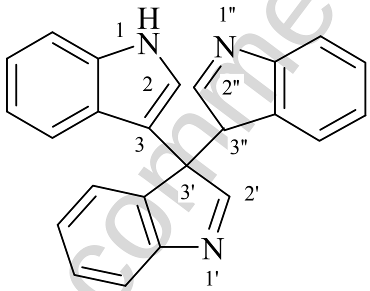
1,2′-biindole (PIN)
(no indicated hydrogen needed)



1*H*,3′*H*-4,4′-biazepine (PIN)



2*H*-1,2′-biisoindole (PIN)

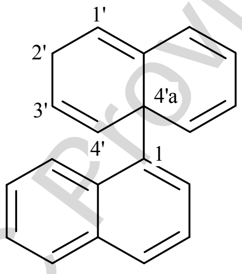


1^2*H*-1^3,2^3:2^3,3^3-terindole (PIN)
1*H*-3,3′:3′,3″-terindole

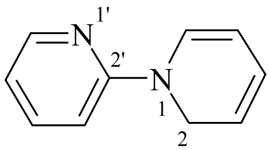
P-28.4.2 Ring assemblies of identical cyclic systems requiring added hydrogen

The ‘added hydrogen method’ (see P-14.6) is used when needed to accommodate the junction of the valence bond. The added hydrogen symbol is enclosed in parentheses and placed immediately after the locant of the point of attachment of the junction bond to which it relates.

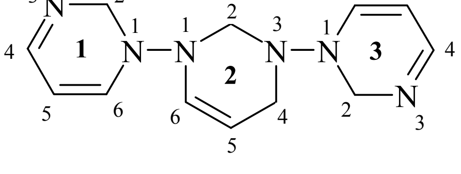
Examples:



1,4′a (2′*H*)-binaphthalene (PIN)

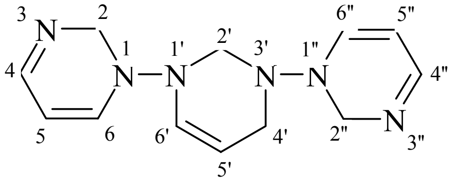


1(2*H*),2′-bipyridine (PIN)



$1^1,2^1(1^2\textit{H},2^2\textit{H}):2^3,3^1(2^4\textit{H},3^2\textit{H})$-terpyrimidine (PIN)
[name method (1), P-28.2.1; numbering method (a), P-28.3.1]

or

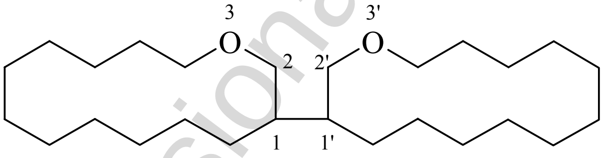


1,1′(2*H*,2′*H*):3′,1″(4′*H*,2″*H*)-terpyrimidine
[name method (1), P-28.2.1; numbering method (b), P-28.3.1]

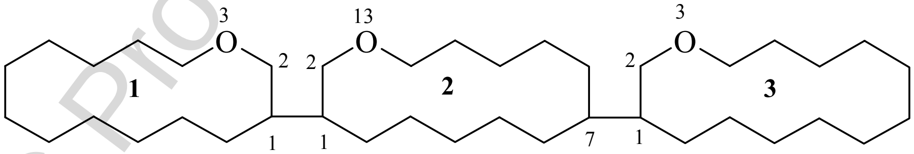
P-28.5 Ring assemblies composed of identical cyclic systems modified by skeletal replacement (‘a’) nomenclature

P-28.5.1 Assemblies composed of identical heterocyclic compounds are named by using the names of parent hydrides, except in the case of heterocyclic compounds of the von Baeyer type and of monocyclic compounds having more than 10 members that are named by using skeletal replacement (‘a’) nomenclature. In this case, the ‘a’ prefixes are placed at the front of the name of the hydrocarbon ring assembly.

Examples:

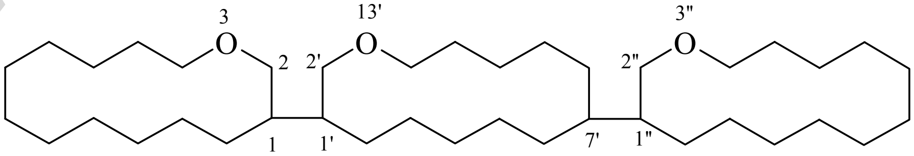


1,1′-dioxa-3,3′-bi(cyclotetradecane) (PIN)

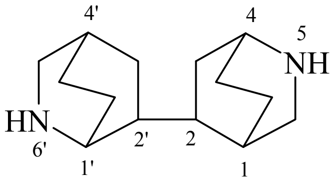


$1^3,2^{13},3^3$-trioxa-$1^1,2^1:2^7,3^1$-tercyclotetradecane (PIN)
[name method (1), P-28.2.1;numbering method (a), P-28.3.1]

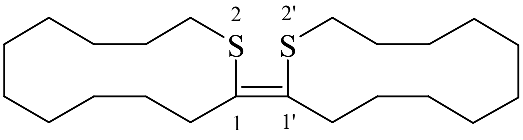
or



3′,3″,13′-trioxa-1,1′:7′,1″-tercyclotetradecane
[name method (1), P-28.2.1;numbering method (b), P-28.3.1]



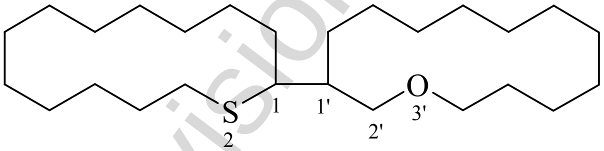
5,6′-diaza-2,2′-bibicyclo[2.2.2]octane (PIN)



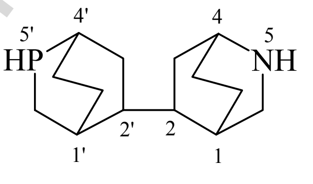
2,2′-dithia-1,1′-bi(cyclododecan-2-ylidene) (PIN)

P-28.5.2 Since hydrocarbon ring assemblies are the parent structures for the application of skeletal replacement (‘a’) nomenclature, heteroatoms do not need to be identical or present in the same number. When heteroatoms of different elements are present, normal skeletal replacement (‘a’) nomenclature is used to name the heterocycles. Low locants are assigned to heteroatoms as a set, then in the order: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Examples:



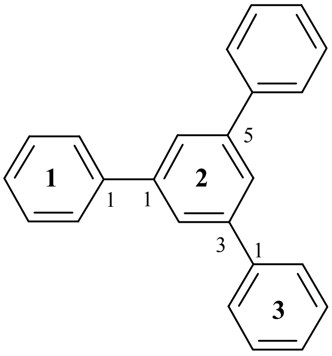
3′-oxa-2-thia-1,1′-bi(cyclotetradecane) (PIN)
[not 3-oxa-2′-thia-1,1′-bi(cyclotetradecane)]
(the locant set 2,3′ is lower than 3,2′)



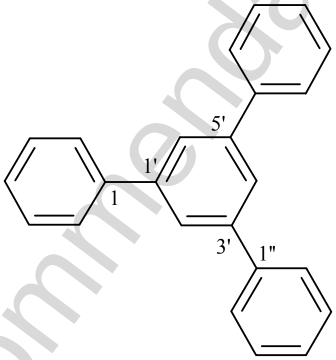
5-aza-5′-phospha-2,2′-bibicyclo[2.2.2]octane (PIN)
(not 5′-aza-5-phospha-2,2′-bibicyclo[2.2.2]octane)
(the locant 5 is lower than 5′ and the prefix ‘aza’ has priority to be assigned the lower locant)

P-28.6 Branched ring assemblies of identical cyclic systems are named by substituting the longest unbranched assembly. The names of substituent groups are formed in accord with the methods described in P-29.3.5 and 29.6.1. If necessary, the criteria for selecting the principal chain are applied: longest chain, maximum number of substituents, lowest locants for substituents considered together, then in alphanumerical order.

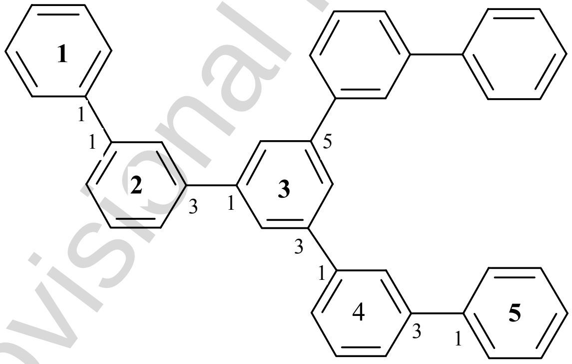
Examples:



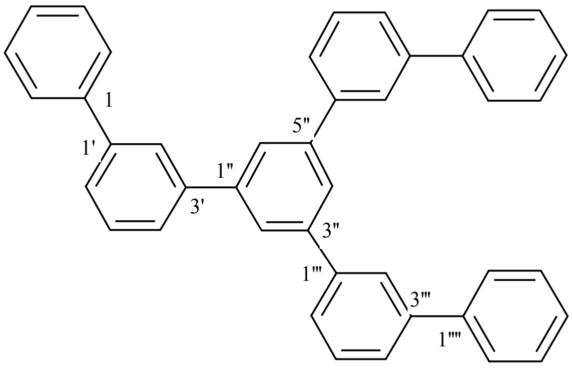
2^{5}-phenyl-1^{1},2^{1}:2^{3},3^{1}-terphenyl (PIN)
[name method (2), P-28.2.1;
numbering method (a), P-28.3.1]



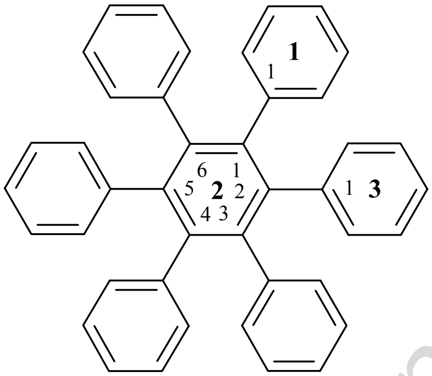
5′-phenyl-1,1′:3′,1″-terphenyl
[name method (2), P-28.2.1;
numbering method (b), P-28.3.1]



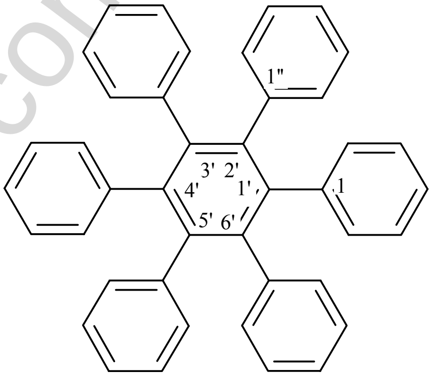
3^{5}-(biphenyl-3-yl)-1^{1},2^{1}:2^{3},3^{1}:3^{3},4^{1}:4^{3},5^{1}-quinquephenyl
[name method (2), P-28.2.1; numbering method (a), P-28.3.1]
or



5″-(biphenyl-3-yl)-1,1′:3′1″:3″-1‴:3‴,1⁗- quinquephenyl
[name method (2), P-28.2.1; numbering method (a), P-28.3.1]



or



2^{3},2^{4},2^{5},2^{6}-tetraphenyl-1^{1},2^{1}:2^{2},3^{1}-terphenyl (PIN)
[name method (2), P-28.2.1;
numbering method (a), P-28.3.1]

3′,4′,5′,6′-tetraphenyl-1,1′:2′,1″-terphenyl
[name method (2), P-28.2.1;
numbering method (b), P-28.3.1]

P-28.7 Assemblies of nonidentical cyclic systems

Assemblies of cyclic systems that cannot be treated as ring assemblies as described above (P-28.1 and P-28.2) are simply nonidentical assemblies and are named by regular substitutive nomenclature principles. Such cyclic hydrocarbon assemblies are discussed in Section P-61.2.1 and nonidentical cyclic assemblies containing heteroatoms, such as Si, N, B, in Section 68. Phane nomenclature (see P-26), where applicable, is used to name ring assemblies composed of identical or nonidentical cyclic systems.

Ring assemblies of identical cyclic systems that are partially unsaturated or partially saturated can be modified either by the endings ‘ene’ or ‘yne’ (introduction of double bonds in saturated systems) or by using the prefixes ‘hydro/dehydro’ in mancude systems (see Section P-31). In some cases, especially in the case of benzene ring assemblies, assemblies of nonidentical cyclic systems result from such operations.

P-29 Prefixes denoting substituent groups derived from parent hydrides

P-29.0 Introduction

This Section includes the names of substituent groups derived from the parent hydrides described in Sections P-21 to P-28 and used as prefixes in substitutive nomenclature. The methodology for forming systematic names is fully described in this Section; the selection of preferred names is treated in Chapter 5, Section P-56.

P-29.1 Definitions

Prefixes derived from parent hydrides are used in many ways in the nomenclature of organic compounds and may be classified as simple prefixes, compound prefixes, and complex prefixes. The definitions given below differ from those that were previously recommended (see A-2.3 in ref. 1 and R-4.1 in ref. 2).

P-29.1.1 A simple substituent group has a name consisting of one part that describes an atom or group of atoms as a unit. Normally, the basic multiplying prefixes 'di', 'tri', 'tetra', etc, denote the presence of more than one identical simple substituent group in a compound, but see P-16.3.

P-29.1.2 A compound substituent group consists of a simple substituent group (the parent substituent group) to which is attached one or more simple substituent groups. Compound substituent group names are formed by combining the names of two or more simple substituent groups. There are two ways to do this:

(1) by an additive operation

(2) by the substitutive operation

Names for compound substituent groups are formed by the substitution operation rather than by an additive operation unless the simple parent substituent group does not have a name that is acceptable for substitution. Compound substituent groups formed by substitution are cited in names as prefixes, often called 'substituted prefixes'. Compound substituent groups formed by addition are cited in names as prefixes, often called 'concatenated prefixes'. Derived multiplying prefixes 'bis', 'tris', 'tetrakis' are used to multiply compound prefixes and to avoid ambiguity when the basic multiplying prefixes are already part of the name of a parent hydride (see P-16.3).

P-29.1.3 A complex substituent group consists of a parent substituent group to which is attached at least one compound substituent group. In a complex substituent group, the parent substituent group of a component compound substituent group is called a subsidiary parent substituent group. Multiplicative prefixes, used as central part in multiplicative nomenclature (see P-15.3.2.3), are formed by the additive operation and when they consist of three or more parts are often considered as ‘complex concatenated prefixes’.

P-29.2 General methodology for naming substituent groups

The presence of free valences formally derived from the loss of one or more hydrogen atoms from a parent hydride are denoted by suffixes ‘yl’, ‘ylidene’, and ‘ylidyne’, together with the multiplying prefixes indicating the number of free valences; lowest locants are assigned to all free valences as a set, then in the order ‘yl’, ‘ylidene’, ‘ylidyne’. In names, the suffixes are cited in the order ‘yl’, ‘ylidene’, ‘ylidyne’. In these recommendations, the suffixes ‘ylidene’ and ‘ylidyne’ are used only to indicate the attachment of a substituent to a parent hydride or parent substituent by a double or triple bond, respectively.

Systematic names are formed by using the suffixes ‘yl’, ‘ylidene’ and ‘ylidyne’, with elision of the final letter ‘e’ of parent hydrides, when present, according to two methods as follows:

Monovalent	Divalent	Trivalent	Tetravalent	etc.
-yl	-diyl	-triyl	-tetrayl	
	-ylidene	-ylidyne	-ylylidyne	
		-ylylidene	-diylidene	etc.
			-diylylidene	

P-29.2.1 Specific method. The suffixes ‘yl’, ‘ylidene’, and ‘ylidyne’ replace the ending ‘ane’ of the parent hydride name. The atom with the free valence terminates a chain and always has the locant ‘1’, which is omitted from the name. This method is recommended only for saturated acyclic and monocyclic hydrocarbon substituent groups and for the mononuclear hydrides of silicon, germanium, tin, and lead.

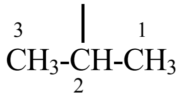
The specific method is no longer applicable to boron.

Examples:

CH_3−	methyl (PIN)	C_6H_{11}−	cyclohexyl (PIN)
SiH_3−	silyl (PIN)	CH_3-CH_2-CH=	propylidene (PIN)
CH_2=	methylidene (PIN)	CH_3-C≡	ethylidyne (PIN)

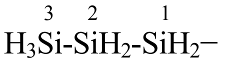
P-29.2.2 General method. Any of the suffixes ‘yl’, ‘ylidene’, and ‘ylidyne’ is added to the name of the parent hydride with elision of the terminal letter ‘e’, if present, when followed immediately by the letter ‘y’. The locants for the atoms of free valences are as low as is consistent with any established numbering of the parent hydride and except for mononuclear parent hydrides or the suffix ‘ylidyne’, the locant ‘1’ must be cited.

Examples:



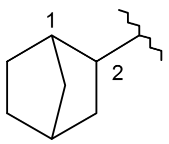
$\overset{3}{CH_3}\text{-}\underset{2}{CH}\text{-}\overset{1}{CH_3}$

propan-2-yl (PIN)

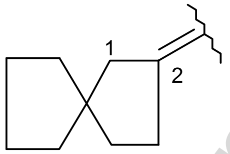


$H_3\overset{3}{Si}\text{-}\overset{2}{Si}H_2\text{-}\overset{1}{Si}H_2-$

trisilan-1-yl (PIN)



bicyclo[2.2.1]heptan-2-yl (PIN)



spiro[4.4]nonan-2-ylidene (PIN)

P-29.3 Systematic names of substituents derived from saturated parent hydrides

P-29.3.1 Substituent groups derived from mononuclear hydrides

Substituent groups are formed by applying the specific method, P-29.2.1, to the mononuclear parent hydrides of carbon, silicon, germanium, tin, and lead (boron is no longer included); the general method, P-29.2.2, is applied to other mononuclear parent hydrides with the exception of oxygen. Thus, method P-29.2.2 is limited to mononuclear hydrides containing S, Se, Te, N, P, As, Sb, Bi, B, Al, Ga, In, and Tl.

This rule is more restrictive than Rule 2.5 cited in the Guide (ref. 2) because it is not necessary to generate names that are not used as preferred names, nor used to generate those of complex substituent groups, as indicated in Section P-29.4 below. The prefixes boryl, borylidene and borylidyne have been replaced by boranyl, boranylidene,, and boranylidyne, respectively

Examples:

CH_3-	GeH_3-	BH_2-
methyl (PIN)	germyl (PIN)	boranyl (PIN) (not boryl)

$CH_2=$	$SnH_2=$	$BH=$
methylidene (PIN)	stannylidene (PIN)	boranylidene (PIN) (not borylidene)
$SH-$	PH_2-	AlH_2-
sulfanyl (PIN) (no longer mercapto)	phosphanyl (PIN) (not phosphino)	alumanyl (PIN)
$S=$	$AsH=$	$AlH=$
sulfanylidene (PIN) thioxo	arsanylidene (PIN) (not arsinidine)	alumanylidene (PIN)

P-29.3.2 Substituent groups derived from acyclic parent hydrides

Names of substituent groups are derived from those of the acyclic parent hydride and formed by the specific and general methods described in P-29.2.

P-29.3.2.1 The specific method P-29.2.1 generates ‘alkyl’, ‘alkylidene’, and ‘alkylidyne’ substituent groups. The free valences denoted by the suffixes ‘yl,’ ‘ylidene’, and ‘ylidyne’ are always situated at an extremity of the chain that is assigned the locant 1. This locant is omitted in names.

Examples:

$\overset{2}{C}H_3\text{-}\overset{1}{C}H_2-$	ethyl (PIN)
$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2-$	propyl (PIN)
$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2-$	butyl (PIN)
$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H=$	propylidene (PIN)
$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}\equiv$	butylidyne (PIN)

P-29.3.2.2 The general method, P-29.2.2, is used to generate names of substituent groups other than those described in P-29.3.2.1. In contrast to alkyl, alkylidene, and alkylidyne groups in carbon compounds, those substituents named by the general method P-29.2.2 are called ‘alkanyl’, ‘alkanylidene’, ‘alkanylidyne’, ‘alkanediyl’, ‘alkanylylidene’, etc., substituent groups Low locants are assigned to free valences considered as a set, in accordance with the numbering of the chain. If there is a choice, low locants are assigned, in order, to the suffixes ‘yl’, ‘ylidene’, and ‘ylidyne’. In names, the suffixes are cited in the order ‘yl’, ‘ylidene’, and ‘ylidyne’.

Examples:

$\overset{3}{\mathrm{CH_3}}\text{-}\underset{2}{\overset{|}{\mathrm{C}}}\mathrm{H}\text{-}\overset{1}{\mathrm{CH_3}}$

propan-2-yl (PIN)

$\overset{4}{\mathrm{CH_3}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\underset{2}{\overset{|}{\mathrm{C}}}\mathrm{H}\text{-}\overset{1}{\mathrm{CH_3}}$

butan-2-yl (PIN)

$\overset{3}{\mathrm{CH_3}}\text{-}\underset{2}{\overset{\|}{\mathrm{C}}}\text{-}\overset{1}{\mathrm{CH_3}}$

propan-2-ylidene (PIN)

$\overset{5}{\mathrm{CH_3}}\text{-}\overset{4}{\mathrm{CH_2}}\text{-}\underset{3}{\overset{\|}{\mathrm{C}}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{CH_3}}$

pentan-3-ylidene (PIN)

$-\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{CH_2}}-$

propane-1,3-diyl (PIN)

$\overset{2}{\mathrm{CH_3}}\text{-}\overset{1}{\mathrm{CH}}<$

ethane-1,1-diyl (PIN)

$-\overset{1}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CH}}=$

ethan-1-yl-2-ylidene (PIN)

$\overset{3}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\underset{1}{\overset{|}{\mathrm{C}}}=$

propan-1-yl-1-ylidene (PIN)

$\overset{4}{\mathrm{CH_3}}\text{-}\underset{3}{\overset{|}{\mathrm{C}}}\mathrm{H}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{CH}}=$

butan-3-yl-1-ylidene (PIN)

$\overset{1}{\mathrm{CH_3}}\text{-}\underset{2}{\overset{|}{\mathrm{C}}}\mathrm{H}\text{-}\underset{3}{\overset{\|}{\mathrm{C}}}\text{-}\overset{4}{\mathrm{CH_3}}$

butan-2-yl-3-ylidene (PIN)

$\mathrm{AsH_3\text{-}AsH_2}-$

diarsanyl (PIN)

$\mathrm{SiH_3\text{-}SiH_2}-$

disilanyl (PIN)

$\overset{3}{\mathrm{NH_2}}\text{-}\overset{2}{\mathrm{NH}}\text{-}\overset{1}{\mathrm{NH}}-$

triazan-1-yl (PIN)

$\overset{3}{\mathrm{SiH_3}}\text{-}\underset{2}{\overset{|}{\mathrm{Si}}}\mathrm{H}\text{-}\overset{1}{\mathrm{SiH_3}}$

trisilan-2-yl (PIN)

$\overset{3}{\mathrm{SiH_3}}\text{-}\overset{2}{\mathrm{O}}\text{-}\overset{1}{\mathrm{SiH_2}}-$

disiloxanyl (PIN)

$\overset{5}{\mathrm{SiH_3}}\text{-}\overset{4}{\mathrm{NH}}\text{-}\underset{3}{\overset{|}{\mathrm{Si}}}\mathrm{H}\text{-}\overset{2}{\mathrm{NH}}\text{-}\overset{1}{\mathrm{SiH_3}}$

trisilazan-3-yl (PIN)

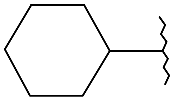
$$\overset{1}{C}H_3\text{-}\overset{2}{O}\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{5}{O}\text{-}\overset{6}{C}H_2\text{-}\overset{7}{C}H_2\text{-}\overset{8}{O}\text{-}\overset{9}{C}H_2\text{-}\overset{10}{C}H_2\text{-}\overset{11}{O}\text{-}\overset{12}{C}H_2\text{-}\overset{13}{C}H_2\text{-}\overset{14}{C}H_2\text{–}$$

2,5,8,11-tetraoxatetradecan-14-yl (PIN)

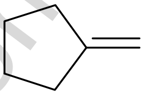
P-29.3.3 Substituent groups derived from saturated cyclic parent hydrides

With the exception of substituent groups derived from cycloalkanes that are named by the specific method P-29.2.1 only, all other substituent groups derived from saturated cyclic parent hydrides are named by the general method, P-29.2.2. Low locants are assigned to free valences 'yl', 'ylidene', and 'ylidyne' in accordance with the numbering of the parent hydride. If there is a choice, the suffixes are assigned low locants, in that order. Suffixes are cited in the order 'yl', 'ylidene', and 'ylidyne'.

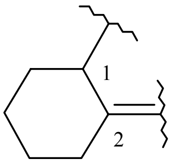
Examples:



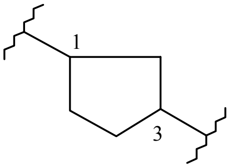
cyclohexyl (PIN)



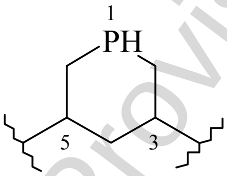
cyclopentylidene (PIN)



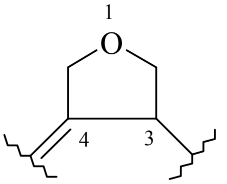
cyclohexan-1-yl-2-ylidene (PIN)



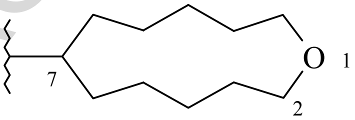
cyclopentane-1,3-diyl (PIN)



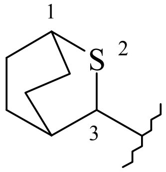
phosphinane-3,5-diyl (PIN)



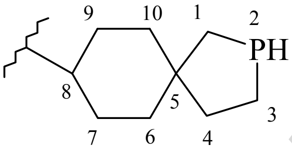
oxolane-3-yl-4-ylidene (PIN)



1-oxacyclododecan-7-yl (PIN)



2-thiabicyclo[2.2.2]octan-3-yl (PIN)

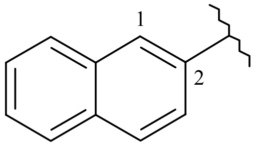


2-phosphaspiro[4.5]decan-8-yl (PIN)

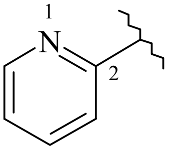
P-29.3.4 Substituent groups derived from mancude parent hydrides

P-29.3.4.1 The general method, P-29.2.2, is applied to all mancude rings and ring systems. There is no difficulty when one hydrogen atom is present to derive a monovalent substituent. When none is present or when an 'ylidene' type substituent group is needed, it is necessary to use 'added hydrogen' (see P-14.6). Formally, this method involves the adding of one hydrogen atom to the atom from which the substituent group is derived and another hydrogen atom that can be located on any atom of the ring or ring system. This 'added hydrogen atom' is expressed by the symbol *H*, preceded by a locant denoting its position.

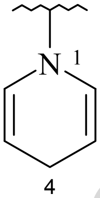
Examples:



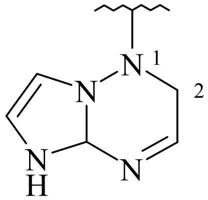
naphthalen-2-yl (PIN)



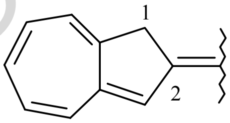
pyridin-2-yl (PIN)



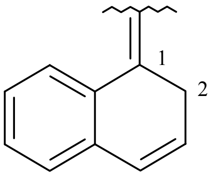
pyridin-1(4*H*)-yl (PIN)



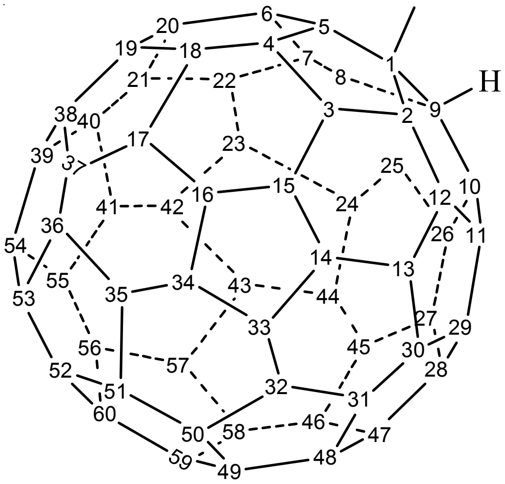
imidazo[1,2-*b*][1,2,4]triazin-1(2*H*)-yl (PIN)



azulen-2(1*H*)-ylidene (PIN)



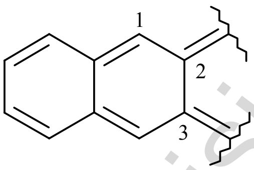
naphthalen-1(2*H*)-ylidene (PIN)



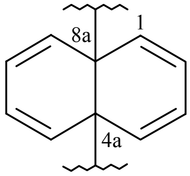
(C_{60}-I_h)[5,6]fulleren-1(9*H*)-yl (PIN)

P-29.3.4.2 ‘Diylidene’ substituent groups derived from mancude compounds by conversion of two
−CH= groups into free valences with any necessary rearrangement of double bonds to a quinoid structure are named by adding two ‘ylidene’ suffixes, i.e. 'diylidene', to the parent hydride; no added hydrogen is necessary. No added hydrogen is necessary either in the case of the formation of a substituent group of the ‘diyl’ type, when the free valences are located at fusion atoms.

Examples:



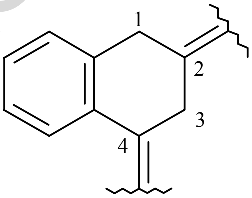
naphthalene-2,3-diylidene (PIN)



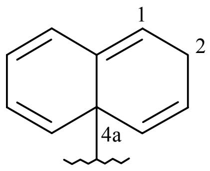
naphthalene-4a,8a-diyl (PIN)

When no quinoid structure results from the introduction of free valences, added hydrogen atoms must be cited in names. They receive the lowest possible locants. When one free valence of the ‘yl’ type is present at a fusion atom, added hydrogen must also be cited in names.

Examples:



naphthalene-2,4(1*H*,3*H*)-diylidene (PIN)



naphthalen-4a(2*H*)-yl (PIN)

P-29.3.5 Substituent groups derived from ring assemblies

Names of substituent groups derived from ring assemblies composed of saturated rings are formed as described in Section P-28.2, and those derived from ring assemblies composed of mancude compounds as described in P-28.3.4.1. Low locants are assigned to ring junctions, then to free valences.

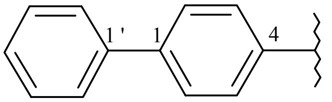
Names of substituent groups derived from ring assemblies are written in two ways.

(a) Suffixes ‘yl’ and ‘ylidene’ are added to the name biphenyl;

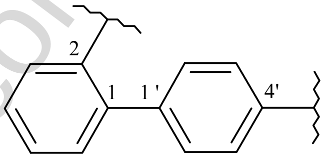
(b) Names denoted by locants are placed in brackets; the suffixes ‘yl’ and ‘ylidene’ are added with elision of the final letter ‘e’ in the name of the parent hydride.

For choice of preferred IUPAC names see Chapter 5..

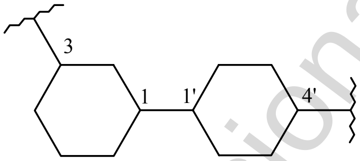
Examples:



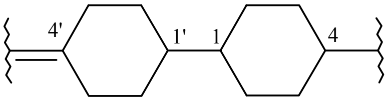
[1,1′-biphenyl]-4-yl (PIN)



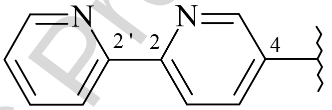
[1,1′-biphenyl]-2,4′-diyl (PIN)



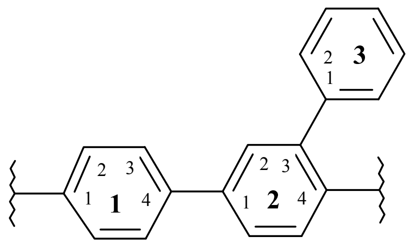
[1,1′-bicyclohexane]-3,4′-diyl (PIN)
[1,1′-bi(cyclohexyl)]-3,4′-diyl



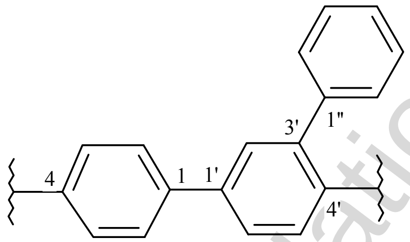
[1,1′-bicyclohexan]-4-yl-4′-ylidene (PIN)
[1,1′-bi(cyclohexyl)]-4-yl-4′-ylidene



[2,2′-bipyridin]-4-yl (PIN)
[2,2′-bipyridyl]-4-yl

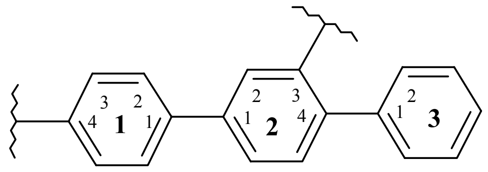


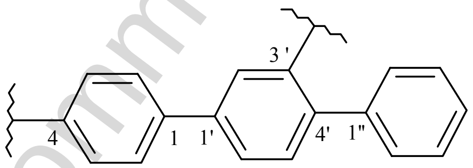
or



(2a) $[1^1,2^1{:}2^3,3^1$-terphenyl$]$-$1^4,2^4$-diyl (PIN)
(see P-28.3.1)

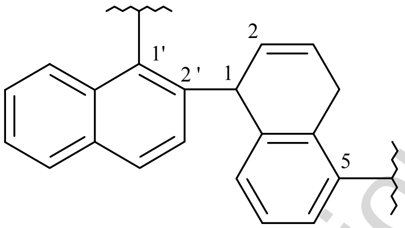
(2b) [1,1′:3′,1″]-terphenyl]-4′,4-diyl
(see P-28.3.1)

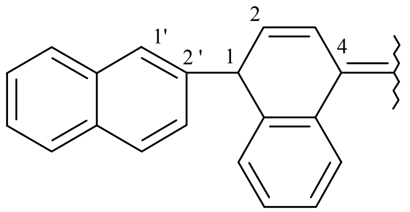




(2a) $[1^1,2^1{:}2^4,3^1$-terphenyl$]$-$1^4,2^3$-diyl (PIN)
(see P-28.3.1)

(2b) [1,1′:4′,1″-terphenyl]-3′,4-diyl
(see P-28.3.1)





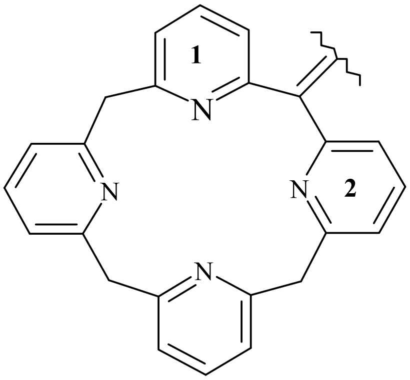
[1,2′-binaphthalene]-1′,5-diyl (PIN)
[1,2′-binaphthyl]-1′,5-diyl

[1,2′-binaphthalen]-4(1*H*)-ylidene (PIN)
[1,2′-binaphthyl]-4(1*H*)-ylidene

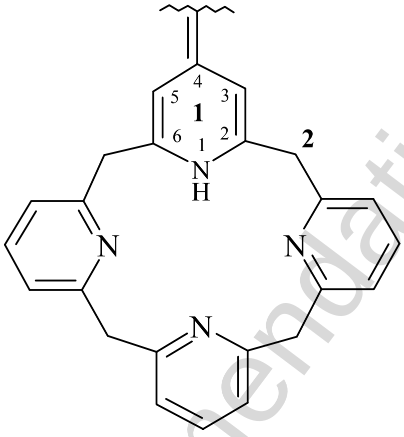
P-29.3.6 Substituent groups derived from cyclophanes

Substituent groups derived from cyclophanes are formed by applying the principles described above.

Examples:



(I)



(II)

(I) 1,5,7(2,6)-tetrapyridinacyclooctaphan-2-ylidene (PIN)
(II) 1,3,5,7(2,6)-tetrapyridinacyclooctaphan-1^4(1^1*H*)-ylidene (PIN)

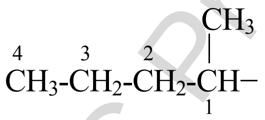
P-29.4 Compound substituent groups

A compound substituent group is formed by substituting one or more simple substituents into another simple substituent considered as the principal chain. The choice of the principal chain is fully discussed in Section P-47. The first criterion to be applied is that the principal chain is the longest chain.

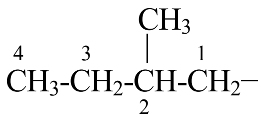
Monovalent branched substituent groups derived from homogeneous chains are named by prefixing the designation of the side chains to the name of the unbranched substituent group possessing the longest possible chain starting from the atom having the free valence, the atom with the free valence being numbered ‘1’. The presence of identical simple substituent groups is indicated by the appropriate multiplying prefix ‘di’, ‘tri, ‘tetra’, etc.

Names of substituent groups are formed in accordance with P-29.3.

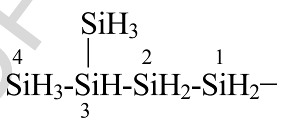
Examples:


$\overset{4}{\mathrm{CH_3}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\underset{1}{\overset{\overset{\mathrm{CH_3}}{|}}{\mathrm{CH}}}-$

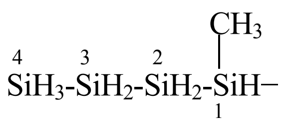
1-methylbutyl
pentan-2-yl (PIN, see P-29.2.2)


$\overset{4}{\mathrm{CH_3}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\underset{2}{\overset{\overset{\mathrm{CH_3}}{|}}{\mathrm{CH}}}\text{-}\overset{1}{\mathrm{CH_2}}-$

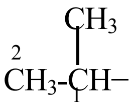
2-methylbutyl (PIN)


$\overset{4}{\mathrm{SiH_3}}\text{-}\underset{3}{\overset{\overset{\mathrm{SiH_3}}{|}}{\mathrm{SiH}}}\text{-}\overset{2}{\mathrm{SiH_2}}\text{-}\overset{1}{\mathrm{SiH_2}}-$

3-silyltetrasilan-1-yl (PIN)

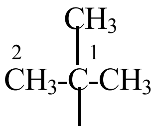

$\overset{4}{\mathrm{SiH_3}}\text{-}\overset{3}{\mathrm{SiH_2}}\text{-}\overset{2}{\mathrm{SiH_2}}\text{-}\underset{1}{\overset{\overset{\mathrm{CH_3}}{|}}{\mathrm{SiH}}}-$

1-methyltetrasilan-1-yl (PIN)



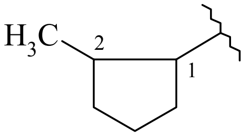
$\overset{2}{CH_3}\text{-}\underset{1}{\overset{\overset{CH_3}{|}}{C}}H-$

1-methylethyl
propan-2-yl (PIN, see P-29.2.2)

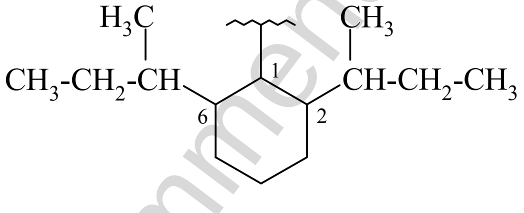


$\overset{2}{CH_3}\text{-}\underset{|}{\overset{\overset{CH_3}{|}\,1}{C}}\text{-}CH_3$

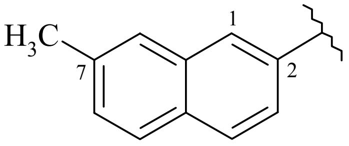
1,1-dimethylethyl (numbering shown)
2-methylpropan-2-yl (PIN, see P-29.2.2)



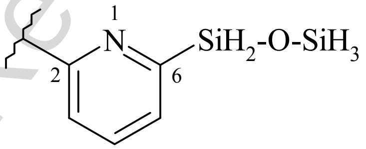
2-methylcyclopentyl (PIN)



2,6-bis(1-methylpropyl)cyclohexyl
2,6-di(butan-2-yl)cyclohexyl (PIN)



7-methylnaphthalen-2-yl (PIN)



6-disiloxanylpyridin-2-yl (PIN)_

P-29.5 Compound catenated substituent groups

Compound catenated substituent groups are used only in multiplicative nomenclature (see P-15.3). Names are formed by adding di- or polyvalent substituent groups to one another, specifically by adding the names of peripheral substituent groups to that of the central substituent group, as prescribed in multiplicative nomenclature.

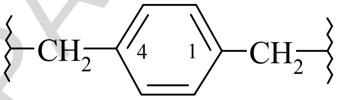
Examples:

$-CH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}CH_2-$

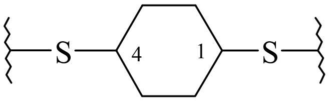
silanediyldiethane-1,2-diyl (PIN)

$-SiH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}SiH_2-$

methylenebis(disilane-1,2-diyl) (PIN)



1,4-phenylenebis(methylene) (PIN)
(1,4-phenylene is a preferred
retained IUPAC name, see P-29.6)



cyclohexane-1,4-diylbis(sulfanediyl) (PIN)

P-29.6 Retained names for substituent groups derived from parent structures.

This Section describes retained names of substituent groups derived from parent structures. Some are IUPAC preferred names as well as names to be used in general nomenclature. The substitutability of each structure is indicated in the same manner as for the parent structures of P-34 and P-55. These types are more fully described in P-46.

Substitutability of substituent groups derived from parent structures with retained names is classified into three main types:

Type 1. Unlimited substitution by substituent groups cited as suffixes or prefixes;

Type 2. Limited substitution classified as follows:

Type 2a. Substitution limited to substituent groups cited as prefixes in recognition of functional groups explicitly expressed or implied in the functional parent compound name;

Type 2b. Substitution limited to substituent groups cited as compulsory prefixes;

Type 2c. Substitution for parent structures not covered by Type 2a or 2b.

Type 3. Substitution of any kind not allowed

Table 2.9 lists retained names for substituent groups derived from parent structures and their substitutability as defined above for use in general nomenclature and as the preferred IUPAC name, if the retained name is also the preferred IUPAC name.

To facilitate the choice of preferred IUPAC prefix names, all usual prefixes, including those described below, are listed in Appendix 2, with clear indications as to their preferred status in IUPAC nomenclature of organic compounds

In retained names, when a locant is necessary to identify a position, it is placed at the front of the name.

Table 2.10 Retained names for substituent groups derived from parent hydrides.

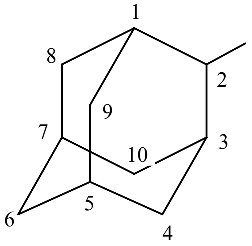
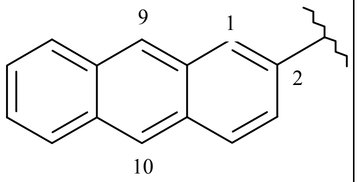
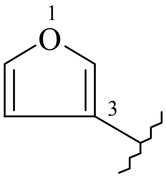
Retained Name	Structure	Substitution Type for General Nomenclature	PIN	Substitution Type for PIN
2-adamantyl (also 1-isomer)		Type 2a	adamantan-2-yl (also 1-isomer)	
2-anthryl (also 1- and 9- isomers)		Type 2a	anthracen-2-yl (also 1- and 9- isomers	
benzyl	C_6H_5-CH_2–	Type 2c	benzyl	Type 3
benzylidene	C_6H_5-CH=	Type 2c	benzylidene	Type 3
benzylidyne	C_6H_5-C≡	Type 2a	benzylidyne	Type 3
tert-butyl	$(CH_3)_3C$–	Type 3	*tert*-butyl	Type 3
ethylene	–CH_2CH_2–	Type 2a	ethane-1,2-diyl	
3-furyl (also 2- isomer)		Type 2a	furan-3-yl (also 2- isomer)	
hydrazinyl	NH_2-NH–	Type 2a	hydrazinyl	Type 2a
isopropyl	$(CH_3)_2$CH–	Type 3	propan-2-yl	

Table 2.9 (cont'd.)

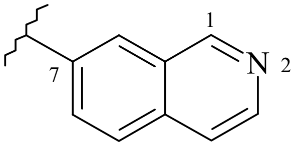
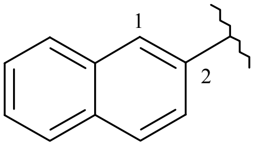
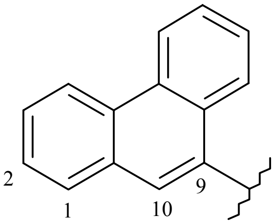
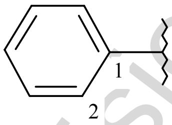
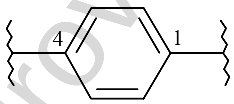
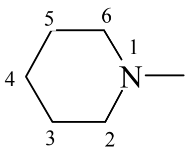
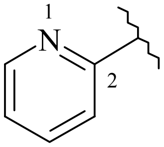
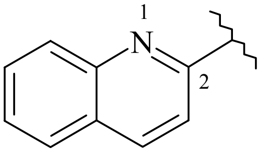
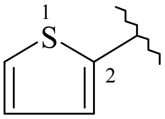
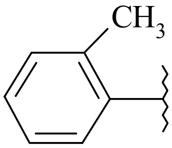
isopropylidene	$(CH_3)_2C=$	Type 3	propan-2-ylidene	
7-isoquinolyl (also 1-, 3-, 4-, 5-, 6-, and 8-isomers)		Type 2a	isoquinolin-7-yl (also 1-, 3-, 4-, 5-, 6-, and 8- isomers)	
methylene	–CH₂–	Type 2a	methylene	Type 2a
2-naphthyl (also 1- isomer)		Type 2a	naphthalen-2-yl (also 1- isomer)	
9-phenanthryl (also 1-, 2-, 3-, and 4- isomers)		Type 2a	phenanthren-9-yl (also 1-, 2-, 3-, and 4- isomers)	
phenyl		Type 2a	phenyl	Type 2a
1,4-phenylene (also 1,2- and 1,3-isomers) (not *o*-, *m*-, or *p*-isomers)		Type 2a	1,4-phenylene (also 1,2- and 1,3-isomers) (not *o*-, *m*-, or *p*-isomers)	Type 2a
1-piperidyl (not piperidino) (also 2-,3-,and 4-isomers)		Type 2a	piperidin-1-yl (also 2-, 3-, and 4- isomers)	

Table 2.9 (cont'd.)

2-pyridyl (also 3- and 4- isomers)		Type 2a	pyridin-2-yl (also 3- and 4- isomers)
2-quinolyl (also 3-, 4-, 5-, 6-, 7-, and 8- isomers)		Type 2a	quinolin-2-yl (also 3-, 4-, 5-, 6-, 7-, and 8- isomers)
styryl	C_6H_5-CH=CH–	Type 3	2-phenylethenyl
2-thienyl (also 3- isomer)		Type 2a	thiophen-2-yl (also 3- isomer) (CAS uses thiophene-2-yl)
o-tolyl (also *m*- and *p*- isomers		Type 3	2-methylphenyl (also 3- and 4- isomers)
trityl	$(C_6H_5)_3C$–	Type 3	triphenylmethyl

CHAPTER P-3 CHARACTERISTIC (FUNCTIONAL) GROUPS

P-30 Introduction

The prefixes and/or suffixes attached to a parent name specify a particular molecular structure and usually represent **substituents** of various types, which are considered to take the place of hydrogen atoms of the parent hydride or parent structure. It has been customary to regard such substituents as **characteristic** (or **functional**) when the link between substituent and parent is not a carbon-carbon bond, for example, −OH, =O and $-NH_2$, but exceptions are recognized, such as −COOH and −CN. It seems appropriate to retain the general view of **functionality** as implying the presence of heteroatoms, but it would not be helpful to attempt to define precisely the limits of application of the term.

Carbon-carbon unsaturation in acyclic and alicyclic compounds is regarded by IUPAC as a special type of functionality and is therefore treated here in Chapter P-3 rather than in Chapter P-2 (Parent hydrides). Its presence here and that of the hydrogenation of parent hydrides having the maximum number of noncumulative double bonds (mancude parent hydrides) is logical for nomenclature, as the unsaturation in acyclic and alicyclic parent hydrides expressed by endings and the saturation of mancude parent hydrides by hydro-dehydro prefixes are essentially equivalent.

This Chapter also deals with **functional parent compounds**, i.e., structures that may be treated as parent structures, having substitutable hydrogen atoms, but possessing characteristics normally associated with functionality, e.g., acetic acid, CH_3-COOH and phosphonic acid $HP(O)(OH)_2$. Functional parent compounds must be distinguished from compounds having a characteristic group systematically introduced as a suffix attached to a parent hydride, for example butanoic acid and ethanol. The latter compounds may be called ‘functionalized parent hydrides’.

Although, strictly speaking, **ions** and **radicals** do not fall within the concept of functionality as described above, an ionic center or a radical center is treated like a function and expressed in the same way as characteristic groups, i.e., by suffixes and prefixes. This treatment is introduced in this Chapter and fully discussed in Chapter P-7.

Any characteristic group is expressed in a name either as suffix or as prefix. As prefixes, they are detachable (alphabetizable) prefixes, as are the prefixes derived from parent hydrides discussed in section P-29.

P-31 Modification of the degree of hydrogenation of parent hydrides

P-31.0 Introduction

Parent hydrides are divided into two groups, fully saturated or fully unsaturated. Fully unsaturated cyclic parent hydrides are, by convention, defined as having the maximum number of noncumulative double bonds, also called ‘mancude’ compounds (an acronym for MAximum Number of nonCUmulated DoublE bonds). Thus a degree of hydrogenation different from those denoting these two groups must be expressed by an additive or subtractive operation corresponding to the addition or the subtraction of hydrogen atoms. Specific rules are devised for compounds having saturated and unsaturated parts, such as cyclophanes, spiro compounds, etc.

The state of hydrogenation of parent hydrides is modified in two ways: (a) by a subtractive operation (subtraction of two or more hydrogen atoms) denoted by the ‘ene’ and ‘yne’ endings or by the prefix ‘dehydro’; or (b) by an additive operation (addition of two or more hydrogen atoms) denoted by the prefix ‘hydro’.

It is important to take note that endings ‘ene’ and ‘yne’ and ‘hydro’ and ‘dehydro’ prefixes are detachable. When used to modify parent hydrides, they are regulated by the principle of lowest locants, in accord with the numbering of the parent hydride and after priority has been given to indicated hydrogen, added hydrogen, and suffixes, when present, as specified in the general rules for numbering (P-14.4).

P-31.1 The endings ‘ene’ or ‘yne’

P-31.1.1 General methodology

P-31.1.1.1 The presence of one or more double or triple bonds in an otherwise saturated parent hydride (except for parent hydrides with Hantzsch-Widman names or retained names denoting partial hydrogenation as indicated later) is denoted by changing the ending ‘ane’ of the name of a saturated parent hydride to ‘ene’ or ‘yne’. Locants as low as possible are given to multiple bonds as a set, even though this may at times give ‘yne’ endings lower locants than ‘ene’ endings. If a choice remains, preference for low locants is given to the double bonds. In names, the ending ‘ene’ always precedes ‘yne’, with elision of the final letter ‘e’ in ‘ene’. Only the lower locant for a multiple bond is cited except when the numerical difference between the two locants is greater than one, in which case the higher locant is enclosed in parentheses.

Examples:

$\overset{1}{C}H_2=\overset{2}{C}H-\overset{3}{C}H_2-\overset{4}{C}H_3$

but-1-ene (PIN)

$H\overset{1}{C}\equiv\overset{2}{C}-\overset{3}{C}H_3$

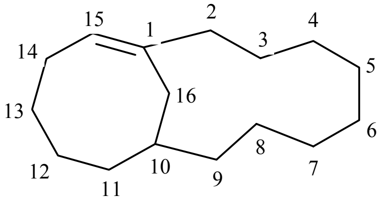
prop-1-yne (PIN)

$\overset{1}{C}H\equiv\overset{2}{C}-\overset{3}{C}H=\overset{4}{C}H-\overset{5}{C}H_3$

pent-3-en-1-yne (PIN)

$\overset{1}{C}H_2=\overset{2}{C}H-\overset{3}{C}H_2-\overset{4}{C}\equiv\overset{5}{C}H$

pent-1-en-4-yne (PIN)



bicyclo[8.5.1]hexadec-1(15)-ene (PIN)

P-31.1.1.2 The multiplying prefixes ‘di’, ‘tri’, etc., are placed before endings denoting unsaturation to indicate the number of multiple bonds of each kind, as required, for example ‘diene’ and ‘triyne’. For euphonic reasons, when the endings ‘ene’ and ‘yne’ are preceded by a multiplying prefix and a locant, the letter ‘a’ is inserted. There is no elision of the final letter ‘a’ of a multiplying prefix before ‘ene’ or ‘yne’, for example, ‘tetraene’ and ‘pentayne’.

Examples:

$\overset{1}{C}H_2=\overset{2}{C}H-\overset{3}{C}H=\overset{4}{C}H_2$

buta-1,3-diene (PIN)

$\overset{1}{C}H_2=\overset{2}{C}H-\overset{3}{C}H=\overset{4}{C}H-\overset{5}{C}H=\overset{6}{C}-\overset{7}{C}H=\overset{8}{C}H-\overset{9}{C}H_3$

nona-1,3,5,7-tetraene (PIN)

The method of P-31.1.1 is applicable to the following saturated hydrocarbon parent hydrides and to the corresponding hydrides modified by skeletal replacement (‘a’) nomenclature that are described in Chapter 2.

P-31.1.2 Acyclic parent hydrides
P-31.1.3 Monocyclic parent hydrides
P-31.1.4 Bi- and polycyclic von Baeyer parent hydrides
P-31.1.5 Spiro parent hydrides composed of monocyclic rings
P-31.1.6 Phane parent hydrides
P-31.1.7 Ring assembly parent hydrides (under specific conditions)

The method is not used to modify Hantzsch-Widman names for saturated heterocyclic compounds or totally or partially hydrogenated mancude compounds having retained names (indane, imidazolidine, indoline, isoindoline, morpholine, piperazine, piperidine, pyrazolidine, pyrrolidine, quinuclidine, and also chromane, isochromane, and their chalcogen analogues).

When necessary, the corresponding mancude compounds are modified by using prefixes ‘hydro’ or ‘dehydro’, as indicated in P-31.2, below.

P-31.1.2 Acyclic parent hydrides

P-31.1.2.1 Retained names

The name acetylene is retained for the compound HC≡CH. It is the preferred IUPAC name, but substitution of any kind is not allowed. Substitution is allowed in general nomenclature, but not by alkyl groups or any other group that extends the carbon chain, or by characteristic groups expressed by suffixes.

The name allene, for $CH_2=C=CH_2$, is retained for general use only. Substitution is allowed, but not by alkyl or any other group that extends the carbon chain, or characteristic groups expressed by suffixes.

The name isoprene, for $CH_2=C(CH_3)-CH=CH_2$, is retained but only for general nomenclature No substitution of any kind is allowed.

P-31.1.2.2 Systematic names

P-31.1.2.2.1 Homogeneous acyclic parent hydrides and acyclic parent hydrides composed of alternating heteroatoms are modified by the general method of P-31.1.1.

Examples:

1 2 3 4 5 6
$CH_2\text{-}CH=CH\text{-}CH_2\text{-}CH_2\text{-}CH_3$

hex-2-ene (PIN)

1 2 3 4
$CH_3\text{-}C\equiv C\text{-}CH_3$

but-2-yne (PIN)
(not dimethylacetylene)

1 2 3 4 5 6
$CH_3\text{-}CH=C=C\text{-}CH_2\text{-}CH_3$

hexa-2,3-diene (PIN)
(not 1-ethyl-3-methylallene)

1 2 3 4 5 6
$CH_2=CH\text{-}CH=CH\text{-}C\equiv CH$

hexa-1,3-dien-5-yne (PIN)

1 2 3 4 5
$H_2N\text{-}N=N\text{-}NH\text{-}NH_2$

pentaaz-2-ene
(preselected name, see P-12.2)

1 2 3 4 5 6
$SiH_3\text{-}SiH=SiH\text{-}SiH_2\text{-}SiH_2\text{-} SiH_3$

hexasil-2-ene
(preselected name, see P-12.2)

1 2
$HSi\equiv SiH$

disilyne
(preselected name, see P-12.2)

1 2 3 4 5
$HP=N\text{-}P=N\text{-}PH_2$

triphosphaza-1,3-diene
(preselected name, see P-12.2)

P-31.1.2.2.2 Acyclic parent hydrides modified by skeletal replacement (‘a’) nomenclature

Locants are assigned to unsaturation sites in chains in accordance with the fixed numbering of the hetero chain. If a choice remains, then lowest locants are assigned to unsaturated sites.

Examples:

1 2 3 4 5 6 7 8 9 10 11 12 13 14
$CH_3\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH{=}CH_2$

2,5,8,11-tetraoxatetradec-13-ene (PIN)

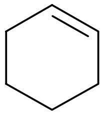
12 11 10 9 8 7 6 5 4 3 2 1
$CH_3\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH{=}CH\text{-}O\text{-}CH_3$

2,5,8,11-tetraoxadodec-3-ene (PIN)

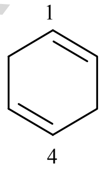
P-31.1.3 Monocyclic parent hydrides

P-31.1.3.1 In monocyclic homogeneous unsaturated compounds, one double or triple bond is always allocated the locant ‘1’. When alone, locant ‘1’ is omitted in names.

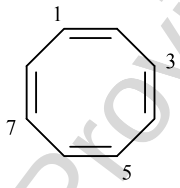
Examples:



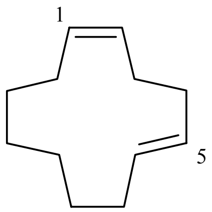
cyclohexene (PIN)



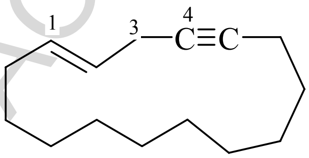
cyclohexa-1,4-diene (PIN)



cycloocta-1,3,5,7-tetraene (PIN)

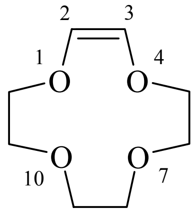


cyclododeca-1,5-diene (PIN)

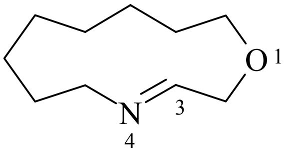


cyclopentadec-1-en-4-yne (PIN)

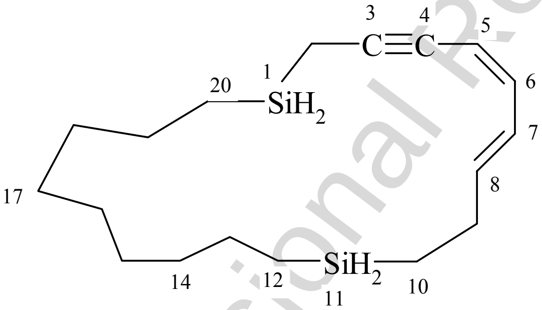
P-31.1.3.2 In rings modified by skeletal replacement (‘a’) nomenclature, low locants are assigned first to heteroatoms and then to unsaturated sites.
Examples:



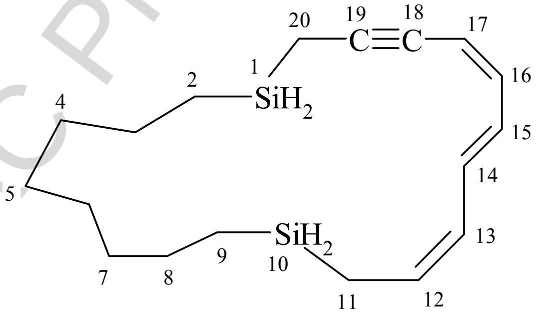
1,4,7,10-tetraoxacyclododec-2-ene (PIN)



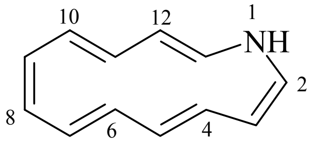
1-oxa-4-azacyclododec-3-ene (PIN)



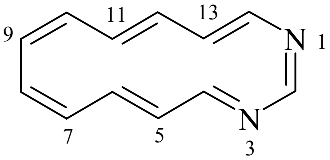
1,11-disilacycloicosa-5,7-dien-3-yne (PIN)
(not 1,11-disilacycloicosa-4,6-dien-8-yne; the locant set ‘3,5,7’ is lower than ‘4,6,8’)



1,10-disilacycloicosa-12,14,16-trien-18-yne (PIN)



1-azacyclotrideca-2,4,6,8,10,12-hexaene (PIN)
1*H*-1-aza[13]annulene



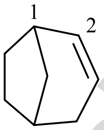
1,3-diazacyclotetradeca-1,3,5,7,9,11,13-heptaene (PIN)
1,3-diaza[14]annulene

P-31.1.4 Bi- and polycyclic von Baeyer parent hydrides

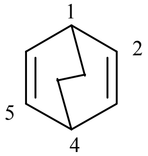
It should be noted that some bi- and polycyclic von Baeyer parent hydrides qualify for phane names as preferred IUPAC names.

P-31.1.4.1 Low locants are allocated first in accordance with the fixed numbering of the ring system. Low locants are allocated for double bonds when the atoms of each bond have consecutive locants.

Examples:



bicyclo[3.2.1]oct-2-ene (PIN)

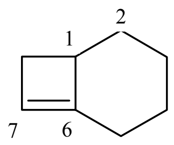


bicyclo[2.2.2]octa-2,5-diene (PIN)

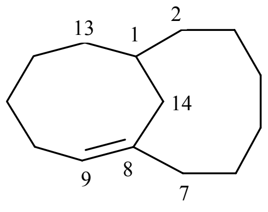
P-31.1.4.2 If there is a choice of names and numbering, the following criteria are considered in order until a decision is reached.

(1) Minimum number of compound locants. A compound locant is used for a double bond if the locants of the atoms at each end of the bond do not differ by a value of one. When a compound locant is required, the higher locant is cited in parentheses. A benzene ring is shown and described as a cyclohexatriene corresponding to the Kekulé structure. Other aromatic rings are treated similarly, when required.

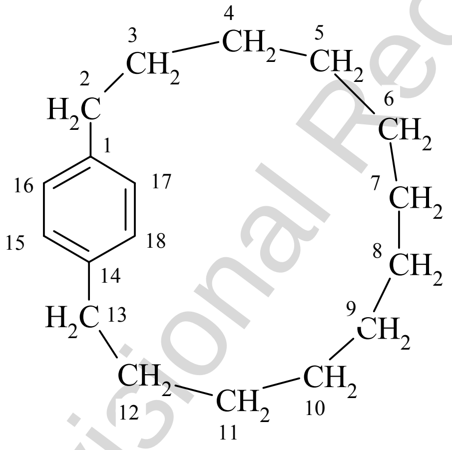
Examples:



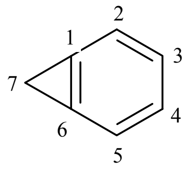
bicyclo[4.2.0]oct-6-ene (PIN)
[not bicyclo[4.2.0]oct-1(8)-ene]



bicyclo[6.5.1]tetradec-8-ene (PIN)
[not bicyclo[6.5.1]tetradec-1(13)-decene;
this is a change from R-3.1.1 in the Guide(ref. 2)]



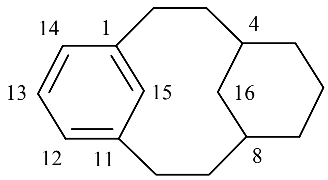
bicyclo[12.2.2]octadeca-1(16),14,17-triene
[not bicyclo[12.2.2]octadeca-1(17),14(18),15-triene]
1(1,4)-benzenacyclotridecaphane (PIN, see P-52.5.2.2)



bicyclo[4.1.0]hepta-1,3,5-triene (PIN)
[not bicyclo[4.1.0]hepta-1(6),2,4-triene]

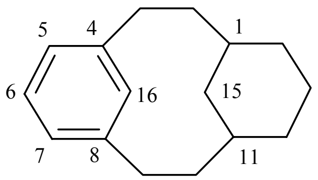
(2) When comparing double bond locants including compound locants any number in parentheses is ignored.

Examples:



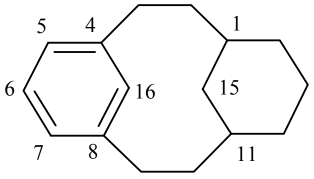
(I)

not



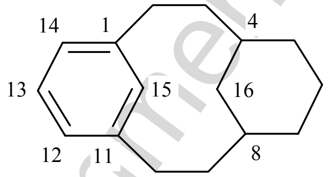
(II)

nor



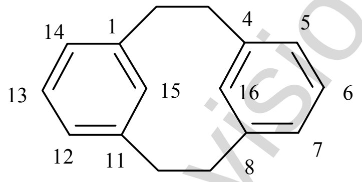
(III)

nor



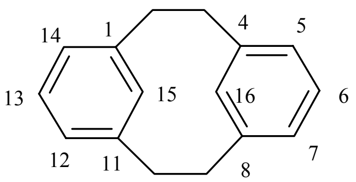
(IV)

tricyclo[9.3.1.1^{4,8}]hexadeca-1(15),11,13-triene (**I**)
[not tricyclo[9.3.1.1^{4,8}]hexadeca-4(16),5,7-triene (**II**)**;**
nor tricyclo[9.3.1.1^{4,8}]hexadeca-4,6,8(16)-triene (**III**);
nor tricyclo[9.3.1.1^{4,8}]hexadeca-1(14),11(15),12-triene (**IV**)]
[the set of locants 1,11,13 in (**I**) is lower than 4,5,7 in (**II**) and 4,6,8 in (**III**);
(**IV**) has two compound locants whereas (**I**) has only one compound locant]
1(1,3)-cyclohexana-4(1,3)-benzenacyclohexaphane (PIN, see P-52.5.2.2)



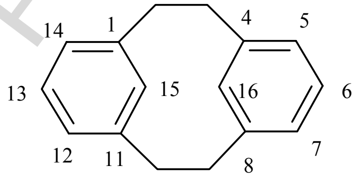
(I)

not



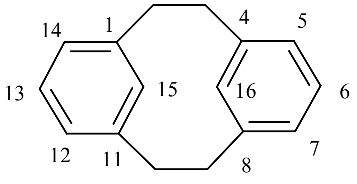
(II)

nor



(III)

nor



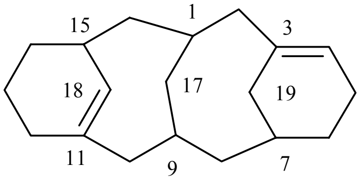
(IV)

tricyclo[9.3.1.1^{4,8}]hexadeca-1(15),4(16),5,7,11,13-hexaene (**I**) (PIN)
[not tricyclo[9.3.1.1^{4,8}]hexadeca-1(15),4,6,8(16),11,13-hexaene (**II**);

nor tricyclo[9.3.1.1^{4,4}]hexadeca-1(14),4,6,8(16),11(15),12-hexaene (**III**);
nor tricyclo[9.3.1.1^{4,8}]hexadeca-1(14),4(16)5,7,11(15)12-hexaene (**IV**)]
[the set of locants in (**I**), '1,4,5,7,11,13' is lower than '1,4,6,8,11,13' in (**II**); and also name (**I**) has two compound locants compared to three in names (**III**) and (**IV**)]
1,4(1,3)-dibenzenecyclohexaphane (PIN, see P-52.5.2.2)

(3) if there is still a choice, low locants are selected considering all locants as a set.

Example:



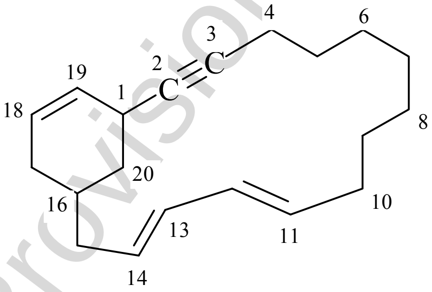
tetracyclo[7.7.1.1^{3,7}.1^{11,15}]nonadeca-3,11(18)-diene (PIN)
[not tetracyclo[7.7.1.1^{3,7}.1^{11,15}]nonadeca-3(19),11-diene;
the locant set 3,11,18 is lower than 3,11,19]

P-31.1.4.3 Bi- and polycyclic von Baeyer structures with both double and triple bonds

If there are double and triple bonds present, the following criteria for numbering are considered, in order, until a decision is reached.

(1) Lower locants are assigned to multiple bonds as a set.

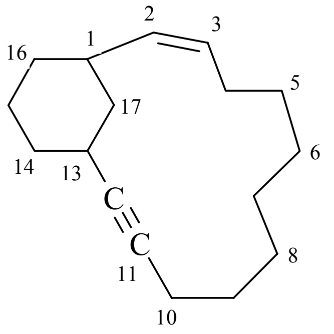
Example:



bicyclo[14.3.1]icosa-11,13,18-trien-2-yne (PIN)
(not bicyclo[14.3.1]icosa-3,5,17-trien-14-yne;
the locant set 2,11,13,18 is lower than 3,5,14,17)

(2) Lower locants are assigned to double bonds.

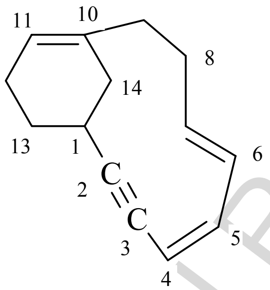
Example:



bicyclo[11.3.1]heptadec-2-en-11-yne (PIN)
(not bicyclo[11.3.1]heptadec-11-en-2-yne)

(3) Compound locants are kept to a minimum.

Example:

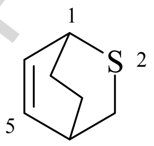


bicyclo[8.3.1]tetradeca-4,6,10-trien-2-yne (PIN)
(not bicyclo[8.3.1]tetradeca-1(13),4,6-trien-8-yne)

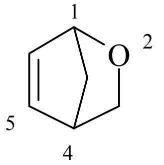
P-31.1.4.4 Bi- and polycyclic von Baeyer heterocycles names by skeletal replacement (‘a’) nomenclature

In heterocyclic compounds formed by using skeletal replacement (‘a’) nomenclature, low locants are assigned to heteroatoms, in accord with the fixed numbering of the system, then to unsaturated sites.

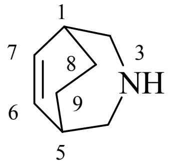
Examples:



2-thiabicyclo[2.2.2]oct-5-ene (PIN)



2-oxabicyclo[2.2.1]hept-5-ene (PIN)



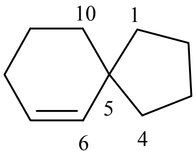
3-azabicyclo[3.2.2]non-6-ene (PIN)

P-31.1.5 Spiro compounds

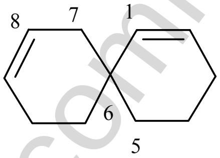
P-31.1.5.1 Spiro compounds composed of saturated rings

P-31.1.5.1.1 Low locants are assigned to double bonds in accordance with the fixed numbering of the spiro compound.

Examples:



spiro[4.5]dec-6-ene (PIN)

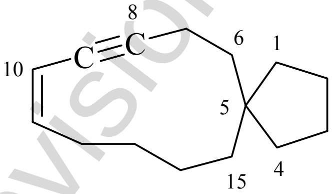


spiro[5.5]undeca-1,8-diene (PIN)

P-31.1.5.1.2 If there are double and triple bonds present, the following criteria are considered, in order, until a decision is reached.

(1) Lower locants are assigned to multiple bonds as a set..

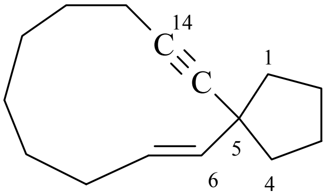
Example:



spiro[4.10]pentadec-10-en-8-yne (PIN)

(2) If there is still a choice, low locants are assigned to double bonds.

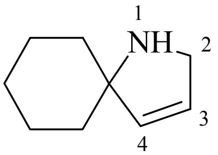
Example:



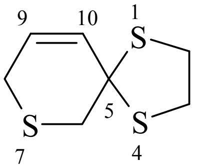
spiro[4.10]pentadec-6-en-14-yne (PIN)

P-31.1.5.1.3 Heteroatoms in spiro compounds consisting of monocyclic rings denoted by skeletal replacement ('a') nomenclature have priority for low locants.

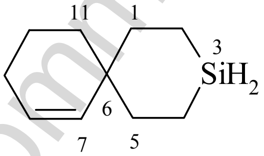
Example:



1-azaspiro[4.5]dec-3-ene (PIN)



1,4,7-trithiaspiro[4.5]dec-9-ene (PIN)

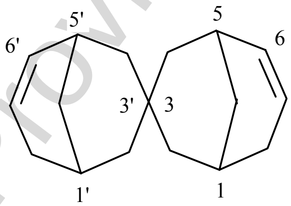


3-silaspiro[5.5]undec-7-ene (PIN)

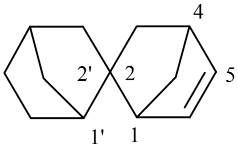
P-31.1.5.2 Spiro compounds composed of identical polycyclic von Baeyer components

Unsaturation in a spiro ring system with one or more components named by the von Baeyer system is indicated by the endings 'ene', 'diene', etc. They are cited after the last bracket of the spiro name; only the final letter 'e' of the saturated hydrocarbon name is elided if followed by a vowel. If there is a choice, low locants are assigned, in order, to spiro junction(s), heteroatoms and double bonds. This is a change from the Guide (ref. 2; see ref. 7)

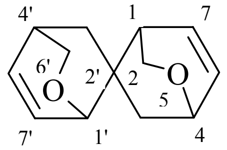
Examples:



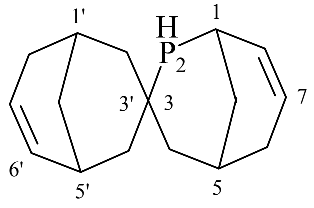
3,3′-spirobi[bicyclo[3.3.1]nonane]-6,6′-diene (PIN)



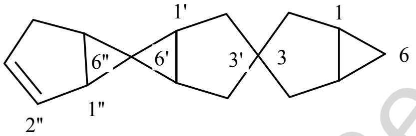
2,2′-spirobi[bicyclo[2.2.1]heptan]-5-ene (PIN)



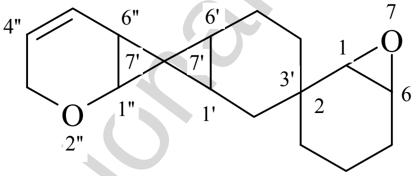
5,6′-dioxa-2,2′-spirobi[bicyclo[2.2.2]octane]-7,7′-diene (PIN)



2-phospha-3,3′-spirobi[bicyclo[3.3.1]nonane]-6′,7-diene (PIN)



3,3′:6′,6″-dispiroter[bicyclo[3.1.0]hex]-2″-ene (PIN)



2″,7-dioxa-2,3′:7′,7″-dispiroter[bicyclo[4.1.0]hexan]-4″-ene (PIN)
[not 5″,7-dioxa-2,3′:7′,7″-dispiroter[bicyclo[4.1.0]hexan]-2″-ene; the locant set ‘2″,7’ is lower than ‘5″,7’ for the ‘oxa’ prefixes]

P-31.1.6 Phane parent hydrides

P-31.1.6.1 Double bonds in amplificants and in simplified phane skeletons

The presence of one or more double or triple bonds in an otherwise saturated phane parent hydride, except in amplificants with Hantzsch-Widman names, is denoted by changing the final letter ‘e’ of the phane parent hydride name to ‘ene’ or ‘yne’, with appropriate multiplying prefixes to indicate the multiplicity of each kind of unsaturated site.

Low locants are allocated for double or triple bonds in accordance with the fixed numbering of the phane parent hydride and of phane parent hydrides that are modified by skeletal replacement (‘a’) nomenclature. Three types of locants are used to fully describe compounds derived from phane parent hydrides:

(1) primary locants, i.e. arabic number locants that denote the atoms and superatoms of the phane parent skeleton;

(2) composite locants, i.e. primary locants with a superscript arabic number locant denoting positions in amplificants (see P-26.4.3);

(3) compound locants, which are primary or composite locants followed by another locant in parentheses, indicating that a double bond is not located between two consecutive locants.

In phane nomenclature, double and triple bonds are denoted in two ways:

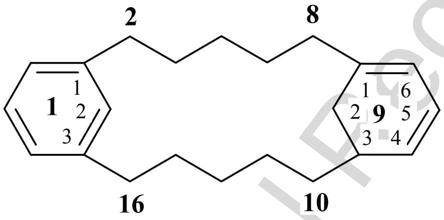
(1) by the lowest locant of a double or triple bond when two consecutive locants are:

   (a) primary locants; or

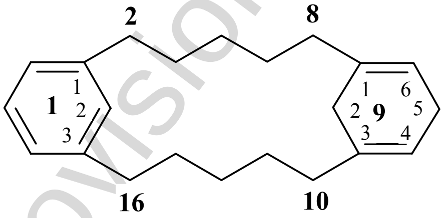
   (b) composite locants, neither of which is adjacent to a primary locant;

(2) by a compound locant, when one locant is a composite locant adjacent to a primary locant.

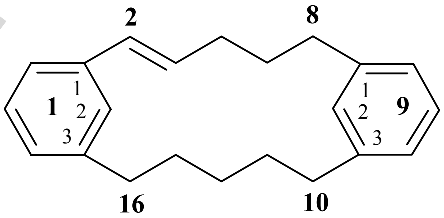
Examples:



1(1,3)-benzena-9(1,3)-cyclohexanacyclohexadecaphane-$9^1(9^6),9^4$-diene (PIN)



1(1,3)-benzena-9(1,3)-cyclohexanacyclohexadecaphane-$9^1(9^6),9^3(9^4)$-diene (PIN)

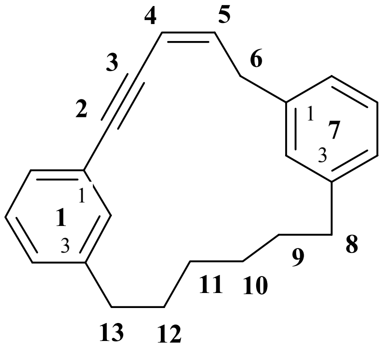


1,9(1,3)-dibenzenacyclohexadecaphan-2-ene (PIN)

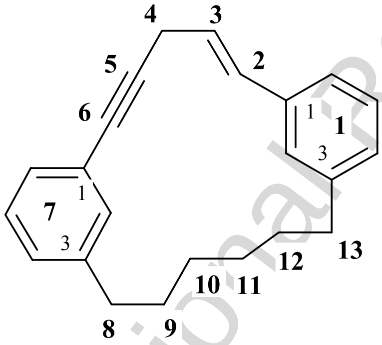
P-31.1.6.2 Phane structures with both double and triple bonds

Double and triple bonds in a phane structure are described by the method of P-31.1.4.4. Low locants are allocated to double and triple bonds first when considered together as a set in ascending order and, if a choice is still needed, to double bonds.

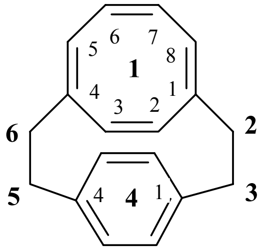
Examples:



1,7(1,3)-dibenzenacyclotridecaphan-4-en-2-yne (PIN)



1,7(1,3)-dibenzenacyclotridecaphan-2-en-5-yne (PIN)

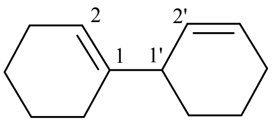


1(1,4)-cyclooctana-4(1,4)-benzenacyclohexaphane-$1^1(1^8)$,2,4,6-tetraene (PIN)

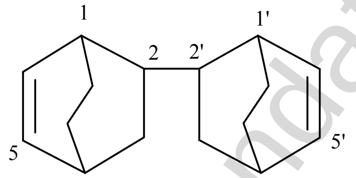
P-31.1.7 Ring assemblies of unsaturated components. Names identified by (1) and (2) are formed according to the two methods given in P-28.2.1. The numbering method is indicated by the letters (a) or (b) according to the two methods given in P-28.3.1.

P-31.1.7.1 Ring assemblies composed of saturated components, monocyclic or alicyclic, are modified by ‘ene’ endings (‘yne’ endings, and any combination of ‘ene’ and ‘yne’ endings are also used when appropriate, in accordance with the general rule P-31.1.1). Low locants are assigned, in order, to ring junctions, heteroatoms and multiple bonds.

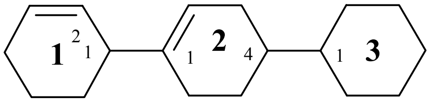
Examples:



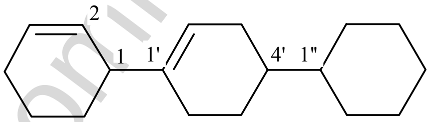
[1,1′-bicyclohexane]-1,2′-diene (PIN)



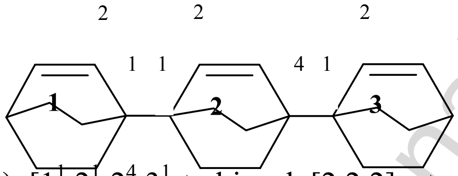
[2,2′-bibicyclo[2.2.2]octane]-5,5′-diene (PIN)



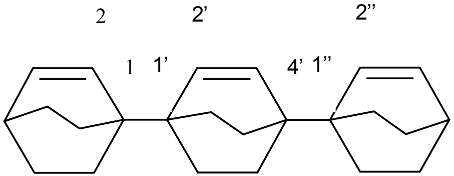
(1a) [$1^1,2^1:2^4,3^1$-tercyclohexane]-$1^2,2^1$-diene (PIN)
(see P-28.2.1; P-28.3.1)



(1b) [1,1′:4′,1″-tercyclohexane]-1′,2-diene
(see P-28.2.1; P-28.3.1)



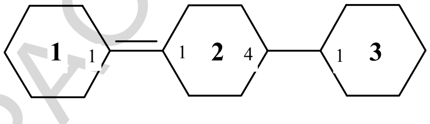
(1a) [$1^1,2^1:2^4,3^1$-terbicyclo[2.2.2]octane]-$1^2,2^2,3^2$-triene (PIN) (see P-28.2.1; P-28.3.1)



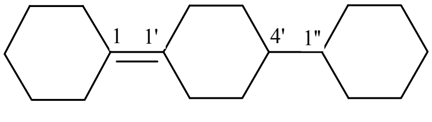
(1b) [1,1′:4′,1″-terbicyclo[2.2.2]octane]-2,2′,2″-triene (see P-28.2.1; P-28.3.1)

P-31.1.7.2 Double bonds linking two rings or ring systems are named in the same way in assemblies composed of three or more identical saturated components. Locants for the terminal position of such bonds are enclosed in parentheses (compound locants).

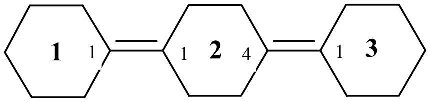
Examples:



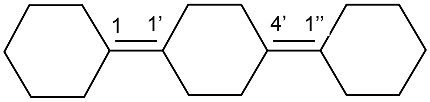
(1a) [$1^1,2^1:2^4,3^1$-tercyclohexan]-$1^1(2^1)$-ene (PIN)
(see P-28.2.1; P-28.3.1)



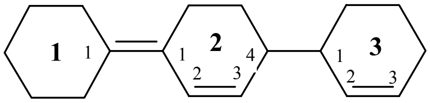
(1b) [1,1′:4′,1″-tercyclohexan]-1(1′)-ene
(see P-28.2.1; P-28.3.1)



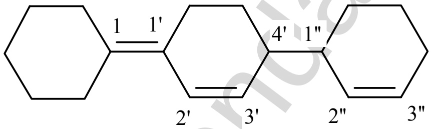
(1a) [1^1,2^1:2^4,3^1-tercyclohexane]-1^1(2^1),2^4(3^1)-diene (PIN)
(see also P-28.2.1; P-28.3.1)



(1b) [1,1′:4′,1″-tercyclohexane]-1(1′),4′(1″)-diene (see also P-28.2.1; P-28.3.1)



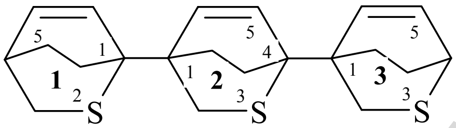
(1a) [1^1,2^1:2^4,3^1-tercyclohexane]-1^1(2^1),2^2,3^2-triene (PIN)
(see also P-28.2.1; P-28.3.1)



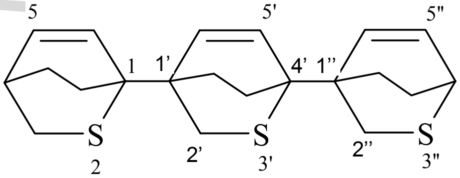
(1b) [1,1′:4′,1″-tercyclohexane]-1(1′),2′,2″-triene (see also P-28.2.1; P-28.3.1)

P-31.1.6.3 When heterocyclic ring assemblies consisting of monocyclic or bi- or polycyclic alicyclic components are named by skeletal replacement ('a') nomenclature, low locants are assigned, in order, to ring junctions, heteroatoms and then unsaturation sites.

Example:



(1a) 1^2,2^3,3^3-trithia[1^1,2^1:2^4,3^1-terbicyclo-[2.2.2]octane]-1^5,2^5,3^5-triene (PIN)
(see also P-28.2.1; P-28.3.1)



(1b) 2,3′,3″-trithia-[1,1′:4′,1″-terbicyclo-[2.2.2]octane]-5,5′,5″-triene
(see P-28.2.1; P-28.3.1)

P-31.2 'Hydro/dehydro' prefixes

P-31.2.1 The prefixes 'hydro/dehydro' are used to indicate addition and subtraction, respectively, of hydrogen atoms to or from mancude compounds.

It is recommended that 'hydro/dehydro' prefixes be considered as detachable prefixes but not included in those prefixes that are cited in alphanumerical order. In names, they are cited immediately at the front of the name of the parent hydride, after alphabetized prefixes and before nondetachable prefixes.

The starting point and direction of numbering of a compound are chosen so as to give lowest locants to the following structural features (if present) considered successively in the order listed until a decision can be made.

(a) fixed numbering of a polycyclic ring system, as in naphthalene, quinoline, etc.

(b) heteroatoms in heterocycles; and heteroatoms in chains modified by skeletal replacement ('a') nomenclature

(c) indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with structural feature (d)].

(d) principal group named as suffix and cumulative suffixes denoting free valences and radical or ionic sites

(e) added hydrogen (consistent with the structure of the compound and in accordance with further substitution)

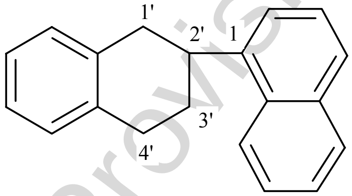
(f) unsaturation-saturation ('ene/yne' endings, and 'hydro/dehydro' prefixes)

(g) substituents named as prefixes (low locants are allocated for substituents regardless of kind; then, if necessary, in the order of citation in the name).

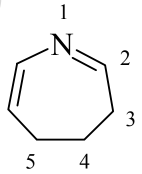
P-31.2.2 General methodology

'Hydro' and 'dehydro' prefixes are associated with the hydrogenation and the dehydrogenation, respectively, of a double bond; thus, multiplying prefixes of even values, as 'di', 'tetra', etc. are used to indicate the saturation of double bond(s), for example 'dihydro', 'tetrahydro', or creation of double bonds, as 'didehydro', etc.. In names, they are placed immediately in front of the name of the parent hydride and any nondetachable prefixes. Indicated hydrogen atoms have priority over 'hydro' prefixes for low locants. If indicated hydrogen atoms are present in a name, the 'hydro' prefixes precede them.

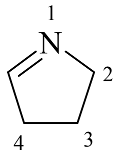
Examples:



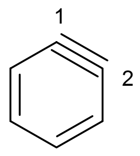
1′,2′,3′,4′-tetrahydro-1,2′-binaphthalene (PIN)



4,5-dihydro-3*H*-azepine (PIN)



3,4-dihydro-2*H*-pyrrole (PIN)



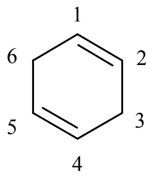
1,2-didehydrobenzene (PIN, see P-31.4.1)
cyclohexa-1,3-dien-5-yne
(not benzyne)

P-31.2.3 The prefix ‘hydro’

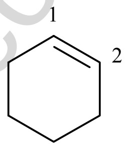
P-31.2.3 Saturation of double bonds in monocyclic mancude compounds

P-31.2.3.1 ‘Hydro’ prefixes are used to modify the degree of hydrogenation of monocyclic mancude compounds having retained or systematic names, except for benzene, for which the traditional names ‘cyclohexene’ and ‘cyclohexadiene’ are recommended.

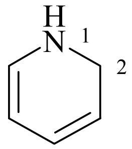
Examples:



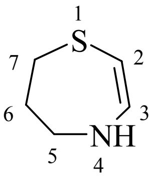
cyclohexa-1,4-diene (PIN)
(not 1,4-dihydrobenzene)



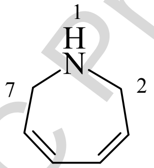
cyclohexene (PIN)
(not 1,2,3,4-tetrahydrobenzene)



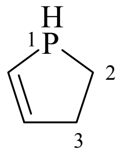
1,2-dihydropyridine (PIN)



4,5,6,7-tetrahydro-1,4-thiazepine (PIN)



2,7-dihydro-1*H*-azepine (PIN)



2,3-dihydro-1*H*-phosphole (PIN)

P-31.2.3.2 Retained names for fully hydrogenated monocyclic parent hydrides

Names listed in Table 2.3 (P-22.2.1) are retained names used as preferred IUPAC names and in general nomenclature. They are treated as parent hydrides in all respects, except for the use of suffixes such as ‘-ene’ or ‘-yne’.

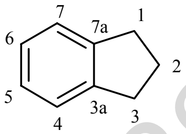
P-31.2.3.3 Saturation of double bonds in polycyclic mancude compounds

P-31.2.3.3.1 Retained names of partially saturated mancude compounds
P-31.2.3.3.2 Polycyclic mancude compounds
P-31.2.3.3.3 Spiro compounds
P-31.2.3.3.4 Phane compounds
P-31.2.3.3.5 Ring assemblies

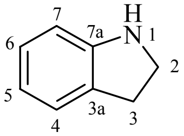
P-31.2.3.3.1 Retained names of partially saturated mancude compounds

Names listed in Table 3.1 are retained names that are not used as preferred IUPAC names. They are, however acceptable in general nomenclature with full substitution, including characteristic groups expressed as suffixes, but not as fusion components nor as amplificants in Phane Nomenclature.

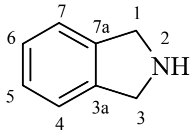
Table 3.1 Retained names of partially saturated polycyclic parent hydrides



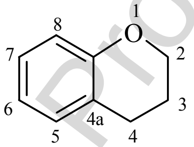
indane
(formerly indan)
2,3-dihydro-1*H*-indene (PIN)



indoline
2,3-dihydro-1*H*-indole (PIN)



isoindoline
2,3-dihydro-1*H*-isoindole (PIN)

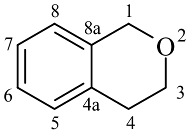


chromane
3,4-dihydro-2*H*-1-benzopyran (PIN)

thiochromane (S instead of O)
3,4-dihydro-2*H*-1-benzothiopyran (PIN)

selenochromane (Se instead of O)
3,4-dihydro-2*H*-1-benzoselenopyran (PIN)

tellurochromane (Te instead of O)
3,4-dihydro-2*H*-1-benzotelluropyran (PIN)



isochromane
3,4-dihydro-1*H*-2-benzopyran (PIN)

isothiochromane (S instead of O)
3,4-dihydro-1*H*-2-benzothiopyran (PIN)

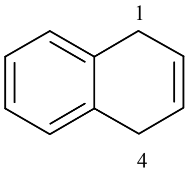
isoselenochromane (Se instead of O)
3,4-dihydro-1*H*-2-benzoselenopyran (PIN)

isotellurochromane (Te instead of O)
3,4-dihydro-1*H*-2-benzotelluropyran (PIN)

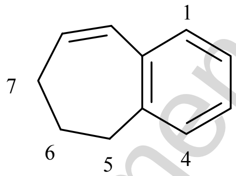
P-31.2.3.3.2 Polycyclic mancude compounds

The degree of hydrogenation of individual mancude ring systems, carbocyclic or heterocyclic, is given by 'hydro' prefixes, in accordance with the general methodology described in P-31.2.2. Total hydrogenation is indicated by the appropriate multiplicative prefixes indicating the total number of hydrogen atoms attached, but locants are omitted [see P-14.3.3 (c)].

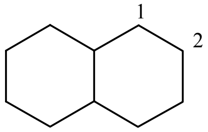
Examples:



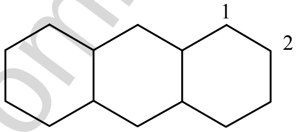
1,4-dihydronaphthalene (PIN)



6,7-dihydro-5*H*-benzo[7]annulene (PIN)



decahydronaphthalene (PIN)

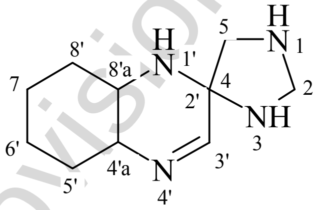


dodecahydroanthracene (PIN)

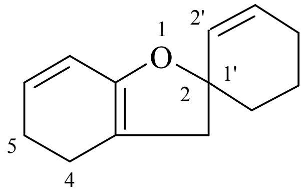
P-31.2.3.3.3 Spiro compounds

Spiro compounds including mancude components are modified in accordance with the general methodology described in P-31.2.2.

Examples:



4′a,5′,6′,7′,8′,8′a-hexahydro-1′*H*-spiro[imidazolidine-4,2′-quinoxaline] (PIN)



4,5-dihydro-3*H*-spiro[1-benzofuran-2,1′-cyclohexan]-2′-ene (PIN)

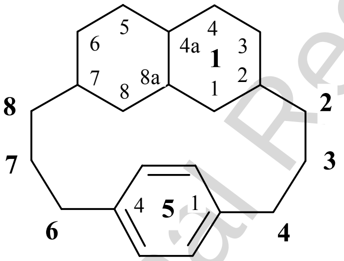
P-31.2.3.3.4 Phane compounds

When the name of an amplificant implies the presence of a maximum number of noncumulated double bonds, other states of hydrogenation are indicated by use of the prefix 'hydro'. This method is applied as follows:

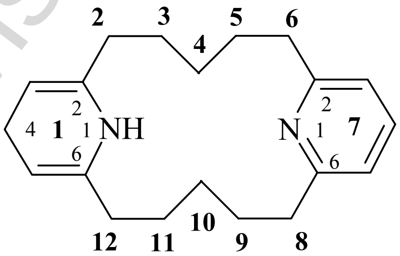
(1) 'Hydro' prefixes are used to modify mancude heteromonocycles having retained names or named in accordance with the extended Hantzsch-Widman system. However, names for the fully saturated heteromonocycles that have retained names or Hantzsch-Widman names are preferred to those expressed by 'hydro' prefixes, for example, oxolane and piperidine are preferred to tetrahydrofuran and hexahydropyridine, respectively.

(2) 'Hydro' prefixes are used to indicate all modifications of the degree of unsaturation of carbocyclic or heterocyclic mancude parent hydrides, except for benzene. Retained names of partially hydrogenated parent hydrides, such as indane and chromane (see P-31.2.3.3.1), are not recommended as amplificants in phane nomenclature.

Examples:



$1^1,1^2,1^3,1^4,1^{4a},1^5,1^6,1^7,1^8,1^{8a}$-decahydro-1(2,7)-naphthalena-5(1,4)-benzenacyclooctaphane (PIN)



$1^1,1^4$-dihydro-1,7(2,6)-dipyridinacyclododecaphane (PIN)

P-31.2.3.5 Ring assemblies

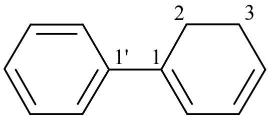
The degree of hydrogenation of ring assemblies composed of mancude components is given by 'hydro' prefixes, in accordance with the general methodology described in P-31.2.2. Since assemblies are considered as parent hydrides, the degree of hydrogenation of the different components can be modified, to a certain extent, in a way that is not allowed for the individual component. This is the case of assemblies composed of monocyclic components, in which the names are different for the mancude and the saturated component. Thus, assemblies composed of monocyclic components and those composed of ring systems are treated differently. In the examples that follow, names identified by (1) and (2) are formed according to the two methods given in P-28.2.1; the numbering method is indicated by the letter (a) or (b) according to the two methods given in P-28.3.1.

P-31.2.3.3.5.1 Ring assemblies composed of monocyclic components
P-31.2.3.3.5.2 Ring assemblies composed of ring systems

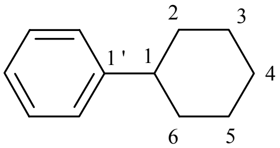
P-31.2.3.3.5.1 Ring assemblies composed of monocyclic components

(a) Ring assemblies composed of monocyclic mancude or saturated hydrocarbons. Low locants are assigned to 'hydro' prefixes in accordance with the fixed numbering of each assembly. In biphenyl and polyphenyl assemblies, one benzene ring must remain in the assembly; otherwise, the starting point is the saturated assembly and the ending 'ene' is used to denote unsaturation (see P-31.1.6). Furthermore, when the modified ring assembly is composed of benzene rings and saturated rings, substitutive nomenclature is preferred (see Chapter 5).

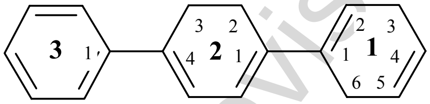
Examples:



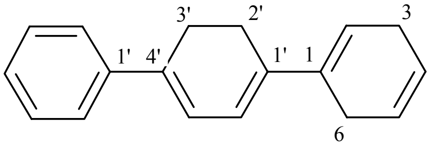
2,3-dihydro-1,1′-biphenyl (PIN)
(numbering shown)
1-(cyclohexa-1,3-dien-1-yl)benzene



cyclohexylbenzene (PIN)
1,2,3,4,5,6-hexahydro-1,1′-biphenyl
(numbering shown)



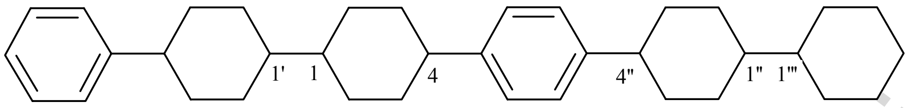
(2a) $1^3,1^6,2^2,2^3$-tetrahydro-$1^1,2^1:2^4,3^1$-terphenyl
(PIN; see also P-28.2.1 and P-28.3.1)



(2b) 2′,3,3′,6-tetrahydro-1,1′:4′,1″-terphenyl
(see also P-28.2.1 and P-28.3.1)

[4-(cyclohexa-1,4-dien-1-yl)cyclohexa-1,3-dien-1-yl]benzene (substitutive name)

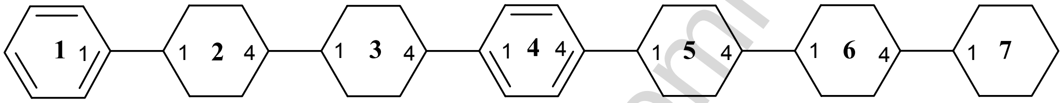
For the following example, the phane name is the preferred IUPAC name (see P-26.4.1.2)



4′-phenyl-4,4″-(1,4-phenylene)di(1,1′-bicyclohexane)
(substitutive name: numbering shown)

(2a) $1^1,1^2,1^3,1^4,1^5,1^6,2^1,2^2,2^3, 2^4, 2^5,2^6,4^1,4^2,4^3,4^4,4^5,4^6,5^1,5^2,5^3,5^4,5^5,5^6$-tetracosahydro-$1^1,2^1,2^4, 3^1,3^4,4^1,4^4,5^1,5^4,6^1$-sexiphenyl (see also P-28.2.1 and P-28.3.1)

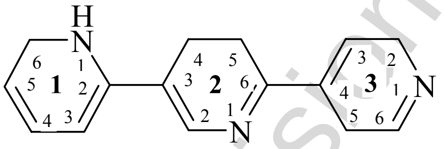
(2b) 1,1′,1‴,1⁗,2,2′,2‴,2⁗,3,3′,3‴,3⁗,4,4′,4‴,4⁗,5,5′,5‴,5⁗,6,6′,6‴,6⁗-tetracosahydro-1,1′:4′,1″:4″,1‴:4‴,1⁗:4⁗,1⁗′-sexiphenyl (see also P-28.2.1 and P-28.3.1)



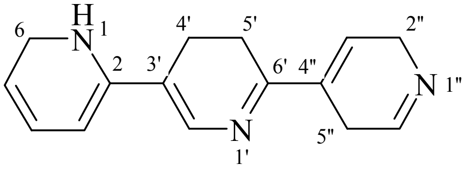
1(1),4(1,4)-dibenzena-2,3,5,6(1,4),7(1)-pentacyclohexanaheptaphane (PIN)

(b) Ring assemblies composed of heteromonocycles. Low locants are assigned to the junctions between rings, then to indicated hydrogen, if any, and finally to ‘hydro’ prefixes.

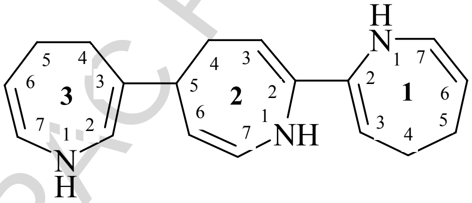
Examples:



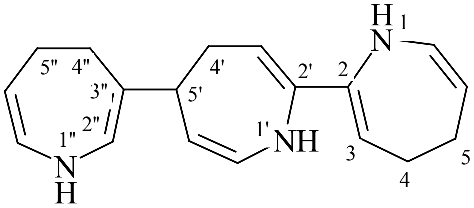
(1a) $1^1,1^6,2^4,2^5,3^2,3^5$-hexahydro-$1^2,2^3:2^6,3^4$-terpyridine (PIN, see also P-28.2.1 and P-28.3.1)



(1b) 1,2″,4′,5′,5″,6-hexahydro-2,3′:6′,4″-terpyridine (see also P-28.2.1 and P-28.3.1)



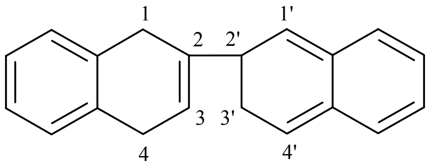
(1a) $1^4,1^5,2^4,2^5,3^4,3^5$-hexahydro-$1^1H,2^1H,3^1H$-$1^2,2^2:2^5,3^3$-terazepine (PIN, see also P-28.2.1 and P-28.3.1)



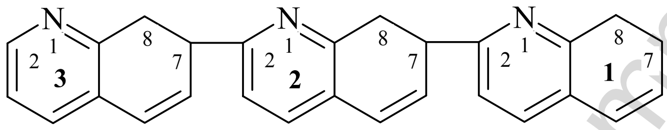
(1b) 4,4′,4″,5,5′,5″-hexahydro-1*H*,1′*H*,1″*H*-2,2′:5′:3″- terazepine (see also P-28.2.1 and P-28.3.1)

P-31.2.3.3.5.2 Ring assemblies composed of polycyclic compounds Low locants are assigned to the junctions between components, then to indicated hydrogen atoms, if any, and finally to ‘hydro’ prefixes.

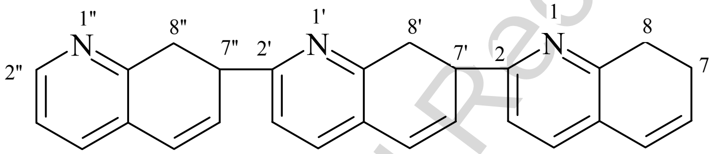
Examples:



1,2′,3′,4-tetrahydro-2,2′-binaphthalene (PIN)



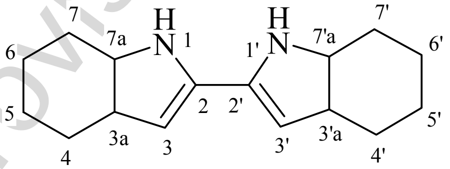
(1a)



(1b)

(1a) $1^7,1^8,2^7,2^8,3^7,3^8$-hexahydro-$1^2,2^7:2^2,3^7$-terquinoline (PIN, see also P-28.2.1 and P-28.3.1)

(1b) 7,7′,7″,8,8′,8″-hexahydro-2,7′:2′,7″-terquinoline (see also P-28.2.1 and P-28.3.1)

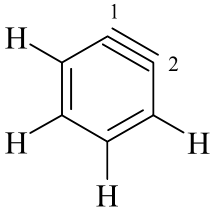


3a,3′a,4,4′a,5, 5′,6,6′,7, 7a,7′,7′a-dodecahydro-1*H*,1′*H*-2,2′-biindole (PIN)

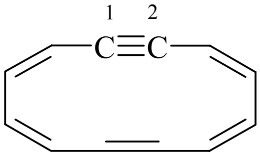
P-31.3 The ‘dehydro’ prefix

P-31.3.1 The subtractive prefix ‘dehydro’ is used to denote the removal of hydrogen atoms and the formation of multiple bonds. Its use is very limited in systematic nomenclature of organic compounds. Applied to benzene, it leads to the name ‘1,2-didehydrobenzene’, that must be used in place of ‘benzyne’ that was formerly used. Applied to annulenes, it leads to didehydro[*n*]annulenes not used in preferred IUPAC names, but acceptable for use in general nomenclature.

Examples:



1,2-didehydrobenzene (PIN)
cyclohexa-1,3-dien-5-yne
(formerly called 'benzyne')

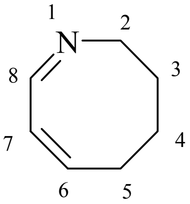


1,2-didehydro[12]annulene
cyclododeca-1,3,5,7,9-pentaen-11-yne (PIN)

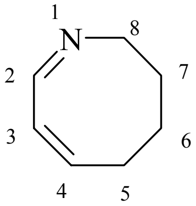
P-31.3.2 The 'dehydro' prefix is more widely used in natural product nomenclature in order to preserve semisystematic names of stereoparents (see P-101.6.6). It is also used in the nomenclature of carbohydrates (ref. 22).

P-31.3.3 The use of the 'dehydro' prefix is not recommended to denote double bond unsaturation in heterocyclic rings having Hantzsch-Widman names. Names must be formed by using the 'hydro' prefix, as shown in the following examples.

Example:



2,3,4,5-tetrahydroazocine (PIN) not



1,2,3,4-tetradehydroazocane

P-32 Substituent prefixes for substituents derived from parent hydrides with a modified degree of hydrogenation

P-32.0 Introduction

Names of substituents derived from the names of the corresponding unsaturated compounds described in Section P-31 are formed by using the appropriate suffixes 'yl', 'ylidene' or 'ylidyne', as described for the formation of substituent prefixes in Section P-29. These names of substituents may contain the endings 'ene' or 'yne', or the prefixes 'hydro' or 'dehydro' in the case of mancude compounds.

P-32.1 Substituent groups derived from parent hydrides with ‘ene’ or ‘yne’ endings

P-32.1.1 Substituents derived from unsaturated acyclic compounds are named in two ways.

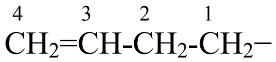
(1) As suffixes have priority for low locants, the position(s) of multiple bonds must be selected in accord with low locants assigned to free valences. These free valences can be in any position of modified parent structure(s). Accordingly, for acyclic parent structures, all locants for the free valences, including ‘1’, must be cited. All locants must be cited for acyclic and cyclic parent structures.

(2) Names can also be formed by substituting simple substituents into larger ones, in a manner similar to saturated prefixes described in Section 29.

> A major change is now recommended to this traditional method. The longest chain must be chosen as the principal chain, not the most unsaturated one. The following examples illustrate this methodology (for preferred IUPAC names see also Chapter 5).

Method (1) leads to preferred IUPAC names

Examples:

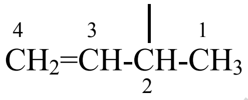


$\overset{4}{CH_2}=\overset{3}{CH}-\overset{2}{CH_2}-\overset{1}{CH_2}-$

(1) but-3-en-1-yl (PIN)

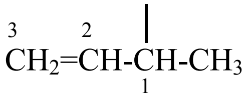
$\overset{3}{CH_2}=\overset{2}{CH}-\overset{1}{CH_2}-$

(1) prop-2-en-1-yl (PIN)



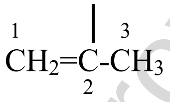
$\overset{4}{CH_2}=\overset{3}{CH}-\underset{2}{\overset{|}{CH}}-\overset{1}{CH_3}$

(1) but-3-en-2-yl (PIN)



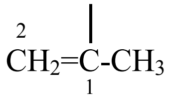
$\overset{3}{CH_2}=\overset{2}{CH}-\underset{1}{\overset{|}{CH}}-CH_3$

(2) 1-methylprop-2-en-1-yl



$\overset{1}{CH_2}=\underset{2}{\overset{|}{C}}-\overset{3}{CH_3}$

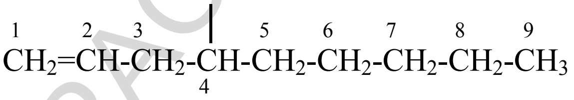
(1) prop-1-en-2-yl (PIN)



$\overset{2}{CH_2}=\underset{1}{\overset{|}{C}}-CH_3$

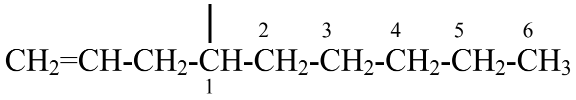
(2) 1-methyleth-1-en-1-yl

isopropenyl (retained name, but not substitutable, see P-32.3)



$\overset{1}{CH_2}=\overset{2}{CH}-\overset{3}{CH_2}-\underset{4}{\overset{|}{CH}}-\overset{5}{CH_2}-\overset{6}{CH_2}-\overset{7}{CH_2}-\overset{8}{CH_2}-\overset{9}{CH_3}$

(1) non-1-en-4-yl (PIN)



$CH_2=CH-CH_2-\underset{1}{\overset{|}{CH}}-\overset{2}{CH_2}-\overset{3}{CH_2}-\overset{4}{CH_2}-\overset{5}{CH_2}-\overset{6}{CH_3}$

(2) 1-(prop-2-en-1-yl)hexyl
(not 1-pentylbut-3-en-1-yl)

$$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{CH}}\text{=}\overset{3}{\mathrm{CH}}\text{-}\underset{4}{\overset{|}{\mathrm{C}}}\mathrm{H}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{CH_2}}\text{-}\overset{7}{\mathrm{CH_3}} \qquad \overset{4}{\mathrm{CH_3}}\text{-}\overset{3}{\mathrm{CH}}\text{=}\overset{2}{\mathrm{CH}}\text{-}\underset{1}{\overset{|}{\mathrm{C}}}\mathrm{H}\text{-}\mathrm{CH_2}\text{-}\mathrm{CH_2}\text{-}\mathrm{CH_3}$$

(1) hept-2-en-4-yl (PIN) (2) 1-propylbut-2-en-1-yl

$$\overset{1}{\mathrm{CH_2}}\text{=}\ \overset{2}{\mathrm{CH}}\text{-}\underset{3}{\overset{|}{\mathrm{C}}}\mathrm{H}\text{-}\overset{4}{\mathrm{CH_2}}\text{-}\underset{5}{\overset{|}{\mathrm{C}}}\mathrm{H}\text{-}\overset{6}{\mathrm{CH}}\text{=}\overset{7}{\mathrm{CH_2}} \qquad \mathrm{CH_2}\text{=}\ \mathrm{CH}\text{-}\underset{1}{\overset{|}{\mathrm{C}}}\mathrm{H}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\underset{3}{\overset{|}{\mathrm{C}}}\mathrm{H}\text{-}\mathrm{CH}\text{=}\mathrm{CH_2}$$

(1) hepta-1,6-diene-3,5-diyl (PIN) (2) 1,3-diethenylpropane-1,3-diyl

$$\overset{4}{\mathrm{CH}}{\equiv}\overset{3}{\mathrm{C}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{CH_2}}-$$

(1) but-3-yn-1-yl (PIN)

$$\overset{8}{\mathrm{CH_3}}\text{-}\overset{7}{\mathrm{C}}{\equiv}\overset{6}{\mathrm{C}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\underset{4}{\overset{\|}{\mathrm{C}}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CH}}\text{=}\overset{1}{\mathrm{CH_2}} \qquad \overset{5}{\mathrm{CH_3}}\text{-}\overset{4}{\mathrm{C}}{\equiv}\overset{3}{\mathrm{C}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\underset{1}{\overset{\|}{\mathrm{C}}}\text{-}\mathrm{CH_2}\text{-}\mathrm{CH}\text{=}\mathrm{CH_2}$$

(1) oct-1-en-6-yn-4-ylidene (PIN) (2) 1-(prop-2-en-1-yl)pent-3-yn-1-ylidene

$$\overset{7}{\mathrm{CH}}{\equiv}\overset{6}{\mathrm{C}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\underset{4}{\overset{|}{\mathrm{C}}}\mathrm{H}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CH}}\text{=}\overset{1}{\mathrm{CH_2}} \qquad \mathrm{CH}{\equiv}\mathrm{C}\text{-}\mathrm{CH_2}\text{-}\underset{1}{\overset{|}{\mathrm{C}}}\mathrm{H}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{3}{\mathrm{CH}}\text{=}\overset{4}{\mathrm{CH_2}}$$

(1) hept-1-en-6-yn-4-yl (PIN) (2) 1-(prop-2-yn-1-yl)but-3-en-1-yl

[In (1) lowest locants are assigned to the double bond;
in (2) the principal chain includes the double bond]

$$\overset{2}{\mathrm{HN}}\text{=}\overset{1}{\mathrm{N}}- \qquad\qquad -\mathrm{N}\text{=}\mathrm{N}-$$

(1) diazenyl
(preselected name, see P-12.2)

(1) diazenediyl
(preselected name, see P-12.2)

$$\overset{3}{\mathrm{HN}}\text{=}\overset{2}{\mathrm{N}}\text{-}\overset{1}{\mathrm{NH}}- \qquad\qquad \overset{2}{\mathrm{HSb}}\text{=}\overset{1}{\mathrm{SbH}}-$$

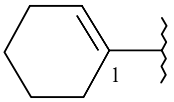
(1) triaz-2-en-1-yl
(preselected name, see P-12.2)

(1) distibenyl
(preselected name, see P-12.2)

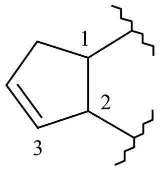
P-32.1.2 Monocyclic substituent groups

Method (1) described in P-32.1.1 is used to name monocyclic substituent groups.

Examples:



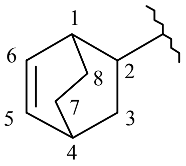
cyclohex-1-en-1-yl (PIN)



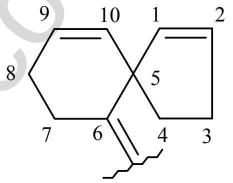
cyclopent-3-ene-1,2-diyl (PIN)

P-32.1.3 Substituent groups derived from parent hydrides having a fixed numbering. Lowest possible locants are assigned first to free valence(s), then to unsaturated sites, in accordance with the fixed numbering of the parent hydride.

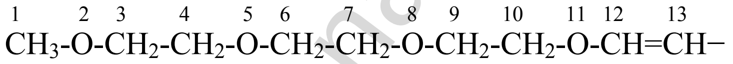
Examples:



bicyclo[2.2.2]oct-5-en-2-yl (PIN)



spiro[4.5]deca-1,9-dien-6-ylidene (PIN)



$$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{O}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{CH_2}}\text{-}\overset{5}{\mathrm{O}}\text{-}\overset{6}{\mathrm{CH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{8}{\mathrm{O}}\text{-}\overset{9}{\mathrm{CH_2}}\text{-}\overset{10}{\mathrm{CH_2}}\text{-}\overset{11}{\mathrm{O}}\text{-}\overset{12}{\mathrm{CH}}{=}\overset{13}{\mathrm{CH}}-$$

2,5,8,11-tetraoxatridec-12-en-13-yl (PIN)
(not 3,6,9,12-tetraoxatridec-1-en-1-yl; the suffix '-yl' is added to the parent hydride name 2,5,8,11-tetraoxatridecane)

P-32.2 Substituent groups derived from partially hydrogenated mancude parent hydrides

Names of substituent groups are formed in accord with the following order of seniority (see P-14.4) for assigning lowest possible locants. Indicated and added hydrogen atoms must be cited in names.

(a) fixed numbering (naphthalene, bicyclo[2.2.2]octane, etc.)

(b) heteroatoms in heterocycles

(c) indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with the structural feature (d)]

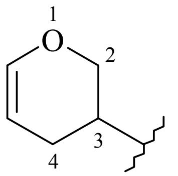
(d) free valence suffix

(e) added hydrogen (consistent with the structure of the compound and in accordance with further substitution)

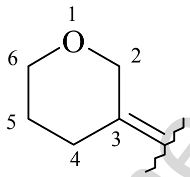
(f) saturation (‘hydro’/‘dehydro’ prefixes) or unsaturation (‘ene’, ‘yne’ endings)

(g) substituents named as prefixes (low locants are allocated for substituents regardless of kind; then, if necessary, in the order of citation).

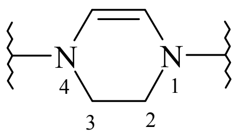
Examples:



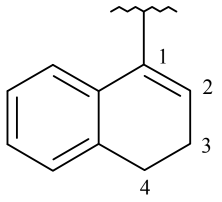
3,4-dihydro-2*H*-pyran-3-yl (PIN)



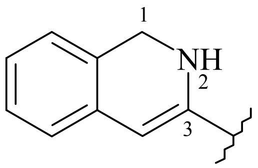
5,6-dihydro-2*H*-pyran-3(4*H*)-ylidene (PIN)



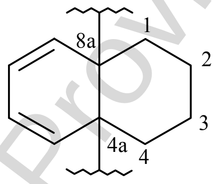
2,3-dihydropyrazine-1,4-diyl (PIN)



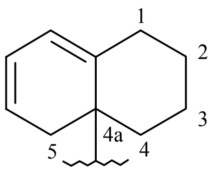
3,4-dihydronaphthalen-1-yl (PIN)



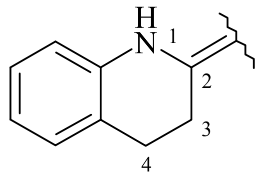
1,2-dihydroisoquinolin-3-yl (PIN)



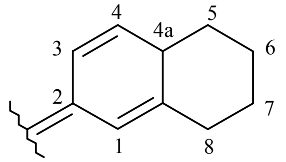
1,2,3,4-tetrahydronaphthalene-4a,8a-diyl (PIN)



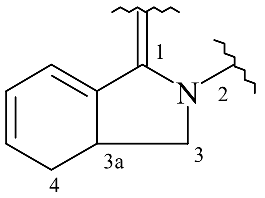
1,3,4,5-tetrahydronaphthalen-4a(2*H*)-yl (PIN)



3,4-dihydroquinolin-2(1*H*)-ylidene (PIN)



5,6,7,8-tetrahydronaphthalen-2(4a*H*)-ylidene (PIN)



3a,4-dihydro-1*H*-isoindol-2(3*H*)-yl-1-ylidene (PIN)

P-32.3 Retained names for prefixes derived from unsaturated acyclic parent hydrides

The following names are retained but are not used as preferred IUPAC names, which are formed systematically; these names are acceptable for general use, with substitution as defined in P-29.6.

$CH_2{=}CH{-}$

vinyl
ethenyl (PIN)

$CH_2{=}C{=}$

vinylidene
ethenylidene (PIN)

$\overset{3}{CH_2}{=}\overset{2}{CH}{-}\overset{1}{CH_2}{-}$

allyl
prop-2-en-1-yl (PIN)

$\overset{3}{CH_2}{=}\overset{2}{CH}{-}\overset{1}{CH}{=}$

allylidene
prop-2-en-1-ylidene (PIN)

$\overset{3}{CH_2}{=}\overset{2}{CH}{-}\overset{1}{C}{\equiv}$

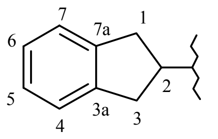
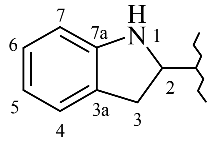
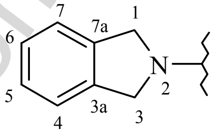
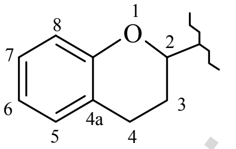
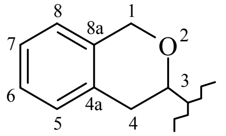
allylidyne
prop-2-en-1-ylidyne (PIN)

The retained name isopropenyl, for $CH_2{=}C(CH_3){-}$, is not used as a preferred IUPAC name. It is acceptable for general use, but no substitution is allowed. The preferred IUPAC name is prop-1-en-2-yl.

P-32.4 Retained names for prefixes derived from partially saturated mancude parent hydrides.

The names in Table 3.2 are retained but are not used as preferred IUPAC names, which are formed systematically; these names are acceptable for general use, with full substitution.

Table 3.2 Retained names of prefixes for partially saturated polycyclic parent hydrides

 indan-2-yl (also 1-, 4-, and 5- isomers) 2,3-dihydro-1*H*-inden-2-yl (PIN) (also, 1-, 4-, and 5- isomers)	
 indolin-2-yl (also 1-, 3-, 4-, 5-, 6-, and 7- isomers) 2,3-dihydro-1*H*-indol-2-yl (PIN) (also, 1-, 3-, 4-, 5-, 6-,and 7- isomers)	 isoindolin-2-yl (also 1-, 4-, and 5- isomers) 2,3-dihydro-1*H*-isoindol-2-yl (PIN) (also, 1-, 4-, and 5- isomers)
 chroman-2-yl (also 3-, 4-, 5-, 6-, 7-, and 8- isomers) 3,4-dihydro-2*H*-1-benzopyran-2-yl (PIN) (also 3-, 4-, 5-, 6-, 7-, and 8- isomers) thiochroman-2-yl (S instead of O) (also 3-, 4-, 5-, 6-, 7-, and 8- isomers) 3,4-dihydro-2*H*-1-benzothiopyran-2-yl (PIN) (also 3-, 4-, 5-, 6-, 7-, and 8- isomers) selenochroman-2-yl (Se instead of O) (also 3-, 4-, 5-, 6-, 7-, and 8- isomers) 3,4-dihydro-2*H*-1-benzoselenopyran-2-yl (PIN) (also 3-, 4-, 5-, 6-, 7-, and 8- isomers) tellurochroman-2-yl (Te instead of O) (also 3-, 4-, 5-, 6-, 7-, and 8- isomers) 3,4-dihydro-2*H*-1-benzotelluropyran (PIN) (also 3-, 4-, 5-, 6-, 7-, and 8- isomers)	 isochroman-3-yl (also 1-, 4-, 5-, 6-, 7-, and 8- isomers) 3,4-dihydro-1*H*-2-benzopyran-3-yl (PIN) (also 1-, 4-, 5-, 6-, 7-, and 8- isomers) isothiochroman-3-yl (S instead of O) (also 1-, 4-, 5-, 6-, 7-, and 8- isomers) 3,4-dihydro-1*H*-2-benzothiopyran-3-yl (PIN) (also 1-, 4-, 5-, 6-, 7-, and 8- isomers) isoselenochroman-3-yl (Se instead of O) (also 1-, 4-, 5-, 6-, 7-, and 8- isomers) 3,4-dihydro-1*H*-2-benzoselenopyran-3-yl (PIN) (also 1-, 4-, 5-, 6-, 7-, and 8- isomers) tellurochroman-2-yl (Te instead of O) (also 1-, 4-, 5-, 6-, 7-, and 8- isomers) 3,4-dihydro-1*H*-2-benzotelluropyran (PIN) (also 1-, 4-, 5-, 6-, 7-, and 8- isomers)

P-33 Suffixes

P-33.0 Introduction

This Section includes names of substituents denoting characteristic groups expressed as suffixes. These characteristic groups are essentially those having free valence(s) on atoms such as the chalcogens (O, S, Se, Te) and nitrogen. The concept is extended to carbon atoms linked to halogens, chalcogens and nitrogen, such as −CO-Cl, −CO-OH, −CS-SH, −CHO, −CN. Radicals and ions are expressed by suffixes in substitutive nomenclature although they are not classified as characteristic groups.

Suffixes describing characteristic groups are divided into 'functional suffixes' and 'cumulative suffixes'. Functional suffixes are used to denote characteristic groups; they are exclusive because only one of them can be placed at the end of a name to represent the principal characteristic group or function. Suffixes designating radicals and ions, on the other hand, can be used in association with each other and also in association with functional suffixes. In names, functional suffixes are always attached to the name of the parent hydride. Cumulative suffixes can be attached directly to the names of parent hydrides; but when functional suffixes are present, cumulative suffixes are attached to them.

Examples:

$CH_4 \longrightarrow CH_5^+$

methane (PIN) methanium (PIN)
(the suffix '-ium' indicates addition of H^+)

$CH_4 \longrightarrow CH_3\text{-}NH_2 \longrightarrow CH_3\text{-}NH_4^+$

methane (PIN)
methanamine (PIN)
(the suffix '-amine' indicates substitution)
methanaminium (PIN)
(the suffix '-ium' indicates addition of H^+)

P-33.1 Functional suffixes

Functional suffixes are classified as 'basic suffixes' and 'derived suffixes'.

P-33.1.1 Basic suffixes

Basic suffixes are those composed only of oxygen and/or nitrogen, with or without association with carbon, as in the case of carboxylic acids, amides, nitriles and aldehydes, and also with sulfur to denote sulfonic acids and sulfinic acids, and the corresponding amides and hydrazides. They are listed in Table 3.3

The suffix ‘peroxol’, for –OOH, has been added to the list of basic suffixes. It is modified by functional replacement generating the suffixes ‘–*OS*-thioperoxol’ for –OSH, and ‘–*SO*-thioperoxol’ for –SOH. The suffix ‘sulfenic acid’, for –SOH, was abandoned in the 1993 Recommendations.

Table 3.3 Basic suffixes, in decreasing order of seniority for citation as the principal characteristic group

	Formula	Basic suffix		Formula	Basic suffix
(1)	–CO-OH	carboxylic acid (PIN)	(9)	–CN	carbonitrile (PIN)
(2)	–(C)O-OH	oic acid (PIN)	(10)	–(C)N	nitrile (PIN)
(3)	–SO$_2$-OH	sulfonic acid (PIN)	(11)	–CHO	carbaldehyde (PIN)
(4)	–SO-OH	sulfinic acid (PIN)	(12)	–(C)HO	al (PIN)
(5)	–CO-NH$_2$	carboxamide (PIN)	(13)	=O	one (PIN)
(6)	–(C)O-NH$_2$	amide (PIN)	(14)	–OH	ol (PIN)
(7)	–CO-NNH$_2$	carbohydrazide (PIN)	(15)	–OOH	peroxol (PIN)
(8)	–(C)O-NNH$_2$	hydrazide (PIN)	(16)	–NH$_2$	amine (PIN)
			(17)	=NH	imine (PIN)

P-33.1.2 Derived suffixes

Derived suffixes are formed in various ways by modifying basic suffixes.

(1) Suffixes including a carbon atom are modified by functional replacement by using infixes to indicate the replacement of oxygen atoms by –OO–, –S–, =S, –Se–, =Se, –Te–, =Te, =NH and =NNH$_2$, as indicated in P-15.5; it is to be noted that the letter ‘x’ of ‘carboxylic’ is maintained before a vowel and that the letter ‘o’ is not elided before amide and aldehyde.

Examples:

–CO-OH	carboxylic acid (PIN)	–C(O)-OOH	carboperoxoic acid (PIN)
		–C(O)-SH	carbothioic *S*-acid (PIN)
		–C(Se)-OH	carboselenoic *O*-acid (PIN)
		–C(=NH)-OH	carboximidic acid (PIN)
		–C(=NNH$_2$)-OH	carbohydrazonic acid (PIN)
		–C(=NH)-SH	carboximidothioic acid (PIN)
–CO-NH$_2$	carboxamide (PIN)	–C(Te)-NH$_2$	carbotelluroamide (PIN)
–CO-NHNH$_2$	carbohydrazide (PIN)	–C(S)-NHNH$_2$	carbothiohydrazide (PIN)
–CHO	carbaldehyde (PIN)	–CHS	carbothioaldehyde (PIN)

(2) Suffixes not including a carbon atom are modified by functional replacement, by using prefixes to indicate the replacement of oxygen atoms by –OO–, –S–, =S, –Se–, =Se, –Te–, =Te, =NH and =NNH$_2$, as indicated in P-15.5; it is to be noted that the letter ‘o’ is not elided before amide and that an additional ‘o’ is elided from ‘imido’ before ‘oic’.for euphonic reasons.

Examples:

–(C)O-OH	oic acid (PIN)	–(C)O-OOH	peroxoic acid (PIN)
		–(C)O-SH	thioic *S*-acid (PIN)
		–(C)Te-OH	telluroic *O*-acid (PIN)
		–(C)(=NH)-OH	imidic acid (PIN) (not imidoic acid)
		–(C)(=NNH$_2$)-OH	hydrazonic acid (PIN)
		–(C)(=NH)-SeH	imidoselenoic acid (PIN)
–(C)O-NH$_2$	amide (PIN)	–(C)S-NH$_2$	thioamide (PIN)
–(C)O-NHNH$_2$	hydrazide (PIN)	–(C)S-NHNH$_2$	thiohydrazide (PIN)
–(C)HO	al (PIN)	–(C)HSe	selenal (PIN)
=O	one (PIN)	=S	thione (PIN)
		=Se	selone (PIN) (not selenone)
		=Te	tellone (PIN) (not tellurone)
–OH	ol (PIN)	–SH	thiol (PIN)
–OOH	peroxol (PIN)	–OSH	*OS*-thioperoxol (PIN)

(3) The stem ‘sulf’ is replaced by ‘selen’ and ‘tellur’ to generate the selenium and tellurium analogues of sulfonic and sulfinic acids.

Examples:

–SO$_2$-OH	sulfonic acid (PIN)	–SeO$_2$-OH	selenonic acid (PIN)
–SO-OH	sulfinic acid (PIN)	–TeO-OH	tellurinic acid (PIN)

(4) Suffixes of the type ‘sulfonic acid’ and analogues are modified by functional replacement by using infixes to indicate the replacement of oxygen atoms by –OO–, –S–, =S, –Se–, =Se, –Te–, =Te, =NH and =NNH$_2$, as indicated in P-15.5.

Examples:

–SO$_2$-OH	sulfonic acid (PIN)	−SO$_2$-OOH	sulfonoperoxoic acid (PIN)
		−S(=NNH)$_2$-OH	sulfonodihydrazonic acid (PIN)
−SeO-OH	seleninic acid (PIN)	−SeO-SH	seleninothioic *S*-acid (PIN)
−TeO$_2$-OH	telluronic acid (PIN)	−Te(=NH)-OH	telluronimidic acid (PIN)
−SO-OH	sulfinic acid (PIN)	−SO(=NNH$_2$)-OH	sulfinohydrazonic acid (PIN)

(5) Names of amides and hydrazides are formed by replacing the ‘ic acid’ ending in suffixes by ‘amide’ or ‘hydrazide’, respectively ; a euphonic letter ‘o’ is added as required:

Examples:

−(C)(=NH)-OH	imidic acid (PIN)
−(C)(=NH)-NH$_2$	imidamide (PIN)
−C(=NH)-OH	carboximidic acid (PIN)
−C(=NH)-NH$_2$	carboximidamide (PIN)
−(C)(=NNH$_2$)-OH	hydrazonic acid (PIN)
−(C)(=NNH$_2$)-NHNH$_2$	hydrazonohydrazide (PIN)
−SO$_2$-OH	sulfonic acid (PIN)
−SO$_2$-NH$_2$	sulfonamide (PIN)
−SeO-OH	seleninic acid (PIN)
−SeO-NHNH$_2$	seleninohydrazide (PIN)

(6) Suffixes with −NH$_2$ and =NH groups substituted by an −OH group are no longer named by using the ‘carbohydroxamic acid’ and ‘carbohydroximic acid’ suffixes. They are now named as *N*-hydroxy derivatives of amides or imides.

Examples:

CH$_3$-CH$_2$-CO-NH$_2$ propanamide (PIN)	CH$_3$-CH$_2$-CO-NH-OH *N*-hydroxypropanamide (PIN) (formerly propanehydroxamic acid)
CH$_3$-CH$_2$-C(=NH)-OH propanimidic acid (PIN)	CH$_3$-CH$_2$-C(=N-OH)-OH *N*-hydroxypropanamidic acid (PIN) (formerly propanehydroximic acid)

P-33.2 Cumulative suffixes

Suffixes used to denote radical and ionic centres in a parent structure are given in Table 3.4. They are classified in decreasing order of seniority, radicals > anions > cations.

Suffixes are added to the name of a parent hydride in the customary mannner, or to suffixes expressing another type of radical or ion, or to suffixes denoting characteristic groups. Names of radicals are formed in the same manner as substituent groups (see P-29.2), with the exception that di- and trivalent radicals centered on a single atom are denoted by the suffixes ‘ylidene’ and ‘ylidyne’, respectively, and never by ‘diyl’ or ‘triyl’.

Table 3.4 Affixes for radical and ionic centers in parent structures

	Operation	Suffix
Radicals	Loss of $H^•$	yl
	Loss of 2 $H^•$	
	from one atom	ylidene
	from different atoms	diyl
	Loss of $3H^•$	
	from one atom	ylidyne
	from different atoms	triyl or ylylidene
	etc.	
Anions	Loss of H^+	ide
		ate
	Addition of H^-	uide
Cations	Loss of H^-	ylium
	Addition of H^+	ium

Examples:

$CH_3\text{-}CH_3$
ethane (PIN)

$CH_3\text{-}CH_2^•$
ethyl (PIN)

$\overset{2}{^-CH_2}\text{-}\overset{1}{CH_2^•}$
ethan-2-id-1-yl (PIN)

$CH_3\text{-}NH_2$
methanamine (PIN)

$CH_3\text{-}NH_3^+$
methanaminium (PIN)

$CH_3\text{-}NH_2^{+}–$
methanaminiumyl (PIN)

P-34 Functional parent structures

P-34.0 Introduction

Many trivial and semisystematic names have been used in organic chemistry. As systematic names have increasingly been preferred, the number of trivial and semisystematic names has been gradually reduced, in the 1979 Rules and again in the 1993 Recommendations. This Section describes the 2005 codification for parent compounds with an implied characteristic group or class.

P-34.1 Definitions

A functional parent is a structure whose name implies the presence of one or more characteristic groups and that has one or more hydrogen atoms attached to at least one of its skeletal atoms or one of its characteristic groups, or in which at least one of its characteristic groups can form at least one kind of functional modification.

Examples:

CH_3-COOH	acetic acid (PIN) (see P-34.4.1)
C_6H_5-NH_2	aniline (PIN) (see P-34.5)
HP(O)$(OH)_2$	phosphonic acid (preselected name, see P-12.2; see Section P-67 for oxo acids of Groups 13, 14, 15, 16 and 17)

A parent hydride bearing a characteristic group denoted by a suffix, for example cyclohexanol, is not considered to be a functional parent compound but may be described as a 'functionalized parent hydride'.

In these Recommendations, parent hydrides whose degree of hydrogenation has been modified are broadly classified as functional parents, for example acetylene and allene (see P-31.1.2.1 and P-32.3), and partially hydrogenated mancude ring systems, for example, indane and indoline (see P- P-31.2.3.3.1 and P-32.4)

P-34.1.1 Functional parents with substitutable hydrogen atoms, i.e., the structure has one or more substitutable hydrogen atoms attached to at least one skeletal atom or one characteristic group

Examples of functional parents and substituent groups:

CH_3-COOH	acetic acid (PIN)	Cl-CH_2-COOH	2-chloroacetic acid (PIN)
H_2N-CO-NH_2	urea (PIN)	NH_2-CO-NH-CH_3	methylurea (PIN)
HP(O)$(OH)_2$	phosphonic acid (preselected name; see P-12.2)		

C_6H_5-P(O)$(OH)_2$ phenylphosphonic acid (PIN)

P-34.1.2 Functional parents having no substitutable hydrogen atoms, i.e., their structure has at least one characteristic group that can form at least one kind of functional modification, for example, formation of esters. These are given preselected names (see P-12).

Examples:

P(O)$(OH)_3$	phosphoric acid (preselected name, see P-12.2)	P(O)$(OCH_3)_3$	trimethyl phosphate (PIN)
N(O)-OH	nitrous acid (preselected name, see P-12.2)	N(O)-O-$[CH_2]_4$-CH_3	pentyl nitrite (PIN)

P-34.2 Types of retained names for functional parent structures

Parent structures are divided into types related to their substitutability, which may differ according to whether the name is required for a preferred IUPAC name or for general nomenclature (see P-46).

Substitutability of functional parent structures with retained names is classified into three types as follows:

Type 1. Unlimited substitution by substituent groups cited as suffixes or prefixes;

Type 2. Limited substitution classified as follows:

Type 2a. Substitution limited to substituent groups cited as prefixes in recognition of functional groups explicitly expressed or implied in the functional parent compound name;

Type 2b. Substitution limited to substituent groups cited as compulsory prefixes;

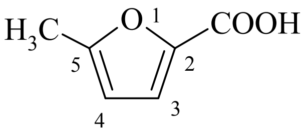
Type 2c. Substitution for parent structures not covered by Type 2a or 2b.

Type 3. Substitution of any kind not allowed.

Type 1 substitution is not common for functional parent compounds. It is used mainly for parent hydrides and their derived substituent prefixes (see P-29.6 and P-46)

Examples of substituted functional parents:

Type 2a:

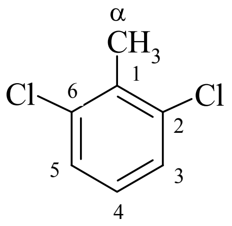


5-methyl-2-furoic acid
5-methylfuran-2-carboxylic acid (PIN)

$Cl_3C\text{-}C\equiv N$

trichloroacetonitrile (PIN)

Type 2c



2,6-dichlorotoluene [no substitution by principal characteristic groups or additional acyclic hydrocarbon groups (see P-46.3)]
1,3-dichloro-2-methylbenzene (PIN)

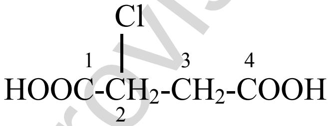
Br-COOH

carbonobromidic acid (PIN)
(not bromoformic acid; formic acid cannot be substituted by an atom or group used in functional replacement nomenclature)

$O_2N\text{-}COOH$

nitroformic acid (PIN, the nitro group is not a group used in functional replacement nomenclature)

Type 3



$\overset{1}{HOOC}\text{-}\underset{2}{\overset{Cl}{C}}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}OOH$

2-chlorobutanedioic acid (PIN)
(not 2-chlorosuccinnic acid)

. $Br\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

3-bromobutanoic acid (PIN)
(not 3-bromobutyric acid)

$H_2N\text{-}\overset{4}{C}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}NH\text{-}CH_3$

N-methylbutanediamide (PIN)
(not *N*-methylsuccinamide; even *N*-substitution is not allowed)

Replacement of the hydrogen atom of a hydroxy group is considered a functionalization rather than a substitution, for instance, in the formation of an ester, and is allowed.

Example:

CH_3-CH_2-CO-O-CH_2-Cl	$(CH_3$-CH_2-CH_2-$CO)_2O$
chloromethyl propanoate (PIN) chloromethyl propionate	butanoic anhydride (PIN) butyric anhydride

P-34.3 Retained names for functional parent compounds having implied characteristic groups or classes

Names of functional parents are trivial names identified as 'retained names'. Some are retained as preferred names and also for use in general nomenclature. Others are not used as preferred names but are acceptable for general use. The complete list of retained names is given in Section P-46. Retained names for unsaturated parent structures and partially saturated parent structures are given in P-31.1.2.1 and P-31.2.3.3.1, respectively. Functional parents are also discussed in Chapter 6 along with systematic names for each class of compounds. The list of names given here is to be considered limiting; however, use of trivial and semisystematic names for compounds covered by special rules, for example amino acids and carbohydrates, is allowed. The substitutability of each structure is indicated by the classification described in P-34.2 above.

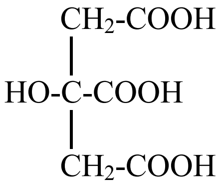
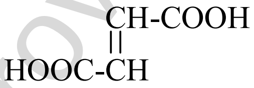
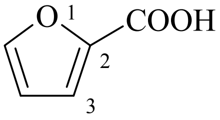
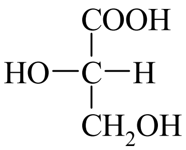
For acid names, functionalization, i.e., the formation of esters, salts, and anhydrides, does not constitute substitution. Similarly, for hydroxy compound names, esters and salts do not constitute substitution. Amides, acyl halides and halogenoids, hydrazides, aldehydes, and nitriles derived from retained names for acids follow the same substitution rules as the corresponding acid.

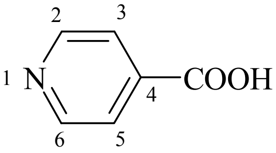
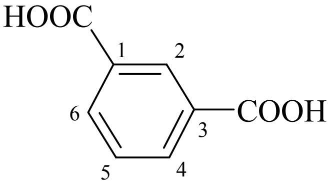
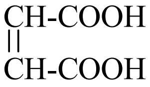
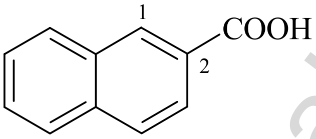
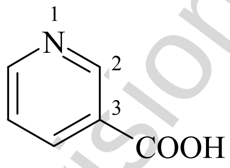
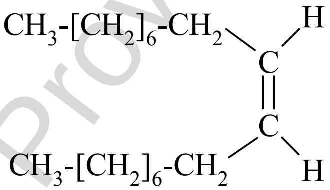
P-34.3.1 Acids
P-34.3.2 Ketones and aldehydes
P-34.3.3 Hydroxy compounds and ethers
P-34.3.4 Amines, amides and other nitrogen compounds

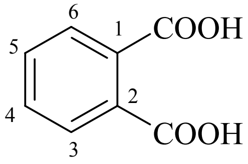
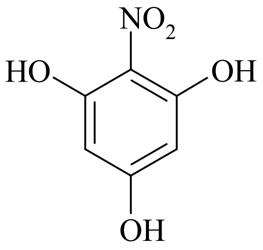
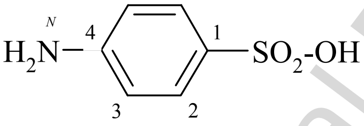
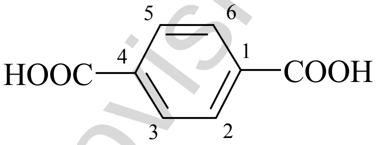
P-34.3.1 Acids

The names of the following carboxylic acids and related classes (amic acids, amides, and acyl groups, etc.) are used, as indicated, as preferred names or in general nomenclature They may be used to form the corresponding imidic acids (see P-65.1.1.3.1.1), hydrazonic acids (see P-65.1.1.3.2.1), amic acids (see P-65.1.1.6.1), aldehydic acids (see P-65.1.1.6.3), acyl groups (see P-65.2), salts and esters (see P-65.4), anhydrides P-65.5), amides (see P-66.1.1.11), imides see P-66.2), hydrazides (see P-66.3.1), amidines (see P-66.4.1), amidrazones (see P-66.4.2), hydrazidines (see P-66.4.3), nitriles (see P-66.5), and aldehydes (see P-66.6).

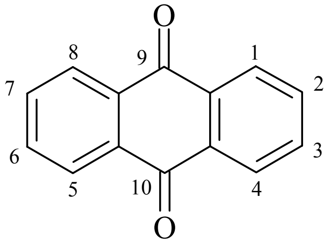
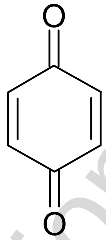
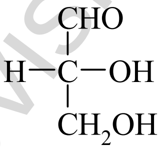
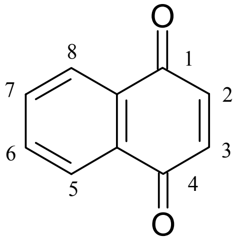
In the following table, 'NA' means 'not applicable'.

Retained Name	Structure	Substitution Type in General Nomenclature	PIN	Substitution Type for PIN
acetic acid	$CH_3\text{-}COOH$	Type 2a	acetic acid	Type 2a
acrylic acid	$CH_2\text{=}CH\text{-}COOH$	Type 3	prop-2-enoic acid	
adipic acid	$HOOC\text{-}[CH_2]_4\text{-}COOH$	Type 3	hexanedioic acid	
benzoic acid	$C_6H_5\text{-}COOH$	Type 2a	benzoic acid	Type 2a
butyric acid	$CH_3\text{-}CH_2\text{-}CH_2\text{-}COOH$	Type 3	butanoic acid	
carbamic acid	$H_2N\text{-}COOH$	Type 2a	carbamic acid	Type 2a
carbonic acid	HO-CO-OH	NA	carbonic acid	NA
citric acid	 $\begin{matrix} CH_2\text{-}COOH \\ \vert \\ HO\text{-}C\text{-}COOH \\ \vert \\ CH_2\text{-}COOH \end{matrix}$	Type 3	2-hydroxypropane-1,2,3-tricarboxylic acid	
cinnamic acid	$C_6H_5\text{-}CH\text{=}CH\text{-}COOH$	Type 3	3-phenylprop-2-enoic acid	
cyanic acid	NCOH	NA	cyanic acid	NA
formic acid	HCOOH	Type 2c	formic acid	Type 2c
fumaric acid	 $\begin{matrix} & CH\text{-}COOH \\ & \Vert \\ HOOC\text{-}CH & \end{matrix}$	Type 3	(*E*)-but-2-enoic acid	
2-furoic acid (also 3- isomer)		Type 2a	furan-2-carboxylic acid	
glutaric acid	$HOOC\text{-}[CH_2]_3\text{-}COOH$	Type 3	pentanedioic acid	
glyceric acid	 $\begin{matrix} & COOH & \\ & \vert & \\ HO- & C & -H \\ & \vert & \\ & CH_2OH & \end{matrix}$	Type 3	2,3-dihydroxypropanoic acid	

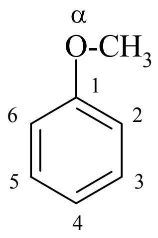
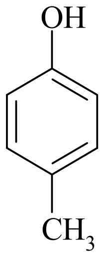
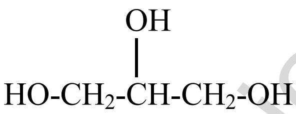
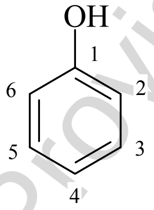
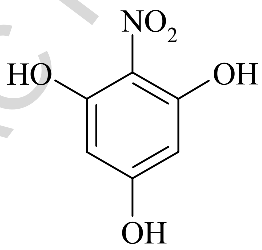
isonicotinic acid		Type 2a	pyridine-4-carboxylic acid	
isophthalic acid		Type 2a	benzene-1,3-dicarboxylic acid	
lactic acid	CH_3-CH(OH)-COOH	Type 3	2-hydroxypropanoic acid	
maleic acid	 $\begin{array}{l}\text{CH-COOH}\\ \text{\|\|}\\ \text{CH-COOH}\end{array}$	Type 3	(*Z*)-but-2-enoic acid	
malonic acid	HOOC-CH_2-COOH	Type 3	propanedioic acid	
methacrylic acid	CH_2=C(CH_3)-COOH	Type 3	2-methylprop-2-enoic acid	
2-naphthoic acid (also 1- isomer)		Type 2a	naphthalene-2-carboxylic acid (also 3- isomer)	
nicotinic acid		Type 2a	pyridine-3-carboxylic acid	
oleic acid		Type 3	(*Z*)-octadec-9-enoic acid	
oxalic acid	HO-CO-CO-OH	NA	oxalic acid	NA
oxaldehydic acid	HCO-COOH	Type 2c	oxaldehydic acid	Type 2a
oxamic acid	H_2N-CO-CO-OH	Type 2a	oxamic acid	Type 2a
palmitic acid	CH_3-[CH_2]$_{14}$-COOH	Type 3	hexadecanoic acid	

phthalic acid		Type 2a	benzene-1,2-dicarboxylic acid
picric acid		Type 3	2-nitrobenzene-1,3,5-triol
propionic acid	CH_3-CH_2-COOH	Type 3	propanoic acid
pyruvic acid	CH_3-CO-COOH	Type 3	2-oxopropanoic acid
stearic acid	CH_2-$[CH_2]_{16}$-COOH	Type 3	octadecanoic acid
succinic acid	HOOC-CH_2-CH_2-COOH	Type 3	butanedioic acid
sulfanilic acid (*p*-isomer only)		Type 3	4-aminobenzenesulfonic acid
tartaric acid	HOOC-$[CH(OH)]_2$-COOH	Type 3	2,3-dihydroxybutanedioic acid
terephthalic acid		Type 2a	benzene-1,4-dicarboxylic acid

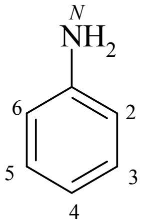
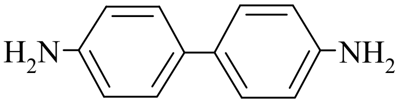
P-34.3.2 Ketones and Aldehydes

Retained Name	Structure	Substitution Type in General Nomenclature	PIN	Substitution Type for PIN
acetone	CH_3-CO-CH_3	Type 2a	propan-2-one	
acetophenone	C_6H_5-CO-CH_3	Type 3	1-phenylethan-1-one	
9,10-anthraquinone (also 1,2-, 1,4-, and 2,3- isomers)		Type 2a	anthracene-9,10-dione (also 1,2-, 1,4-, and 2,3- isomers	
benzophenone	C_6H_5-CO-C_6H_5	Type 3	diphenylmethanone	
1,4-benzoquinone (also 1,2- isomer)		Type 2a	cyclohexa-2,5-diene-1,4-dione (also 3,4-diene-1,2-dione)	
glyceraldehyde	 $\begin{array}{c} \text{CHO} \\ \vert \\ \text{H}-\text{C}-\text{OH} \\ \vert \\ \text{CH}_2\text{OH} \end{array}$	Type 3	2,3-dihydroxypropanal	
ketene	H_2C=C=O	Type 2b	1-ethen-1-one	
1,4-naphthoquinone (also 1,2-, and 2,3- isomers		Type 2a	naphthalene-1,4-dione (also 1,2-, and 2,3- isomers	
oxaldehyde	OCH-CHO	Type 2a	oxaldehyde	Type 2a

P-34.3.3 Hydroxy compounds and ethers

Retained Name	Structure	Substitution Type in General Nomenclature	PIN	Substitution Type for PIN
anisole		Type 2c	anisole	Type 3
p-cresol (also *o*- and *m*- isomers)		Type 3	4-methylphenol (also 2- and 3- isomers)	
ethylene glycol	$HO-CH_2-CH_2-OH$	Type 3	ethane-1,2-diol	
glycerol	 $HO-CH_2-\overset{\overset{OH}{\vert}}{CH}-CH_2-OH$	Type 3	propane-1,2,3-triol	
phenol		Type 2a	phenol	Type 2a
picric acid		Type 3	2-nitrobenzene-1,3,5-triol	

P-34.3.4 Amines and Other Nitrogen Compounds

Retained Name	Structure	Substitution Type in General Nomenclature	PIN	Substitution Type for PIN
aniline		Type 2a	aniline	Type 2a
benzidine		Type 3	[1,1′-biphenyl]-4,4′-diamine	
biguanide	$H_2N-C(=NH)-NH-C(=NH)-NH_2$	Type 2b	1,2,3-triimidodicarbonic diamide	
biuret	$H_2N-C(O)-NH-CO-NH_2$	Type 2b	imidodicarbonic diamide	
formazan	$\overset{1}{HN}=\overset{2}{N}-\overset{3}{C}H=\overset{4}{N}-\overset{5}{N}H_2$	Type 2b	formazan	Type 2b
guanidine	$H_2\overset{1}{N}-C(=\overset{2}{N}H)-\overset{3}{N}H_2$	Type 2b	guanidine	Type 2b
hydroxylamine	NH_2-OH	Type 2c	hydroxylamine	Type 2c
oxalonitrile	NC-CN	NA	oxalonitrile	NA
oxamide	$H_2N-CO-CO-NH_2$	Type 2b	oxamide	Type 2b
semicarbazide	$H_2\overset{1}{N}\overset{2}{N}H-\overset{3}{C}O-\overset{4}{N}H_2$	Type 2b	hydrazinecarboxamide	
urea	$H_2\overset{1}{N}-\overset{2}{C}O-\overset{3}{N}H_2$	Type 2b	urea	Type 2b

P-34.4 Prefixes derived from functional parent compounds

P-34.4.0 Introduction

Names of prefixes derived from functional parent compounds are trivial names identified as 'retained names'. Some are retained as preferred IUPAC names and are also used in general nomenclature. Others are not used as preferred IUPAC names but are acceptable for general use. The complete list of retained names is given in Section P-46. Retained names for prefixes derived from unsaturated parent structures and partially saturated parent structures are given in P-31.1.2.2 and P-31.2.3.3.2, respectively.

P-34.4.1 Acyl groups.

Except as given below, the names of prefix groups derived from the acids and related classes. imidic acids, amic acids, hydrazonic acids, and aldehydic acids given in P-34.3.1 are formed by changing the '–ic acid' or '–oic acid' ending of the name of the acid to 'oyl'. They are preferred IUPAC names and may be used in general nomenclature. Substitution follows the type given above for the acid.

Retained Name	Structure	Substitution Type in General Nomenclature	PIN	Substitution Type for PIN
acetyl	CH_3-CO–	Type 2a	acetyl	Type 2a
butyryl	CH_3-CH_2-CH_2-CO–	Type 3	butanoyl	
carbonyl	–CO–	NA	carbonyl	NA
cyano	NC	NA	cyano	NA
formyl	HCO–	Type 2c	formyl acid	Type 2c
glutaryl	–OC-$[CH_2]_3$-CO–	Type 3	pentanedioyl	
malonyl	–OC-CH_2-CO–	Type 3	propanedioyl	
oxalo	HO-CO-CO–	NA	oxalo	NA
oxalyl	–CO-CO–	NA	oxalyl	NA
oxaldehydoyl	OCH-CO–	Type 2c	oxaldehydoyl	Type 2c

oxamoyl	H_2N-CO-CO–	Type 2a	oxamoyl	Type 2a
propionyl	CH_3-CH_2-CO–	Type 3	propanoyl	
succinyl	–OC-CH_2-CH_2-CO–	Type 3	butanedioyl	

P-34.4.2 Alkoxy groups

Retained Name	Structure	Substitution Type in General Nomenclature	PIN	Substitution Type for PIN
butoxy	CH_3-CH_2-CH_2-CH_2-O–	Type 2a	butoxy	Type 2a
sec-butoxy	CH_3-CH_2-CH(CH_3)-O–	Type 3	butan-2-yloxy	
tert-butoxy	$(CH_3)_3$C-O–	Type 3	2-(methylpropan-2-yl)oxy	
ethoxy	CH_3-CH_2-O–	Type 2a	ethoxy	Type 2a
isopropoxy	$(CH_3)_2$CH-O–	Type 3	propan-2-yloxy	
methoxy	CH_3-O–	Type 2a	methoxy	Type 2a
phenoxy	C_6H_5-O–	Type 2a	phenoxy	Type 2a
propoxy	CH_3-CH_2-CH_2-O–	Type 2a	propoxy	Type 2a

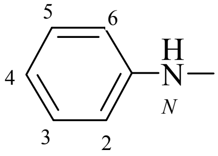
P-34.4.3 Carbonyl compounds

The only retained name for prefixes derived from the retained names for aldehydes and ketones (see P-34.3.2) is acetonyl, CH_3-CO-CH_2–. It is not used as a preferred IUPAC name, but can be used in general nomenclature; it belongs to the Type 2 class for substitution. No substituent prefix groups are retained from benzoquinone, naphthoquinone, anthraquinone, aceophenone, benzophenone, or ketene for either general nomenclature or as IUPAC preferred names.

P-34.4.4 Amido, imido, amino, and other nitrogeneous groups

Retained names for amide and imido prefixes derived from the acids given in P-34.3.1 are formed by changing the name of the ....amide or ....imide' ending to ...amido or ...imido, respectively, for example, acetamido, phthalamido, succinimido. These names follow the same substitution rules as the corresponding acid given above.

Other nitrogeneous prefix groups follow.

Retained Name	Structure	Substitution Type in General Nomenclature	PIN	Substitution Type for PIN
anilino		Type 2a	anilino	Type 2a
formazan-1-yl* (also the 3- and 5-yl isomers)	$\overset{5}{H_2N}\text{-}\overset{4}{N}\text{=}\overset{3}{CH}\text{-}\overset{2}{N}\text{=}\overset{1}{N}\text{–}$	Type 2a*	formazan-1-yl* (also the 3- and 5-yl isomers)	Type 2a*

- The -1,5-diyl, the -3,5-diyl, the -1-yl-5-ylidene, the -3-yl-5-ylidene, the -1,3,5-triyl, and the -1,3-diyl-5-ylidene substituent prefix names follow the same pattern.

P-35 Prefixes corresponding to characteristic groups

P-35.0 Introduction

Prefixes used to designate characteristic groups in substitutive nomenclature are those having free valence(s) attached to an atom of Group 17 (F, Cl, Br, and I) or Group 16 (O, S, Se, and Te), or to nitrogen. Oxygen and nitrogen atoms can also be attached to a carbon atom, for example –CO-OH, –CO-NH_2, and –CO-CH_2-CH_3, or to a chalcogen atom, for example –S(O_2)-OH, –Se(O_2)-OH. These prefixes correspond to suffixes listed in P-33, for example the prefix 'hydroxy' for –OH correspond to the suffix 'ol' for the same group; they also correspond to functionalized parents, for example '2-carboxyethyl' for –CH_2-CH_2-COOH, derived from propanoic acid, CH_3-CH_2-COOH. Prefixes are also derived from functional parents as defined in Section P-34, in particular acyl groups such as 'acetyl', for –CO-CH_3, derived from acetic acid.

Prefixes may have both a retained name and a systematic name only one of which can be a preferred name. In order to facilitate the selection of preferred names, clear indications are given in Chapter 6 for each class of compounds. The prefixes are also alphabetically listed in Appendix 2, with indications concerning their status as preferred names as well as their use in substitutive nomenclature and as functional replacement prefixes.

In this Section, the different types of prefixes used in substitutive nomenclature are described.

P-35.1 General methodology

Substitutive prefixes corresponding to characteristic groups and functional parent compounds may be classified as simple (see P-29.1.1), compound (see P-29.1.2) and complex (see P-29.1.3),; mixed substituent groups are complex substituent groups formed by the combination of substitutive and additive operations.

The multiple occurrence of simple prefixes is denoted by the basic multiplying terms ‘di’, ‘tri’, etc., or by derived prefixes, ‘bis’, ‘tris’, ‘tetrakis’, etc., in order to distinguish between two simple prefixes and those including a basic multiplying term, for example disulfanyl, ‘−SSH’ and bis(sulfanyl), two −SH groups. Compound and mixed substituent prefixes require the derived multiplying terms, ‘bis’, ‘tris’, ‘tetrakis’, etc., to designate their multiplicity in substitutive nomenclature..

Simple prefixes are either retained or systematically formed as follows:

(1) by subtraction of hydrogen atom(s) from parent hydrides (described as substituent groups derived from parent hydrides in Section 29), for example, ‘sulfanyl’, −SH, and ‘diselanyl’,–SeSeH; from functional parents, for example, acetonyl, CH_3-CO-CH_2–; or from a contracted name, for example, ‘phenoxy’, C_6H_5-O−;

(2) acyl groups are formed by subtraction of all −OH groups from oxo acids for example, ‘acetyl’, CH_3-CO− and ‘carbonyl’, >C=O.

P-35.2 Simple prefixes denoting characteristic groups

P-35.2.1 Retained traditional prefixes

Examples:

−F	–Cl
fluoro (preselected name)	chloro (preselected name)
−Br	−I
bromo (preselected name)	iodo (preselected name)

−OH	=O	–O–
hydroxy (preselected name)	oxo (preselected name)	oxy (preselected name)

$-\mathrm{COOH}$

carboxy (PIN)

$-\mathrm{SO_2\text{-}OH}$

sulfo (preselected name)
selenono (Se instead of S; preselected name)
tellurono (Te instead of S)

$-\mathrm{SO\text{-}OH}$

sulfino (preselected name)
selenino (Se instead of S)
tellurino (Te instead of S)

$-\mathrm{NH_2}$
amino (preselected name)

$=\mathrm{NH}$
imino (to the same atom; preselected name)

$-\mathrm{N}<$

nitrilo (to different atoms; preselected name)

$=\mathrm{N_2}$

diazo (preselected name)

$-\mathrm{N_3}$

azido (preselected name)

$-\mathrm{CN}$

cyano (PIN)

$-\mathrm{NC}$

isocyano (PIN)

$-\mathrm{NCO}$

isocyanato (PIN)
isothiocyanato (S instead of O; PIN))
isoselenocyanato (Se instead of O; PIN)
isotellurocyanato (Te instead of O; PIN)

P-35.2.2 Substituents formed by the subtraction of one or more hydrogen atoms from mono- and dinuclear parent hydrides (see P-21). Systematic names are formed by the general methodology described in P-28.2.

Examples:

$-\mathrm{IH_2}$

λ^3-iodanyl (preselected name)

$-\mathrm{SH}$

sulfanyl (preselected name)
(not mercapto-)

$-\mathrm{S}-$

sulfanediyl (preselected name)
thio

–SS–

disulfanediyl (preselected name)
dithio

>NH

azanediyl (preselected name)
(to different atoms)

–N=

azanylylidene (preselected name)
(to different atoms)

N≡

azanylidyne (to the same atom)

P-35.2.3 Simple prefixes derived from functional parents

A few simple prefixes are derived from functional parents. They are described in Section P-34.

Examples:

–CO–

carbonyl (PIN; see P-65.1.1.5.1.5)

–PO<

phosphoryl (preselected name;
see P-67.1.4.1.2)

$-SO_2-$

sulfonyl (preselected name;
sulfuryl
(see P-65.3.2.3.1)

–SO–

sulfinyl (preselected name;
thionyl
(see P-65.3.2.3.1)

$-SeO_2-$

selenonyl (preselected name;
(see P-65.3.2.3.1)

–SeO–

seleninyl (preselected name;
(see P-65.3.2.3.1)

$-TeO_2-$

telluronyl (preselected name;
(see P-65.3.2.3.1)

–TeO–

tellurinyl (preselected name;
(see P-65.3.2.3.1)

P-35.3 Compound substituent prefixes

P-35.3.1 Names of compound prefixes derived from suffixes or functional parent compounds may be formed by substituting simple prefixes into other simple prefixes.

Examples:

$-SSeH$	selanylsulfanyl (preselected name)
$-NH\text{-}Cl$	chloroamino (preselected name)
$-NH\text{-}CH_3$	methylamino (PIN)

P-35.3.2 Names of compound prefixes derived from suffixes or functional parent compounds may be formed by the additive operation called concatenation. It is used to assemble simple mono-, di-, tri-, and tetravalent prefixes. Hydrocarbyl divalent substituents can be attached to prefixes expressing characteristic groups.

Examples:

$-O\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3$	pentyloxy (PIN)
$-O\text{-}CH_2\text{-}C_6H_5$	benzyloxy (PIN)
$-CO\text{-}Cl$	carbonochloridoyl (PIN) chlorocarbonyl
$-C(=NH)\text{-}OH$	*C*-hydroxycarbonimidoyl (PIN)
$-C(=N\text{-}NH_2)\text{-}OH$	*C*-hydroxycarbonohydrazonoyl (PIN)
$-CO\text{-}NH\text{-}NH_2$	hydrazinylcarbonyl (PIN)
$-O\text{-}CH_2\text{-}CH_2\text{-}O-$	ethane-1,2-diylbis(oxy) (PIN)
$>N\text{-}CH_2\text{-}N<$	methylenedinitrilo (PIN)

P-35.3.3 Mixed substituent prefix names are formed by combining substitutive and additive operations.

Examples:

$CH_3\text{-}CH_2\text{-}O\text{-}SO\text{-}NH-$	(ethoxysulfinyl)amino (PIN)
$CH_3\text{-}CO\text{-}S\text{-}CO-$	(acetylsulfanyl)carbonyl (PIN)
$CH_3\text{-}CO\text{-}O\text{-}NH\text{-}SO\text{-}O-$	{[(acetyloxy)amino]sulfinyl}oxy (PIN)

P-35.4 Complex substituent prefixes

P-35.4.1 Names of complex substituent prefixes may be formed by substituting a simple or compound substituent prefix into a compound substituent prefix.

Examples:

−NH-S-SeH	(selanylsulfanyl)amino (preselected name)
$-CH_2$-NH-Cl	(chloroamino)methyl (PIN)

P-35.4.2 Names of complex substituent prefixes may be formed by adding simple or compound substituent prefixes to a compound substituent prefix by the process called ‘concatenation.

Examples:

−CO-O-CH_2-C_6H_5	(benzyloxy)carbonyl (PIN)
−O-CO-$NHNH_2$	(hydrazinylcarbonyl)oxy (PIN)

P-35.4.3 Complex mixed substituent prefix names are formed by combining the substitutive and additive operations. .

Examples:

CH_3-CH_2-O-SO-NH−	(ethoxysulfinyl)amino (PIN)
CH_3-CO-S-CO−	(acetylsulfanyl)carbonyl (PIN)
CH_3-CO-O-NH-SO-O−	{[(acetyloxy)amino]sulfinyl}oxy (PIN)

CHAPTER P-4 RULES FOR NAME CONSTRUCTION

P-40 Introduction

In this Chapter, principles regarding name construction are presented. It is recognized that in chemical discussions it may sometimes be convenient to depart from rigorous rules in order to provide a name more appropriate to the chemical intent or to avoid obscuring an important feature. However, such deviations should not be done without good reason, and names so derived are not recommended for general use in publications.

The application of the principles and rules described in this Chapter has been devised to lead to a preferred IUPAC name. Preferred IUPAC names are not necessarily the aim of a practicing chemist who wants to communicate with his colleagues in familiar, well understood terms, but it may be appropriate to those who cite chemical names in legislative documents, in international trade and commerce, or for preparing programs for index purposes, databases and retrieval systems.

This Chapter includes the general rules and orders of seniority used in substitutive nomenclature and functional class nomenclature.

P-41 Order of seniority of classes

The order of seniority of classes is given in Table 4-1. It ranks classes expressed by suffixes (classes 1 through 20) and classes based on the senior atom in compounds (classes 21 to 35).

Table 4.1 General compound classes listed in decreasing order of seniority for choosing and naming the principal class (radicals and ions) or characteristic group in an organic compound*

Ionic classes

1 Radicals

2 Radical anions

3 Radical cations

4 Anions

5 Zwitterions

6 Cations

Classes expressed by characteristic groups

7 Acids.

7a ‘Suffix’ acids in the order carboxylic (not including carbonic, oxalic, or polycarbonic acids, which belong to sub-class ‘7b’), sulfonic, sulfinic, selenonic, seleninic, telluronic, tellurinic, each followed in turn by the corresponding peroxy, imidic, and hydrazonic acids. Chalcogen analogues follow each of the corresponding oxygen acids and, in each case, the chalcogen analogue with the greater number of the preferred chalcogen atom (O > S > Se > Te), considered first in −OOH groups, then in −OH groups as necessary. (See P-42 for the complete list of seniority of acids, P-43 for suffixes modified by functional replacement, and Appendix 1 for an extensive list of the order of seniority of these suffixes).

7b Carbon acids with no substitutable hydrogen atoms in the order polynuclear carbonic acids (tricarbonic acid, dicarbonic acid), then oxalic acid, and carbonic acid

7c Oxoacids having substitutable hydrogen atoms attached to their central atoms and their acidic derivatives in the following decreasing order of seniority: azonic, azinic, phosphonic, phosphinic, phosphonous, phosphinous acids, etc. (see P-42 for the complete list).

7d Mononuclear and polynuclear oxoacids other than carbon acids without substitutable hydrogen atoms attached to their central atom (see 7b, above), but that may be functionalized or may form derivatives by functional replacement having substitutable hydrogen atoms.

7e Other monobasic ‘oxo acids’ used as functional parent compounds.

8 Anhydrides [substitutive nomenclature is used for cyclic anhydrides (see 16 below); functional class names are given to acyclic anhydrides and to a few cyclic anhydrides corresponding to acids having retained names; cyclic anhydrides are preferred over noncyclic anhydrides, when functional names are used].

9 Esters (functional class names are given to noncyclic esters; lactones and other cyclic esters are named as heterocycles; see 16 below).

10 Acid halides and pseudohalides [first in the order of the corresponding acid given above, then in the order of the halogen atoms (−F > −Cl > −Br > −I); then in the following order of pseudohalogen groups ($-N_3$ > −CN > −NC > −NCO > −NCS > −NCSe > −NCTe > −CNO).

11 Amides [in the order of the corresponding acids; cyclic amides are named as heterocycles (see 16 below)].

12 Hydrazides (in the order of corresponding acids).

13 Imides (includes only cyclic imides derived from organic di- or polybasic acids having retained names).

14 Nitriles.

15 Aldehydes and chalcogen analogues.

16 Ketones (of the type −C-CO-C−), pseudoketones (of the type −C-CO-X , X-CO-X, or −CO-X-CO−, where X ≠ C, halogen, pseudohalogen, or NH_2) and heterones. See Classes 8, 9 and 10, on lactones, lactams, anhydrides, imides.

17 Hydroxy compounds and chalcogen analogues (includes alcohols and phenols, which no longer have a separate ranking order).

18 Hydroperoxides (peroxols), i.e., −OOH.

19 Amines (defined as having three single covalent attachments to a nitrogen atom, i.e., NR_3).

20 Imines, R=NH or R=N-R′.

Classes denoted by the senior atom in heterane nomenclature

21 Nitrogen compounds: heterocycles, polyazanes, hydrazines (except for hydrazides), diazenes, hydroxylamines, azanes (except for amides and amines)

22 Phosphorus compounds: heterocycles, polyphosphanes, phosphanes

23 Arsenic compounds: heterocycles, polyarsanes, arsanes

24 Antimony compounds: heterocycles, polystibanes, stibanes

25 Bismuth compounds: heterocycles, polybismuthanes, bismuthanes

26 Silicon compounds: heterocycles, polysilanes, silanes

27 Germanium compounds: heterocycles, polygermanes, germanes

28 Tin compounds: heterocycles, polystannanes, stannanes

29 Lead compounds: heterocycles, polyplumbanes, plumbanes

30 Boron compounds: heterocycles, polyboranes, boranes

31 Aluminium compounds: heterocycles, polyalumanes, alumanes

32 Gallium compounds: heterocycles, polygallanes, gallanes

33 Indium compounds: heterocycles, polyindiganes, indiganes

34 Thallium compounds: heterocycles, polythallanes, thallanes

35 Oxygen compounds: heterocycles, polyoxidanes (trioxidane but not peroxides or ethers)

36 Sulfur compounds: heterocycles, polysulfanes (trisulfane, λ^4 and λ^6 mono and disulfanes, but not disulfides or sulfides)

37 Selenium compounds: heterocycles, polyselanes (triselane but not diselenides, selenides)

38 Tellurium compounds: heterocycles, polytellanes (tritellane but not ditellurides, tellurides)

39 λ^3, λ^5, and λ^7 halogen compounds in the order $F > Cl > Br > I$.

40 Carbon compounds: rings, chains

41 λ^1 Halogen compounds in the order $F > Cl > Br > I$

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* In this table, the the symbol ‘ >’ means ‘is senior to’.

Examples:

$HOOC\text{-}CH_2\text{-}CH_2{-}$

2-carboxyethyl (PIN)
[free valence (radical) > carboxylic acid]

$(CH_3)_3N^+\text{-}CH_2\text{-}COO^-$

(trimethylazaniumyl)acetate (PIN)
(anion > cation)

$HO\text{-}CH_2\text{-}CH_2\text{-}CONH_2$

3-hydroxypropanamide (PIN)
(amide > alcohol)

$OHC\text{-}CH_2\text{-}CH_2\text{-}CN$

4-oxobutanenitrile (PIN)
(nitrile > aldehyde)

$HSSS\text{-}SiH_3$

trisulfanylsilane (preselected name, see P-12.2)
(Si > S)

$BH_2\text{-}PH_2$

boranylphosphane (preselected name, see P-12.2)
(P > B)

$(CH_3)_4Si$

tetramethylsilane (PIN)
(Si > C)

$(C_6H_5)_3P$

triphenylphosphane (PIN)
(P > C)

P-42 Order of seniority of acids and derivatives

Acids of class 7 (see Table 4.1) in the order of classes of compounds are further classified into subclasses. They correspond to acids expressed by suffixes and acids used as functional parents (see P-34). The following subsections complete the brief description given in Class 7; the acids are described in decreasing seniority order.

P-42.1 Class 7a. Acids expressed by suffixes (excludes carbonic, oxalic, and polycarbonic acids)

carboxylic acids	$-COOH$	-carboxylic acid
	$-(C)(O)OH$	-oic acid
sulfonic acids	$-SO_2\text{-}OH$	-sulfonic acid
sulfinic acids	$-SO\text{-}OH$	-sulfinic acid
selenonic acids	$-SeO_2\text{-}OH$	-selenonic acid
seleninic acids	$-SeO\text{-}OH$	-seleninic acid
telluronic acids	$-TeO_2\text{-}OH$	-telluronic acid
tellurinic acids	$-TeO\text{-}OH$	-tellurinic acid

P-42.2 Class 7b. Carbon acids with no substitutable hydrogen atoms

polycarbonic acids
dicarbonic acid
oxalic acid
carbonic acid
cyanic acid

P-42.3 Class 7c. Noncarbon acids having substitutable hydrogen atoms on the central atom.

All these names are preselected names. In this class, criteria for seniority are, in descending order:

(a) the central atom first in the list N > P > As > Sb > B;
(b) maximum number of central atoms;
(c) homopolyacids (isopolyacids) (see ref. 14);
(d) having contiguous central atoms;
(e) maximum number of acidic (−OH) groups;
(f) highest oxidation number for the central atom

azonic acid	$NH(O)(OH)_2$
azinic acid	$NH_2(O)(OH)$
polyphosphonic acids	$(HO)PH(O)\text{-}O\text{-}[PH(O)\text{-}O\text{-}]_nPH(O)(OH)$
diphosphonic acid	$(HO)PH(O)\text{-}O\text{-}PH(O)(OH)$
hypodiphosphonic acid (see P-67.2.1)	$(HO)(O)HP\text{-}PH(O)(OH)$
phosphonic acid	$PH(O)(OH)_2$
polyphosphonous acids	$(HO)PH\text{-}O\text{-}[PH\text{-}O\text{-}]_nPH(OH)$
diphosphonous acid	$(HO)PH\text{-}O\text{-}PH(OH)$
hypodiphosphonous acid (see P-67.2.1)	$(HO)HP\text{-}PH(OH)$
phosphonous acid	$PH(OH)_2$
phosphinic acid	$PH_2(O)(OH)$
phosphinous acid	$PH_2(OH)$
polyarsonic acids > diarsonic acid > hypodiarsonic acid (see P-67.2.1)	
arsonic acid	$AsH(O)(OH)_2$
polyarsonous acids > diarsonous acid > hypodiarsonous acid (see P-67.2.1)	
arsonous acid	$AsH(OH)_2$
arsinic acid	$AsH_2(O)(OH)$

arsinous acid	$AsH_2(OH)$

polystibonic acids > distibonic acid > hypodistibonic acid (see P-67.2.1)

stibonic acid	$SbH(O)(OH)_2$

polystibonous acids > distibonous acid > hypodistibonous acid (see P-67.2.1)

stibonous acid	$SbH(OH)_2$
stibinic acid	$SbH_2(O)(OH)$
stibinous acid	$SbH_2(OH)$
diboronic acid	$(HO)BH\text{-}O\text{-}BH\text{-}(OH)$
hypodiboronic acid (see P-67.2.1)	$(HO)HB\text{-}BH(OH)$
boronic acid	$BH(OH)_2$
borinic acid	$BH_2(OH)$

P-42.4 Class 7d. Noncarbon acids used to generate derivatives having substitutable hydrogen atoms. All these names are preselected names. In this class, criteria for seniority are, in descending order:

(a) the central atom first in the list: P > As > Sb > Si > B > S > Se > Te;

(b) maximum number of central atoms;

(c) homopolyacids (isopolyacids) (see ref. 14);

(d) polyacids having contiguous central atoms;

(e) maximum number of acidic groups (-OH) groups);

(f) highest oxidation number for the central atom.

> For consistency in the names of polynuclear oxoacids, the numerical infix ‘di’ has been uniformly used in naming dinuclear ‘hypo’ acids, for example, hypodiphosphorous acid, rather than hypophosphorus acid.

polyphosphorous acids	$(HO)_2P\text{-}O\text{-}[P(OH)\text{-}O]_n\text{-}P(OH)_2$
tetraphosphoric acid	$(HO)_2P(O)\text{-}O\text{-}P(O)(OH)\text{-}O\text{-}P(O)(OH)\text{-}O\text{-}P(O)(OH)_2$
triphosphoric acid	$(HO)_2P(O)\text{-}O\text{-}P(O)(OH)\text{-}O\text{-}P(O)(OH)_2$
diphosphoric acid	$(HO)_2P(O)\text{-}O\text{-}P(O)(OH)_2$
diphosphorous acid	$(HO)_2P\text{-}O\text{-}P(OH)_2$
hypodiphosphoric acid (see P-67.2.1)	$(HO)_2(O)P\text{-}P(O)(OH)_2$
hypodiphosphorous acid (see P-67.2.1)	$(HO)_2P\text{-}P(OH)_2$
phosphoric acid	$P(O)(OH)_3$
phosphorous acid	$P(OH)_3$

polyarsoric acids > polyarsorous acids > diarsoric acid > diarsorous acid > hypodiarsoric acid (see P-67.2.1) > hypodiarsorous acid (see P-67.2.1)

arsoric acid	$As(O)(OH)_3$
arsorous acid	$As(OH)_3$

polystiboric acids > polystibonous acid > distiboric acid > distibonous acid > hypodistiboric acid (see P-67.2.1) > hypodistibonous acid (see P-67.2.1)

stiboric acid	$Sb(O)(OH)_3$
stiborous acid	$Sb(OH)_3$
orthosilicic acid	$Si(OH)_4$
diboric acid	$(HO)_2B-O-B(OH)_2$
hypodiboric acid (see P-67.2.1)	$(HO)_2B-B(OH)_2$
boric acid	$B(OH)_3$
polysulfuric acids	$(HO)SO_2-O-[SO_2(OH)-O-]_nSO_2(OH)$
polysulfurous acids	$(HO)SO-O-[SO(OH)-O-]_nSO(OH)$
disulfuric acid	$(HO)SO_2-O-SO_2(OH)$
disulfurous acid	$(HO)S(O)-O-S(O)(OH)$
dithionic acid (hypodisulfuric acid)	$(HO)O_2S-SO_2(OH)$
dithionous acid (hypodisulfurous acid)	$(HO)(O)S-S(O)(OH)$
sulfuric acid	$S(O)_2(OH)_2$
sulfurous acid	$S(O)(OH)_2$

polyselenic acids > polyselenous acids > diselenic acid > diselenous acid > hypodiselenic acid (see P-67.2.1) > hypodiselenous acid (see P-67.2.1)

selenic acid	$Se(O)_2(OH)_2$
selenous acid	$Se(O)(OH)_2$

polytelluric acids > polytellurous acids > ditelluric acid > ditellurous acid > hypoditelluric acid (see P-67.2.1) > hypoditellurous acid (see P-67.2.1)

telluric acid	$Te(O)_2(OH)_2$
tellurous acid	$Te(O)(OH)_2$

P-42.5 Class 7e Other monobasic 'oxo' acids used as functional parents. All these names are preselected names. In this class, criteria for seniority are, in descending order.

(a) the central atom first in the list N > Cl > Br > I;
(b) highest oxidation number for the central atom.

nitric acid	$HO-NO_2$
nitrous acid	$HO-NO$
perfluoric acid	$F(O)_3OH$
fluoric acid	$F(O)_2OH$

fluorous acid	F(O)OH
hypofluorous acid	FOH
perchloric acid	$Cl(O)_3OH$
chloric acid	$Cl(O)_2OH$
chlorous acid	Cl(O)OH
hypochlorous acid	ClOH
perbromic acid	$Br(O)_3OH$
bromic acid	$Br(O)_2OH$
bromous acid	Br(O)OH
hypobromous acid	BrOH
periodic acid	$I(O)_3OH$
iodic acid	$I(O)_2OH$
iodous acid	I(O)OH
hypoiodous	IOH

P-43 Order of seniority of suffixes

P-43.0 Introduction

The order of seniority for suffixes is described in this Section. It is based on the seniority of classes 7 through 20 given in Table 4.1 and includes suffixes modified by functional replacement.

P-43.1 General methodology of functional replacement

Suffixes are modified as indicated in Table 4.3. Prefixes and infixes are used as indicated in Table 4.2. Prefixes are used to modify suffixes such as ‘ol’, ‘al’, for example ‘thiol’ and ‘thial’. Infixes are recommended to modify the suffixes ‘carboxylic acid’, ‘sulfonic acid’, and related suffixes, for example ‘carboperoxoic acid’ and ‘sulfonothioic acid’.

Table 4.2 Prefixes and infixes, in decreasing order of seniority, used to generate suffixes in preferred IUPAC names by functional replacement

Prefix	Infix	Replaced atom(s)	Replacing atom(s)
peroxy-	-peroxo-	−O−	−OO−
thioperoxy-	-(thioperoxo)-	−O−	−OS− or −SO−
dithioperoxy-	-(dithioperoxo)-	−O−	−SS−
thio-	-thio-	−O− or =O	−S− or =S
seleno-	-seleno-	−O− or =O	−Se− or =Se

telluro-	-telluro-	−O− or =O	−Te− or =Te
imido-	-imido-	=O	=NH
hydrazono-	-hydrazono-	=O	$=NNH_2$

When several oxygen atoms are replaceable, the following criteria are applied, in order, until a decision is reached:

(a) maximum number of oxygen atoms, then S, Se, and Te atoms, then =NH and $=NNH_2$ groups;

(b) maximum number of oxygen atoms, then S, Se, and Te atoms, in −OO− groups;

(c) oxygen atoms, then S, Se and Te atoms, in −(O)OH and −OH groups.

The order of seniority is described, in the case of carboxylic acids, sulfonic acids and sulfinic acids, by indicating, after the name of the modified suffix the number and kind of atoms used in the replacement operation (see Table 4.2).

Table 4.3 gives the list, in decreasing order, of the seniority of suffixes and suffixes modified by functional replacement for carboxylic and sulfonic acids. Sulfinic acid suffixes are similar to sulfonic acids. Selenium and tellurinum acid suffixes are formed by replacing 'sulf' by 'selen' or 'tellur'.

Table 4.3 Carboxylic and sulfonic acid suffixes generated for IUPAC preferred names by functional replacement, in decreasing order of seniority

1 Carboxylic acids

–COOH	carboxylic acid	
–CO-OOH	carboperoxoic acid	(3O)
–CS-OOH	carboperoxothioic *OO*-acid	(2O,1S; OO)
–CSe-OOH	carboperoxoselenoic acid	(2O,1Se; OO)
–CO-SOH	carbo(thioperoxoic) *SO*-acid	(2O,1S; OS; OH)
–CO-OSH	carbo(thioperoxoic) *OS*-acid	(2O,1S; OS; SH)
–CO-SeOH	carbo(selenoperoxoic) *SeO*-acid	(2O,1Se; OSe; OH)
–CO-OSeH	carbo(selenoperoxoic) *OSe*-acid	(2O,1Se; OSe; SeH)
–CS-SOH	carbothio(thioperoxoic) *SO*-acid	(1O,2S; OS; OH)
–CS-OSH	carbothio(thioperoxoic) *OS*-acid	(1O,2S; OS; SH)
–CSe-OSH	carboseleno(thioperoxoic) *OS*-acid	(1O,1S,1Se; OS; SH)
–CS-SeOH	carbo(selenoperoxo)thioic *SeO*-acid	(1O,1S,1Se; OSe: OH)
–CS-OSeH	carbo(selenoperoxo)thioic *OSe*-acid	(1O,1S,1Se; OSe; eH)
–CS-SSH	carbo(dithioperoxo)thioic acid	(3S)

–CSe-SeSeH	carbo(diselenoperoxo)selenoic acid	(3Se)
–CTe-TeTeH	carbo(ditelluroperoxo)telluroic acid	(3Te)
–CS-OH	carbothioic *O*-acid	(1O,1S; OH)
–CO-SH	carbothioic *S*-acid	(1O,1S; SH)
–CS-SH	carbodithioic acid	(2S)
–CSe-SH	carboselenothioic *S*-acid	(1S,1Se; SH)
–CS-SeH	carboselenothioic *Se*-acid	(1S,1Se; SeH)
–CSe-SeH	carbodiselenoic acid	(2Se)
–CTe-SeH	carboselenotelluroic *Se*-acid	(1Se,1Te; SeH
–CTe-TeH	carboditelluroic acid	(2Te)
–C(=NH)-OH	carboximidic acid	
–C(=NH)-OOH	carbimidoperoxoic acid	(2O,1N; OO)
–C(=NH)-SOH	carbimido(thioperoxoic) *SO*-acid	(1O,1S,1N; OS; OH)
–C=(NH)-OSH	carbimido(thioperoxoic) *OS*-acid	(1O,1S,1N; OS; SH)
–C(=NH)-SSH	carbo(dithioperox)imidic acid	(2S,1N; SS)
–C(=NH)-SeSH	carbimido(selenothioperoxoic) *SeS*-acid	(1S,1Se,1N; SSe; SH)
–C(=NH)-SH	carbimidothioic acid	(1S,1N)
–C(=NH)-SeH	carbimidoselenoic acid	(1Se,1N)
–C(=NH)-TeH	carbimidotelluroic acid	(1Te,1N)
–C(=NNH$_2$)-OH	carbohydrazonic acid	
–C(=NNH$_2$)-OOH	carbohydrazonoperoxoic acid	(2O,1NN; OO)
–C(=NNH$_2$)-SOH	carbohydrazono(thioperoxoic) *SO*-acid	(1O,1S,1NN; OS; OH)
–C(=NNH$_2$)-OSH	carbohydrazono(thioperoxoic) *OS*-acid	(1O,1S,1NN; OS; SH)
–C(=NNH$_2$)-TeTeH	carbo(ditelluroperoxo)hydrazonoic acid	(2Te,1NN; TeTe)

2 Sulfonic acids

–SO$_2$-OH	sulfonic acid	
–SO$_2$-OOH	sulfonoperoxoic acid	(4O)
–S(O)(S)-OOH	sulfonoperoxothioic *OO*-acid	(3O,1S; OO)
–S(O)(Se)-OOH	sulfonoperoxoselenoic *OO*-acid	(3O,1Se; OO)
–SO$_2$-SOH	sulfono(thioperoxoic) *SO*-acid	(3O,1S; OS; OH)
–SO$_2$-OSH	sulfono(thioperoxoic) *OS*-acid	(3O,1S; OS; SH)
–SS$_2$-OOH	sulfonoperoxodithioic *OO*-acid	(2O,2S; OO)

–S(O)(S)-SOH	sulfonothio(thioperoxoic) *SO*-acid	(2O,2S; OS; OH)
–S(S)(Se)-OOH	sulfonoperoxoselenothioic *OO*-acid	(2O,1S,1Se; OO)
–SSeSe-SSH	sulfino(dithioperoxo)diselenoic acid	(2S,2Se; SS)
–SS$_2$-SeSeH	sulfono(diselenoperoxo)dithioic acid	(2S,2Se; SeSe)
–STe$_2$-TeTeH	sulfono(ditelluroperoxo)ditelluroic acid	(4Te)
–S(O)(S)-OH	sulfonothioic *O*-acid	(2O,1S; OH)
–SO$_2$-SH	sulfonothioic *S*-acid	(2O,1S; SH)
–SO$_2$-SeH	sulfonoselenoic *Se*-acid	(2O,1Se; SeH)
–SS$_2$-OH	sulfonodithioic *O*-acid	(1O,2S; OH)
–S(O)(S)-SH	sulfonodithioic *S*-acid	(1O,2S; SH)
–S(Se)(Te)-OH	sulfonoselenotelluroic *O*-acid	(1O,1Se,1Te; OH
–S(O)(Te)-SeH	sulfonoselenotelluroic *Se*-acid	(1O,1Se,1Te; SeH)
–S(O)(Se)-TeH	sulfonoselenotelluroic *Te*-acid	(1O,1Se.1Te; TeH)
–SS$_2$-SH	sulfonotrithioic acid	(3S)
–S(O)(=NH)-OH	sulfonimidic acid	
–S(O)(=NH)-OOH	sulfonimidoperoxoic acid	(3O,1N; OO)
–S(S)(=NH)-OOH	sulfonimidoperoxothioic *OO*-acid	(2O,1S,1N; OO; OH)
–S(O)(=NH)-SOH	sulfonimido(thioperoxoic) *OO*-acid	(2O,1S,1N; OS; OH)
–S(O)(=NH)-OSH	sulfonimido(thioperoxoic) *OS*-acid	(2O,1S,1N; OS; SH)
-S(S)(=NH)-OH	sulfonimidothioic *O*-acid	(1O,1S; OH)
–S(O)(=NH)-SH	sulfonimidothioic *S*-acid	(1O,1S; SH)
–S(S)(=NH)-SH	sulfoimidodithioic acid	(2S)
–S(Se)(=NH)-SH	sulfonimidoselenothioic *S*-acid	(1S,1Se; SH)
–S(S)(=NH)-SeH	sulfonimidoselenothioic *Se*-acid	(1S,1Se; SeH)
–S(Te)(=NH)-TeH	sulfonimidoditelluroic acid	(2Te)
–S(=NH)$_2$-OH	sulfonodiimidic acid	
–S(=NH)$_2$-OOH	sulfonodiimidoperoxoic acid	(2O,2N; OO)
–S(=NH)$_2$-SOH	sulfonodiimido(thioperoxoic) *SO*-acid	(1O,1S,2N: OS; OH)
–S(=NH)$_2$-OSH	sulfonodiimido(thioperoxoic) *OS*-acid	(1O,1S,2N; OS; SH)
–S(=NH)$_2$-SeH	sulfonodiimidoselenoic acid	(1Se,2N)
–S(=NH)$_2$-TeH	sulfonodiimidotelluroic acid	(1Te,2N)
–S(O)(=NNH$_2$)-OH	sulfonohydrazonic acid	

–S(O)(=NNH$_2$)-OOH	sulfonohydrazonoperoxoic acid	(3O,1NN; OO)
–S(S)(=NNH$_2$)-OOH	sulfonohydrazonoperoxothioic acid	(2O,1S,1NN; OO)
–S(S)(=NH$_2$)-OH	sulfonohydrazonothioic *O*-acid	(1O,1S,1NN; OH)
–S(O)(=NNH$_2$)-SH	sulfonohydrazonothioic *S*-acid	(1O,1S,1NN; SH)
–S(=NNH$_2$)$_2$OH	sulfonodihydrazonic acid	
–S(=NNH$_2$)$_2$-OOH	sulfonodihydrazonoperoxoic acid	(2O,2NN; OO)
–S(=NNH$_2$)$_2$-SOH	sulfonodihydrazono(thioperoxoic) *SO*-acid	(1O,1S,2NN; SO, OH)
–S(=NNH$_2$)$_2$-SH	sulfonodihydrazonothioic acid	(1S,2NN)

Table 4.4 Complete list of suffixes and functional replacement analogues for IUPAC preferred names, in decreasing order of seniority

1. Carboxylic acids	–CO-OH –(C)O-OH	carboxylic acid oic acid
Carboperoxoic acids	–CO-OOH –(C)O-OH	carboperoxoic acid peroxoic acid
Carboperoxoic acids modified by replacement with S, Se and/or Te		
	–CS-OOH –(C)S-OOH	carboperoxothioic acid peroxothioic acid
	–CSe-OOH –(C)Se-OOH	carboperoxoselenoic acid peroxoselenoic acid
	–CO-SOH –(C)O-SOH	carbo(thioperoxoic) *SO*-acid (thioperoxoic) *SO*-acid
	–CO-OSH –(C)O-OSH	carbo(thioperoxoic) *OS*-acid (thioperoxoic) *OS*-acid
Carboxylic acids modified by replacement with S, Se, and/or Te		
	–CS-OH –(C)S-OH	carbothioic *O*-acid thioic *O*-acid
	–CO-SH –(C)O-SH	carbothioic *S*-acid thioic *S*-acid
	–CO-SeH –CO-SeH	carboselenoic *Se*-acid selenoic *Se*-acid
	–CS-SH –C(S)-SH	carbodithioic acid dithioic acid

2. Carboximidic acids	–C(=NH)-OH	carboximidic acid
	–(C)(=NH)-OH	imidic acid
Carboximidoperoxoic acids	–C(=NH)-OOH	carboximidoperoxoic acid
	–(C)=(NH)-OOH	imidoperoxoic acid

Carboximidoperoxoic acids modified by replacement with S, Se and/or Te

–C=(NH)-SOH	carboximido(thioperoxoic) *SO*-acid
–(C)(=NH)-SOH	imido(thioperoxoic) *SO*-acid
–C(=NH)-OSH	carboximido(thioperoxoic) *OS*-acid
–(C)(=NH)-OSH	imido(thioperoxoic) *OS*-acid
–C=(NH)-SSH	carbo(dithioperox)imidic acid
–(C)(=NH)-SSH	(dithioperox)imidic acid
–C(=NH)-SeSH	carboximido(selenothioperoxoic) *SeS*-acid
–(C)(=NH)-SeSH	carboximido(selenothioperoxoic) *SeS*-acid

Carboximidic acids modified by replacement with S, Se and/or Te

–C(=NH)-SH	carboximidothioic acid
–(C)(=NH)-SH	carboximidothioic acid

3. Carbohydrazonic acids	–C(=NNH$_2$)-OH	carbohydrazonic acid
	–(C)(=NHNH$_2$)	hydrazonic acid
Carbohydrazonoperoxoic acids	–C(=NNH$_2$)-OOH	carbohydrazonoperoxoic acid
	–(C)(=NNH$_2$)-OOH	hydrazonoperoxoic acid

Carbohydrazonoperoxoic acids modified by replacement with S, Se and/or Te

–C(=NNH$_2$)-SOH	carbohydrazono(thioperoxoic) *SO*-acid
–(C)(=NNH$_2$)-SOH	hydrazono(thioperoxoic) *SO*-acid
–C(=NNH$_2$)-OSH	carbohydrazono(thioperoxoic) *OS*-acid
–(C)(=NNH$_2$)-OSH	hydrazono(thioperoxoic) *OS*-acid
–C(=NNH$_2$)-TeTeH	carbo(ditelluroperoxo)hydrazonoic acid
–(C)(=NNH$_2$)-TeTeH	(ditelluroperoxo)hydrazonoic acid

Carbohydrazonic acids modified by replacement with S, Se and/or Te

–C(=NHNH$_2$)-SH	carbohydrazonothioic acid
–(C)(=NHNH$_2$)-SH	carbohydrazonothioic acid

4. Sulfonic acids	−SO$_2$-OH	sulfonic acid
Sulfonoperoxoic acids	−SO$_2$-OOH	sulfonoperoxoic acid

Sulfonoperoxoic acids modified by replacement with S, Se and/or Te

–S(O)(S)-OOH	sulfonoperoxothioic acid
–SO$_2$-SOH	sulfono(thioperoxoic) *SO*-acid

–SO$_2$-OSH	sulfono(thioperoxoic) *OS*-acid
–SS$_2$-OOH	sulfonoperoxodithioic acid

Sulfonic acids modified by replacement with S, Se and/or Te

–SO$_2$-SH	sulfonothioic *S*-acid
–S(O)(S)-OH	sulfonothioic *O*-acid
–S(S)(S)-SH	sulfonotrithioic acid

5. Sulfonimidic acids	–S(O)(=NH)-OH	sulfonimidic acid
Sulfonimidoperoxoic acids	–S(O)(=NH)-OOH	sulfonimidoperoxoic acid

Sulfonimidoperoxoic acids modified by replacement with S, Se and/or Te

–S(O)(=NH)-SOH	sulfonimido(thioperoxoic) *SO*-acid
–S(O)(=NH)-OSH	sulfonimido(thioperoxoic) *OS*-acid

Sulfonimidic acids modified by replacement with S, Se and Te

–S(O)(=NH)-SH	sulfonimidothioic *S*-acid

6. Sulfonodiimidic acids	–S(=NH)$_2$-OH	sulfonodiimidic acid
Sulfonodiimidoperoxoic acids	–S(=NH)$_2$-OOH	sulfonodiimidoperoxoic acid

Sulfonodiimidoperoxoic acids modified by replacement with S, Se and/or Te

–S(=NH)$_2$-SOH	sulfonodiimido(thioperoxoic) *SO*-acid
–S(=NH)$_2$-OSH	sulfonodiimido(thioperoxoic) *OS*-acid

Sulfonodiimidic acids modified by replacement with S, Se and/or Te

–S(=NH)$_2$-SeH	sulfonodiimidoselenoic acid

7. Sulfonohydrazonic acids	–S(O)(=NNH$_2$)-OH	sulfonohydrazonic acid
Sulfonohydrazonoperoxoic acids	–S(O)=(NNH$_2$)-OOH	sulfonohydrazonoperoxoic acid

Sulfonohydrazonoperoxoic acids modified by replacement with S, Se and/or Te

–S(S)(=NNH$_2$)-OOH	sulfonohydrazonoperoxothioic acid

Sulfonohydrazonic acids modified by replacement with S, Se and/or Te

–S(S)(=NNH$_2$)-OH	sulfonohydrazonothioic *O*-acid
–S(O)(=NNH$_2$-SH	sulfonohydrazonothioic *S*-acid

8. Sulfonodihydrazonic acids	−S(=NNH$_2$)$_2$OH	sulfonodihydrazonic acid
Sulfonodihydrazonoperoxoic acids	–S(=NNH$_2$)$_2$-OOH	sulfonodihydrazonoperoxoic acid

Sulfonodihydrazonoperoxoic acids modified by replacement by S, Se and/or Te

–S(=NNH$_2$)$_2$-SOH	sulfonodihydrazono(thioperoxoic) *O*-acid

Sulfonodihydrazonic acids modified replacement with S, Se and/or Te

$-S(=NNH_2)_2$-SH   sulfonodihydrazonothioic acid

9. Sulfinic acids   –SO-OH   sulfinic acid

Sulfinoperoxoic acid   –SO-OOH   sulfinoperoxoic acid

Sulfinoperoxoic acid modified by replacement with S, Se and/or Te

–S(O)(S)-OOH   sulfinoperoxothioic acid

–SO-SOH   sulfino(thioperoxoic) *SO*-acid

–SO-OSH   sulfino(thioperoxoic) *OS*-acid

Sulfinic acids modified by replacement with S, Se and/or Te

–SS-OH   sulfinothioic *O*-acid

–SO-SeH   sulfinoselenoic *Se*-acid

10. Sulfinimidic acids   –S(=NH)-OH   sulfinimidic acid

Sulfinoimidoperoxoic acids   –S(=NH)-OOH   sulfinimidoperoxoic acid

Sulfinoimidoperoxoic acids modified by replacement with S, Se and/or Te

–S(=NH)-OSH   sulfinimido(thioperoxoic) *S*-acid

Sulfinimidic acids modified by replacement with S, Se and/or Te

–S(=NH)-SH   sulfinimidothioic acid

11. Sulfinohydrazonic acids $-S(=NNH_2)$-OH   sulfinohydrazonic acid

Sulfinohydrazonoperoxoic acids $-S(=NNH_2)$-OOH   sulfinohydrazonoperoxoic acid

Sulfinohydrazonoperoxoic acids modified by replacement with S, Se and/or Te

$-S(=NNH_2)$-SSeH   sulfinohydrazono(selenothioperoxoic) *Se*-acid

Sulfinohydrazonic acids modified by replacement with S, Se and/or Te

$-S(=NNH_2)$-TeH   sulfinohydrazonotelluroic acid

12. Selenonic acids $-SeO_2$-OH   selenonic acid (as for sulfonic acids)

13. Seleninic acids   –SeO-OH   seleninic acid (as for sulfinic acids)

14. Telluronic acids $-TeO_2$-OH   telluronic acid (as for sulfonic acids)

15. Tellurinic acids   –TeO-OH   tellurinic acid (as for sulfinic acids)

16. Carboxamides $-CO\text{-}NH_2$ carboxamide

–(C)O-NH_2	amide

Carboxamides modified by replacement with S, Se and/or Te

–CS-NH_2	carbothioamide
–(C)S-NH_2	thioamide

17. Carboximidamides	–C(=NH)-NH_2	carboximidamide
	–(C)(=NH)-NH_2	imidamide
18. Carbohydrazonamides	$\text{–C(=NNH}_2\text{)-NH}_2$	carbohydrazonamide
	$\text{–(C)(=NNH}_2\text{)-NH}_2$	hydrazonamide
19. Sulfonamides	$\text{–SO}_2\text{-NH}_2$	sulfonamide

Sulfonamides modified by replacement with S, Se and/or Te

–S(O)(S)-NH_2	sulfonothioamide
–S(S)(Se)-NH_2	sulfonoselenothioamide

20. Sulfonimidamides	–S(O)(=NH)-NH_2	sulfonimidamide

Sulfonimidamides modified by replacement with S, Se and/or Te

–S(S)(=NH)-NH_2	sulfonimidothioamide

21. Sulfonodiimidamides	$\text{–S(=NH)}_2\text{-NH}_2$	sulfonodiimidamide
22. Sulfonohydrazonamides	$\text{–S(O)(=NNH}_2\text{)-NH}_2$	sulfonohydrazonamide

Sulfonohydrazonamides modified by replacement with S, Se and/or Te

–S(S)(=NH)-NH_2	sulfonohydrazonothioamide

23. Sulfonodihydrazonamides	$\text{–S(=NNH}_2\text{)}_2\text{-NH}_2$	sulfonodihydrazonamide
24. Sulfinamides	–SO-NH_2	sulfinamide

Sulfinamides modified by replacement with S, Se and/or Te

–S(Se)-NH_2	sulfinoselenoamide

25. Sulfinimidamides	–S(=NH)-NH_2	sulfinimidamide
26. Sulfinohydrazonamides	$\text{–S(=NNH}_2\text{)-NH}_2$	sulfinohydrazonamide
27. Selenonamides	$\text{–SeO}_2\text{-NH}_2$	selenonamide (as for sulfonamides)
28. Seleninamides	–SeO-NH_2	seleninamide (as for sulfinamides)
29. Telluronamides	$\text{–TeO}_2\text{-NH}_2$	telluronamide (as for sulfonamides)
30. Tellurinamides	–TeO-NH_2	tellurinamide (as for sulfinamide)

31. Carbohydrazides –CO-NHNH_2 carbohydrazide –(C)O-NHNH_2 hydrazide

Carbohydrazides modified by replacement with S, Se and/orTe

–CS-NHNH_2 carbothiohydrazide

32. Carboximidohydrazides –C(=NH)-NHNH_2 carboximidohydrazide
–(C)(=NH)-NHNH_2 imidohydrazide

33. Carbohydrazonohydrazides $\text{–C(=NNH}_2\text{)-NHNH}_2$ carbohydrazonohydrazide
$\text{–(C)(=NNH}_2\text{)-NHNH}_2$ hydrazonohydrazide

34. Sulfonohydrazides $\text{–SO}_2\text{-NHNH}_2$ sulfonohydrazide

Sulfonohydrazides modified by replacement with S, Se and/or Te

–S(O)(S)-NHNH_2 sulfonothiohydrazide

35. Sulfonimidohydrazides –S(O)(=NH)-NHNH_2 sulfonimidohydrazide

Sulfonimidohydrazides modified by replacement with S, Se and/or Te

$\text{–S(Se)(=NH)-NHNH}_2$ sulfonimidoselenohydrazide

36. Sulfonodiimidohydrazides $\text{–S(=NH)}_2\text{-NHNH}_2$ sulfonodiimidohydrazide

37. Sulfonohydrazonohydrazides $\text{–S(O)(=NNH}_2\text{)-NHNH}_2$ sulfonohydrazonohydrazide

Sulfonohydrazonohydrazides modified by replacement with S, Se andor Te
$\text{-S(Te)(=NNH}_2\text{)-NHNH}_2$ sulfonohydrazonotellurohydrazide

38. Sulfonodihydrazonohydrazides $\text{–S(=NNH}_2\text{)}_2\text{-NHNH}_2$ sulfonodihydrazonohydrazide

39. Sulfinohydrazides –S(O)-NHNH_2 sulfinohydrazide

Sulfinohydrazides modified by replacement with S, Se and/or Te

–S(Se)-NHNH_2 sulfinoselenohydrazide

40. Sulfinimidohydrazides –S(=NH)-NHNH_2 sulfinimidohydrazide

41. Sulfinohydrazonohydrazides $\text{–S(=NNH}_2\text{)-NHNH}_2$ sulfinodihydrazonohydrazides

42. Selenonohydrazides $\text{–SeO}_2\text{-NHNH}_2$ selenonohydrazide (as for sulfonohydrazides)

43. Seleninohydrazides –Se(O)-NHNH_2 seleninohydrazides (as for sulfinohydrazides)

44. Telluronohydrazides $\text{–TeO}_2\text{-NHNH}_2$ telluronohydrazides (as for sulfonohydrazides)

45. Tellurinohydrazides –Te(O)-NHNH_2 tellurinohydrazides (as for sulfinohydrazides)

46. Nitriles	$-CN$	carbonitrile
	$-(C)N$	nitrile
47. Aldehydes	$-CHO$	carbaldehyde
	$-(C)HO$	al

Aldehydes modified by replacement with S, Se and/or Te

$-CHS$	carbothialdehyde
$-(C)HS$	thial
$-CHSe$	carboselenaldehyde
$-(C)HSe$	selenal
$-CHTe$	carbotelluraldehyde
$-(C)HTe$	tellural

48. Ketones, pseudoketones, and heterones	$>(C)=O$	one

Ketones, pseudoketones, and heterones modified by replacement with S, Se and/or Te

$>(C)=S$	thione
$>(C)=Se$	selone (not selenone)
$>(C)=Te$	tellone (not tellurone)

49. Hydroxy compounds	$-OH$	ol

Hydroxy compounds modified by replacement with S, Se and/or Te

$-SeH$	selenol
$-TeH$	tellurol

50. Hydroperoxides	$-OOH$	peroxol

Hydroperoxides modified by replacement with S, Se and/or Te

$-OSH$	*OS*-thioperoxol
$-SOH$	*SO*-thioperoxol (not sulfenic acid)

51. Amines	$-NH_2$	amine
52. Imines	$=NH$	imine

P-44 Seniority order of parent structures

P-44.0 Introduction

The selection of parent hydrides is based on the seniority of classes (see P-41), giving priority to suffixes. This order of seniority is also used to choose a parent hydride when different classes are present and between rings and chains. Section P-44.1 covers the selection of parent hydrides when different classes are involved and between rings and chains in the same class. When there is a choice among cyclic parent hydrides, the senior ring or ring system is chosen in accord with the seniority order of rings and ring systems (see P-44.2). When there is a choice among acyclic parent hydrides a principal chain must be chosen (see P-44.3). The three seniority orders, for classes, rings and ring systems, and the principal chain, are expressed in a general seniority order called 'seniority order of parent structures'. Section P-44.4 covers more criteria applicable to both rings and chains.

A thorough revision and extension of the seniority order of classes, of rings and ring systems, and for selecting the principal chain was needed in the context of preferred names.

This revision leads to a major change. In this document, it is recommended to invert the traditional order of seniority between unsaturation and length in the case of acyclic compounds; thus, the first criterion is concerned with the length of the chain and unsaturation is second to length.

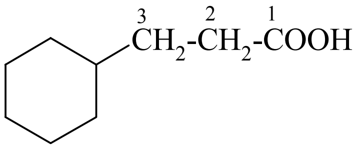
P-44.1 Seniority order of parent structures

When there is a choice, the senior parent structure is chosen by applying the following criteria, in order, until a decision is reached. These criteria must always be applied before those applicable to rings and ring systems (see P-44.2 and P-44.4) and to chains (see P-44.3 and P-44.4).

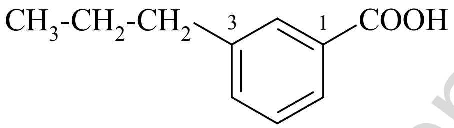
P-44.1.1 The senior parent structure has the maximum number of substituents corresponding to the principal characteristic group (suffixes) in accord with the seniority of classes (P-41) and the seniority of suffixes (P-43).

Suffixes are used to designate the principal function when attached to chains, rings or ring systems and to any atom, carbon atom or heteroatom.

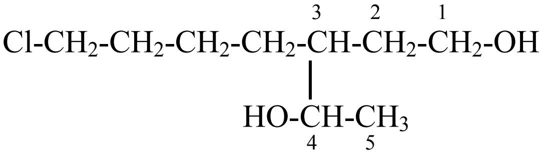
Examples:



3-cyclohexylpropanoic acid (PIN)



3-propylbenzoic acid (PIN)



$$\mathrm{Cl{-}CH_2{-}CH_2{-}CH_2{-}CH_2{-}\underset{\underset{\displaystyle HO{-}\underset{4}{C}H{-}\underset{5}{C}H_3}{|}}{\overset{3}{C}H}{-}\overset{2}{C}H_2{-}\overset{1}{C}H_2{-}OH}$$

3-(4-chlorobutyl)pentane-1,4-diol (PIN)

$H_2N\text{-}NH\text{-}COOH$

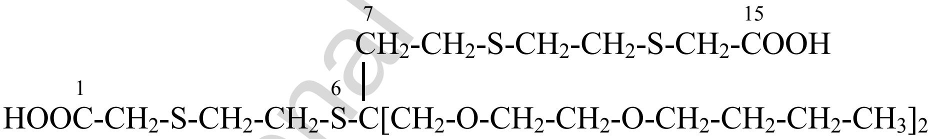
hydrazinecarboxylic acid (PIN)

$H_3Si\text{-}CH_2\text{-}CH_2\text{-}COOH$

3-silylpropanoic acid (PIN)

$HOOC\text{-}SiH_2\text{-}CH_2\text{-}CH_3$

ethylsilanecarboxylic acid (PIN)



$$\mathrm{HO\overset{1}{O}C{-}CH_2{-}S{-}CH_2{-}CH_2{-}\overset{6}{S}{-}\overset{\overset{\displaystyle \overset{7}{C}H_2{-}CH_2{-}S{-}CH_2{-}CH_2{-}S{-}CH_2{-}\overset{15}{C}OOH}{|}}{C}[CH_2{-}O{-}CH_2{-}CH_2{-}O{-}CH_2{-}CH_2{-}CH_2{-}CH_3]_2}$$

7,7-bis[(2-butoxyethoxy)methyl]-3,6,10,13-tetrathiapentadecanedioic acid (PIN)

P-44.1.2 The senior parent structure, whether cyclic or acyclic, has the senior atom in accordance with the seniority of classes (see P-41) expressed by the following decreasing element order: N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl > O > S > Se > Te > C. This criterion is applied to select the senior atom in chains and to choose between rings and chains. It is not used to choose between rings (see P-44.2) or to select the principal chain modified by skeletal replacement (‘a’) nomenclature (see P-15.4).

P-44.1.2.1 When two or more atoms denoting different classes are present in a compound directly bonded to each other, and when the choice for parent compound is between these atoms, the parent compound is the one belonging to the class cited first in the seniority of classes given above. A single senior atom is sufficient to give seniority to the parent hydride.

Examples:

$Si(CH_3)_4$

tetramethylsilane (PIN)

$Al(CH_2\text{-}CH_3)_3$

triethylalumane (PIN)

$CH_3\text{-}PH\text{-}SiH_3$

methyl(silyl)phosphane (PIN)

$HS\text{-}S\text{-}S\text{-}S\text{-}S\text{-}SiH_2\text{-}SiH_2\text{-}SiH_3$

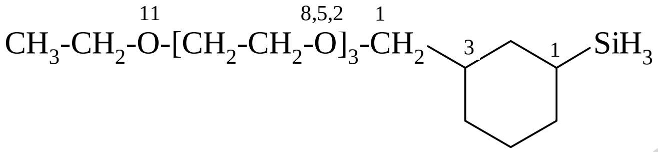
1-pentasulfanyltrisilane (preselected name)

$H_3Si\text{-}SiH_2\text{-}CH_2\text{-}CH_2\text{-}PH_3$

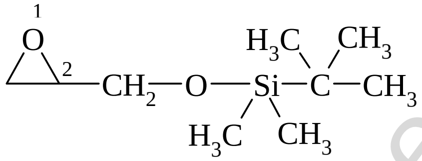
(2-disilanylethyl)phosphane (PIN)

$H_3Sb\text{-}CH_2\text{-}AsH_3$

(stibanylmethyl)arsane (PIN)



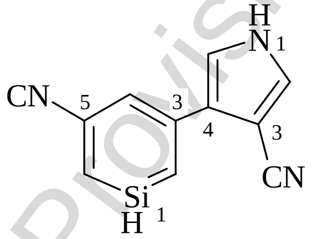
3-[(2,5,8,11-tetraoxatridecan-1-yl)cyclohexyl]silane (PIN)
(among classes, Si is senior to O, and both are senior to C)



tert-butyldimethyl(oxiran-2-ylmethoxy)silane (PIN)

$HOOC\text{-}\overset{1}{Si}H_2\text{-}\overset{2}{Si}H_2\text{-}CH_2\text{-}CH_2\text{-}COOH$

2-(2-carboxyethyl)disilane-1-carboxylic acid (PIN)



4-(5-cyanosilin-3-yl)pyrrole-3-carbonitrile (PIN)

P-44.1.2.2 Systems composed of rings and chains

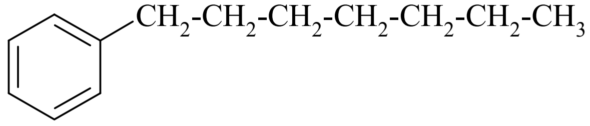
Two methods are recognized to name systems composed of rings and chains

Method (a). Within the same class, a ring or ring system has seniority over a chain. When a ring and a chain contain the same senior element, the ring is chosen as parent. Rings and chains are chosen regardless of their degree of hydrogenation. As a consequence, this approach prefers the choice of a ring over a chain in systems composed of cyclic and acyclic hydrocarbons.

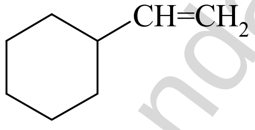
Method (b) The context may favor the ring or the chain, so that, for example, substituents may be treated alike or an unsaturated acyclic structure may be recognized, or the one chosen has the greater number of skeletal atoms in the ring or in the principal chain of the acyclic structure.

In the examples that follow, when a choice is possible, names formed by both methods are given; for preferred IUPAC names method (a) is the choice (see also Chapter 5).

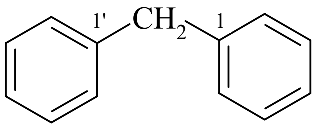
Examples:



(a) heptylbenzene (PIN)
(ring preferred to chain)
(b) 1-phenylheptane
(chain has greater number of skeletal atoms)

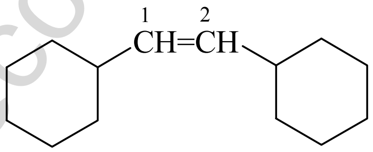


(a) vinylcyclohexane (PIN)
(ring preferred to chain)
(b) cyclohexylethene
(emphasizes unsaturation)

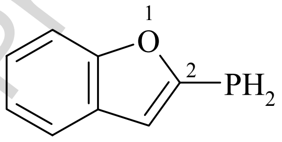


(a) 1,1′-methylenedibenzene (PIN)
(ring preferred to chain as preferred parent)

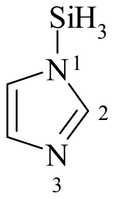
(b) diphenylmethane
(treats phenyl groups alike as substituents)



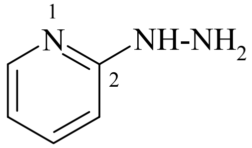
(a) ethene-1,2-diyldicyclohexane (PIN)
(ring preferred to chain)
(b) 1,2-dicyclohexylethene
(emphasizes unsaturation)



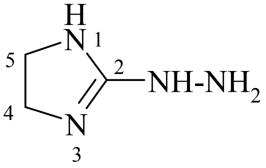
1-benzofuran-2-ylphosphane (PIN)
(P preferred to O)



1-(trimethylsilyl)-1*H*-imidazole (PIN)
(N preferred to Si)



(a) 2-hydrazinylpyridine (PIN)
(ring preferred to chain)



(a) 2-hydrazino-4,5-dihydro-1*H*-imidazole (PIN)
(ring preferred to chain)

P-44.1.3 Senior ring or ring system. Criteria that apply only when the choice for parent structure is between two or more rings are given in P-44.2.

P-44.1.4 The principal chain. Criteria that apply only when the choice for parent structure is between two or more chains are given in P-44.3

P-44.1.5 Identical parent structures may differ only in the presence of skeletal atoms with different bonding orders, isotopic modification, or stereochemical configuration. The criteria for such a choice, applicable to either chains or rings, are given in P-44.4.

P-44.2 Seniority order of rings and ring systems

P-44.2.1 General criteria for determining ring seniority given below are applied successively until there are no alternatives remaining. These criteria are listed first and then separately illustrated.

The senior ring or ring system:

(a) is a heterocycle;

(b) has at least one nitrogen atom;

(c) has at least one heteroatom (in the absence of nitrogen) that occurs earlier in the following sequence: F > Cl > Br > I > O > S > Se > Te > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;

(d) has the greater number of rings;

(e) has the greater number of ring atoms;

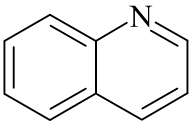
(f) has the greater number of heteroatoms of any kind;

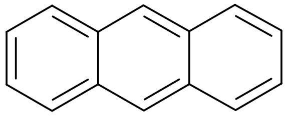
(g) has the greater number of heteroatoms occurring earlier in the sequence listed in (c), above.

Each of these criteria is illustrated below.

(a) The senior ring or ring system is a heterocycle.

Example:

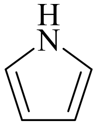


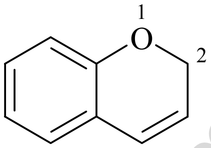


quinoline (PIN) > anthracene (PIN)

(b) The senior ring or ring system has at least one nitrogen ring atom.

Example:

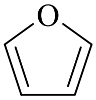


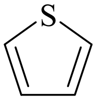


1*H*-pyrrole (PIN) > 2*H*-chromene (PIN)

(c) The senior ring or ring system has at least one heteroatom (in the absence of nitrogen) that occurs earlier in the following sequence: F > Cl > Br > I > O > S > Se > Te > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl

Example:

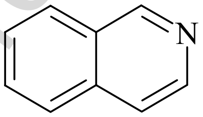


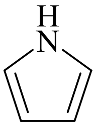


furan (PIN) > thiophene (PIN)

(d) The senior ring or ring system has the greater number of rings.

Example:

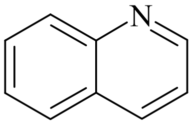


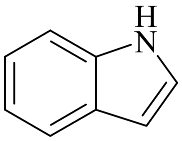


isoquinoline (PIN) > 1*H*-pyrrole (PIN)

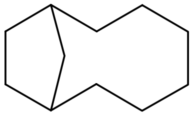
(e) The senior ring or ring system has the greater number of atoms.

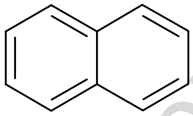
Examples:



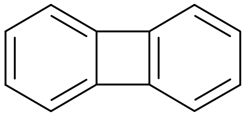


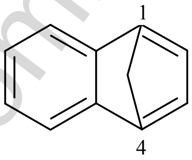
quinoline (PIN) > 1*H*-indole (PIN)





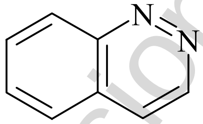
bicyclo[6.2.1]undecane (PIN) > naphthalene (PIN)

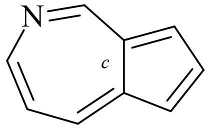




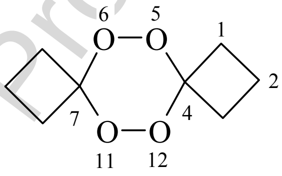
biphenylene (PIN) > 1,4-methanonaphthalene (PIN)

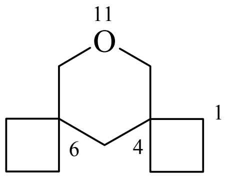
(f) The senior ring or ring system has the greater number of heteroatoms of any kind.
Examples:



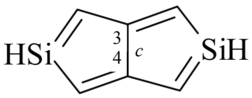


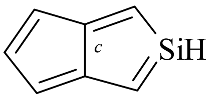
cinnoline (PIN) > cyclopenta[*c*]azepine (PIN)



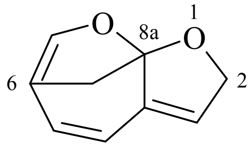


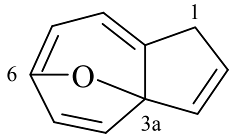
5,6,11,12-tetraoxadispiro[$3.2.3^{7}.2^{4}$]dodecane (PIN) > 1-oxadispiro[$3.1.3^{6}.3^{4}$]dodecane (PIN)



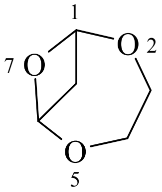


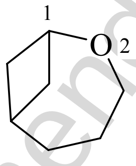
2*H*,5*H*-silolo[3,4-*c*]silole (PIN) > 2*H*-cyclopenta[*c*]silole (PIN)





2*H*-6,8a-methanofuro[2,3-*b*]oxepine (PIN) > 1*H*-3a,6-epoxyazulene (PIN)

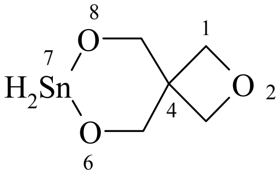


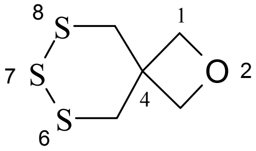


2,5,7-trioxabicyclo[4.1.1]octane (PIN) > 2-oxabicyclo[4.1.1]octane (PIN)

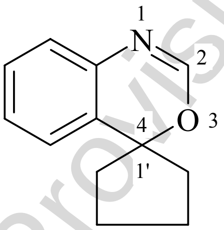
(g) The senior ring or ring system has the greater number of heteroatoms that occur earlier in the following sequence: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

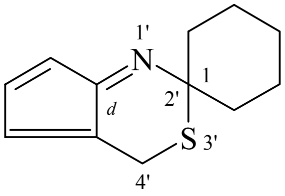
Examples:



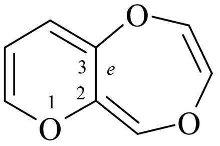


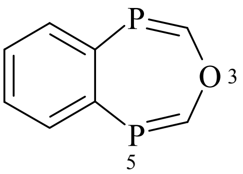
2,6,8-trioxa-7-stannaspiro[3.5]nonane (PIN) > 2-oxa-6,7,8-trithiaspiro[3.5]nonane (PIN)



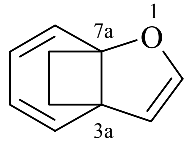


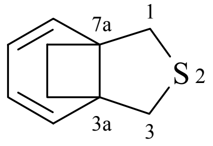
spiro[3,1-benzoxazine-4,1′-cyclopentane] (PIN) > 4′*H*-spiro[cyclohexane-1,2′-cyclopenta[*d*][1,3]thiazine] (PIN)



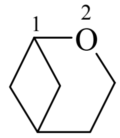


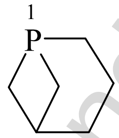
pyrano[3,2-*e*]-1,4-dioxepine (PIN) > 3,1,5-benzoxadiphosphepine (PIN)





3a,7a-ethano-1-benzofuran (PIN) > 1*H*,3*H*-3a,7a-ethano-2-benzothiophene (PIN)





2-oxabicyclo[3.1.1]heptane (PIN) > 1-phosphabicyclo[3.1.1]heptane (PIN)

P-44.2.2 Senority criteria for determining ring seniority applicable to particular types of ring or ring system.

(1) Monocycles (see P-22)

(2) Polycyclic systems. The senior ring system occurring first in the following list of ring system types.

(a) a spiro ring system (see P-23);

(b) a cyclic phane system (see P-26);

(c) a fused ring system (see P-25);

(d) a bridged fused ring system (see P-25);

(e) a nonfused bridged ring system (see P-24);

(f) an acyclic (linear) phane system (see P-26);

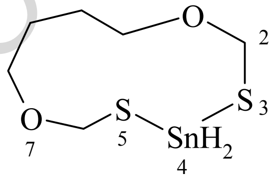
(g) a ring assembly (see P-28).

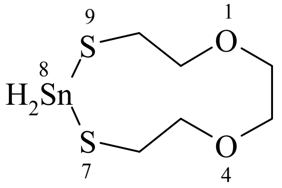
P-44.2.2.1 Senority criteria for determining ring seniority of monocycles.

The senior monocycle:

(a) has the lower locants for the heteroatoms compared as a set without regard to kind;

Example:



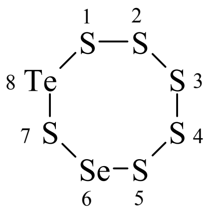


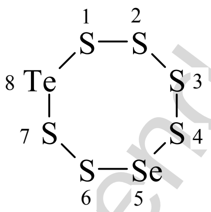
1,7-dioxa-3,5-dithia-4-stanna-cycloundecane (PIN) > 1,4-dioxa-7,9-dithia-8-stanna-cycloundecane (PIN)

(the set of locants 1,3,4,5,7 is lower than 1,4,7,8,9)

(b) has the lower locants for heteroatoms occuring earlier in the following sequence: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Example:





1,2,3,4,5,7,6,8-hexathiaselenatellurocane (preselected name, see P-12.2) > 1,2,3,4,6,7,5,8-hexathiaselenatellurocane (preselected name, see P-12.2)

P-44.2.2.2 The senior ring system occurs earliest in the following listing:

(a) a spiro ring system (see P-44.2.2.2.1);

(b) a cyclic phane system (see P-44.2.2.2.2);

(c) a fused ring system (see P-44-2.2.2.3);

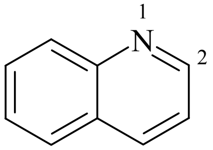
(d) a bridged fused ring system see(P-44.2.2.2.4);

(e) a nonfused bridged ring system (see P-44.2.2.2.5);

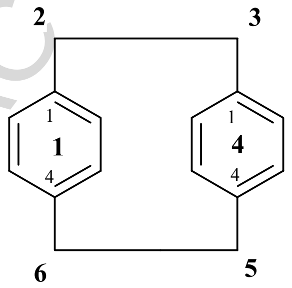
(f) an acyclic (linear) phane system (see P-44.2.2.2.6);

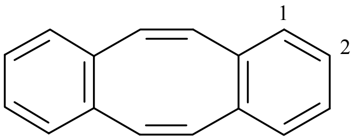
(g) a ring assembly (see P-44.2.2.2.7).

Examples:

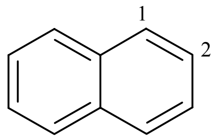


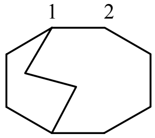
8-azaspiro[4.5]decane (PIN) > quinoline (PIN)



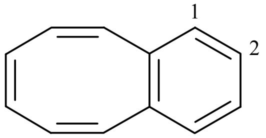


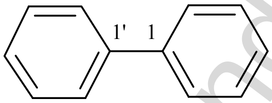
1,4(1,4)-dibenzenacyclohexaphane (PIN) > dibenzo[*a*,*e*][8]annulene (PIN)





naphthalene (PIN) > bicyclo[4.2.2]decane (PIN)





benzo[8]annulene (PIN) > 1,1′-biphenyl (PIN)

P-44.2.2.2.1 Senority criteria for spiro ring systems are applied successively until there are no alternatives remaining. These criteria are listed first and then separately illustrated.

The senior spiro system:

(a) has the greater number of spiro fusions;

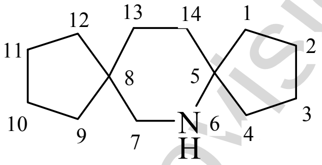
(b) consists of saturated rings;

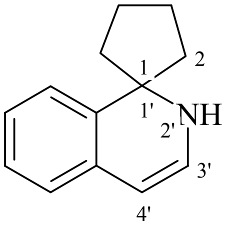
(c) consists of only discrete components.

Each of these criteria is illustrated below.

(a) The senior spiro system has the greater number of spiro fusions.

Example:



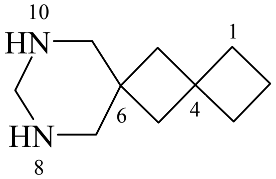


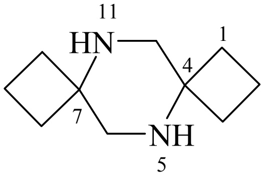
6-azadispiro[4.2.4^{8}.2^{5}]tetradecane (PIN) > 2′*H*-spiro[cyclopentane-1,1′-isoquinoline] (PIN)

(b) The senior spiro system consists of only saturated monocyclic rings and:

(i) has the lower locant(s) for spiro atom(s);

Example:

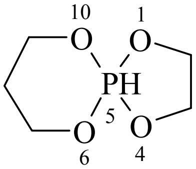


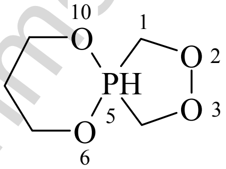


8,10-diazadispiro[3.1.5^6.1^4]dodecane (PIN) > 5,11-diazadispiro[3.2.3^7.2^4]dodecane (PIN)

(ii) has the lower locants for the heteroatoms compared as a set without regard to kind;

Example:

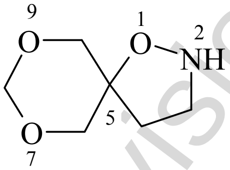


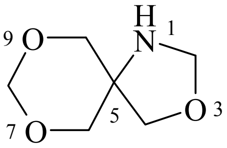


1,4,6,10-tetraoxa-5λ^5-phospha-spiro[4.5]decane (PIN) > 2,3,6,10-tetraoxa-5λ^5-phospha-spiro[4.5]decane (PIN)

(iii) has the lower locants for heteroatoms that occur earlier in the following sequence; F > Cl > Br > I > O > S > Se > Te > N > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Example:



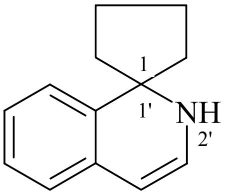


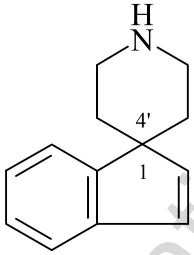
1,7,9-trioxa-2-azaspiro[4.5]decane (PIN) > 3,7,9-trioxa-1-azaspiro[4.5]decane (PIN)

(c) The senior spiro system consists only of discrete components and:

(i) has the preferred component determined by criteria above and below for the appropriate kind of ring system when the components are compared in their order of seniority;

Example:

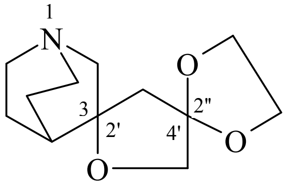


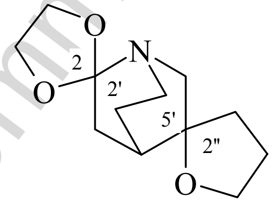


2′*H*-spiro[cyclopentane-1,1′-isoquinoline] (PIN) > spiro[indene-1,4′-piperidine] (PIN)

(ii) has the senior component when compared in their order of citation in the name;

Example:



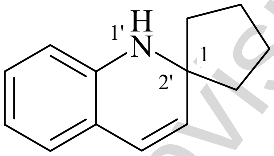


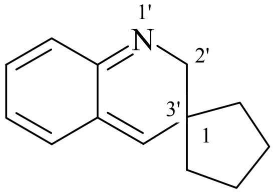
I > **II**

I dispiro[[1]azabicyclo[2.2.2]octane-3,2′-oxolane-4′,2″-[1,3]dioxolane] (PIN)
II dispiro[[1,3]dioxolane-2,2′-[1]azabicyclo[2.2.2]octane-5′,2″-oxolane] (PIN)

(iii) has the lower locants for the spiro atoms in the order of citation in the name.

Example:





1′*H*-spiro[cyclopentane-1,2′-quinoline] (PIN) > 2′*H*-spiro[cyclopentane-1,3′-quinoline] (PIN)

P-44.2.2.2.2 Senority criteria for cyclic phane systems given below are applied sucessively until there are no alternatives remaining. These criteria are listed first and then separately illustrated.

The senior cyclic phane system:

(a) is the one occurring earlier in the following list of phane skeletal ring systems: spiro, von Baeyer, monocyclic;

(b) has the senior amplificant, as defined by P-44.2.1.1 through P-44.2.1.7;

(c) has the lowest superatom locants for all amplificants;

(d) has the lowest locants for senior amplificants;

(e) has the lowest attachment locants considered as a set when compared term by term in order of increasing numerical value;

(f) has the lowest attachment locants when compared term by term in their order of citation in the name;

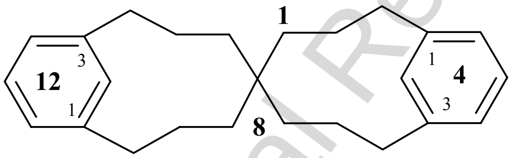
(g) has the lowest locants for heteroatoms introduced by skeletal replacement ('a') nomenclature without regard to kind;

(h) has the lowest locants for heteroatoms introduced by skeletal replacement ('a') nomenclature first cited in the following order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

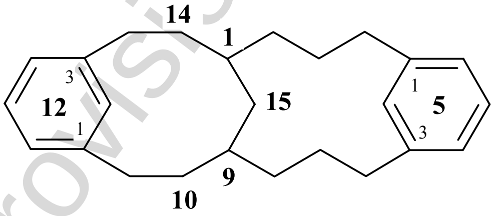
Each of these criteria is illustrated below.

(a) The senior cyclic phane system occurs earlier in the following list of basic phane skeletal ring systems: spiro, von Baeyer, monocyclic.

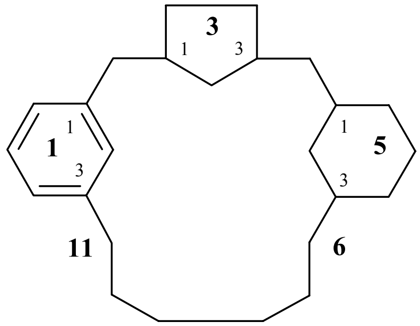
Examples (in order of decreasing seniority according to the above list):



4,12(1,3)-dibenzenaspiro[7.7]pentadecaphane (PIN)



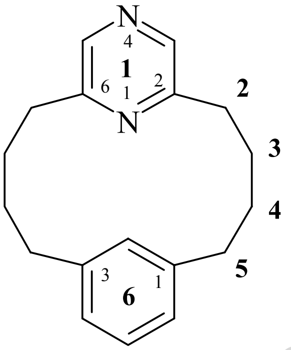
5,12(1,3)-dibenzenabicyclo[7.5.1]pentadecaphane (PIN)

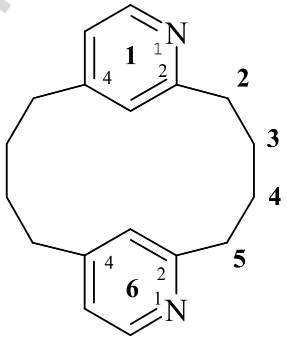


1(1,3)-benzena-5(1,3)-cyclohexana-3(1,3)-cyclopentanacycloundecaphane (PIN)

(b) The senior cyclic phane system has the senior amplificant, as defined by P-44.2.1.1 through P-44.2.1.7.

Example:



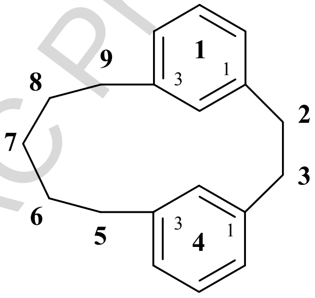


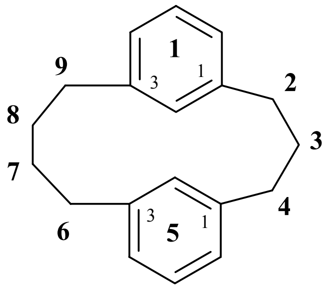
1(2,6)-pyrazina-6(1,3)-benzena-cyclodecaphane (PIN) > 1,6(2,4)-dipyridinacyclodecaphane (PIN)

(pyrazine senior to pyridine)

(c) The senior cyclic phane system has the lowest superatom locants for all amplificants.

Example:

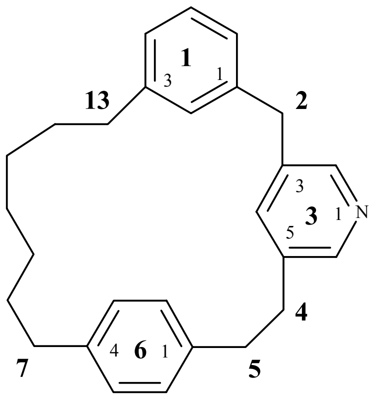




1,4(1,3)-dibenzenacyclononaphane (PIN) > 1,5(1,3)-dibenzenacyclononaphane (PIN)

(d) The senior cyclic phane system has the lowest locants for senior amplificants

Example:



I

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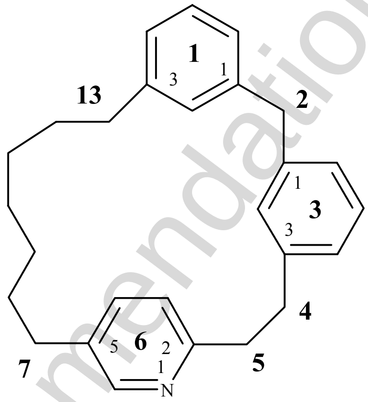
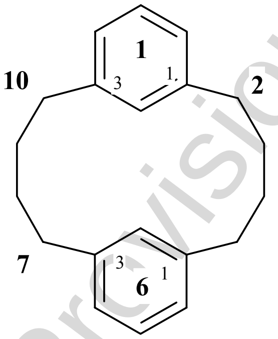


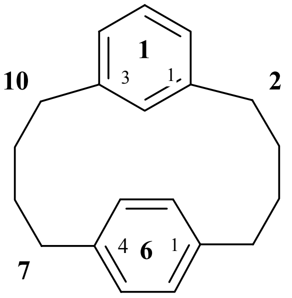
II

I 3(3,5)-pyridina-1(1,3),6(1,4)-dibenzenacyclotridecaphane (PIN)
II 6(2,5)-pyridina-1,3(1,3)-dibenzenacyclotridecaphane (PIN)

(e) The senior cyclic phane system has the lowest attachment locants considered as a set when compared term by term in order of increasing numerical value.

Example:

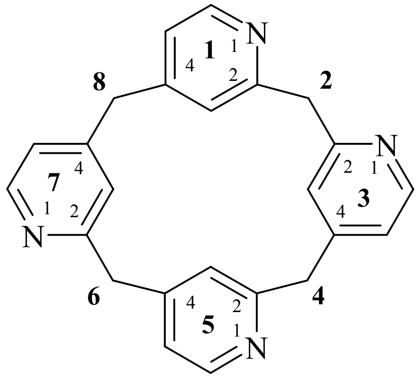




1,6(1,3)-dibenzenacyclodecaphane (PIN) > 1(1,3),6(1,4)-dibenzenacyclodecaphane (PIN)

(f) The senior cyclic phane system has the lowest attachment locants when compared term by term in their order of citation in the name.

Example:



I

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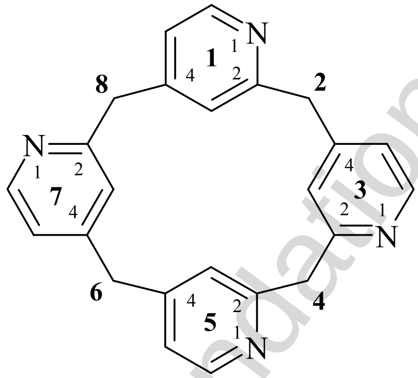
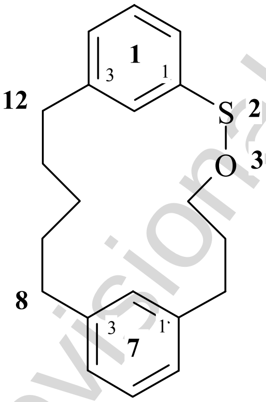


II

I 1,3,5,7(2,4)-tetrapyridinacyclooctaphane (PIN)
II 1,5(2,4),3,7(4,2)-tetrapyridinacyclooctaphane (PIN)

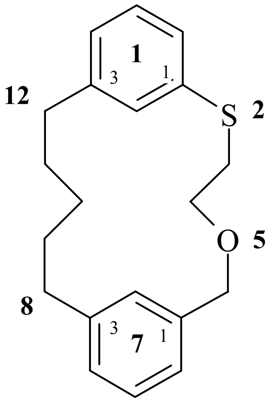
(g) The senior cyclic phane system has the lowest locants for heteroatoms specified by 'a' prefixes without regard to kind

Example:



I

>

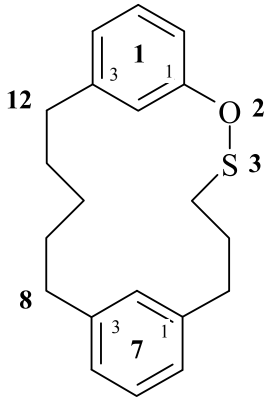


II

I 3-oxa-2-thia-1,7(1,3)-dibenzenacyclododecaphane (PIN)
II 5-oxa-2-thia-1,7(1,3)-dibenzenacyclododecaphane (PIN)

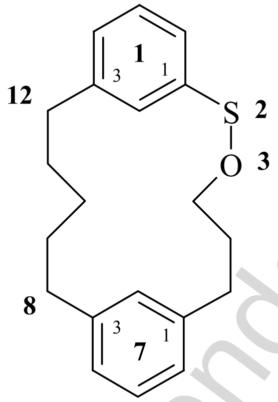
(h) The senior cyclic phane system has the lowest locants for heteroatoms specified by 'a' prefixes first cited in the following order: F > Cl > B > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Example:



I

>



II

I 2-oxa-3-thia-1,7(1,3)-dibenzenacyclododecaphane (PIN)
II 3-oxa-2-thia-1,7(1,3)-dibenzenacyclododecaphane (PIN)

P-44.2.2.2.3 Senority criteria for fused ring systems are applied successively until there are no alternatives remaining. These criteria are listed first and then separately illustrated.

The senior fused ring system:

(a) has the larger individual ring component at first point of difference when their ring sizes are compared in order of decreasing size;

(b) has the greater number of rings in a horizontal row (see P-25.3.2.3.2)

(c) has the lower letters in the expression for ring fusion when compared as a set; letters omitted in names are taken into consideration in the application of this criterion;

(d) has the lower numbers in the expression for ring fusion, in the order of appearance in a name; locants omitted in names are taken into consideration in application of this criterion;

(e) has the senior ring system component according to P-44.2.2.5.1 through P-44.2.2.5.4 when its components are compared in order of decreasing seniority;

(f) has the lower locants for heteroatoms the heteroatoms being compared as a set without regard to kind;

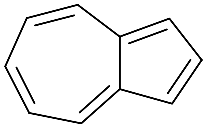
(g) has the lower locants for heteroatoms occurring earlier in the following sequence: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;

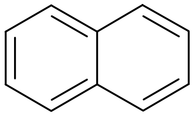
(h) has the lower locants for carbon atoms at fusion sites.

Each of these criteria is illustrated below.

(a) The senior fused ring system has the larger individual ring component at first point of difference when their ring sizes are compared in order of decreasing size.

Example:

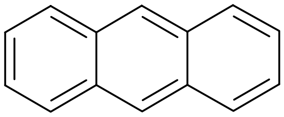


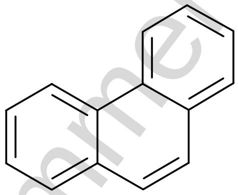


azulene (PIN) > naphthalene (PIN)

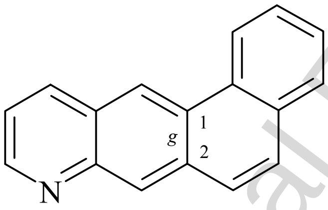
(b) The senior fused ring system has the greater number of rings in a horizontal row

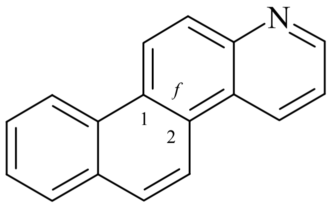
Examples:





anthracene (PIN) > phenanthrene (PIN)

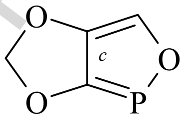


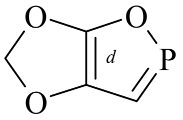


naphtho[1,2-*g*]quinoline (PIN) > naphtho[2,1-*f*]quinoline (PIN)

(c) The senior fused ring system has the lower letters in the expression for ring fusion when compared as a set; letters omitted in names are taken into consideration in the application of this criterion. [This criterion is valid only for comparing names that have letters; when letters are absent in all names or present in only one name, go to P-44.2.2.4.6 below.]

Example:

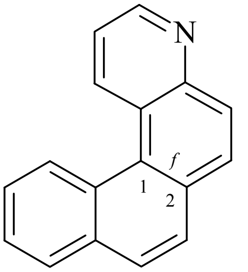


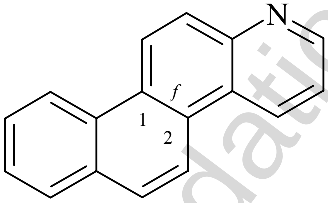


[1,3]dioxolo[*c*][1,2]oxaphosphole (PIN) > [1,3]dioxolo[*d*][1,2]oxaphosphole (PIN)

(d) The senior fused ring system has the lower numbers in the expression for ring fusion, in the order of appearance in a name; locants omitted in names are taken into consideration in application of this criterion.

Example:

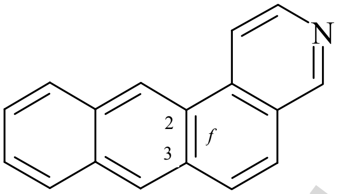


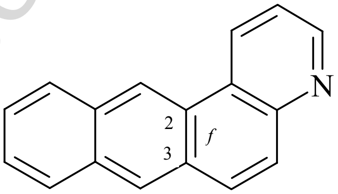


naphtho[1,2-*f*]quinoline (PIN) > naphtho[2,1-*f*]quinoline (PIN)

(e) The senior fused ring system has the senior ring system component according to P-44.2.2.4.1 through P-44.2.2.4.4 when its components are compared in order of decreasing seniority

Example:

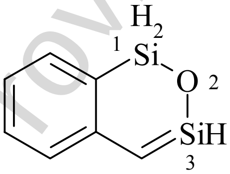


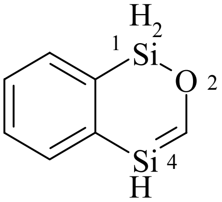


naphtho[2,3-*f*]quinoline (PIN) > naphtho[2,3-*f*]isoquinoline (PIN)

(f) The senior fused ring system has the lower locants for heteroatoms the heteroatoms being compared as a set without regard to kind.

Example:

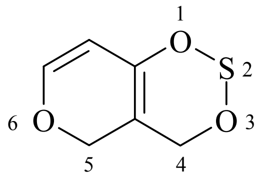


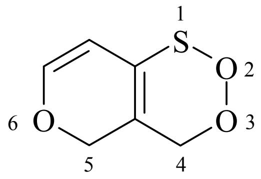


1*H*-2,1,3-benzoxadisiline (PIN) > 1*H*-2,1,4-benzoxadisiline (PIN)

(g) The senior fused ring system has the lower locants for heteroatoms occurring earlier in the following sequence: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Example:

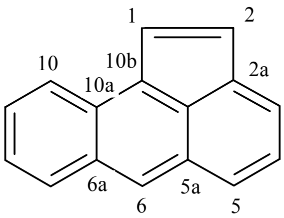


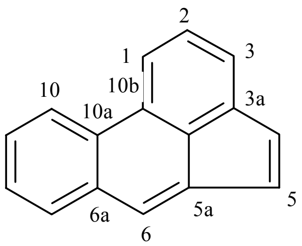


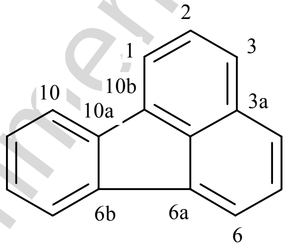
4*H*,5*H*-pyrano[4,3-*d*]-1,3,2-dioxathiine (PIN) > 4*H*,5*H*-pyrano[4,3-*d*]-1,2,3-dioxathiine (PIN)

(h) The senior fused ring system has the lowest locants for carbon atoms at fusion sites

Example:

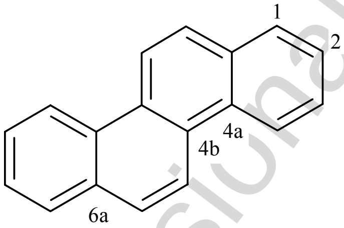


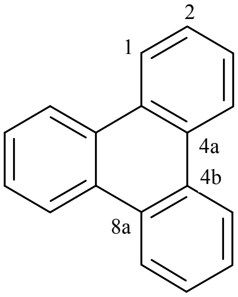




aceanthrylene (PIN) > acephenanthrylene (PIN) > fluoranthene (PIN)

(2a > 3a; 3a,5a > 3a,6a)





chrysene (PIN) > triphenylene (PIN)

(4a,4b,6a > 4a,4b,8a)

P-44.2.2.2.4 Seniority criteria for bridged fused ring systems are applied successively until there are no alternatives remaining. These criteria are listed first and then separately illustrated.

The senior bridged fused ring system:

(a) has the bridged ring system with the greater number of rings before bridging;

(b) is the bridged ring system with the greater number of ring atoms before bridging;

(c) is the bridged ring system with the fewer heteroatoms in the fused ring system;

(d) is the bridged ring system with the senior fused ring system before bridging according to P-44-2.2.4.1 through P-44.2.2.4.5 and P-44.2.2 above;

(e) has the lower locants for bridge attachments;

(f) has the lower locants for heteroatoms in bridges, without regard to kind;

(g) has the lower locants for heteroatoms in bridges, in the order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;

(h) has the fewer composite bridges;

(i) has the fewer dependent bridges;

(j) has fewer atoms in dependent bridges;

(k) has the greater number of divalent bridges;

(l) has lower locants for attachment of independent bridges;

(m) has the lower locants for attachment of dependent bridges;

(n) has the fused ring system with the greater number of noncumulative double bonds before bridging.

Each of these criteria is illustrated below.

(a) The senior bridged fused ring system has the bridged ring system with the greater number of rings before bridging.

Example:

4,7-methanocyclopenta[*a*]indene (PIN) > 1,4:5,8-dimethanonaphthalene (PIN)

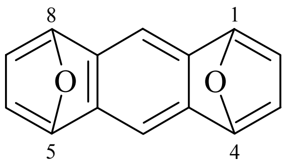
(b) The senior bridged fused ring system is the bridged ring system with the greater number of ring atoms before bridging.

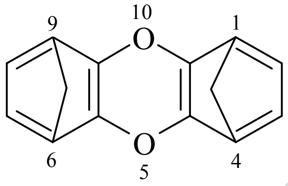
Example:

1H-3,10a-methanophenanthrene (PIN) > 1,4a-ethanofluorene (PIN)

(c) The senior bridged fused ring system is the bridged ring system with the fewer heteroatoms in the fused ring system.

Example:

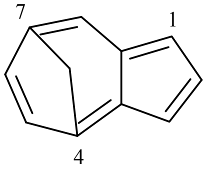


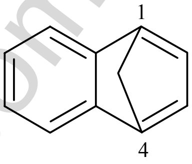


1,4:5,8-diepoxyanthracene (PIN) > 1,4:6,9-dimethanooxanthrene (PIN)

(d) The senior bridged fused ring system is the bridged ring system with the senior fused ring system before bridging according to P-44-2.2.4.1 through P-44.2.2.4.5 and P-44.2.2 above.

Example:

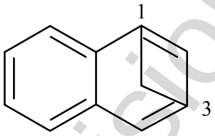


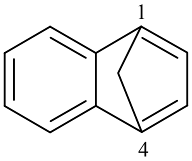


4,7-methanoazulene (PIN) > 1,4-methanonaphthalene (PIN)

(e) The senior bridged ring system has the lowest locants for bridge attachments.

Example:

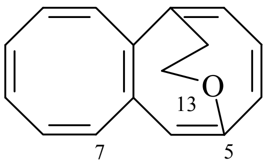


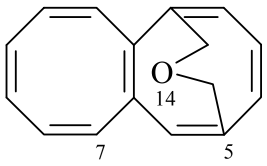


1,3-methanonaphthalene (PIN) > 1,4-methanonaphthalene (PIN)

(f) The senior bridged fused ring system has the lowest locants for heteroatoms in bridges, without regard to kind.

Example:



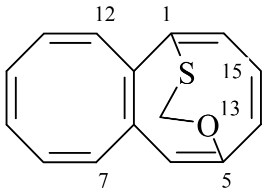


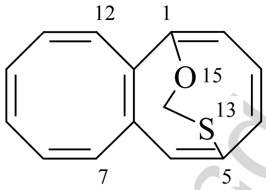
5,1-(epoxyethano)octalene (PIN) > 1,5-(methanooxymethano)octalene (PIN)

(locant 13 for the oxygen atom is lower than 14)

(g) The senior bridged fused ring system has the lowest locants for heteroatoms in bridges, in the order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Example:



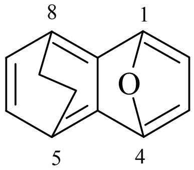


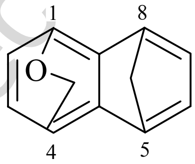
5,1-(epoxymethanosulfano)octalene (PIN) > 1,5-(epoxymethanosulfano)octalene (PIN)

(locant 13 for the oxygen atom is lower than 15)

(h) The senior bridged fused ring system has the fewer composite bridges.

Example:

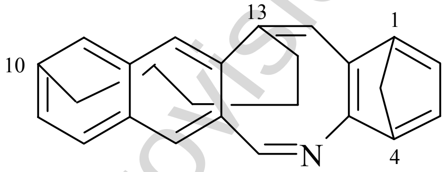


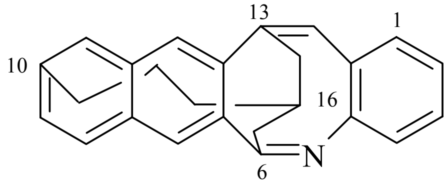


1,4-epoxy-5,8-ethanonaphthalene (PIN) > 1,4-epoxymethano-5,8-methanonaphthalene (PIN)

(i) The senior bridged fused ring system has the fewer dependent bridges.

Example:



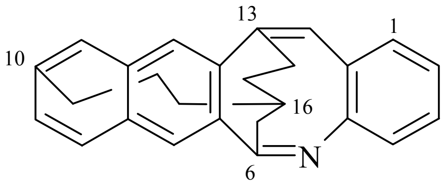


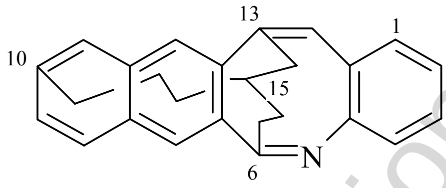
I > **II**

I 1,4-methano-10,13-pentanonaphtho[2,3-*c*][1]benzazocine (PIN)
II 6,16-methano-10,13-pentanonaphtho[2,3-*c*][1]benzazocine (PIN)

(j) The senior bridged fused ring system has fewer atoms in dependent bridges.

Example:



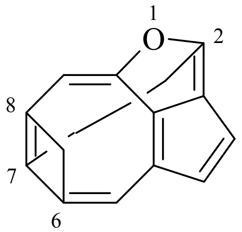


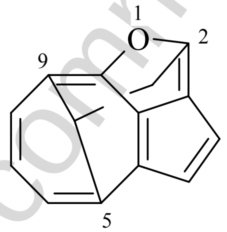
I > **II**

I 6,16-methano-10,13-hexanonaphtho[2,3-*c*][1]benzazocine (PIN)
II 6,15-ethano-10,13-pentanonaphtho[2,3-*c*][1]benzazocine (PIN)

(k) The senior bridged fused ring system has the greater number of divalent bridges.

Example:



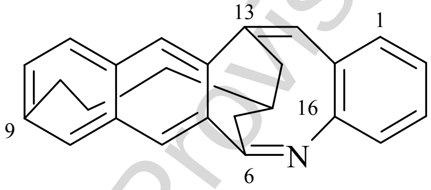


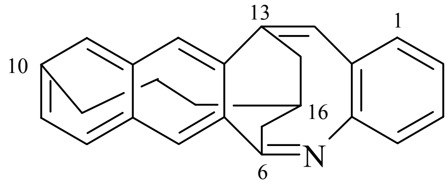
I > **II**

I 1-oxa-2,7:6,8-dimethanocycloocta[1,2,3-*cd*]pentalene (PIN)
II 1-oxa-5,9,2-(ethane[1,1,2]triyl)cycloocta[1,2,3-*cd*]pentalene (PIN)

(l) The senior bridged fused ring system has lower locants for attachment of independent bridges.

Example:



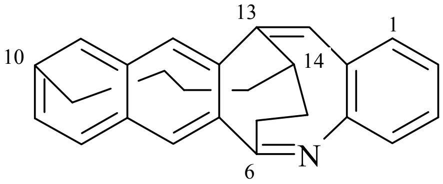


I > **II**

I 6,16-methano-9,13-pentanonaphthaleno[2,3-*c*][1]benzazocine (PIN)
II 6,16-methano-10,13-pentanonaphthaleno[2,3-*c*][1]benzazocine (PIN)

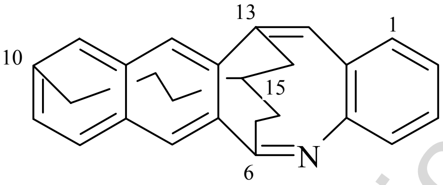
(m) The senior bridged fused ring system has the lower locants for attachment of dependent bridges.

Example:



I

>

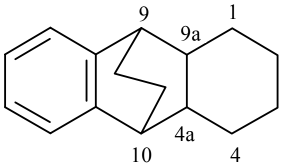


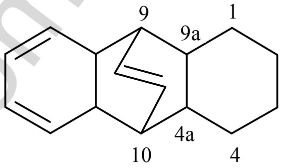
II

I 6,14-ethano-10,13-pentanonaphthaleno[2,3-*c*][1]benzazocine (PIN)
II 6,15-ethano-10,13-pentanonaphthaleno[2,3-*c*][1]benzazocine (PIN)

(n) The senior bridged fused ring system has the fused ring system with the greater number of noncumulative double bonds before bridging.

Example:





1,2,3,4,4a,9,9a,10-octahydro-
9,10-ethanoanthracene (PIN)

>

1,2,3,4,4a,8a,9,9a,10,10a-decahydro-
9,10-ethenoanthracene (PIN)

P-44.2.2.2.5 Senority criteria for bridged nonfused ring systems (von Baeyer ring systems) are applied successively until there are no alternatives remaining. These criteria are listed first and then separately illustrated.

The senior bridged nonfused ring system:

(a) has the lower number at the first point of difference for describing ring sizes in the descriptor in order of citation;

(b) has the lower bridge attachment locants (superscript locants) at the first point of difference when compared term by term in order of increasing numerical value;

(c) has the lower bridge attachment locants (superscript locants) at first point of difference when compared term by term in their order of citation in the name;

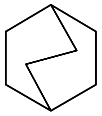
(d) has lowest locants for heteroatoms considered as a set without regard to kind;

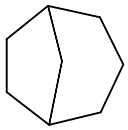
(e) has lowest locants for heteroatoms cited first in the sequence: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Each of these criteria is illustrated below.

(a) The senior bridged nonfused ring system has the lower number at the first point of difference for describing ring sizes in the descriptor in order of citation.

Example:

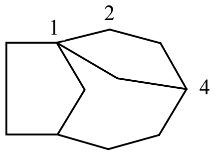


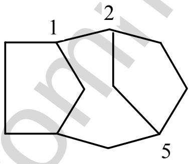


bicyclo[2.2.2]octane (PIN) > bicyclo[3.2.1]octane (PIN)

(b) The senior bridged nonfused ring system has the lower bridge attachment locants (superscript locants) at the first point of difference when compared term by term in order of increasing numerical value.

Example:

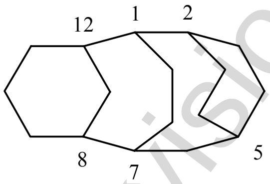


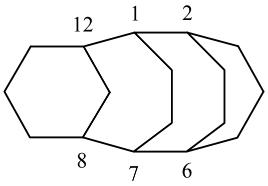


tricyclo[5.2.1.1^{1,4}]undecane (PIN) > tricyclo[5.2.1.1^{2,5}]undecane (PIN)

(c) The senior bridged nonfused ring system has the lower bridge attachment locants (superscript locants) at first point of difference when compared term by term in their order of citation in the name.

Example:

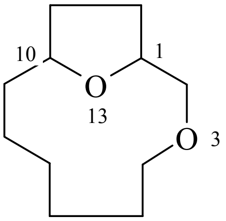


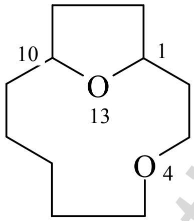


tetracyclo[5.5.2.2^{2,5}.1^{8,12}]heptadecane (PIN) > tetracyclo[5.5.2.2^{2,6}.1^{8,12}]heptadecane (PIN)

(d) The senior bridged nonfused ring system has lowest locants for heteroatoms considered as a set without regard to kind.

Example:

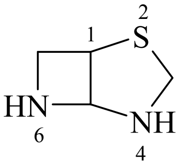


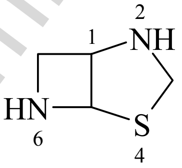


3,13-dioxabicyclo[8.2.1]tridecane (PIN) > 4,13-dioxabicyclo[8.2.1]tridecane (PIN)

(e) The senior bridged nonfused ring system has lowest locants for heteroatoms cited first in the sequence: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Example:





2-thia-4,6-diazabicyclo[3.2.0]heptane (PIN) > 4-thia-2,6-diazabicyclo[3.2.0]heptane (PIN)

P-44.2.2.2.6 Senority criteria for acyclic (linear) phane systems are applied sucessively until there are no alternatives remaining. These criteria are listed first and then separately illustrated.

The senior acyclic (linear) phane system:

(a) has the senior amplificant, as defined by P-44.2.2.1 through P-44.2.2.5;

(b) has the lowest set of superatom locants for all amplificants;

(c) has the lowest locants for senior amplificants;

(d) has the lowest amplificant attachment locants considered as a set when compared term by term in order of increasing numerical value;

(e) has the lowest attachment locants when compared term by term in their order of citation in the name;

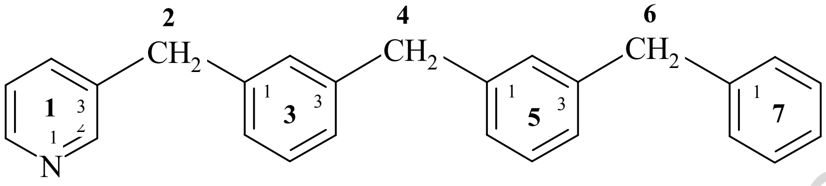
(f) has the lowest locants for heteroatoms described 'a' prefixes without regard to kind;

(g) has the lowest locants for heteroatoms described by 'a' prefixes first cited in the following order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

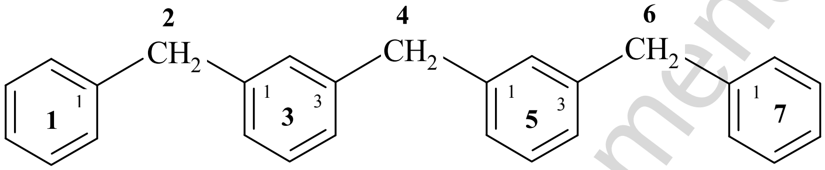
Each of these criteria is illustrated below.

(a) The senior acyclic phane system has the senior amplificant, as defined by P-44.2.2.1 through P-44.2.2.5.

Examples:



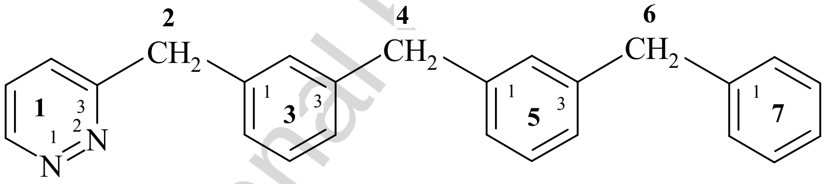
(I)



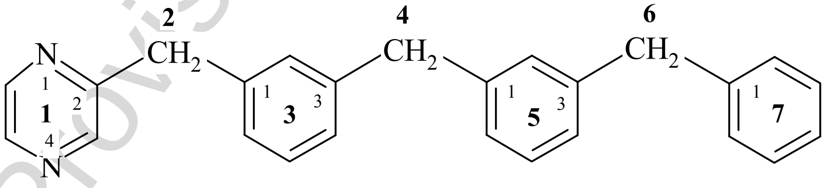
(II)

(**I**) 1(3)-pyridina-3,5(1,3),7(1)-tribenzenaheptaphane (PIN) > (**II**) 1,7(1),3,5(1,3)-tetrabenzenaheptaphane (PIN)

[the amplificant pyridine in (**I**) is senior to the amplificant benzene in (**II**)]



(I)



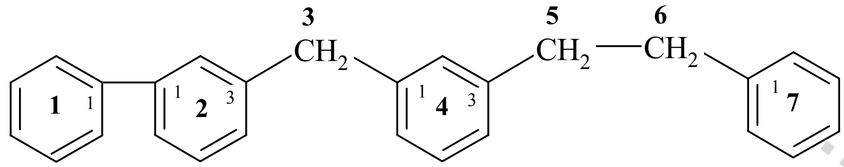
(II)

(I) 1(3)-pyridazina-3,5(1,3),7(1)-tribenzenaheptaphane (PIN) > (II) 1(2)-pyrazina-3,5(1,3),7(1)-tribenzenaheptaphane (PIN)

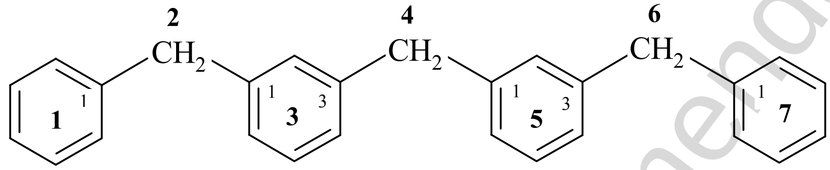
[the amplificant pyridazine in (**I**) is senior to the amplificant pyrazine in (**II**)]

(b) The senior acyclic phane ring system has the lowest set of superatom locants for all amplificants.

Example:



(I)



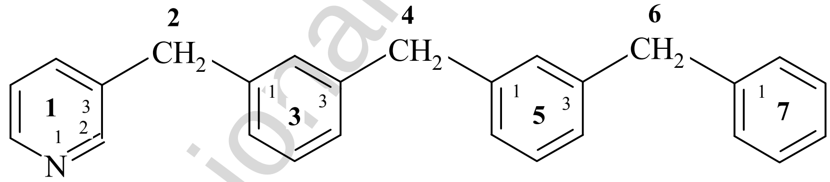
(II)

(**I**) 1,7(1),2,4(1,3)-tetrabenzena-heptaphane (PIN) > (**II**) 1,7(1), 3,5(1,3)-tetrabenzena-heptaphane (PIN)

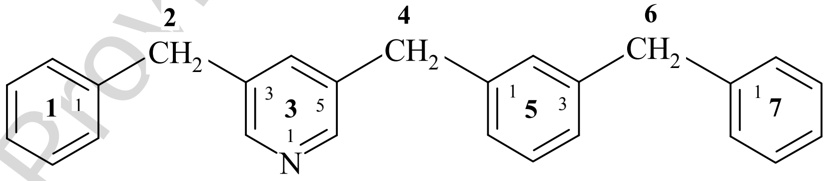
[the locant set '1,2,4,7 ' in (**I)** is lower than '1,3,5,7' in (**II**)]

(c) The senior acyclic phane ring system has the lowest locants for senior amplificants

Example:



(I)



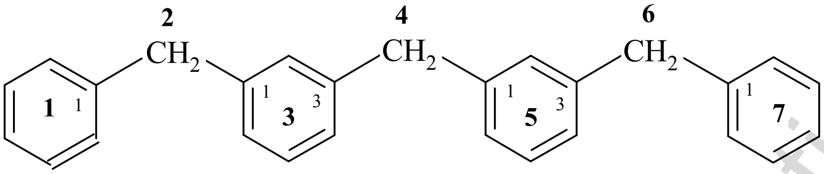
(II)

(**I**) 1(3)-pyridina-3,5(1,3),7(1)-tri-benzenaheptaphane (PIN) > (**II**) 3(3,5)-pyridina-1,7(1),5(1,3)-tribenzenaheptaphane (PIN)

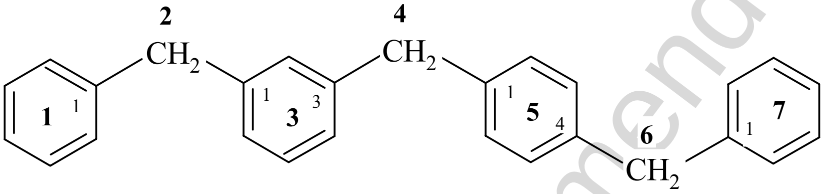
[the senior amplificant, pyridine, has the lower locant '1' in (**I**)]

(d) The senior acyclic phane ring system has the lowest amplificant attachment locants considered as a set when compared term by term in order of increasing numerical value.

Example:



(I)



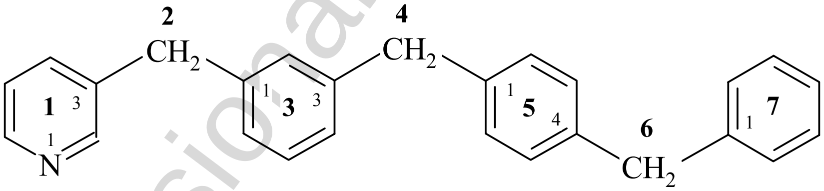
(II)

(**I**) 1,7(1),3,5(1,3)-tetrabenzena-heptaphane (PIN) > (**II**) 1,7(1), 3(1,3),5(1,4)-tetrabenzena-heptaphane (PIN)

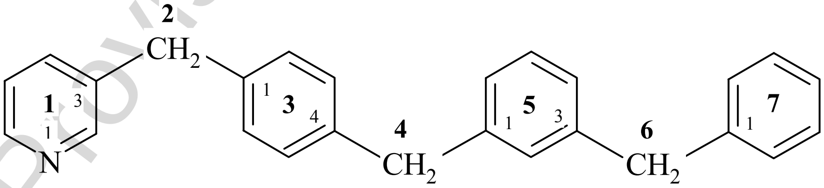
[the locant set ‘1,1,1,1,3,3’ in (**I**) is lower than ‘1,1,1,1,3,4’ in (**II**)]

(e) The senior phane ring system has the lowest attachment locants when compared term by term in their order of citation in the name.

Example:



(I)



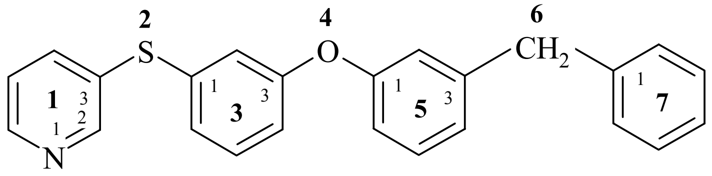
(II)

(**I**) 1(3)-pyridina-3(1,3),5(1,4),7(1)-tribenzenaheptaphane (PIN) > (**II**) 1(3)-pyridina-3(1,4),5(1,3),7(1)-tribenzenaheptaphane (PIN)

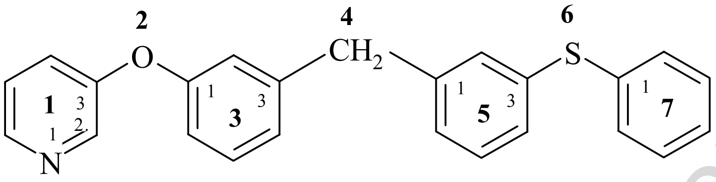
[the locant set ‘3,1,3,1,4’ in **(I)** is lower than ‘3,1,4,1,3’ in (**II**)]

(f) The senior acyclic phane ring system has the lower locants for heteroatoms described by ‘a’ prefixes without regard to kind.

Example:



(I)



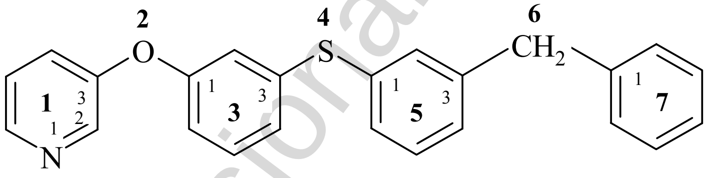
(II)

(**I**) 4-oxa-2-thia-1(3)-pyridina- 3,5(1,3),7(1)-tribenzena- heptaphane (PIN)	>	(**II**) 2-oxa-6-thia-1(3)-pyridina- 3,5(1,3),7(1)-tribenzena- heptaphane (PIN)

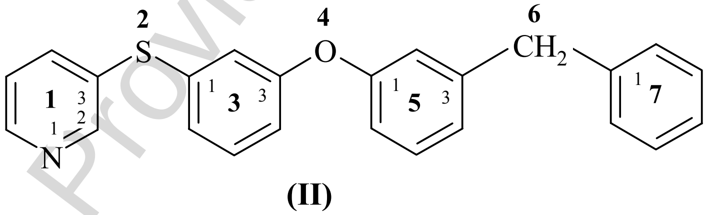
[the locant set ‘2,4’ for S and O in (**I**) is lower than ‘2,6’ in (**II**)]

(g) The senior acyclic phane ring system has the lowest locants for heteroatoms described by (‘a’) prefixes first cited in the following order: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Example:



(I)



(II)

(**I**) 2-oxa-4-thia-1(3)-pyridina- 3,5(1,3),7(1)tribenzena- heptaphane (PIN)	>	(**II**) 4-oxa-2-thia-1(3)-pyridina- 3,5(1,3),7(1)tribenzena- heptaphane (PIN)

[the locant ‘2’ for the senior heteroatom, oxa, in **(I)** is lower than ‘4’ in (**II**)]

P-44.2.2.2.7 Senority criteria for ring assemblies are applied successively until there are no alternatives remaining. These criteria are listed first and then separately illustrated.

The senior bridged nonfused ring system:

(a) has the senior component according to the appropriate criteria for rings and ring systems in P-44.2.2.1 through P-44.2.2.6;

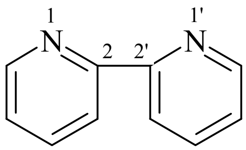
(b) has the lower ring junction locants at the first point of difference when compared term by term in order of increasing numerical value;

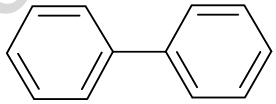
(c) has the lower ring junction locants at the first point of difference when compared term by term in order of their appearance in the name;

Each of these criteria is illustrated below.

(a) The senior ring assembly has the senior component according to the appropriate criteria for rings and ring systems in P-44.2.2.1 through P-44.2.2.6.

Example:

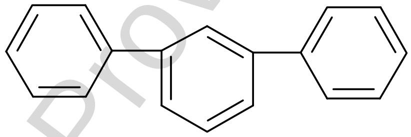


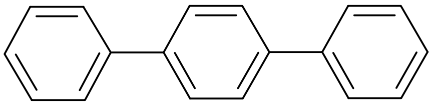


2,2′-bipyridine (PIN) > 1,1′-biphenyl (PIN)

(b) The senior ring assembly has the lower ring junction locants at the first point of difference when compared term by term in order of increasing numerical value. The arabic numbers and letters within parentheses refer to the method of name formation (see P-28.2.1) and the method of numbering (see P-28.3.1)

Example:



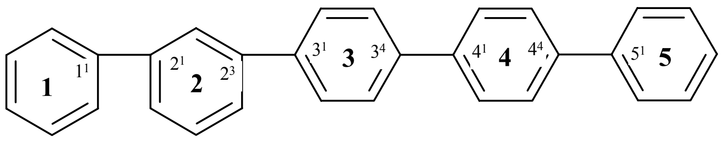


(2a) $1^1,2^1:2^3,3^1$-terphenyl (PIN) > (2a) $1^1,2^1:2^4,3^1$-terphenyl (PIN)
(see P-28.2.1 and P-28.3.1) (see P-28.2.1 and P-28.3.1)
(2b) 1,1′:3′,1″-terphenyl > (2b) 1,1′:4′,1″-terphenyl
(see P-28.2.1 and P-28.3.1) (see P-28.2.1 and P-28.3.1)

(c) The senior ring assembly has the lower ring junction locants at the first point of difference when compared term by term in order of their appearance in the name.

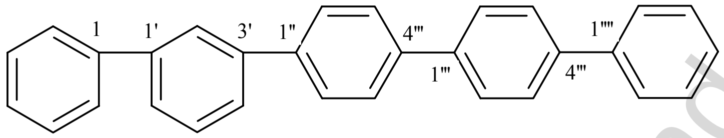
Example:

Ia

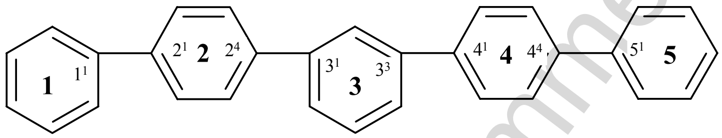


or

Ib

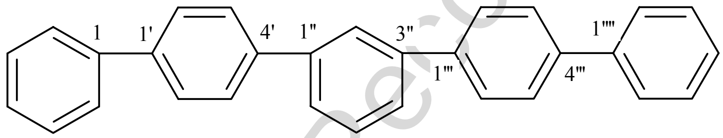


IIa



or

IIb



Ia (2a) $1^1,2^1:2^3,3^1:3^4,4^1:4^4,5^1$-quinquephenyl (PIN) (see P-28.2.1 and P-28.3.1) > **IIa** (2a) $1^1,2^1:2^4,3^1:3^3,4^1:4^4,5^1$-quinquephenyl (PIN) (see P-28.2.1 and P-28.3.1)

or

Ib (2b)1,1′;3′,1″;4″,1‴,4‴,1⁗-quinquephenyl (see P-28.2.1 and P-28.3.1) > **IIb** (2b) 1,1′;4′,1″;3″,1‴;4‴,1⁗-quinquephenyl (see P-28.2.1 and P-28.3.1)

(at the third term, 2^3 in **Ia** or 3′ in **Ib** is lower than 2^4 in **IIb** or 4′ in **IIb**)

P-44.2.3 Senority criteria applicable to all rings and ring systems. They are applied successively until there are no alternatives remaining. These criteria are listed first and then separately illustrated.

The senior ring or ring system:

(a) has the greater number of multiple bonds;

(b) has the greater number of double bonds;

(c) has the lower locants for indicated hydrogen;

(d) has the lower locants for points of attachment (if a substituent group);

(e) has the lower locant for an attached group expressed as suffix;

(f) has the lower locant(s) for endings or prefixes that express changes in the level of hydrogenation, i.e., for ‘ene’ and ‘yne’ endings and ‘hydro/dehydro’ prefixes;

(g) has the maximum number of substituents cited as prefixes;

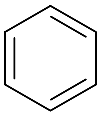
(h) has lower locants for substituents named as prefixes;

(i) has lower locants for the substituent named as a prefix and which is cited first in alphanumerical order.

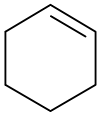
Each of these criteria is illustrated below.

(a) the senior ring or ring system has the greater number of multiple bonds; for the purpose of this criterion, mancude rings or ring systems are considered as consisting of noncumulative double bonds.

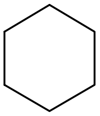
Examples:



benzene (PIN) >

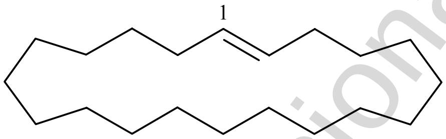


cyclohexene (PIN) >

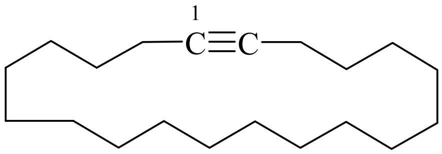


cyclohexane (PIN)

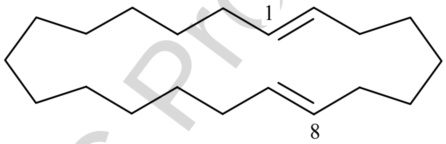
(b) (b) the senior ring or ring system has the greater number of double bonds.



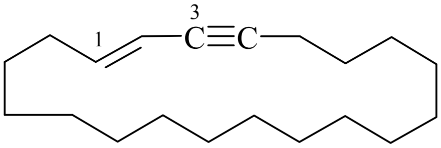
cycloicosene (PIN) >



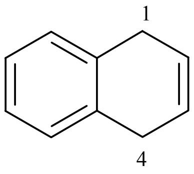
cycloicosyne (PIN)



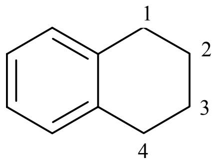
cycloicosa-1,8-diene (PIN) >



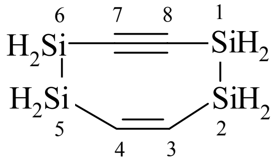
cycloicos-1-en-3-yne (PIN)

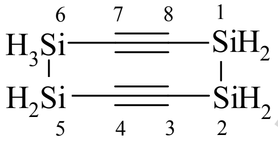


1,4-dihydronaphthalene (PIN) >



1,2,3,4-tetrahydronaphthalene (PIN)

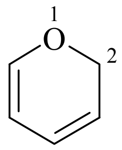


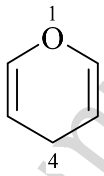


1,2,5,6-tetrasilacyclooct-3-en-7-yne (PIN) > 1,2,5,6-tetrasilacycloocta-3,7-diyne (PIN)

(c) The senior ring or ring system has the lowest locants for indicated hydrogen.

Example:

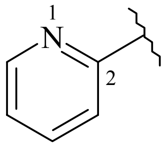


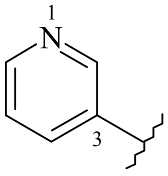


2*H*-pyran (PIN) > 4*H*-pyran (PIN)

(d) The senior ring or ring system has the lowest locants for points of attachment (if a substituent group).

Example:

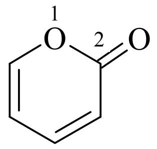


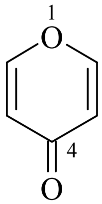


pyridin-2-yl (PIN) > pyridin-3-yl (PIN)

(e) The senior ring or ring system has the lowest locant for an attached group expressed as suffix.

Example:



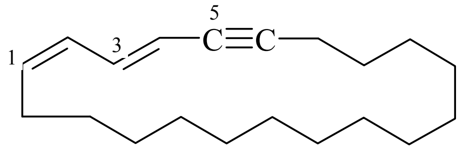


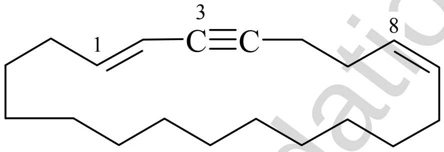
2*H*-pyran-2-one (PIN) > 4*H*-pyran-4-one (PIN)

(f) The senior ring or ring system has the lowest locants for endings or prefixes that express changes in the degree of hydrogenation, i.e., for ‘ene’ and ‘yne’ endings and ‘hydro/dehydro’ prefixes.

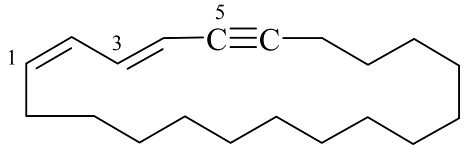
(i) For the endings endings ‘ene’ and ‘yne’ lower locants are assigned first to the endings as a set without regard to type and then to ‘ene’ endings.

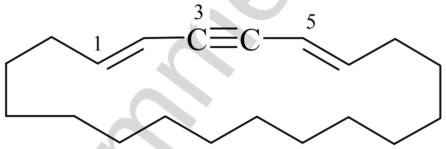
Examples:





cycloicosa-1,3-dien-5-yne (PIN) > cycloicosa-1,8-dien-3-yne (PIN)

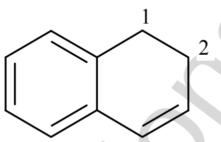


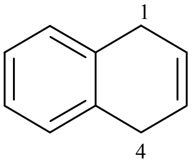


cycloicosa-1,3-dien-5-yne (PIN) > cycloicosa-1,5-dien-3-yne (PIN)

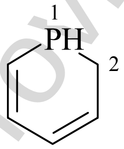
(ii) for ‘hydro/dehydro’ prefixes, lower locants are assigned as described in P-31.2.4.

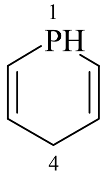
Examples:



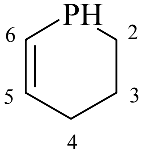


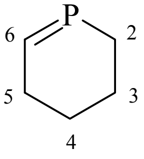
1,2-dihydronaphthalene (PIN) > 1,4-dihydronaphthalene (PIN)



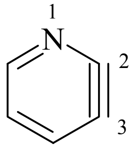


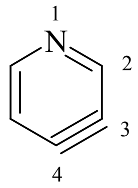
1,2-dihydrophosphinine (PIN) > 1,4-dihydrophosphinine (PIN)





1,2,3,4-tetrahydrophosphinine (PIN) > 2,3,4,5-tetrahydrophosphinine (PIN)

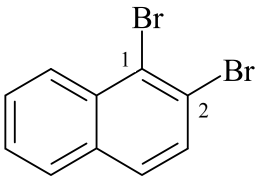


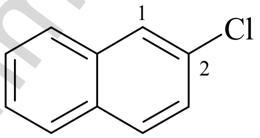


2,3-didehydropyridine (PIN) > 3,4-didehydropyridine (PIN)

(g) The senior ring or ring system has the maximum number of substituents cited as prefixes.

Example:

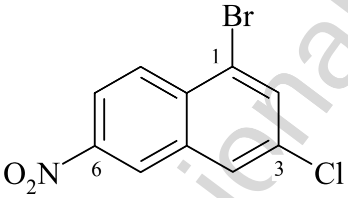


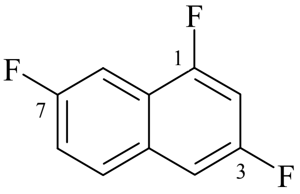


1,2-dibromonaphthalene (PIN) > 2-chloronaphthalene (PIN)

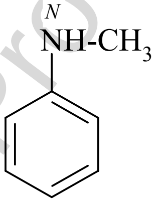
(h) The senior ring or ring system has lower locants for substituents named as prefixes.

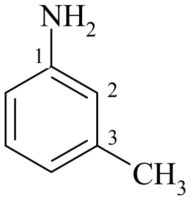
Example:



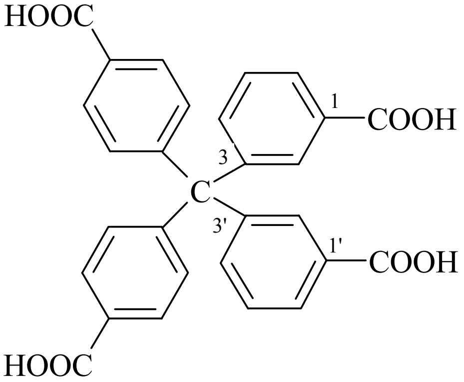


1-bromo-3-chloro-6-nitronaphthalene (PIN) > 1,3,7-trifluoronaphthalene (PIN)





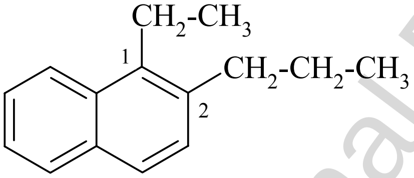
N-methylaniline (PIN) > 3-methylaniline (PIN)

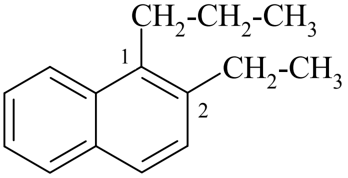


3,3′-[bis(4-carboxyphenyl)methylene]dibenzoic acid (PIN)
[not 4,4′-[bis(3-carboxyphenyl)methylene]dibenzoic acid; the senior parent structure must be the benzene ring substituted in the 1,3-positions]

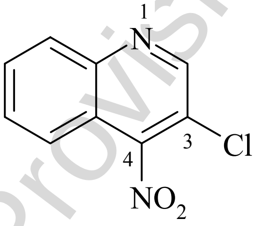
(i) The senior ring or ring system has lower locants for the substituent named as a prefix and which is cited first in alphanumerical order.

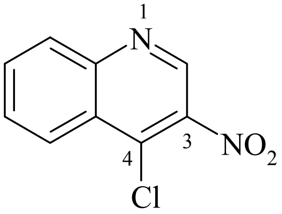
Examples:



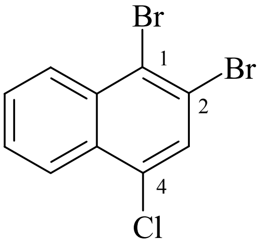


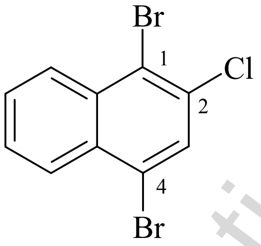
1-ethyl-2-propylnaphthalene (PIN) > 2-ethyl-1-propylnaphthalene (PIN)





3-chloro-4-nitroquinoline (PIN) > 4-chloro-3-nitroquinoline (PIN)





1,2-dibromo-4-chloronaphthalene (PIN) > 1,4-dibromo-2-chloronaphthalene (PIN)

P-44.3 The principal chain

In an acyclic compound, or in a compound composed of chains and rings, the chain on which the nomenclature and numbering is based is called the 'principal chain'. When there is a choice for the principal chain, the following criteria are applied, in the order listed, until a decision is reached.

A change to the traditional order of seniority criteria is recommended; the length of the chain is senior to unsaturation.

The principal chain:

(a) contains the greater number of heteroatoms;

(b) has the greater number of skeletal atoms;

(c) contains the greater number of the most senior acyclic heteroatom in the order: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;

(d) has the greater number of double and triple bonds considered together;

(e) contains the greater number of double bonds;

(f) has lowest locants for heteroatoms considered together as a set without regard to kind;

(g) has lowest locants for heteroatoms appearing first in the order: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;

(h) has lowest locants for the principal group (that is for the suffix);

(i) has lowest locants for multiple bonds;

(j) has lowest locants for double bonds;

(k) has the greater number of substituents (other than the principal characteristic group or 'hydro/dehydro') cited as prefixes;

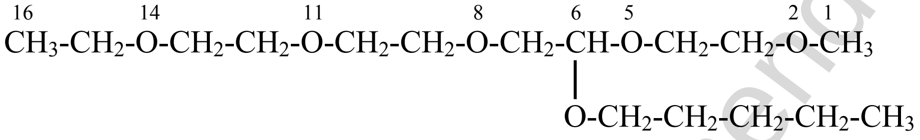
(l) has the lower locant(s) for all substituents (other than the principal characteristic group or 'hydro/dehydro') cited as detachable prefixes;

(m) has the maximum number of substituents (other than principal characteristic groups or ‘hydro/dehydro’) cited as prefixes earlier in alphanumerical order.

Each of these criteria is illustrated below.

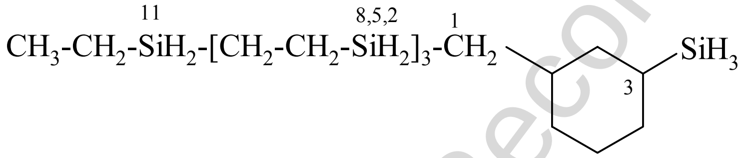
(a) The principal chain contains the greater number of acyclic heteroatoms.

Examples:



$$\overset{16}{C}H_3\text{-}CH_2\text{-}\overset{14}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{11}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{8}{O}\text{-}CH_2\text{-}\overset{6}{C}H(O\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3)\text{-}\overset{5}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{2}{O}\text{-}\overset{1}{C}H_3$$

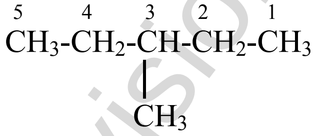
6-(pentyloxy)-2,5,8,11,14-pentaoxahexadecane (PIN)
[not 11-(2-methoxyethoxy)-3,6,9,12-tetraoxaheptadecane]



1-(3-silylcyclohexyl)-2,5,8,11-tetrasilatridecane (PIN)

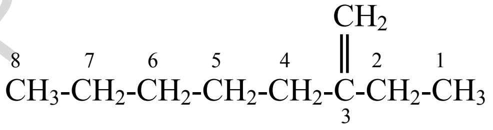
(b) the principal chain has the greater number of skeletal atoms.

Examples:



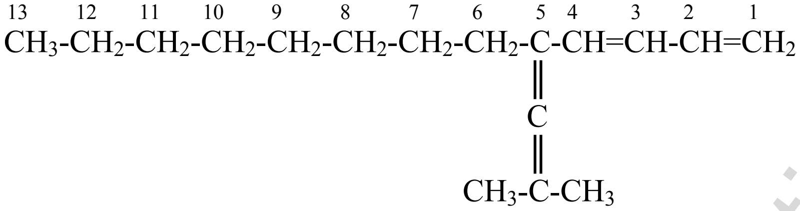
$$\overset{5}{C}H_3\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H(CH_3)\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_3$$

3-methylpentane (PIN)
(not 2-ethylbutane)



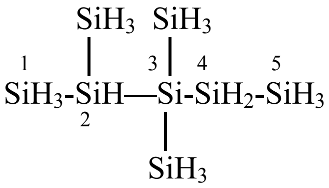
$$\overset{8}{C}H_3\text{-}\overset{7}{C}H_2\text{-}\overset{6}{C}H_2\text{-}\overset{5}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\underset{3}{C}(=CH_2)\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_3$$

3-methylideneoctane (PIN)
(formerly 2-ethylhept-1-ene)



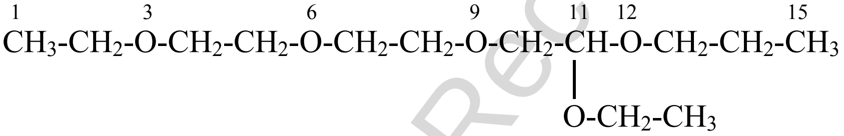
$$\overset{13}{C}H_3\text{-}\overset{12}{C}H_2\text{-}\overset{11}{C}H_2\text{-}\overset{10}{C}H_2\text{-}\overset{9}{C}H_2\text{-}\overset{8}{C}H_2\text{-}\overset{7}{C}H_2\text{-}\overset{6}{C}H_2\text{-}\underset{\substack{\| \\ C \\ \| \\ CH_3\text{-}C\text{-}CH_3}}{\overset{5}{C}}\text{-}\overset{4}{C}H{=}\overset{3}{C}H\text{-}\overset{2}{C}H{=}\overset{1}{C}H_2$$

5-(2-methylprop-1-en-1-ylidene)trideca-1,3-diene (PIN)
(formerly 7-methyl-5-octylocta-1,3,5,6-tetraene)



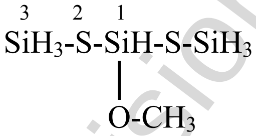
$$\overset{1}{Si}H_3\text{-}\underset{2}{\overset{\overset{SiH_3}{|}}{Si}}H\text{—}\underset{\underset{SiH_3}{|}}{\overset{\overset{SiH_3}{|}}{\overset{3}{Si}}}\text{-}\overset{4}{Si}H_2\text{-}\overset{5}{Si}H_3$$

2,3,3-trisilylpentasilane (preselected name, see P-12.2)



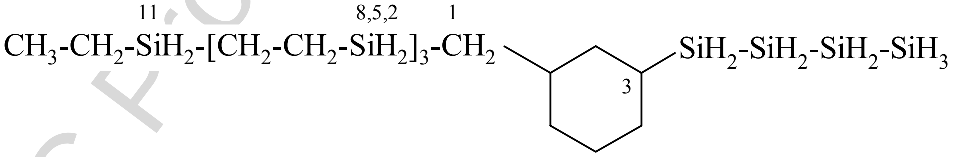
$$\overset{1}{C}H_3\text{-}CH_2\text{-}\overset{3}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{6}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{9}{O}\text{-}CH_2\text{-}\underset{\underset{O\text{-}CH_2\text{-}CH_3}{|}}{\overset{11}{C}H}\text{-}\overset{12}{O}\text{-}CH_2\text{-}CH_2\text{-}\overset{15}{C}H_3$$

11-ethoxy-3,6,9,12-tetraoxapentadecane (PIN)
(not 4-propoxy-3,6,9,12-tetraoxatetradecane)

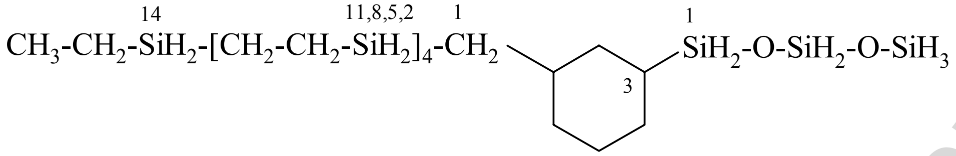


$$\overset{3}{Si}H_3\text{-}\overset{2}{S}\text{-}\underset{\underset{O\text{-}CH_3}{|}}{\overset{1}{Si}H}\text{-}S\text{-}SiH_3$$

3-methoxytrisilathiane (PIN)



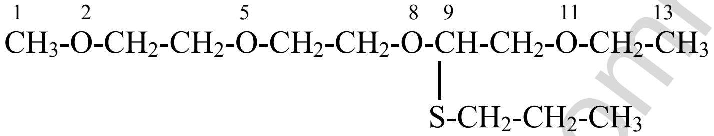
1-(3-tetrasilan-1-ylcyclohexyl)-2,5,8,11-tetrasilatridecane (PIN)
(four heteroatoms in each chain; longest chain is the ‘a’ chain)



1-[3-(trisiloxan-1-yl)cyclohexyl]-2,5,8,11,14-pentasilahexadecane (PIN)
(5 heteroatoms in each chain; longest chain is the 'a' chain)

(c) The principal chain contains the greater number of the most senior acyclic heteroatom in the order: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Examples:

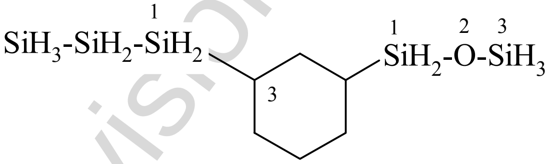


$CH_3\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH(S\text{-}CH_2\text{-}CH_2\text{-}CH_3)\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_3$

9-(propylsulfanyl)-2,5,8,11-tetraoxatridecane (PIN)
(4 O > 3 O,1 S)

$SiH_3\text{-}O\text{-}SiH_2\text{-}S\text{-}SiH_3$

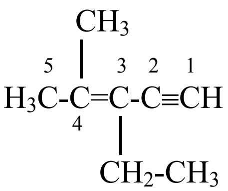
(silylsulfanyl)disiloxane (PIN)
(O > S)



1-[3-(trisilan-1-yl)cyclohexyl]disiloxane (PIN)
(O > Si)

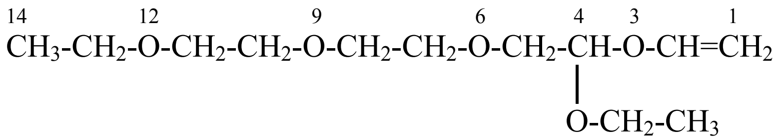
(d) The principal chain has the greater number of unsaturated bonds of any kind

Examples:



$H_3C\text{-}C(CH_3)\text{=}C(CH_2\text{-}CH_3)\text{-}C\equiv CH$

3-ethyl-4-methylpent-3-en-1-yne (PIN)

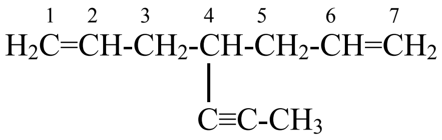


$$\overset{14}{CH_3}-CH_2-\overset{12}{O}-CH_2-CH_2-\overset{9}{O}-CH_2-CH_2-\overset{6}{O}-CH_2-\underset{\substack{|\\ O-CH_2-CH_3}}{\overset{4}{CH}}-\overset{3}{O}-CH=\overset{1}{CH_2}$$

4-ethoxy-3,6,9,12-tetraoxatetradec-1-ene (PIN)

(e) The principal chain contains the greater number of double bonds.

Example:

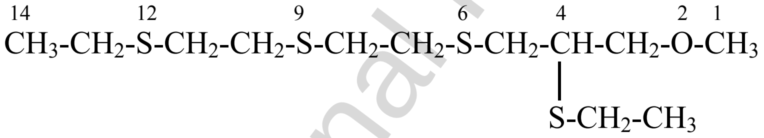


$$H_2\overset{1}{C}=\overset{2}{CH}-\overset{3}{CH_2}-\underset{\substack{|\\ C\equiv C-CH_3}}{\overset{4}{CH}}-\overset{5}{CH_2}-\overset{6}{CH}=\overset{7}{CH_2}$$

4-(prop-1-yn-1-yl)hepta-1,6-diene (PIN)

(f) The principal chain expresses lowest locants for heteroatoms considered together as a set without regard to kind.

Example:

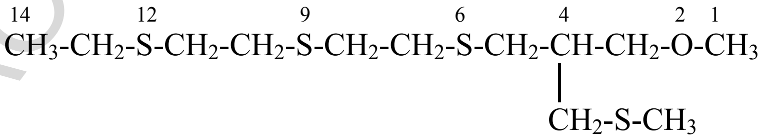


$$\overset{14}{CH_3}-CH_2-\overset{12}{S}-CH_2-CH_2-\overset{9}{S}-CH_2-CH_2-\overset{6}{S}-CH_2-\underset{\substack{|\\ S-CH_2-CH_3}}{\overset{4}{CH}}-CH_2-\overset{2}{O}-\overset{1}{CH_3}$$

4-(ethylsulfanyl)-2-oxa-6,9,12-trithiatetradecane (PIN)
[not 11-(ethylsulfanyl)-13-oxa-3,6,9-trithiatetradecane;
the heteroatom locant set 2,6,9,12 is lower than the
locant set 3,6,9,13]

(g) The principal chain expresses lowest locants for heteroatoms appearing first in the order: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl.

Example:

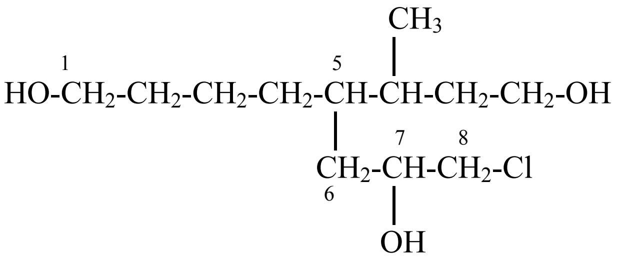


$$\overset{14}{CH_3}-CH_2-\overset{12}{S}-CH_2-CH_2-\overset{9}{S}-CH_2-CH_2-\overset{6}{S}-CH_2-\underset{\substack{|\\ CH_2-S-CH_3}}{\overset{4}{CH}}-CH_2-\overset{2}{O}-\overset{1}{CH_3}$$

4-[(methylsulfanyl)methyl]-2-oxa-6,9,12-trithiatetradecane (PIN)
(O > S for lower locant)

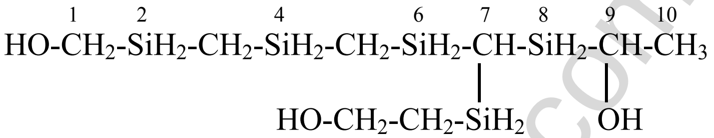
(h) The senior parent chain has the lower locant(s) for the characteristic group expressed as a suffix, i.e., the principal group.

Examples:



$HO\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}\underset{CH_2\text{-}\underset{OH}{CH}\text{-}CH_2\text{-}Cl}{CH}\text{-}\overset{CH_3}{CH}\text{-}CH_2\text{-}CH_2\text{-}OH$

8-chloro-5-(4-hydroxybutan-2-yl)octane-1,7-diol (PIN)
8-chloro-5-(3-hydroxy-1-methylpropyl)octane-1,7-diol

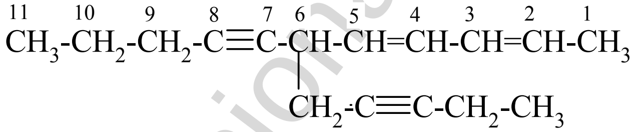


$HO\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}\underset{HO\text{-}CH_2\text{-}CH_2\text{-}SiH_2}{CH}\text{-}SiH_2\text{-}\underset{OH}{CH}\text{-}CH_3$

7-[(2-hydroxyethyl)silyl]-2,4,6,8-tetrasiladecane-1,9-diol (PIN)

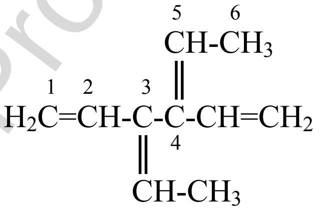
(i) The principal chain has lowest locants for multiple bonds.

Examples:



$CH_3\text{-}CH_2\text{-}CH_2\text{-}C{\equiv}C\text{-}\underset{CH_2\text{-}C{\equiv}C\text{-}CH_2\text{-}CH_3}{CH}\text{-}CH{=}CH\text{-}CH{=}CH\text{-}CH_3$

6-(pent-2-yn-1-yl)undeca-2,4-dien-7-yne (PIN)
(the locant set 2,4,7 is lower than 2,4,8)

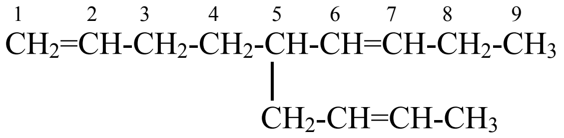


$H_2C{=}CH\text{-}\underset{\overset{\|}{CH\text{-}CH_3}}{C}\text{-}\overset{\underset{\|}{CH\text{-}CH_3}}{C}\text{-}CH{=}CH_2$

4-ethenyl-3-ethylidene-1,4-diene (PIN)

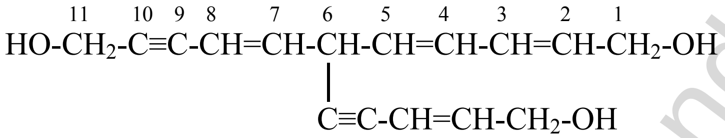
(j) The principal chain has the lowest locants for double bonds.

Examples:



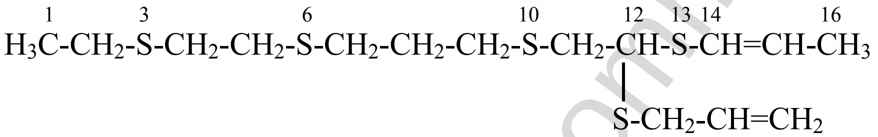
$$CH_2{=}CH\text{-}CH_2\text{-}CH_2\text{-}CH(CH_2\text{-}CH{=}CH\text{-}CH_3)\text{-}CH{=}CH\text{-}CH_2\text{-}CH_3$$

5-(but-2-en-1-yl)nona-1,6-diene (PIN)



$$HO\text{-}CH_2\text{-}C{\equiv}C\text{-}CH{=}CH\text{-}CH(C{\equiv}C\text{-}CH{=}CH\text{-}CH_2\text{-}OH)\text{-}CH{=}CH\text{-}CH{=}CH\text{-}CH_2\text{-}OH$$

6-(5-hydroxypent-3-en-1-yn-1-yl)undeca-2,4,7-trien-9-yne-1,11-diol (PIN)

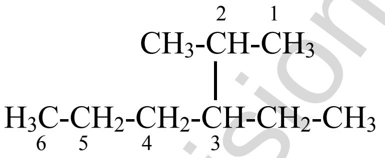


$$H_3C\text{-}CH_2\text{-}S\text{-}CH_2\text{-}CH_2\text{-}S\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}S\text{-}CH_2\text{-}CH(S\text{-}CH_2\text{-}CH{=}CH_2)\text{-}S\text{-}CH{=}CH\text{-}CH_3$$

12-(prop-2-en-1-ylsulfanyl)-3,6,10,13-tetrathiahexadec-14-ene (PIN)
[not 12-(prop-1-en-1-ylsulfanyl)-3,6,10,13-tetrathiahexadec-15-ene]

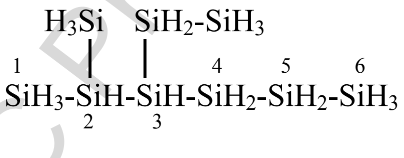
(k) The principal chain has the greater number of substituents (other than the principal characteristic group or ‘hydro/dehydro’) cited as prefixes.

Examples:



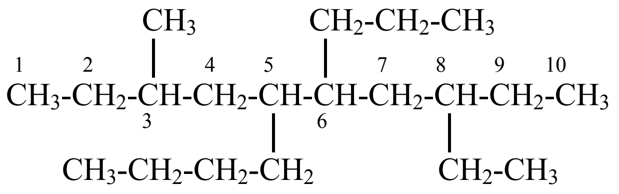
$$H_3C\text{-}CH_2\text{-}CH_2\text{-}CH(CH(CH_3)\text{-}CH_3)\text{-}CH_2\text{-}CH_3$$

3-ethyl-2-methylhexane (PIN)
(not 3-isopropylhexane)



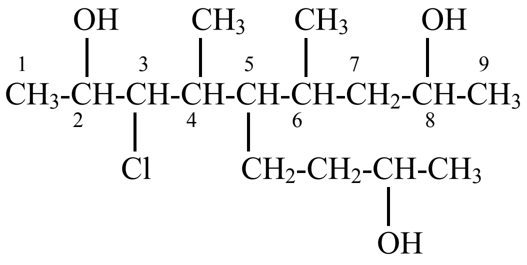
$$SiH_3\text{-}SiH(SiH_3)\text{-}SiH(SiH_2\text{-}SiH_3)\text{-}SiH_2\text{-}SiH_2\text{-}SiH_3$$

3-disilanyl-2-silylhexasilane (preselected name, see P-12.2)



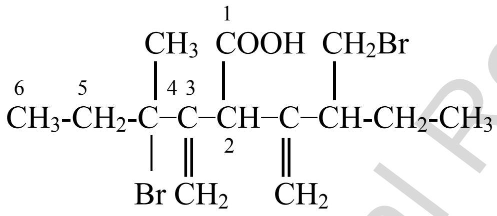
$CH_3\text{-}CH_2\text{-}CH(CH_3)\text{-}CH_2\text{-}CH(CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3)\text{-}CH(CH_2\text{-}CH_2\text{-}CH_3)\text{-}CH_2\text{-}CH(CH_2\text{-}CH_3)\text{-}CH_2\text{-}CH_3$

5-butyl-8-ethyl-3-methyl-6-propyldecane (PIN)



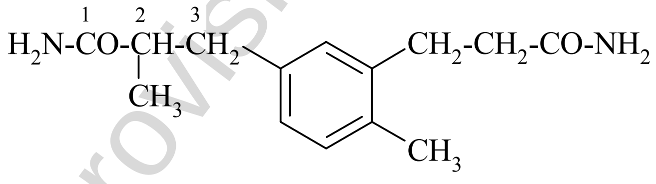
$CH_3\text{-}CH(OH)\text{-}CH(Cl)\text{-}CH(CH_3)\text{-}CH(CH_2\text{-}CH_2\text{-}CH(OH)\text{-}CH_3)\text{-}CH(CH_3)\text{-}CH_2\text{-}CH(OH)\text{-}CH_3$

3-chloro-5-(3-hydroxybutyl)-4,6-dimethylnonane-2,8-diol (PIN)

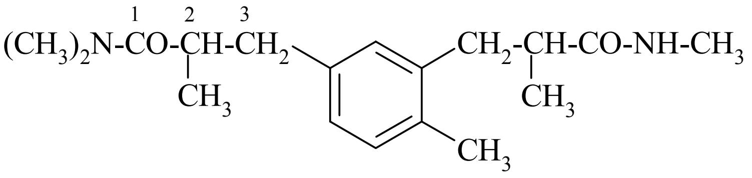


$CH_3\text{-}CH_2\text{-}C(CH_3)(Br)\text{-}C(=CH_2)\text{-}CH(COOH)\text{-}C(=CH_2)\text{-}CH(CH_2Br)\text{-}CH_2\text{-}CH_3$

4-bromo-2-[3-(bromomethyl)pent-1-en-2-yl]-4-methyl-3-methylidenehexanoic acid (PIN)
4-bromo-2-[2-(bromomethyl)-1-methylidenebutyl]-4-methyl-3-methylidenehexanoic acid



3-[3-(3-amino-3-oxopropyl)-4-methylphenyl]-2-methylpropanamide (PIN)
[not 3-[5-(3-amino-2-methyl-3-oxopropyl)-2-methylphenyl]propanamide;
the correct name has 2 substituents; the incorrect name only 1]

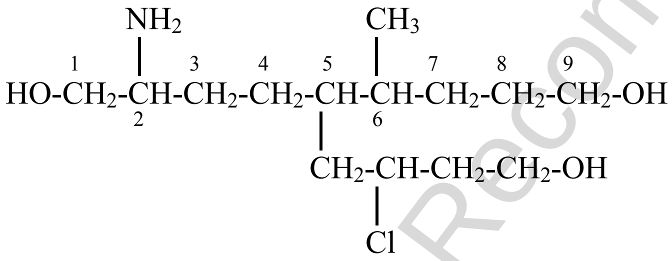


N,N,2-trimethyl-3-{4-methyl-3-[2-methyl-3-(methylamino)-3-oxopropyl]phenyl}-propanamide (PIN)

[not 3-{5-[(3-dimethylamino)-2-methyl-3-oxopropyl]-2-methylphenyl}-*N*,2-dimethylpropanamide; the correct name has 4 substituents, the incorrect name has only 3]

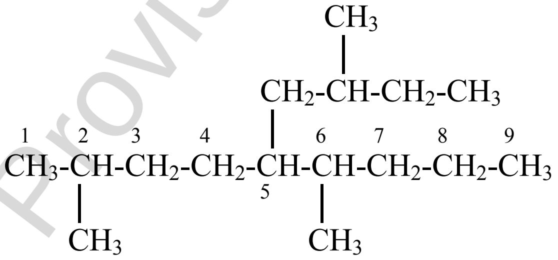
(l) The principal chain has the lower locant(s) for substituents (other than the principal characteristic group or ‘hydro/dehydro’) cited as detachable prefixes.

Examples:



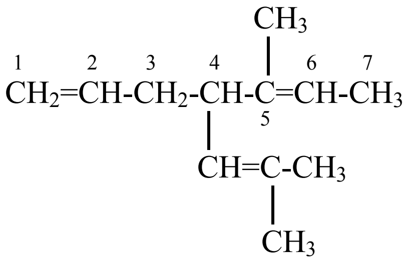
2-amino-5-(2-chloro-4-hydroxybutyl)-6-methylnonane-1,9-diol (PIN)

[not 2-amino-7-chloro-5-(5-hydroxypentan-2-yl)nonane-1,9-diol; nor 5-(3-amino-4-hydroxybutyl)-3-chloro-6-methylnonane-1,9-diol; the locant set ‘2,5,6’ in the correct name is lower than either of the locant sets ‘2,5,7’ or ‘3,5,6’]

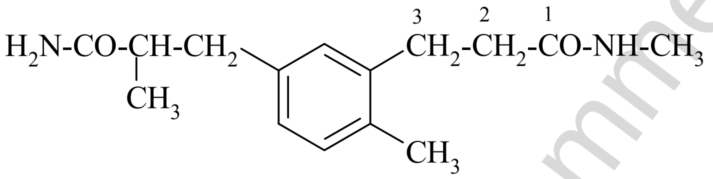


2,6-dimethyl-5-(2-methylbutyl)nonane (PIN)

[not 2,7-dimethyl-5-pentan-2-ylnonane; nor 3,6-dimethyl-5-(3-methylbutyl)nonane; the locant set ‘2,5,6’ in the correct name is lower that either of the locant sets ‘2,5,7’ or ‘3,5,7’]



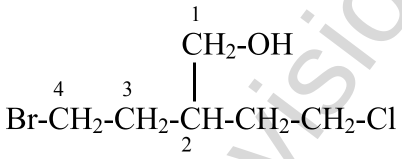
5-methyl-4-(2-methylprop-1-en-1-yl)hepta-1,5-diene (PIN)
[not 4-but-2-en-2-yl-6-methylhepta-1,5-diene; the locant set ‘4,5’ is lower than ‘4,6’]



3-[5-(3-amino-2-methyl-3-oxopropyl)-2-methylphenyl]-*N*-methylpropanamide (PIN)
[not 2-methyl-3-{3-[3-(methylamino)-3-oxopropyl]-4-methylphenyl}propanamide; the locant set *N*,3 in the correct name is lower than 2,3 (see P-14.3.4)]

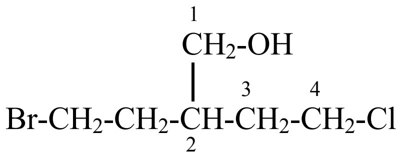
(m) The principal chain has the maximum number of substituents (other than principal characteristic groups or ‘hydro/dehydro’) cited as prefixes earlier in alphanumerical order, i.e., when two series of substituent names in alphanumerical order are compared term by term the series that contains the earlier term at the first difference is preferred.

Examples:



$\mathrm{Br\text{-}CH_2\text{-}CH_2\text{-}\overset{CH_2\text{-}OH}{CH}\text{-}CH_2\text{-}CH_2\text{-}Cl}$

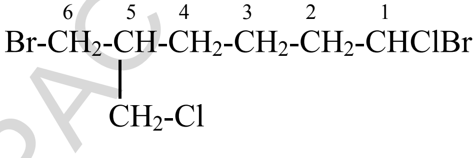
not



$\mathrm{Br\text{-}CH_2\text{-}CH_2\text{-}\overset{CH_2\text{-}OH}{CH}\text{-}CH_2\text{-}CH_2\text{-}Cl}$

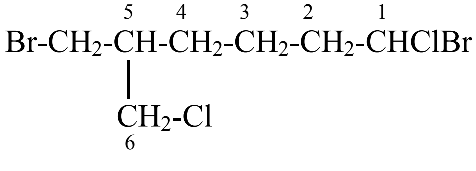
4-bromo-2-(2-chloroethyl)butan-1-ol (PIN) 2-(2-bromoethyl)-4-chlorobutan-1-ol

(‘bromo’ precedes ‘bromoethyl’ in alphanumerical order)



$\mathrm{Br\text{-}CH_2\text{-}\underset{CH_2\text{-}Cl}{CH}\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CHClBr}$

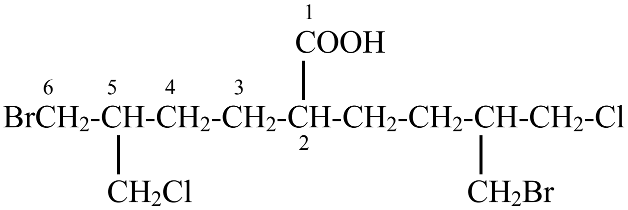
not



$\mathrm{Br\text{-}CH_2\text{-}\underset{CH_2\text{-}Cl}{CH}\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CHClBr}$

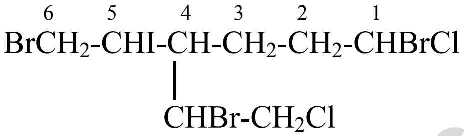
1,6-dibromo-1-chloro-5-(chloromethyl)-hexane (PIN) 1-bromo-5-(bromomethyl)-1,6-dichloro-hexane

[the correct name has two bromo prefixes viewed as bromo-,bromo-, the incorrect name has only one bromo prefix;.the numerical term is ignored and thus the alphanumerical comparison is ‘bromo-,bromo-,chloro’ with ‘bromo-,bromomethyl’]



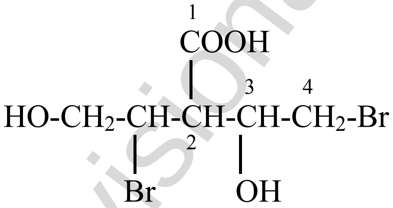
$$\mathrm{BrCH_2\text{-}\underset{CH_2Cl}{CH}\text{-}CH_2\text{-}CH_2\text{-}\overset{COOH}{CH}\text{-}CH_2\text{-}CH_2\text{-}\underset{CH_2Br}{CH}\text{-}CH_2\text{-}Cl}$$

6-bromo-2-[4-bromo-3-(chloromethyl)butyl]-5-(chloromethyl)hexanoic acid (PIN)
[not 2-[4-bromo-3-(chloromethyl)butyl]-5-(bromomethyl)-6-chlorohexanoic acid; ‘bromo’, ‘bromo’, precedes ‘bromo’, ‘chloromethyl’ in alphanumerical order]



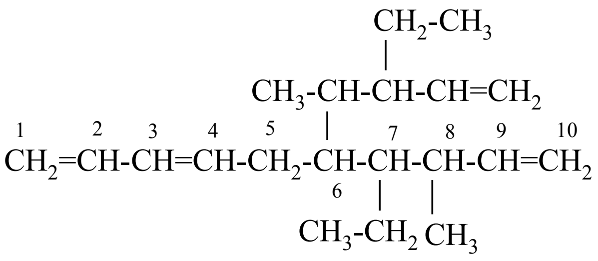
$$\mathrm{BrCH_2\text{-}CHI\text{-}\underset{CHBr\text{-}CH_2Cl}{CH}\text{-}CH_2\text{-}CH_2\text{-}CHBrCl}$$

1,6-dibromo-4-(1-bromo-2-chloroethyl)-1-chloro-5-iodohexane (PIN)
[not 1,5-dibromo-4-(2-bromo-1-iodoethyl)-1,6-dichlorohexane; since the two prefixes first cited are identical in number and in alphanumerical order, the next prefixes in order are considered and ‘(bromo...chloroethyl)’ precedes ‘(bromo...iodoethyl)’]

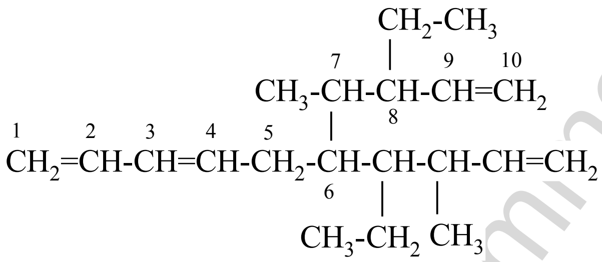


$$\mathrm{HO\text{-}CH_2\text{-}\underset{Br}{CH}\text{-}\overset{COOH}{CH}\text{-}\underset{OH}{CH}\text{-}CH_2\text{-}Br}$$

4-bromo-2-(1-bromo-2-hydroxyethyl)-3-hydroxybutanoic acid (PIN)
[not 3-bromo-2-(2-bromo-1-hydroxyethyl)-4-hydroxybutanoic acid; ‘(1-bromo-2-hydroxyethyl)’ appears earlier in alphanumerical order than ‘(2-bromo-1-hydroxyethyl)’ (see P-14.5).]

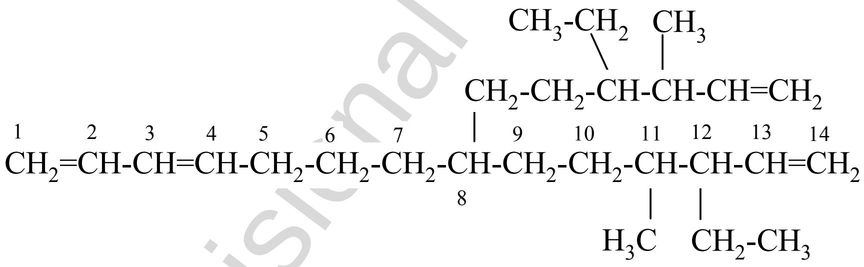


(I)

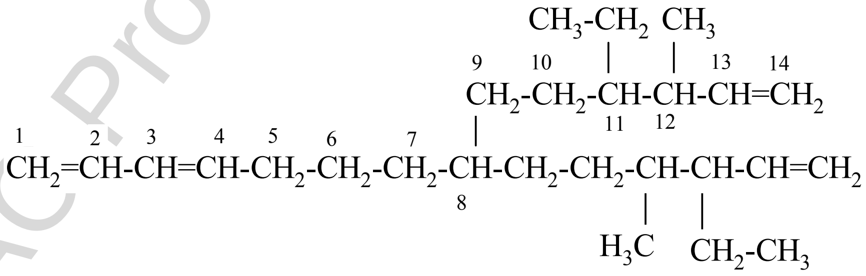


(II)

7-ethyl-6-(3-ethylpent-4-en-2-yl)-8-methyldeca-1,3,9-triene **(I)** (PIN)
[not 8-ethyl-7-methyl-6-(4-methylhex-5-en-3-yl)deca-1,3,9-triene **(II)**; ‘ethylpentenyl’ precedes ‘methyl’ in alphanumerical order]

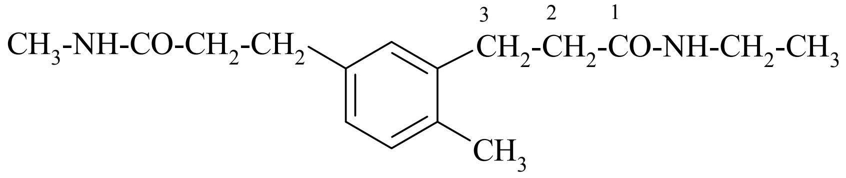


(I)



(II)

12-ethyl-8-(3-ethyl-4-methylhex-5-en-1-yl)-11-methyltetradeca-1,3,13-triene **(I)** (PIN)
[not 11-ethyl-8-(4-ethyl-3-methylhex-5-en-1-yl)-12-methyltetradeca-1,3,13-triene**(II)**; ‘(3-ethyl-4-methylhex-5-en-1-yl)’ must be cited before ‘(4-ethyl-3-ethyl-5-en-1-yl)’]



N-ethyl-3-{2-methyl-5-[3-(methylamino)-3-oxopropyl]phenyl}propanamide (PIN)
[not 3-{3-[3-(ethylamino)-3-oxopropyl]-4-methylphenyl}-*N*-methylpropanamide;
'ethyl' precedes 'ethylamino' in alphanumerical order]

P-44.4 Further criteria applicable to rings, ring systems, and principal chains

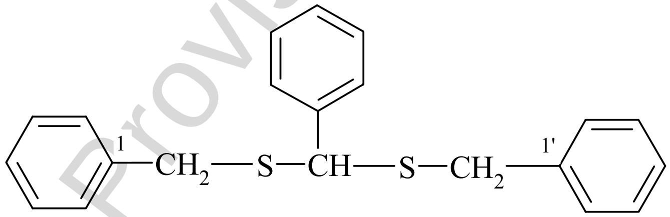
Two or more names may result from using the same parent structures because of multiple occurrences of the parent structure or may differ only in the presence of skeletal atoms with different bonding numbers, isotopic modification, or stereochemical configuration.

P-44.4.1 Multiplied identical parent structures;
P-44.4.2 Selection of preferred IUPAC name according to lowest alphanumerical order;
P-44.4.3 Seniority according to nonstandard bonding numbers;
P-44.4.4 Senority according to isotopic modification;
P-44.4.5 Seniority according to configuration.

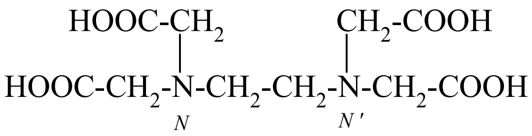
P-44.4.1 Multiplied identical parent structures

When two or more parent structures, rings, ring systems, or chains, satisfy the requirements for multiplicative nomenclature (see P-15.3), the greater number of parent structures is included as the parent structure by multiplication.

Example:

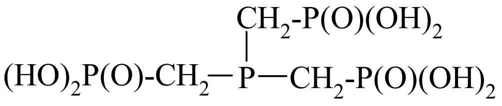


1,1′-[(phenylmethylene)bis(sulfanediylmethylene)]dibenzene (PIN)



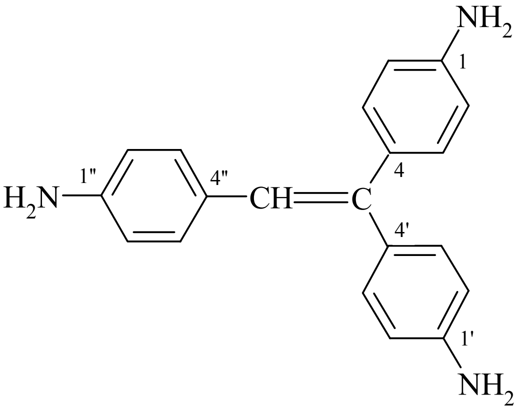
$$HOOC\text{-}CH_2\text{-}\underset{N}{\overset{HOOC\text{-}CH_2}{N}}\text{-}CH_2\text{-}CH_2\text{-}\underset{N'}{\overset{CH_2\text{-}COOH}{N}}\text{-}CH_2\text{-}COOH$$

N,N′-ethane-1,2-diylbis[*N*-(carboxymethyl)glycine] (PIN)
2,2′,2″,2‴-(ethane-1,2-diyldinitrilo)tetraacetic acid



$$(HO)_2P(O)\text{-}CH_2\text{—}\overset{\displaystyle CH_2\text{-}P(O)(OH)_2}{\overset{|}{P}}\text{—}CH_2\text{-}P(O)(OH)_2$$

[phosphanetriyltris(methylene)]tris(phosphonic acid) (PIN)

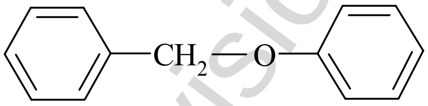


4,4′,4″-(ethene-1,1,2-triyl)trianiline (PIN)

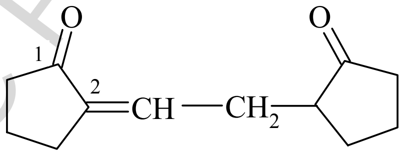
P-44.4.2 Selection of names according to lowest alphanumerical order

When two names can be formed based on the same parent structure, the preferred name is the one that exhibits the lowest alphanumerical order when the names are compared character by character.

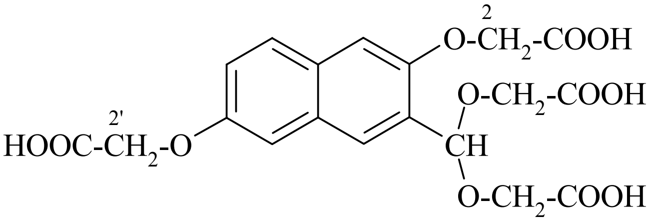
Examples:



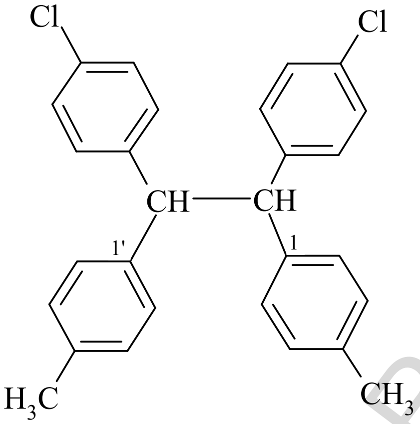
(phenylmethoxy)benzene (PIN)
[not (phenoxymethyl)benzene]



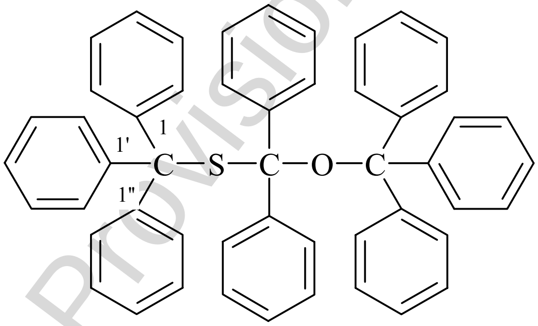
2-[2-(2-oxocyclopentyl)ethylidene]cyclopentan-1-one (PIN)
[not 2-[2-(2-oxocyclopentylidene)ethyl]cyclopentan-1-one]



2,2'-({3-[bis(carboxymethoxy)methyl]naphthalene-2,6-diyl}bis(oxy))diacetic acid (PIN)
[not 2,2′-({[3,7-bis(carboxymethoxy)naphthalene-2-yl]methanediyl}bis(oxy))diacetic acid]



1,1′-[1,2-bis(4-chlorophenyl)ethane-1,2-diyl]bis(4-methylbenzene) (PIN)
[not 1,1′-[1,2-bis(4-methylphenyl)ethane-1,2-diyl]bis(4-chlorobenzene)

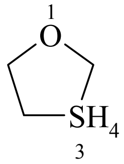


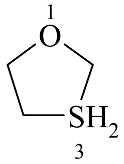
1,1′,1″-({[diphenyl(triphenylmethoxy)methyl]sulfanyl}methanetriyl)tribenzene (PIN)
[not1,1′,1″-({diphenyl[(triphenylmethyl)sulfanyl]methoxy}methanetriyl)tribenzene

P-44.4.3 Parent structures in compounds having atoms with nonstandard bonding numbers (see P-14.1)

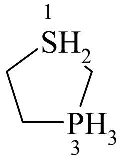
P-44.4.3.1 When a choice is needed between two chains or two rings or ring systems having skeletal atoms with nonstandard bonding numbers, the one having the maximum number of atoms with nonstandard bonding numbers is chosen as principal chain or senior ring or ring system. If a further choice is needed between the same skeletal atom with two different nonstandard bonding numbers, preference for the senior parent structure is given in order of the decreasing numerical value of the bonding number, i.e., λ^6 is preferred to λ^4.

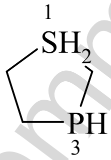
Examples:



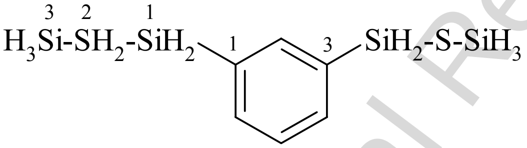


1λ^6-thiolane (PIN) > 1λ^4-thiolane (PIN)

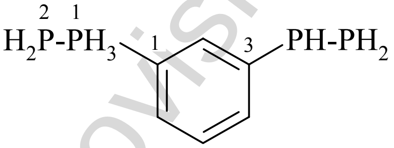




1λ^4,3λ^5-thiaphospholane (PIN) > 1λ^4,3-thiaphospholane (PIN)



1-[3-(disilathian-1-yl)phenyl]-2λ^4-disilathiane (PIN)
(not 1-[3-(2λ^4-disilathian-1-yl)phenyl]disilathiane)



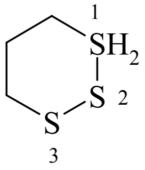
1-[3-(diphosphan-1-yl)phenyl]-1λ^5-diphosphane (PIN)
(not 1-[3-(1λ^5-diphosphan-1-yl)phenyl]diphosphane)

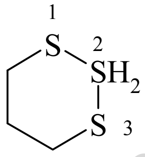
P-44.4.3.2 When a choice is needed between two chains or rings or ring systems having skeletal atoms with nonstandard bonding numbers, the one having the lowest locants for atoms with nonstandard bonding numbers is chosen as principal chain or senior ring or ring system. If a further choice is needed, the atom with the highest bonding number receives the lowest locant.

Examples:

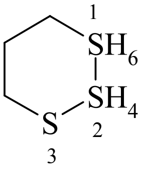
$\overset{1}{H_3S}\text{-}\overset{2}{S}\text{-}\overset{3}{SH}$ $\qquad$ $\overset{1}{HS}\text{-}\overset{2}{SH_2}\text{-}\overset{3}{SH}$

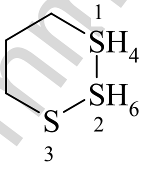
1λ^4-trisulfane (PIN) > 2λ^4-trisulfane (PIN)





1λ^4-1,2,3-trithiane (PIN) > 2λ^4-1,2,3-trithiane (PIN)

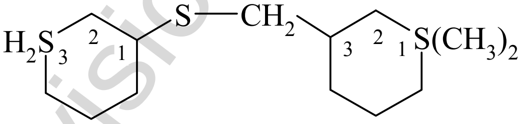




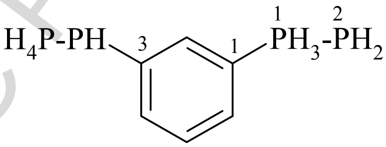
1λ^6,2λ^4-1,2,3-trithiane(PIN) > 1λ^4,2λ^6-1,2,3-trithiane (PIN)

P-44.4.3.3 When a choice between two chains or rings or ring systems having the same skeletal atoms with nonstandard bonding numbers, the parent chain or ring or ring system as that with the greater number of substituents. If a choice still remains, the parent chain or ring or ring system is the one with substituents having the lower locants.

Example:



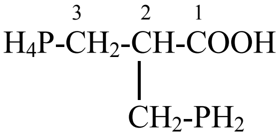
3-{[(dihydro-1λ^4-thiopyran-3(2*H*)-yl)sulfanyl]methyl}-1,1-dimethyltetrahydro-1λ^4-thiopyran (PIN) (greater number of substituents)



1-[3-(1λ^5-diphosphan-2-yl)phenyl]-1λ^5-diphosphane (PIN)
(not 2-[3-(1λ^5-diphosphan-1-yl)phenyl]-1λ^5-diphosphane; lower locant for substituent)

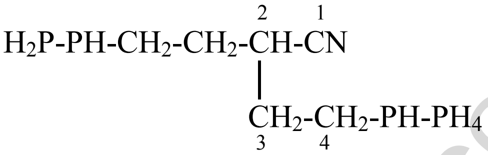
P-44.4.3.4 When a choice for principal chain is needed between two chains having substituent groups differing only by their bonding numbers, that chain having the greater number of substituent group(s) with the higher bonding number is selected as principal chain. If a further choice is needed, that chain having the lowest locants for atoms with the higher bonding number is selected as principal chain.

Examples:



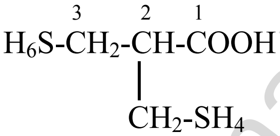
$H_4P\text{-}CH_2\text{-}\underset{CH_2\text{-}PH_2}{CH}\text{-}COOH$

3-(λ^5-phosphanyl)-2-(phosphanylmethyl)propanoic acid (PIN)



$H_2P\text{-}PH\text{-}CH_2\text{-}CH_2\text{-}\underset{CH_2\text{-}CH_2\text{-}PH\text{-}PH_4}{CH}\text{-}CN$

4-(1λ^5-diphosphan-2-yl)-2-(diphosphan-1-ylethyl)butanenitrile (PIN)

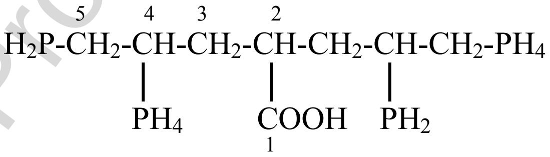


$H_6S\text{-}CH_2\text{-}\underset{CH_2\text{-}SH_4}{CH}\text{-}COOH$

3λ^6-sulfanyl-2-(λ^4-sulfanylmethyl)propanoic acid (PIN)

P-44.4.3.5 When a further choice is needed, that chain having the lowest locants for the substituent group(s) with the higher bonding number is selected as principal chain.

Example:



$H_2P\text{-}CH_2\text{-}\underset{PH_4}{CH}\text{-}CH_2\text{-}\underset{COOH}{CH}\text{-}CH_2\text{-}\underset{PH_2}{CH}\text{-}CH_2\text{-}PH_4$

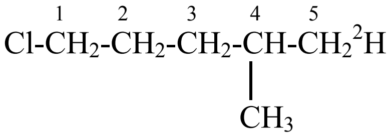
2-(2,3λ^5-diphosphanylpropyl)-4λ^5,5-diphosphanylpentanoic acid (PIN)

P-44.4.4 Parent structures with isotopic modification.

When there is a choice for the senior parent structure between isotopically modified and isotopically unmodified compounds (see Chapter 8), the senior parent structure is chosen according to the following criteria, applied successively until a decision can be made. In structures and names, nuclide symbols enclosed in parentheses describe isotopic substitution; nuclide symbols enclosed in square brackets describe isotopic labeling (see Chapter 8).

(a) The senior parent structure will contain the greater number of isotopically modified atoms or groups.

Example:

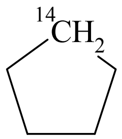


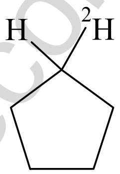
$$\overset{1}{\mathrm{Cl\text{-}CH_2}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\underset{\displaystyle |\atop \mathrm{CH_3}}{\overset{4}{\mathrm{CH}}}\text{-}\overset{5}{\mathrm{CH_2{}^{2}H}}$$

1-chloro-4-methyl(5-$^{2}H_{1}$)pentane (PIN)

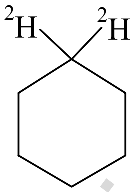
(b) The senior parent structure has the greater number of nuclides of higher atomic number for modified atoms or groups.

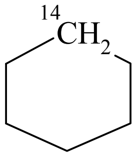
Examples:



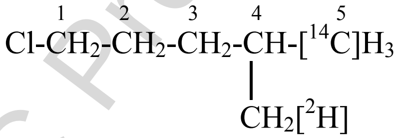


($^{14}C_1$)cyclopentane (PIN) > ($^{2}H_1$)cyclopentane (PIN)





(1,1-$^{2}H_2$)cyclohexane (PIN) > ($^{14}C_1$)cyclohexane (PIN)

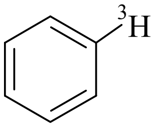


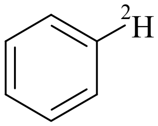
$$\overset{1}{\mathrm{Cl\text{-}CH_2}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\underset{\displaystyle |\atop \mathrm{CH_2[^{2}H]}}{\overset{4}{\mathrm{CH}}}\text{-}\overset{5}{\mathrm{[^{14}C]H_3}}$$

1-chloro-4-([$^{2}H_1$]methyl)[5-^{14}C]pentane (PIN)
[not 1-chloro-4-[^{14}C]methyl[5-^{2}H]pentane]

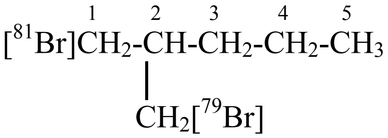
(c) The senior parent structure has the greater number of nuclides of higher mass number for modified atoms or groups.

Example:





($^{3}H_{1}$)benzene (PIN) > ($^{2}H_{1}$)benzene (PIN)

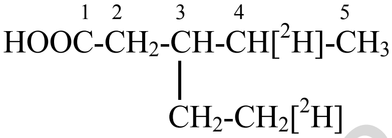


$$[^{81}\mathrm{Br}]\overset{1}{\mathrm{C}}\mathrm{H_2}\text{-}\underset{\substack{|\\ \mathrm{CH_2}[^{79}\mathrm{Br}]}}{\overset{2}{\mathrm{C}}\mathrm{H}}\text{-}\overset{3}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{4}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{5}{\mathrm{C}}\mathrm{H_3}$$

1-([^{81}Br]bromo)-2-([^{79}Br]bromomethyl)pentane (PIN)

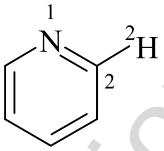
(d) The senior parent structure has the lowest locant(s) for isotopically modified atoms or groups.

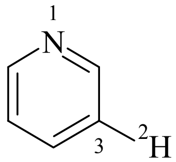
Examples:



$$\mathrm{HOO}\overset{1}{\mathrm{C}}\text{-}\overset{2}{\mathrm{C}}\mathrm{H_2}\text{-}\underset{\substack{|\\ \mathrm{CH_2\text{-}CH_2}[^{2}\mathrm{H}]}}{\overset{3}{\mathrm{C}}\mathrm{H}}\text{-}\overset{4}{\mathrm{C}}\mathrm{H}[^{2}\mathrm{H}]\text{-}\overset{5}{\mathrm{C}}\mathrm{H_3}$$

3-([2-$^{2}H_{1}$]ethyl)[4-$^{2}H_{1}$]pentanoic acid (PIN)

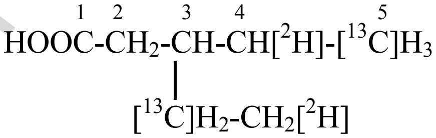




(2-$^{2}H_{1}$)pyridine (PIN) > (3-$^{2}H_{1}$)pyridine (PIN)

(e) The senior parent structure has the lower locant(s) for nuclides of higher atomic number for modified atoms or groups;

Example:

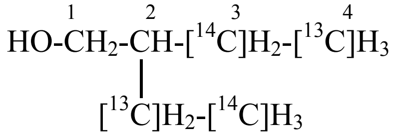


$$\mathrm{HOO}\overset{1}{\mathrm{C}}\text{-}\overset{2}{\mathrm{C}}\mathrm{H_2}\text{-}\underset{\substack{|\\ [^{13}\mathrm{C}]\mathrm{H_2\text{-}CH_2}[^{2}\mathrm{H}]}}{\overset{3}{\mathrm{C}}\mathrm{H}}\text{-}\overset{4}{\mathrm{C}}\mathrm{H}[^{2}\mathrm{H}]\text{-}[^{13}\overset{5}{\mathrm{C}}]\mathrm{H_3}$$

3-([1-^{13}C,2-$^{2}H_{1}$]ethyl)[5-^{13}C,4-$^{2}H_{1}$]pentanoic acid (PIN)

(f) The senior parent structure has the lowest locant(s) for nuclides of higher mass number for modified atoms or groups.

Example:



$$\mathrm{HO{-}\overset{1}{C}H_2{-}\underset{\textstyle |\atop [^{13}C]H_2{-}[^{14}C]H_3}{\overset{2}{C}H}{-}[^{14}\overset{3}{C}]H_2{-}[^{13}\overset{4}{C}]H_3}$$

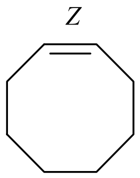
2-([1-^{13}C,2-^{14}C]ethyl)[4-^{13}C,3-^{14}C]butan-1-ol (PIN)

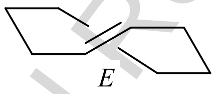
P-44.4.5 Parent structures with different stereochemical configurations

P-44.4.5.1 Choice between ‘*E*’ and ‘*Z*’

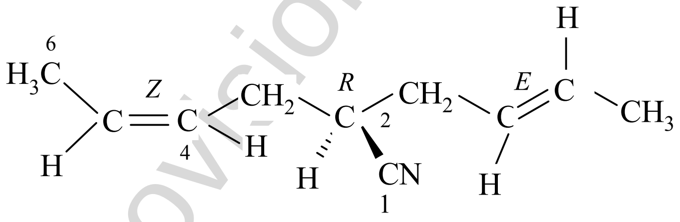
When there is a choice between parent structures that differ only by ‘*Z*’ and ‘*E*’ configurations, the senior parent structure contains the greater number of double bonds with ‘*Z*’ configuration; when a further choice is required, the senior parent structure has the lower locant(s) for the double bond(s) with the ‘*Z*’ configuration. For the meaning of ‘*Z*’, ‘*E*’, ‘*R*’, and ‘*S*’, see Chapter 9.

Examples:

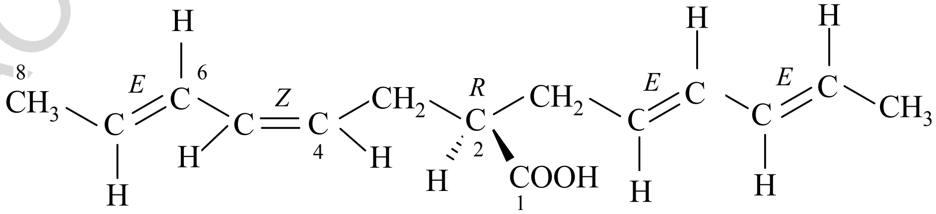




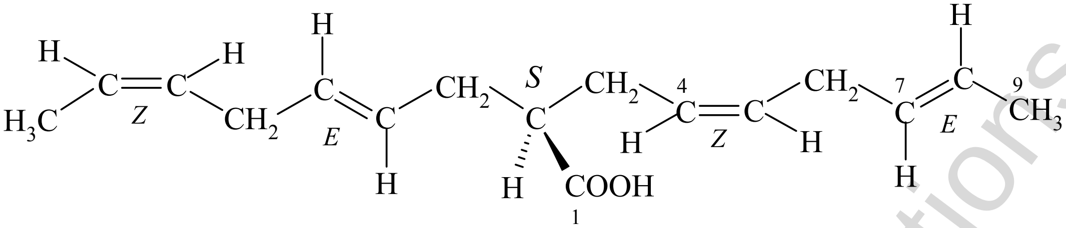
(*Z*)-cyclooctene > (*E*)-cyclooctene



(2*R*,4Z)-[(2*E*)-but-2-en-1-yl]hex-4-enenitrile
(for the symbol ‘*R*’ in position 2, see P-92.3.5)



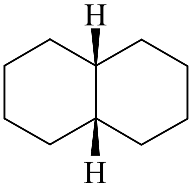
(2*R*,4*Z*,6*E*)-2-[(2*E*,4*E*)-hexa-2,4-dien-1-yl]octa-4,6-dienoic acid
(for the symbol ‘*R*’ in position 2, see P-92.3.5)

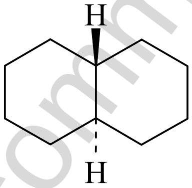


(2*S*,4*Z*,7*E*)-2-[(2*E*,5*Z*)-hepta-2,5-dien-1-yl]nona-4,7-dienoic acid

P-44.4.5.2 In a preferred parent structure, *cis*-configurations are senior to *trans*-configurations.

Example:



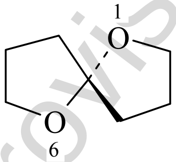


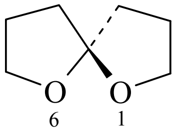
cis-decahydronaphthalene > *trans*-decahydronaphthalene

P-44.4.5.3 Choice among chiral centers

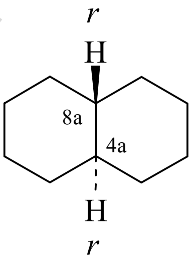
When there is a choice between parent structures differing only by the configurations of the chiral centers, the principal chain or the senior ring system is chosen by applying the CIP sequence rules 4 and 5, in the order: *like* stereodescriptors such as '*RR*', '*SS*' have priority over *unlike* '*RS*' and '*SR*' ('*l*' has priority over '*u*'), the '*r*' over '*s*', then '*R*' over '*S*'. The CIP Rules are described in Chapter 9.

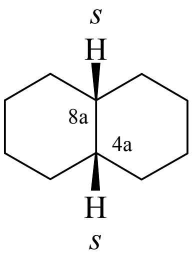
Examples:



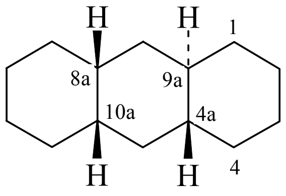


(*R*)-1,6-dioxaspiro[4.4]nonane > (*S*)-1,6-dioxaspiro[4.4]nonane



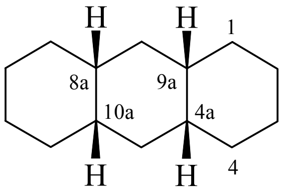


(4a*r*,8a*r*)-decahydronaphthalene > (4a*s*,8a*s*)-decahydronaphthalene



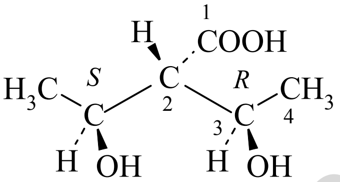
I

>

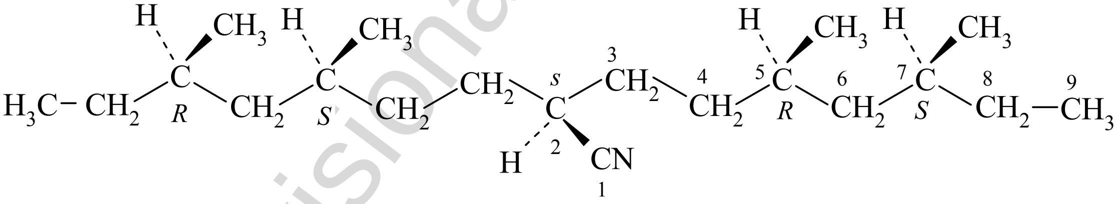


II

I r*el*-(4a*R*,8a*R*,9a*R*,10a*S*)-tetradecahydroanthracene
II *rel*-(4a*R*,8a*R*,9a*S*,10a*S*)-tetradecahydroanthracene
(in the order 4a,8a,9,a,10a the stereodescriptors are '*R*,*R*,*R*,*S*' for compound **I** and '*R*,*R*,*S*,*S*' for compound **II**; the pairs '4a,8a' are '*R*,*R*' (*like*) for both compounds; the pairs '4a,9a' are '*R*,*R*' ('*l*') and '*R*,*S*' (*unlike*), respectively; as *like* precedes *unlike*, compound **I** is senior to compound **II**).



(2*s*,3*R*)-3-hydroxy-2-[(*S*)-1-hydroxyethyl]butanoic acid
(for the symbol '*s*' at position 2, see P-92.3.5)



(2s,5*R*,7*S*)-5,7-dimethyl-2-[(3*S*,5*R*)-3,5-dimethylheptyl]nonanenitrile
(both pairs of stereodescriptors are *unlike* in sequence rule 4; as '*R*' precedes '*S*' in sequence rule 5, the principal chain is chosen that has the '*R*' configuration for the chirality center encountered first along the chain)

P-45 The principal chain in substituent groups

P-45.0 Introduction

Compound acyclic substituents, i.e., substituted acyclic substituents, consist of a principal chain and one or more acyclic substituents. If the substituent to the principal chain also has acyclic substituents, it itself is a compound substituent; the resulting complete substituent is called a complex acyclic substituent. Complex substituents are named by extending the methods given below for compound substituents.

Compound substituents are named in two ways:

(1) by using alkyl substituents (see P-29.2.1);

(1) by using alkanyl substituents (see P-29.2.2).

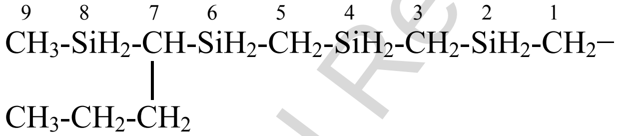
Alkyl and alkanyl substituent groups have been defined in Section P-29. Simple alkyl substituent groups have their free valence(s) denoted by the suffixes ‘yl’, ‘ylidene’ or ‘ylidyne’ only at position 1. Simple alkanyl substituent groups have their free valence(s) denoted by the suffixes ‘yl’ or ‘ylidene’ which may be located at any position of the chain, except position 1. Both alkyl and alkanyl substituent groups can form compound substituent groups. In some cases, a compound substituent group resulting from substitution of the principal chain by alkyl or alkanyl substituent groups results in the same structure that corresponds to a simple alkanyl substituent group.

P-45.1 The principal chain

Selection of the principal chain is accomplished in accordance with the following criteria, applied successively in the order given until a decision is reached.

(a) the principal chain has the greater number of heteroatoms; this criterion is used only in method (b) of P-45.0.

Example:

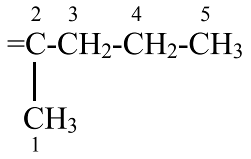


$$\overset{9}{\mathrm{CH_3}}\text{-}\overset{8}{\mathrm{SiH_2}}\text{-}\underset{\mathrm{CH_3\text{-}CH_2\text{-}CH_2}}{\underset{|}{\overset{7}{\mathrm{CH}}}}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{SiH_2}}\text{-}\overset{1}{\mathrm{CH_2}}-$$

7-propyl-2,4,6,8-tetrasilanonan-1-yl (PIN)

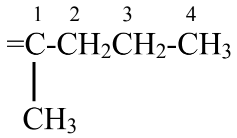
(b) The principal chain has the greater number of skeletal atoms, i.e., it is the longest chain; this criterion is applicable to both methods (a) and (b) of P-45.0; both methods generate simple and compound substituent groups.

Examples:



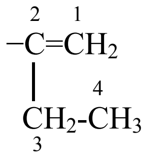
$=\overset{2}{C}(\underset{1}{CH_3})-\overset{3}{C}H_2-\overset{4}{C}H_2-\overset{5}{C}H_3$

pentan-2-ylidene (PIN)
(a simple substituent group)



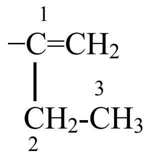
$=\overset{1}{C}(CH_3)-\overset{2}{C}H_2\overset{3}{C}H_2-\overset{4}{C}H_3$

1-methylbutylidene
(a compound substituent group)



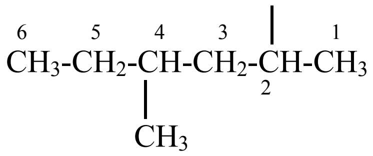
$-\overset{2}{C}(\underset{3}{C}H_2-\overset{4}{C}H_3)=\overset{1}{C}H_2$

but-1-en-2-yl (PIN)
(a simple substituent group)



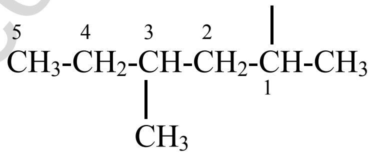
$-\overset{1}{C}(\underset{2}{C}H_2-\overset{3}{C}H_3)=CH_2$

1-methylidenepropyl
(a compound substituent group)



$\overset{6}{C}H_3-\overset{5}{C}H_2-\overset{4}{C}H(CH_3)-\overset{3}{C}H_2-\underset{2}{C}H(-)-\overset{1}{C}H_3$

4-methylhexan-2-yl (PIN)
(a compound substituent group)

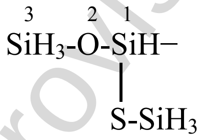


$\overset{5}{C}H_3-\overset{4}{C}H_2-\overset{3}{C}H(CH_3)-\overset{2}{C}H_2-\underset{1}{C}H(-)-CH_3$

1,3-dimethylpentyl
(a compound substituent group)

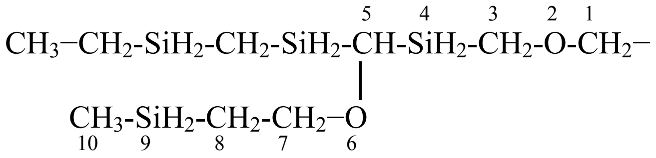
(c) The principal chain has the greater number of heteroatoms in the order: O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl. l.

Examples:



$\overset{3}{Si}H_3-\overset{2}{O}-\overset{1}{Si}H(S-SiH_3)-$

1-(silylsulfanyl)disiloxanyl (PIN)

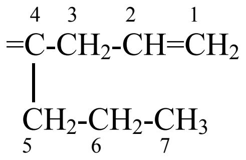


$CH_3-CH_2-SiH_2-CH_2-SiH_2-\overset{5}{C}H(\overset{6}{O}-\overset{7}{C}H_2-\overset{8}{C}H_2-\overset{9}{Si}H_2-\overset{10}{C}H_3)-\overset{4}{Si}H_2-\overset{3}{C}H_2-\overset{2}{O}-\overset{1}{C}H_2-$

5-{[(ethylsilyl)methyl]silyl}-2,6-dioxa-4,9-disiladecan-1-yl (PIN)

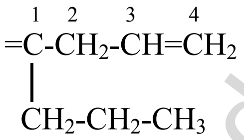
(d) The principal chain has the greater number of multiple bonds regardless of type, then the greater number of double bonds; this criterion is applicable to methods (a) and (b) in P-45.0; both generate simple and compound substituent groups.

Examples:



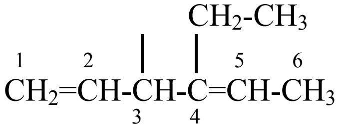
$$\begin{array}{l} ^{4}\,^{3}\quad ^{2}\quad ^{1} \\ {=}C\text{-}CH_2\text{-}CH{=}CH_2 \\ | \\ CH_2\text{-}CH_2\text{-}CH_3 \\ ^{5}\quad ^{6}\quad ^{7} \end{array}$$

hept-1-en-4-ylidene (PIN)
(a simple substituent group)



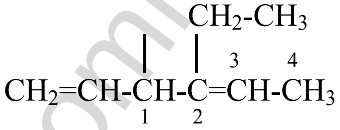
$$\begin{array}{l} ^{1}\,^{2}\quad ^{3}\quad ^{4} \\ {=}C\text{-}CH_2\text{-}CH{=}CH_2 \\ | \\ CH_2\text{-}CH_2\text{-}CH_3 \end{array}$$

1-propylbut-3-en-1-ylidene
(a compound substituent group)



$$\begin{array}{l} \qquad\qquad\quad CH_2\text{-}CH_3 \\ ^{1}\quad ^{2}\quad | \quad | \quad ^{5}\quad ^{6} \\ CH_2{=}CH\text{-}CH\text{-}C{=}CH\text{-}CH_3 \\ \qquad\qquad\ _{3}\quad _{4} \end{array}$$

4-ethylhexa-1,4-dien-3-yl (PIN)
(a compound substituent group)

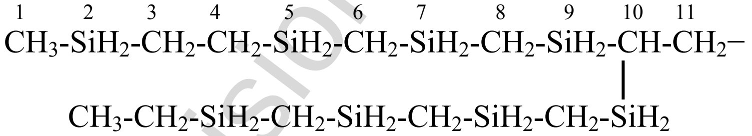


$$\begin{array}{l} \qquad\qquad\quad CH_2\text{-}CH_3 \\ \qquad\qquad | \quad | \quad ^{3}\quad ^{4} \\ CH_2{=}CH\text{-}CH\text{-}C{=}CH\text{-}CH_3 \\ \qquad\qquad\ _{1}\quad _{2} \end{array}$$

1-ethenyl-2-ethylbut-2-en-1-yl
(a compound substituent group)

(e) The principal chain has the lowest locants for heteroatoms; this criterion is used in method (b) of P-45.0 only.

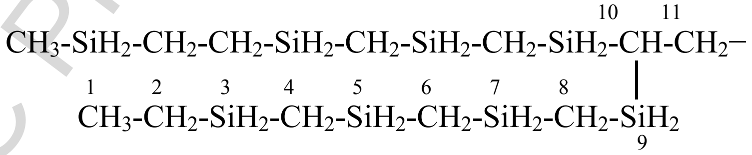
Examples:



$$\begin{array}{l} ^{1}\quad ^{2}\quad ^{3}\quad ^{4}\quad ^{5}\quad ^{6}\quad ^{7}\quad ^{8}\quad ^{9}\quad ^{10}\quad ^{11} \\ CH_3\text{-}SiH_2\text{-}CH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH\text{-}CH_2\text{–} \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad | \\ \quad CH_3\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2 \end{array}$$

10-(1,3,5,7-tetrasilanonan-10-yl)-2,5,7,9-tetrasilaundecan-11-yl (PIN)

not

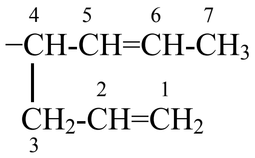


$$\begin{array}{l} \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad ^{10}\quad ^{11} \\ CH_3\text{-}SiH_2\text{-}CH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH\text{-}CH_2\text{–} \\ \quad ^{1}\quad ^{2}\quad ^{3}\quad ^{4}\quad ^{5}\quad ^{6}\quad ^{7}\quad ^{8}\qquad | \\ \quad CH_3\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2 \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad _{9} \end{array}$$

10-(1,3,5,8-tetrasilanonan-10-yl)-3,5,7,9-tetrasilaundecan-11-yl
(the locant set in the correct principal chain ‘2,5,7,9’ is lower than the set ‘3,5,7,9’)

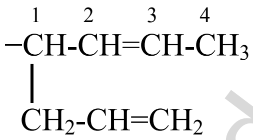
(f) The principal chain has the lower locant(s) for multiple bonds, regardless of type, then the lower locant(s) for double bonds; this criterion is applicable to methods (a) and (b) of P-45.0; both methods generate simple and compound substituent groups.

Examples:



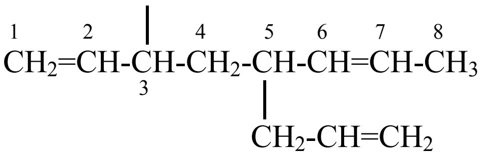
$$\begin{array}{l}-\overset{4}{C}H-\overset{5}{C}H=\overset{6}{C}H-\overset{7}{C}H_3\\ \;|\\ \underset{3}{C}H_2-\overset{2}{C}H=\overset{1}{C}H_2\end{array}$$

hepta-1,5-dien-4-yl (PIN)
(a simple substituent group)



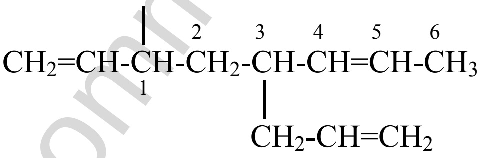
$$\begin{array}{l}-\overset{1}{C}H-\overset{2}{C}H=\overset{3}{C}H-\overset{4}{C}H_3\\ \;|\\ CH_2-CH=CH_2\end{array}$$

1-(prop-2-en-1-yl)but-2-en-1-yl
(a compound substituent group)



$$\begin{array}{l}\overset{1}{C}H_2=\overset{2}{C}H-\underset{3}{\overset{|}{C}}H-\overset{4}{C}H_2-\overset{5}{C}H-\overset{6}{C}H=\overset{7}{C}H-\overset{8}{C}H_3\\ \qquad\qquad\qquad\qquad\quad|\\ \qquad\qquad\qquad\qquad CH_2-CH=CH_2\end{array}$$

5-(prop-2-en-1-yl)octa-1,6-dien-3-yl (PIN)
(a compound substituent group)

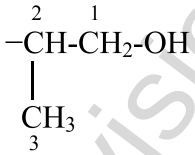


$$\begin{array}{l}CH_2=CH-\underset{1}{\overset{|}{C}}H-\overset{2}{C}H_2-\overset{3}{C}H-\overset{4}{C}H=\overset{5}{C}H-\overset{6}{C}H_3\\ \qquad\qquad\qquad\qquad\quad|\\ \qquad\qquad\qquad\qquad CH_2-CH=CH_2\end{array}$$

1-ethenyl-3-(prop-2-en-1-yl)hex-4-en-1-yl
(a compound substituent group)

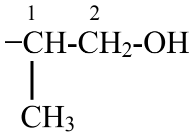
(g) The principal chain has the greater number of substituents; this criterion is applicable to methods (a) and (b); both methods generate simple and compound substituent groups, respectively.

Examples:



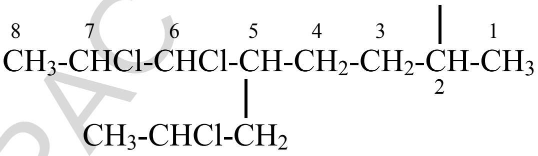
$$\begin{array}{l}-\overset{2}{C}H-\overset{1}{C}H_2-OH\\ \;|\\ \underset{3}{C}H_3\end{array}$$

1 hydroxypropan-2-yl (PIN)
(a substituted simple
substituent group)



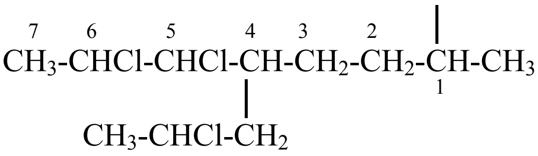
$$\begin{array}{l}-\overset{1}{C}H-\overset{2}{C}H_2-OH\\ \;|\\ CH_3\end{array}$$

2-hydroxy-1-methylethyl
[not 1-(hydroxymethyl)ethyl]
(a substituted compound
substituent group)



$$\begin{array}{l}\overset{8}{C}H_3-\overset{7}{C}HCl-\overset{6}{C}HCl-\overset{5}{C}H-\overset{4}{C}H_2-\overset{3}{C}H_2-\underset{2}{\overset{|}{C}}H-\overset{1}{C}H_3\\ \qquad\qquad\qquad\qquad|\\ \quad CH_3-CHCl-CH_2\end{array}$$

6,7-dichloro-5-(2-chloropropyl)-
octan-2-yl (PIN)
(a substituted compound
substituent)

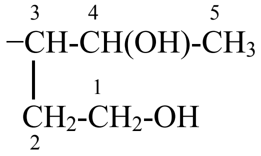


$$\begin{array}{l}\overset{7}{C}H_3-\overset{6}{C}HCl-\overset{5}{C}HCl-\overset{4}{C}H-\overset{3}{C}H_2-\overset{2}{C}H_2-\underset{1}{\overset{|}{C}}H-CH_3\\ \qquad\qquad\qquad\qquad|\\ \quad CH_3-CHCl-CH_2\end{array}$$

5,6-dichloro-4-(2-chloropropyl-
1-methylheptyl
(a substituted compound
substituent)

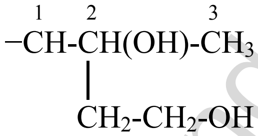
(h) The principal chain has the lowest locants for substituents; this criterion is applicable to methods (a) and (b) of P-45.0; both methods generate simple and compound substituent groups.

Examples:



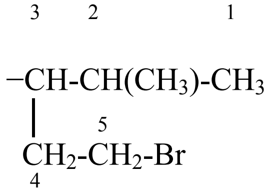
$$\begin{array}{l}-\overset{3}{C}H-\overset{4}{C}H(OH)-\overset{5}{C}H_3\\ \;|\\ \underset{2}{C}H_2-\overset{1}{C}H_2-OH\end{array}$$

1,4-dihydroxypentan-3-yl (PIN)
(a substituted simple substituent)



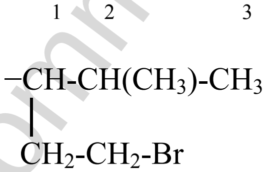
$$\begin{array}{l}-\overset{1}{C}H-\overset{2}{C}H(OH)-\overset{3}{C}H_3\\ \qquad|\\ \qquad CH_2-CH_2-OH\end{array}$$

2-hydroxy-1-(2-hydroxyethyl)propyl
(a substituted compound substituent)



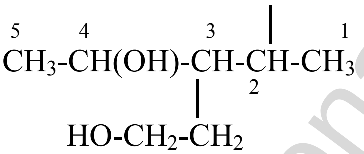
$$\begin{array}{l}-\overset{3}{C}H-\overset{2}{C}H(CH_3)-\overset{1}{C}H_3\\ \;|\\ \underset{4}{C}H_2-\overset{5}{C}H_2-Br\end{array}$$

5-bromo-2-methylpentan-3-yl (PIN)
(a substituted simple substituent)



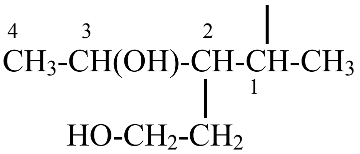
$$\begin{array}{l}-\overset{1}{C}H-\overset{2}{C}H(CH_3)-\overset{3}{C}H_3\\ \;|\\ CH_2-CH_2-Br\end{array}$$

1-(2-bromoethyl)-2-methylpropyl
(a substituted copound substituent)



$$\begin{array}{l}\qquad\qquad\qquad\qquad\quad|\\ \overset{5}{C}H_3-\overset{4}{C}H(OH)-\overset{3}{C}H-\underset{2}{C}H-\overset{1}{C}H_3\\ \qquad\qquad\quad|\\ \qquad HO-CH_2-CH_2\end{array}$$

4-hydroxy-3-(2-hydroxyethyl)
pentan-2-yl (PIN)
(a substituted compound
substituent)

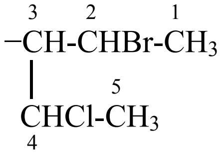


$$\begin{array}{l}\qquad\qquad\qquad\qquad\quad|\\ \overset{4}{C}H_3-\overset{3}{C}H(OH)-\overset{2}{C}H-\underset{1}{C}H-CH_3\\ \qquad\qquad\quad|\\ \qquad HO-CH_2-CH_2\end{array}$$

3-hydroxy-2-(2-hydroxyethyl))-
1-methylbutyl
(a substituted compound
substituent)

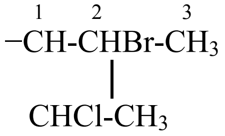
(i) The principal chain has lower locants for the substituent(s) cited earlier in alphanumerical order; this criterion is applicable to methods (a) and (b); both methods generate simple and complex substituent groups.

Examples:



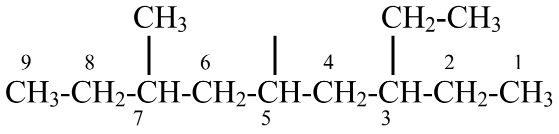
$-CH(CHCl{-}CH_3){-}CHBr{-}CH_3$

2-bromo-4-chloropentan-3-yl (PIN)
(a substituted simple substituent group)
(not 4-bromo-2-chloropentan-3-yl)



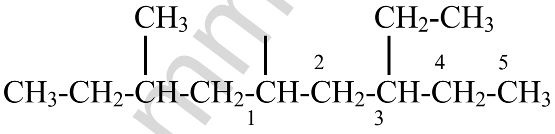
$-CH(CHCl{-}CH_3){-}CHBr{-}CH_3$

2-bromo-1-(1-chloroethyl)propyl
(a substituted compound substituent group)
[not 1-(bromoethyl)-2-chloropropyl; 'bromo...chloro' is preferred to 'bromoethyl']



$CH_3{-}CH_2{-}CH(CH_3){-}CH_2{-}CH{-}CH_2{-}CH(CH_2{-}CH_3){-}CH_2{-}CH_3$

3-ethyl-7-methylnonan-5-yl (PIN)
(a compound substituent)



$CH_3{-}CH_2{-}CH(CH_3){-}CH_2{-}CH{-}CH_2{-}CH(CH_2{-}CH_3){-}CH_2{-}CH_3$

3-ethyl-1-(2-methylbutyl)pentyl
(a substituted compound substituent)

P-46 Substitution rules for parent structures with retained names

The following rules are used for the substitution of parent hydrides having retained names and described in P-22.1.2, P-22.1.3, Tables 2.2, 2.3, 2.7, 2.8 and Tables 3.1, 3.2 for functional parent compounds given in P-34.

Substitutability of parent structures with retained names is classified into three types:

Type 1. Unlimited substitution by substituent groups cited as suffixes or prefixes;

Type 2. Limited substitution classified as follows:

Type 2a. Substitution limited to substituent groups cited as prefixes in recognition of functional groups explicitly expressed or implied in the functional parent compound name;

Type 2b. Substitution limited to substituent groups cited as compulsory prefixes;

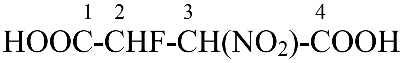
Type 2c. Substitution for parent structures not covered by Types 2a or 2b.

Type 3. Substitution of any kind not allowed

P-46.1 Type 1 substitution rules

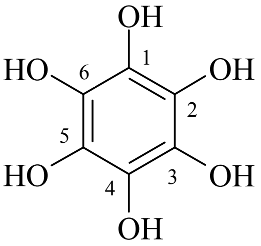
P-46.1.1 Type 1 substitution is recommended for retained names of parent hydrides described in Chapters 2 and 3. There is no limit to the number of substituent groups cited as suffixes or prefixes, like or unlike.

Examples:

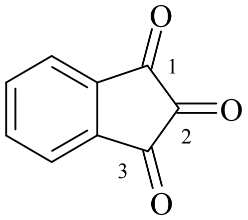


$\overset{1}{\mathrm{HOOC}}\text{-}\overset{2}{\mathrm{CHF}}\text{-}\overset{3}{\mathrm{CH}}(\mathrm{NO_2})\text{-}\overset{4}{\mathrm{COOH}}$

2-fluoro-3-nitrobutanedioic acid (PIN)
(butane is a retained name)



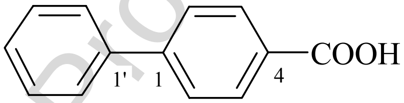
benzene-1,2,3,4,5,6-hexol (PIN)
(not pentahydroxyphenol)
(benzene is a retained name)



indane-1,2,3-trione
1*H*-indene-1,2,3-trione (PIN)

P-46.1.2 Criteria to select the senior ring or ring system and the principal chain must be applied to names of all retained parent structures.

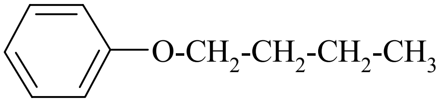
Examples:



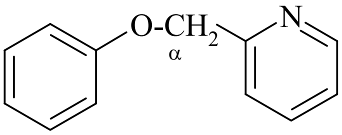
1,1′-biphenyl-4-carboxylic acid (PIN)
(not 4-phenylbenzoic acid)

CH_3-CH_2-C≡CH

but-1-yne
(not ethylacetylene)



butoxybenzene (PIN)
(not α-propylanisole)



2-(phenoxymethyl)pyridine (PIN)
[not α-(pyridin-2-yl)anisole]

P-46.2 Type 2 substitution

Substitution of parent hydrides with retained names or their derived substituent prefixes and of functional parent compounds whose names explicitly or implicitly express the presence of a characteristic group normally expressed as a suffix such as '-one', or a functional class, such as ether is limited in different ways as described in the following subsections Rules for the substitution of inorganic oxo acids used as functional parents and parent structures are described in P-67.

P-46.2.1 Type 2a substitution rules

P-46.2.1.1 Type 2a includes substituent groups having free valences of any type, '-yl', 'ylidene,', 'ylidyne', 'diyl', 'ylylidene', etc. As free valences correspond to the most senior class, any substituent group is cited as a prefix.

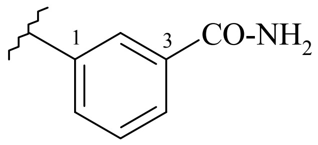
Examples:

$$–\overset{1}{C}H=\overset{2}{C}H\text{-}COOH$$

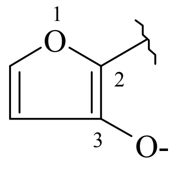
2-carboxyvinyl
2-carboxyeth-1-en-1-yl (PIN)

$$–\overset{1}{C}H_2\text{-}\overset{2}{C}H=\overset{3}{C}H\text{-}\overset{+}{N}(CH_3)_3$$

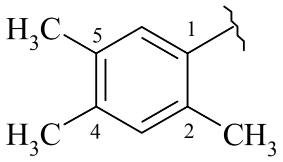
3-(trimethylazaniumyl)allyl
3-(trimethylazaniumyl)prop-2-en-1-yl (PIN)
3-(trimethylammoniumyl)allyl



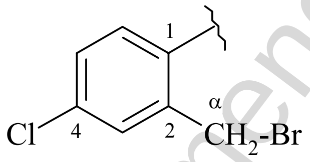
3-carbamoylphenyl (PIN)



3-methoxy-2-furyl
3-methoxyfuran-2-yl (PIN)



2,4,5-trimethylphenyl (PIN)
(not 4,5-dimethyl-*o*-tolyl)



2-(bromomethyl)-4-chlorophenyl (PIN)
(not α-bromo-4-chlorotolyl)

P-46.2.1.2 Type 2a includes functional parent compounds whose name expresses or implies a characteristic group normally expressed as suffix.

P-46.2.1.2.1 Substitution by introducing substituent groups, expressed as prefixes, having lesser seniority than that denoted by the suffix is allowed.

Examples:

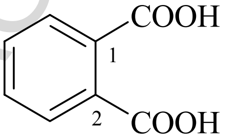
H_2N-CH_2-CO-CH_3
aminoacetone
1-aminopropan-2-one (PIN)

HS-CH_2-COOH
2-sulfanylacetic acid (PIN)

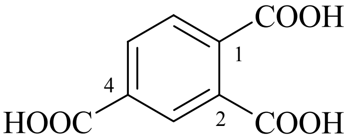
Furthermore, a suffix explicitly or implicitly present cannot be repeated.

Examples:

HOOC-CH_2-COOH
propanedioic acid (PIN)
malonic acid
(not 2-carboxyacetic acid)



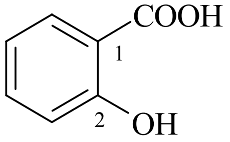
phthalic acid (PIN)
(not 2-carboxybenzoic acid)



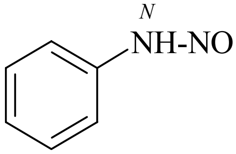
benzene-1,2,4-tricarboxylic acid (PIN)
(not 2,4-dicarboxybenzoic acid, nor
4-carboxyphthalic acid)

P-46.2.1.2.2 The senior functional suffix or class must be expressed in the name.

Examples:



2-hydroxybenzoic acid (PIN)
(not 2-carboxyphenol)



N-phenylnitrous amide (PIN)
(not *N*-nitrosoaniline)

P-46.2.2. Type 2b substitution rules

P-46.2.2.1 Type 2b includes parent compounds explicitly or implicitly devoid of suffixes. Thus, substitution of these parent compounds is possible by using compulsory prefixes only. Acetylene and allene are included in this class.

The following characteristic groups cited as compulsory prefixes can be used to substitute parent structures of Type 2b (ring and the side chain if required): halides −Br, −Cl, −F, −I, pseudohalides $-N_3$, −NCO (and chalcogen analogues), −NC, substituent groups derived from the halogen oxo acids −ClO, $-ClO_2$, $-ClO_3$ (similarly for groups in which Cl is replaced by Br or I), $-NO_2$ and –NO, $-PO_2$ and –PO, and –OR (R = alkyl groups), and chalcogen analogues.

Examples:

Br-C≡C-H

bromoacetylene (PIN)

$\overset{1}{\text{Cl-CH}}=\overset{2}{\text{C}}=\overset{3}{\text{CH}}\text{-Cl}$

1,3-dichloroallene (PIN)

P-46.2.3 Type 2c substitution rules apply to functional parent compounds that are not included in type 2b, for example, hydroxylamine and formic acid.

P-46.2.3.1 Substitution of hydroxylamine

Hydroxylamine can be *O*-substituted by –COOH and $-SO_3OH$ groups, and their derived groups, that are cited as suffixes (see P-68.3.1.1.1.4).

Example:

$H_2N-O-SO_3OH$

hydroxylamine-*O*-sulfonic acid
(preselected name)

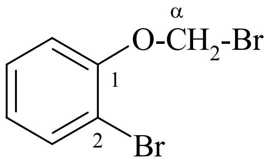
$H_2N-O-CO-NH_2$

hydroxylamine-*O*-carboxamide (PIN)

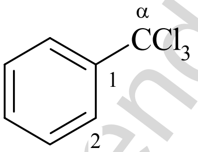
P-46.2.3.2 Substitution of anisole, toluene, benzyl, and benzylidene

The parent compound names anisole, toluene, and benzyl are retained preferred IUPAC names but cannot be substituted (see Type 3 below). However, they can be used in general nomenclature and cannot be substituted by suffixes, only by compulsory prefixes; prefixes derived from suffix groups must lead to names expressing those prefixes as suffixes. In addition, the α-position in all of them cannot be substituted by an acyclic carbon atom which would lengthen the chain. Furthermore, anisole and toluene cannot be substituted by other methoxy or methyl groups, respectively.

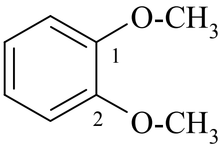
Examples:



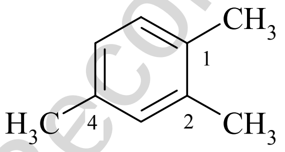
α,2-dibromoanisole
1-bromo-2-(bromomethoxy)benzene (PIN)



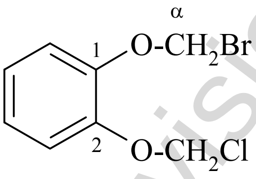
α,α,α-trichlorotoluene
(trichloromethyl)benzene (PIN)



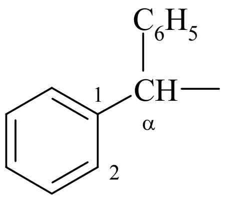
1,2-dimethoxybenzene (PIN)
(not 2-methoxyanisole)



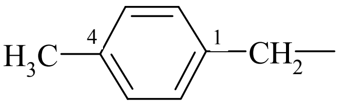
1,2,4-trimethylbenzene (PIN)
(not 4-methyl-*o*-xylene, nor
2,4-dimethyltoluene)



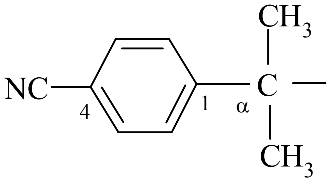
α-bromo-2-(chloromethoxy)anisole
[not 2-(bromomethoxy)-α-chloroanisole;
bromo...chloro is alphabetically preferred
to bromomethoxy]
1-(bromomethoxy)-2-(chloromethoxy)benzene (PIN)



α-phenylbenzyl
(benzyl is a larger structural
unit)
diphenylmethyl (PIN)



4-methylbenzyl
(not *p*-tolylmethyl;
benzyl is a larger
larger structural unit)
(4-methylphenyl)methyl (PIN)



2-(4-cyanophenyl)propan-2-yl (PIN)
1-(4-cyanophenyl)-1-methylethyl
(not 4-cyano-α,α-dimethylbenzyl)

P-46.2.3.2 Substitution rules for formic acid

The hydrogen atom attached to carbon is substitutable under specific conditions. Substitution of the hydrogen atom of formic acid by the following atoms or groups of functional replacement nomenclature, –OOH, –SH, –SeH, –TeH, –F, –Cl, –Br, –I, $–N_3$, –NC, –NCO, –NCS, –NCSe, –NCTe, $–NH_2$, leads to preferred IUPAC names derived from carbonic acid (see P-and by the $–NHNH_2$ group leads to derivatives of hydrazine (see P-). Hence, these groups cannot substitute the hydrogen atom of formic acid. However, atoms or groups not on this list may sybstitute the hydrogen atom of formic acid.

Example:

O_2N-COOH

nitroformic acid (PIN)

P-46.3. For parent hydrides and functional parent compounds of type 3, no substitution of any kind is allowed. Functionalization of characteristic groups, such as the formation of esters, anhydrides, and salts, however, is allowed

CHAPTER 5 CONSTRUCTING PREFERRED IUPAC NAMES

P-50 Introduction

Many compounds can have multiple names in accordance with two or more methods recommended by IUPAC for their formation, one of which is recommended herein as the preferred IUPAC name (PIN). Preferred IUPAC names are part of a systematic approach to nomenclature based on a minimum of principles, rules and conventions that are actually applied. Thus, preferred IUPAC names are not new names, although the continued rationalization of nomenclature has led to some recommended changes. Preferred IUPAC names are essential today to communicate precisely in legal situations with manifestations in patents, and for export-import regulations, health and safety information, etc.

This Chapter summarizes the selection rules that are recommended for generation of preferred IUPAC names.

P-51 Selecting the preferred method of nomenclature

Substitutive nomenclature is by far the preferred method of nomenclature for naming organic compounds. Other methods are used to enhance substitutive nomenclature or to simplify substitutive names.

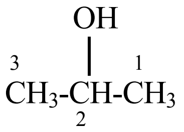
P-51.1 Functional class nomenclature

Substitutive nomenclature is preferred to functional class nomenclature for generating preferred IUPAC names, except for naming esters (see P-65.3.3.1), acyl halides and pseudohalides (see P-65.2), and oximes (see P-68.3.1.2).

Examples:

CH_3Br

bromomethane (PIN)
methyl bromide



$\overset{3}{C}H_3\text{-}\overset{OH}{\underset{2}{C}}H\text{-}\overset{1}{C}H_3$

propan-2-ol (PIN)
isopropyl alcohol

$CH_3\text{-}COO\text{-}CH_3$

methyl acetate (PIN)

$C_6H_5\text{-}CO\text{-}Cl$

benzoyl chloride (PIN)

$CH_3\text{-}CO\text{-}CN$

acetyl cyanide (PIN)

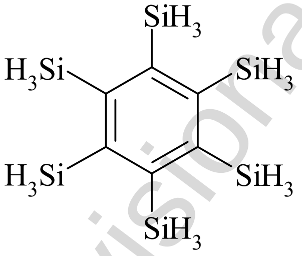
$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH{=}N\text{-}OH$

butanal oxime (PIN)

P-51.2 Multiplicative nomenclature

Multiplicative nomenclature (P-15.3) is preferred to simple substitutive nomenclature for generating preferred IUPAC names to express multiple occurrences of parent hydrides, other than alkanes, functional parents, or functionalized parent hydrides in names.

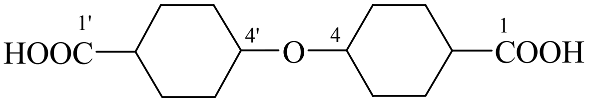
Examples:



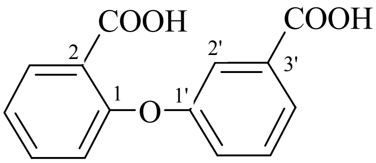
benzenehexaylhexakis(silane) (PIN, multiplicative name)
(2,3,4,5,6-pentasilylphenyl)silane (simple substitutive name)

$HOOC\text{-}\overset{2}{C}H_2\text{-}S\text{-}\overset{2'}{C}H_2\text{-}COOH$

2,2′-sulfanediyldiacetic acid (PIN, multiplicative name)
2-[(carboxymethyl)sulfanyl]acetic acid (simple substitutive name)



4,4'-oxydi(cyclohexane-1-carboxylic acid) (PIN, multiplicative name)
4-[(4-carboxycyclohexyl)oxy]cyclohexane-1-carboxylic acid (simple substitutive name)



2,3′-oxydibenzoic acid (PIN, multiplicative name; see P-15.3)
2-(3-carboxyphenoxy)benzoic acid (simple substitutive name)

CH_3-CH_2-O-CH_2-CH_3

ethoxyethane (PIN, simple substitutive name)
(not 1,1′-oxydiethane; carbon chains are not allowed as parent hydrides in multiplicative nomenclature)

P-51.3 Skeletal replacement ('a') nomenclature

Skeletal replacement ('a') nomenclature is used in two ways to generate preferred IUPAC names:

(1) it is the only recommended method to generate names for certain heterocyclic compounds;

(2) it is used to simplify substitutive nomenclature or multiplicative nomenclature when heteroatoms are present in chains.

P-51.3.1 Skeletal replacement ('a') nomenclature is used to derive preferred IUPAC names for heteromonocyclic compounds having more than ten ring atoms (see P-22.2.3), heterocyclic von Baeyer ring systems (see P-23.3.1), heterocyclic spiro parent hydrides consisting of two or more saturated monocyclic rings (see P-24.2.4.1.1), heteropolycyclic ring systems for which fusion nomenclature based on heterocyclic parent rings is not applicable (see P-25.5.1), heterophane ring systems (see P-26.5), and for heterofullerenes (see P-27.5).

P-51.3.2 Skeletal replacement ('a') nomenclature is used to generate preferred IUPAC names in place of substitutive or multiplicative names for acyclic structures when four and more heterounits are present (see P-15.4.3.2).

Example 1:

$\overset{1}{\mathrm{H_3Si}}\text{-}\mathrm{CH_2}\text{-}\overset{1'}{\mathrm{SiH_3}}$

1,1′-methylenebis(silane) (PIN, multiplicative name)
(silylmethyl)silane (simple substitutive name)

$\mathrm{CH_3}\text{-}\overset{1}{\mathrm{SiH_2}}\text{-}\mathrm{CH_2}\text{-}\overset{1'}{\mathrm{SiH_2}}\text{-}\mathrm{CH_3}$

1,1′-methylenebis(methylsilane) (PIN, multiplicative name)
methyl[(methylsilyl)methyl]silane (simple substitutive name)

$\mathrm{CH_3}\text{-}\overset{1}{\mathrm{SiH_2}}\text{-}\mathrm{CH_2}\text{-}\mathrm{SiH_2}\text{-}\mathrm{CH_2}\text{-}\overset{1'}{\mathrm{SiH_2}}\text{-}\mathrm{CH_3}$

1,1′-[silanediylbis(methylene)]bis(methylsilane) (PIN), multiplicative name)
(treats two silane groups as parent hydrides)
bis[(methylsilyl)methyl]silane
(treats only one silane group as a parent hydride; two silane groups as substituents)

$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{SiH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{SiH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{SiH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{8}{\mathrm{S}}\text{-}\overset{9}{\mathrm{CH_2}}\text{-}\overset{10}{\mathrm{CH_3}}$

8-thia-2,4,6-trisiladecane (PIN, skeletal replacement (‘a’) name)
1-[(ethylsulfanyl)methyl]-1′-methyl-1,1′-[silanediylbis(methylene)]bis(silane)
(multiplicative name)
({[(ethylsulfanyl)methyl]silyl}methyl)[(methylsilyl)methyl]silane
(simple substitutive name)

Example 2:

$\mathrm{HOOC}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\mathrm{O}\text{-}\mathrm{CH_2}\text{-}\mathrm{CH_2}\text{-}\mathrm{O}\text{-}\overset{2'}{\mathrm{CH_2}}\text{-}\mathrm{COOH}$

2,2′-[ethane-1,2-diylbis(oxy)]diacetic acid (PIN, multiplicative name)
2-[2-(carboxymethoxy)ethoxy]acetic acid (simple substitutive name)

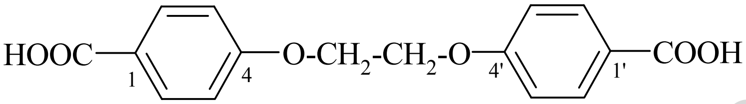
$\mathrm{HOOC}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\mathrm{O}\text{-}\mathrm{CH_2}\text{-}\mathrm{CH_2}\text{-}\mathrm{O}\text{-}\mathrm{CH_2}\text{-}\overset{2'}{\mathrm{CH_2}}\text{-}\mathrm{O}\text{-}\mathrm{CH_2}\text{-}\mathrm{COOH}$

2,2′-[oxybis(ethane-2,1-diyloxy)diacetic acid (PIN, multiplicative name)
2-{2-[2-(carboxymethoxy)ethoxy]ethoxy}acetic acid (simple substitutive name)

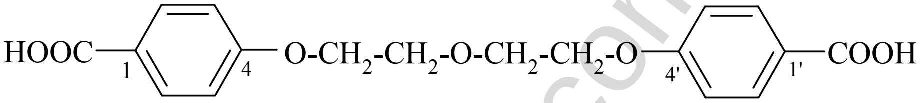
$$\overset{1}{\mathrm{HOOC}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{3}{\mathrm{O}}\text{-}\overset{4}{\mathrm{CH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{O}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{8}{\mathrm{CH_2}}\text{-}\overset{9}{\mathrm{O}}\text{-}\overset{10}{\mathrm{CH_2}}\text{-}\overset{11}{\mathrm{CH_2}}\text{-}\overset{12}{\mathrm{O}}\text{-}\overset{13}{\mathrm{CH_2}}\text{-}\overset{14}{\mathrm{COOH}}$$

3,6,9,12-tetraoxatetradecane-1,14-dioic acid [PIN, skeletal replacement (‘a’) name]
2,2'-{ethane-1,2-diylbis[(oxyethane-2,1-diyl)oxy]}diacetic acid (multiplicative name)
2-(2-{2-[2-(carboxymethoxy)ethoxy]ethoxy}ethoxy)acetic acid (simple substitutive name)

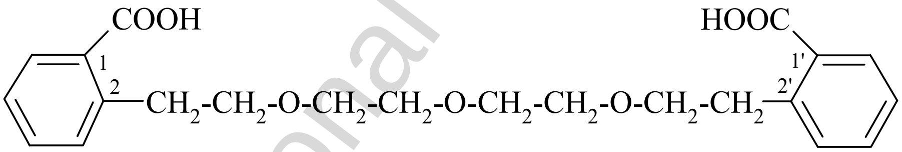
Example 3:



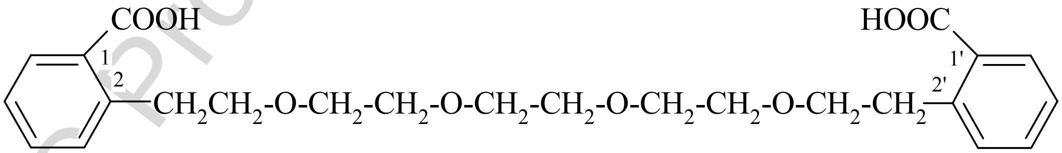
4,4'-[ethane-1,2-diylbis(oxy)]dibenzoic acid (PIN, multiplicative name)
4-[2-(4-carboxyphenoxy)ethoxy]benzoic acid (simple substitutive name)



4,4'-[oxybis(ethane-2,1-diyloxy)]dibenzoic acid (PIN, multiplicative name)
4-{2-[2-(4-carboxyphenoxy)ethoxy]ethoxy}benzoic acid (simple substitutive name)



2,2'-{oxybis[(ethane-2,1-diyloxy)ethane-2,1-diyl]}dibenzoic acid (PIN, multiplicative name)
2-[2-(2-{2-[2-(2-carboxyphenyl)ethoxy]ethoxy}ethoxy)ethyl]benzoic acid
(simple substitutive name)

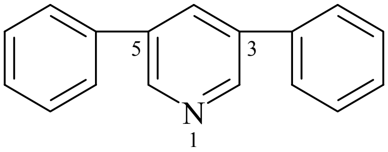


2,2'-(3,6,9,12-tetraoxatetradecane-1,9-diyl)dibenzoic acid (PIN, multiplicative name using the skeletal replacement (‘a’) name for the multiplying substituent group)
2,2′-{[ethane-1,2-diylbis(oxy)]bis(ethane-2,1-diyloxyethane-2,1-diyl)}dibenzoic acid (multiplicative name using simple substitutive nomenclature)
2-{2-[2-(2-{2-[2-(2-carboxyphenyl)ethoxy]ethoxy}ethoxy)ethoxy]ethyl}benzoic acid (simple substitutive name)

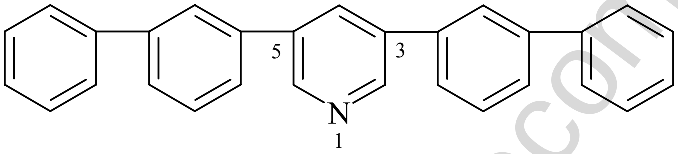
P-51.4 Phane nomenclature

P-51.4.1 Phane nomenclature is used to generate preferred IUPAC names for linear acyclic/cyclic compounds that include a minimum of seven nodes including four rings or ring systems, two of which are terminal, even though these compounds can also be named by substitutive or multiplicative nomenclature.

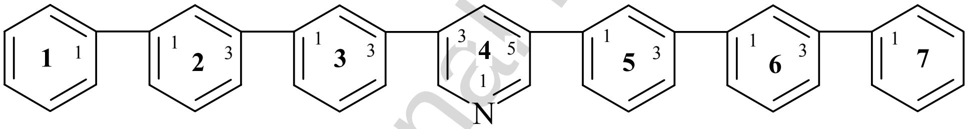
Example 1:



3,5-diphenylpyridine (PIN, substitutive name)

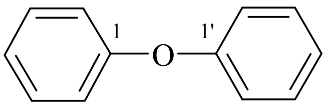


3,5-bis([biphenyl]-3-yl)pyridine (PIN, substitutive name)

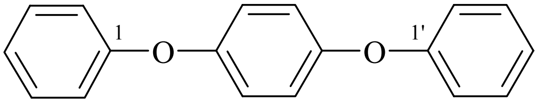


4(3,5)-pyridina-1,7(1),2,3,5,6(1,3)-hexabenzenaheptaphane (PIN, phane name)
3,5-bis([1^1,2^1:2^3,3^1-terphenyl]-1^3-yl)pyridine (simple substitutive name, see P-28.2.1 and P-28.3.1)
3,5-bis([1,1':3',1″-terphenyl]-3-yl)pyridine (simple substitutive name, see P-28.2.1 and P-28.3.1)

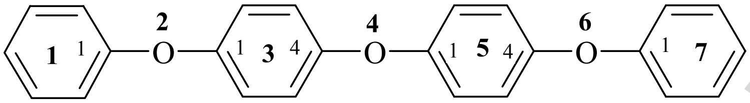
Example 2:



1,1′-oxydibenzene (PIN, multiplicative name)
phenoxybenzene (simple substitutive name)
(not diphenyl ether)

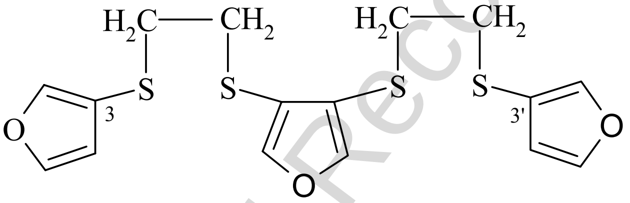


1,1′-[1,4-phenylenebis(oxy)]dibenzene (PIN, multiplicative name)
1,4-diphenoxybenzene (simple substitutive name)

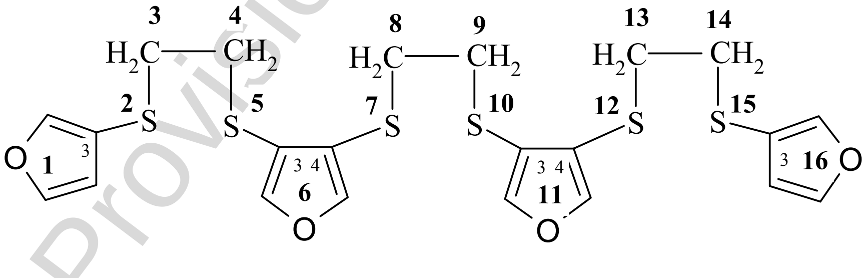


2,4,6-trioxa-1,7(1),3,5(1,4)-tetrabenzenaheptaphane (PIN, phane name)
1,1′-oxybis(4-phenoxybenzene) (multiplicative name)
1-phenoxy-4-(4-phenoxyphenoxy)benzene (simple substitutive name)

Example 3:



3,3′-{furan-3,4-diylbis[(sulfanediylethane-2,1-diyl)sulfanediyl]}difuran
(PIN, multiplicative name)
3,4-bis{[2-(furan-3-ylsulfanyl)ethyl]sulfanyl}furan (simple substitutive name)



2,5,7,10,12,15-hexathia-1,16(3),6,11(3,4)-tetrafuranahexadecaphane (PIN, phane name)
3,3′-[ethane-1,2-diylbis(sulfanediyl)]bis({4-[2-(furan-3-ylsulfanyl)ethyl]sulfanyl}furan)
(multiplicative name)
3-{[2-(furan-3-ylsulfanyl)ethyl]sulfanyl}-4-({2-[(4-{ [2-(furan-3-ylsulfanyl)ethyl]sulfanyl}furan-3-yl)sulfany]ethyl}sulfanyl)furan
(a simple substitutive name)

P-52 Selecting preferred IUPAC names and preselected names (see P-12) for parent hydrides

For naming the parent hydrides described in Chapter 2, when only one method is described, the resulting single names are naturally preferred IUPAC names. When more than one method is recommended for generating the names of parent hydrides, preferred IUPAC names, and in some cases, preselected names, must be chosen. Some retained names are used as preferred IUPAC names and as names for use in general nomenclature.

P-52.1 Selecting preselected names

P-52.1.1 Preselected mononuclear parent hydride names (see P-21.1.1)

fluorane	HF	azane	NH_3	borane	BH_3
chlorane	HCl	phosphane	PH_3	alumane	AlH_3
bromane	HBr	arsane	AsH_3	indigane	InH_3
iodane	HI	stibane	SbH_3	gallane	GaH_3
astatane	HAt	bismuthane	BiH_3	thallane	TlH_3
oxidane	H_2O	silane	SiH_4		
selane	H_2Se	germane	GeH_4		
sulfane	H_2S	stannane	SnH_4		
tellane	H_2Te	plumbane	PbH_4		
polane	H_2Po				

P-52.1.2 Preselected names for homogeneous acyclic polynuclear parent hydrides (see P-21.2.2)

Examples:

NH_2-NH_2
hydrazine (preselected name)

NH_2-$[NH_2]_7$-NH_2
nonaazane (preselected name)

SiH_3-$[SiH_2]_3$-SiH_3
pentasilane (preselected name)

HS-S-S-S-SH
trisulfane (preselected name)

PH_2-PH-PH_2
triphosphane (preselected name)

P-52.1.3 Heterogeneous acyclic parent hydrides composed of alternating atoms [a(ba)$_n$ hydrides], excluding carbon (see P-21.2.3.1)

Examples:

SiH_3-NH-SiH_3
disilazane (preselected name)

SnH_3-O-SnH_2-O-SnH_3
tristannoxane (preselected name)

P-52.1.4 Parent hydrides with nonstandard bonding numbers

Examples:

PH_5
λ^5-phosphane (preselected name)
phosphorane

AsH_5
λ^5-arsane (preselected name)
arsorane

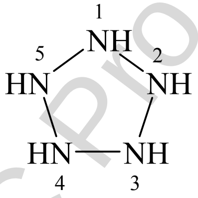
SbH_5
λ^5-stibane (preselected name)
stiborane

$\overset{1}{SH}\text{-}\overset{2}{SH_2}\text{-}\overset{3}{SH}$
2λ^4-trisulfane (preselected name)

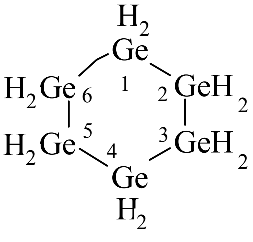
P-52.1.5 Homogeneous heteromonocyclic parent hydrides

Preselected names for homogeneous heteromonocyclic parent hydrides are Hantzsch-Widman names (see P-22.2.2) for rings composed of ten or fewer ring members. Skeletal replacement ('a') names (see P-22.2.3) are preselected names for heterogeneous monoheterocyclic parent hydrides with alternating heteroatoms with more than ten ring members. Alternative names are those formed by using the prefix 'cyclo' (see P-22.2.5).

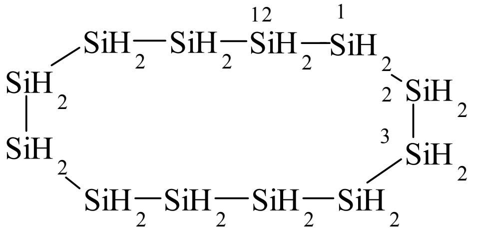
Examples:



pentazolane (preselected name)
cyclopentaazane



hexagerminane (preselected name)
cyclohexagermane

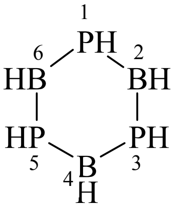


dodecasilacyclododecane (preselected name)
cyclododecasilane

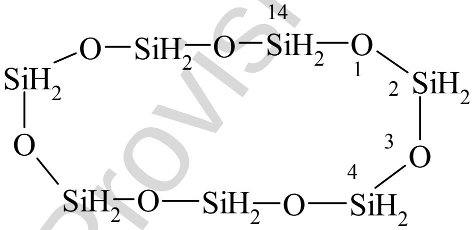
P-52.1.6 Heterogeneous heteromonocyclic parent hydrides consisting of alternating heteroatoms

Preselected names for heterogeneous heteromonocyclic parent hydrides with ten or fewer ring members composed of alternating heteroatoms are Hantzsch-Widman names (see P-22.2.2). Skeletal replacement (‘a’) names (see P-22.2.3) are preselected names for heterogeneous monoheterocyclic parent hydrides with alternating heteroatoms with more than ten ring members. Alternative names are those formed by using the prefix ‘cyclo’ (see P-22.2.5).

Examples:



1,3,5,2,4,6-triphosphatriborinane (preselected name)
cyclotriboraphosphane

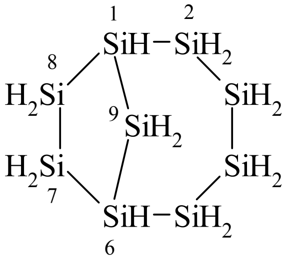


1,3,5,7,9,11,13-heptaoxa-2,4,6,8,10,12,14-heptasilacyclotetradecane (preselected name)
cycloheptasiloxane

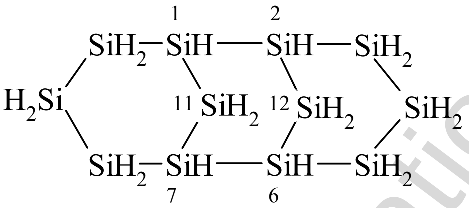
P-52.1.7 Homogeneous heterocyclic von Baeyer systems and spiro compounds

Preselected names for von Baeyer systems and spiro compounds composed entirely of heteroatoms of the same kind, are names formed by using the total number of heteroatoms expressed as mononuclear parent hydrides; alternative names are those formed by skeletal replacement (‘a’) nomenclature (see P-23.3 and P-2.4.2)

Examples:



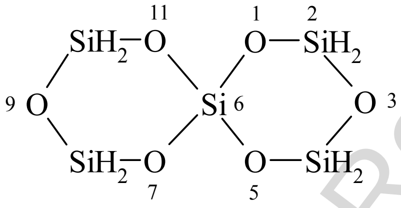
bicyclo[4.2.1]nonasilane (preselected name)
nonasilabicyclo[4.2.1]nonane



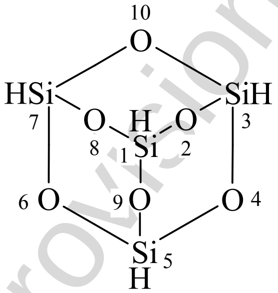
tricyclo[5.3.1.1^{2,6}]dodecasilane (preselected name)
dodecasilatricyclo[5.3.1.1^{2,6}]dodecane

P-52.1.8 Preselected names for bi- and polyalicyclic ring systems (von Baeyer ring systems) and spiro compounds having only monocyclic components composed of alternating heteroatoms are formed by citing the number and the names of the alternating atoms (see P-23.5); alternative names are those formed by skeletal replacement ('a') nomenclature.

Examples:



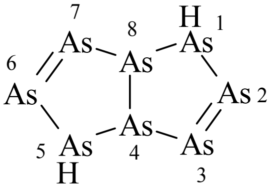
spiro[5.5]pentasiloxane (preselected name)
1,3,5,7,9,11-hexaoxa-2,4,6,8,10-pentasilaspiro[5.5]undecane



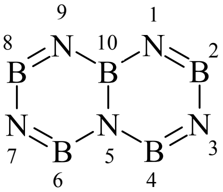
tricyclo[3.3.1.1^{3,7}]tetrasiloxane (preselected name)
2,4,6,8,9,10-hexaoxa-1,3,5,7-tetrasilabicyclo[3.3.1.1^{3,7}]decane

P-52.1.9 Preselected names for homogeneous and heterogeneous heterobi- and polycyclic fused ring systems are appropriate fusion names

Examples:



1*H*,5*H*-pentarsolopentarsole (preselected name)



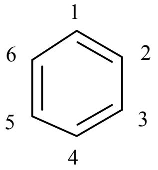
[1,3,5,2,4,6]triazatriborino[1,2-*a*][1,3,5,2,4,6]triazatriborine (preselected name)

P-52.2 Selecting preferred IUPAC names

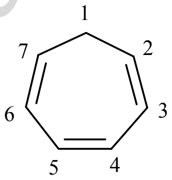
P-52.2.1 Monocyclic hydrocarbons

The name [*n*]annulene is used in preferred IUPAC fusion names as a parent component (see P-25.3.2.1.1) and may be used in general nomenclature as a parent hydride name. Preferred IUPAC names for cycloalkenes and cycloalkapolyenes are generated from cycloalkane names (see P-32.1.3.1).

Examples:



benzene (PIN)
[6]annulene)

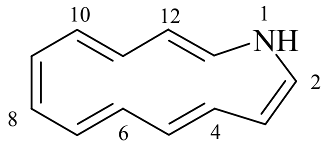


cyclohepta-1,3,5-triene (PIN)
1*H*-[7]annulene (preferred IUPAC name for the parent component in fusion nomenclature, see P-25.3.2.1.1)

P-52.2.2 Unsaturated heteromonocyclic compounds with more than ten ring members

Names derived from cycloalkanes modified by skeletal replacement (‘a’) nomenclature are preferred IUPAC names; [*n*]annulene names (see P-31.1.3.2) may be used in general nomenclature. A modified skeletal replacement (‘a’) name is used to designate these heterocyclic compounds as components in fusion names (see P-25.3.2.1.2) and is found in general nomenclature.

Example:

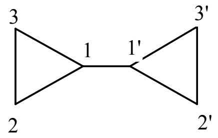


1-azacyclotrideca-2,4,6,8,10,12-hexaene (PIN)
1-azacyclotridecine (preferred IUPAC name for the the principal component in a fusion name, see also P-25.2.2.1.2; 1-azacyclotridecino for an attached component, see P-25.3.2.2.2)
1*H*-1-aza[13]annulene

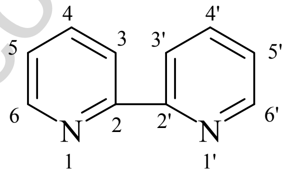
P-52.2.3 Preferred names and numbering for ring assemblies

P-52.2.3.1 Preferred IUPAC names for assemblies of two identical cyclic systems joined by a single bond are formed using the names of parent hydrides, except for benzene assemblies, biphenyl and the polyphenyls, rather than the names of substituent groups.

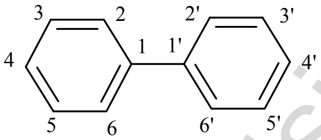
Examples:



1,1'-bi(cyclopropane) (PIN)
1,1'-bi(cyclopropyl)



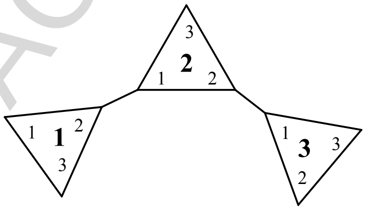
2,2'-bipyridine (PIN)
2,2'-bipyridyl



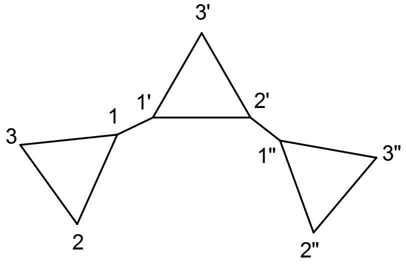
1,1′-biphenyl (PIN)
biphenyl

P-52.2.3.2 The preferred numbering for ring assemblies composed of three or more identical cyclic systems is by composite locants rather than primed locants.

Examples:



$1^1,2^1:2^2,3^1$-tercyclopropane (PIN)



1,1′:2′,1″-tercyclopropane

P-52.5 Selecting a preferred cyclic parent hydride

When two or more cyclic parent hydrides can be chosen to name a cyclic compound, one of them must be selected as the preferred parent hydride.

P-52.5.1 General rule

The preferred parent hydride is one occurring first in the following list given in decreasing order of seniority:

spiro system

cyclic phane system

fused system

bridged fused system

von Baeyer polyalicyclic system

linear phane system

ring assembly.

P-52.5.2 Definitions

P-52.5.2.1 Fused systems, bridged fused systems, spiro systems, bi- and polyalicyclic (von Baeyer) ring systems, and ring assemblies are described in Chapter 2.

It must be noted that for preferred IUPAC names fusion nomenclature is applicable only when two five membered rings are present. Thus, the name octahydropentalene (a fusion name) is preferred to bicyclo[3.3.0]octane. Systems without the required two five membered rings are given von Baeyer names, for example, bicyclo[2.2.0]hexane.

P-52.5.2.2 Cyclic and linear phane systems

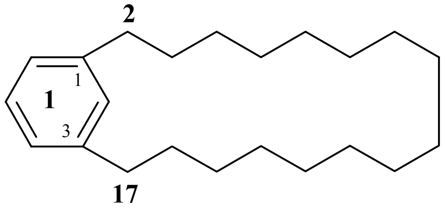
Cyclic and linear phane structures are defined in section P-26. For the purpose of selecting preferred IUPAC names for polycyclic systems and correctly applying P-52.5.1, cyclic and acyclic phane systems are defined more rigorously as follows:

(1) cyclophanes are cyclic phane structures containing one or more rings or ring systems, at least one ring or ring system of which must be a mancude system attached to adjacent components at nonadjacent ring positions;

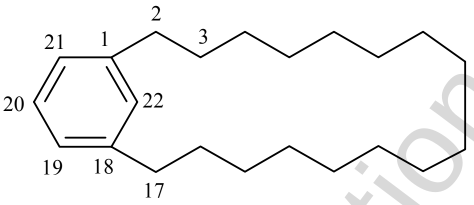
(2) linear phanes consist of four or more rings or ring systems, two of which must be terminal, and together with acyclic atoms or chains must consist of at least seven nodes (components).

P-52.5.3 Name selection. The following examples illustrate the application of P-52.5.1.

Examples:

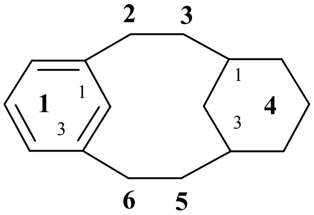


1(1,3)-benzenacycloheptadecane (PIN; phane name)

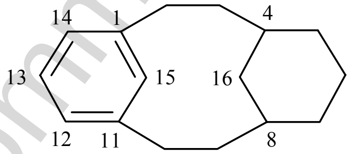


bicyclo[16.3.1]docosane-1(22),18,20-triene (von Baeyer name)

(a fusion name is not possible for this structure; a phane name is preferred to a von Baeyer name)

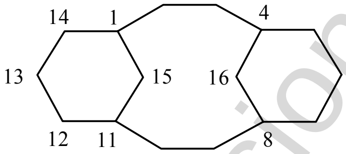


1(1,3)-benzena-4(1,3)-cyclohexanacyclohexaphane (PIN)

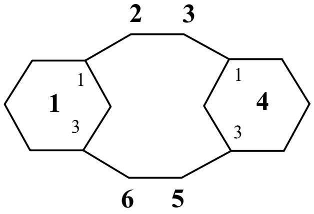


tricyclo[9.3.1.1^{4,8}]hexadeca-1(15),11,13-triene (von Baeyer name)

(a fusion name is not possible for this structure; a phane name is preferred to a von Baeyer name)

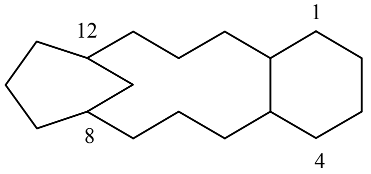


tricyclo[9.3.1.1^{4,8}]hexadecane (PIN)

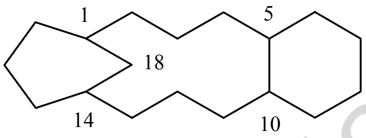


1,4(1,3)-dicyclohexanacyclohexaphane

(a fusion name is not possible; since there is no mancude ring present a phane name is not appropriate; therefore the von Baeyer name is the preferred IUPAC name)



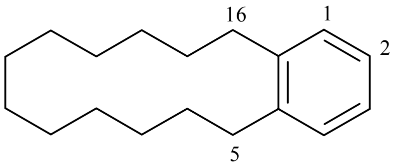
(I)



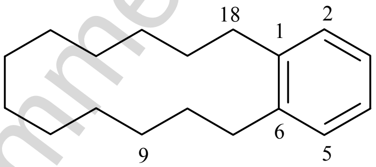
(II)

(I) hexadecahydro-1*H*-8,12-methanobenzo[13]annulene (PIN)
(II) tricyclo[12.3.1.$0^{5,10}$]octadecane

[the bridged fused name (**I**) is preferred to von Baeyer name (**II**); since no mancude ring being present, a phane name is not allowed]

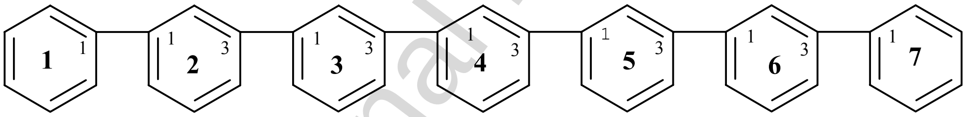


5,6,7,8,9,10,11,12,13,14,15,16-dodecahydro-benzo[14]annulene (PIN)



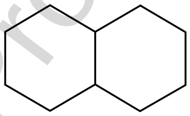
bicyclo[12.4.0]octadeca-1(14),17,19-triene

(a phane name is not allowed according to Rule P-52.5.3.2; a fusion name is preferred to a von Baeyer name)



1,7(1),2,3,4,5,6(1,3)heptabenzenaheptaphane (PIN)
$1^{1},2^{1}.2^{3}.3^{1},3^{3},4^{1},4^{4},5^{1},5^{3},6^{1},6^{3},7^{1}$-septiphenyl
1,1′:3′,1″:3″,1‴:3‴,1⁗:3⁗,1⁗′-septiphenyl

(a phane name, where permitted, is preferred to a ring assembly name)



decahydronaphthalene (PIN)
bicyclo[4.4.0]decane
(a fusion name is preferred to a von Baeyer name)

P-53 Selecting a method for modifying the degree of hydrogenation

Three methods are used to modify the degree of hydrogenation of parent hydrides:

(1) by changing the ending ‘ane’ in acyclic parent hydrides to ‘ene’ and ‘yne’;

(2) by using ‘hydro’ prefixes to saturate one or more double bonds in mancude compounds;

(3) by using ‘dehydro’ prefixes to introduce triple bonds in mancude compounds.

Systematic IUPAC names and retained names may be modified in the same way or in different ways.

P-53.1 Changing the ending ‘ane’ into ‘ene’ and ‘yne’

P-53.1.1 Alkanes, homogenous chains, and heterogenous hetero chains composed in part or entirely of heteroatoms are modified by changing the ending ‘ane’ into ‘ene’ and ‘yne’ to generate preferred IUPAC names (see P-31.1.2.2.1).

Examples:

$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_3$ butane (PIN)	$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H\text{=}\overset{1}{C}H_2$ but-1-ene (PIN)
$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3$ pentane (PIN)	$\overset{5}{C}H_3\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}\equiv\overset{2}{C}\text{-}\overset{1}{C}H_3$ pent-2-yne (PIN)
$H_2N\text{-}NH\text{-}NH_2$ triazane (preselected name)	$H_2\overset{3}{N}\text{-}\overset{2}{N}\text{=}\overset{1}{N}H$ triazene (preselected name)
$H_2P\text{-}NH\text{-}PH_3$ diphosphazane (preselected name)	$H_2\overset{3}{P}\text{-}\overset{2}{N}\text{=}\overset{1}{P}H$ diphosphazene (preselected name)
$CH_3\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_3$ 2,4,6,8-tetrasilanonane (PIN)	$\overset{9}{C}H_3\text{-}\overset{8}{Si}H_2\text{-}\overset{7}{C}H_2\text{-}\overset{6}{Si}H_2\text{-}\overset{5}{C}H_2\text{-}\overset{4}{Si}H\text{=}\overset{3}{C}H\text{-}\overset{2}{Si}H_2\text{-}\overset{1}{C}H_3$ 2,4,6,8-tetrasilanon-3-ene (PIN)

The retained name 'hydrazine' generates the systematic name 'diazene':

$H_2N\text{-}NH_2$

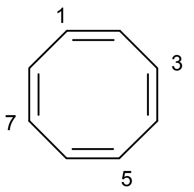
hydrazine (preselected name)
diazane

$H\overset{2}{N}{=}\overset{1}{N}H$

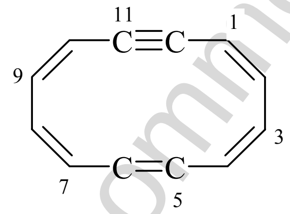
diazene (preselected name)

P-53.1.2 Preferred IUPAC names for monocyclic mancude hydrocarbons (see P-31.1.3.1), von Baeyer polyalicyclic compounds (see P-31.1.4.1), and saturated spiro compounds (see P-31.1.5.1), are formed by modifying the ending 'ane' into 'ene'.

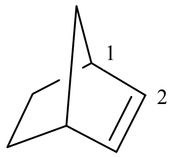
Example:



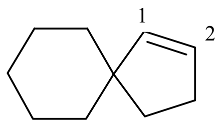
cycloocta-1,3,5,7-tetraene (PIN)
[8]annulene



cyclododeca-1,3,5,7,9-pentaen-11-yne (PIN)
1,2-didehydro[12]annulene

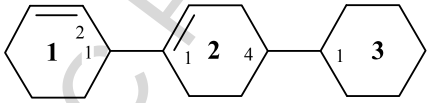


bicycle[2.2.1]hept-2-ene (PIN)

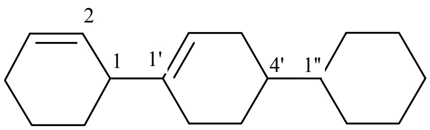


spiro[4.5]dec-1-ene (PIN)

P-53.1.3 Assemblies of identical saturated rings and ring systems are modified by 'ene' and 'yne' endings (see P-31.1.6). Preferred IUPAC names are generated by the use of 'ene' and 'yne' endings using composite locants rather than primed locants (see P-28.3.1).
Example:



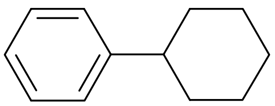
[1^1,2^1:2^4,3^1-tercyclohexane]-1^2,2^1-diene (PIN)
(see also P-28.3.1)



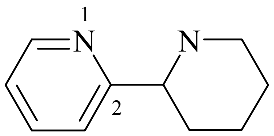
[1,1′:4′,1″-tercyclohexane]-1′,2-diene
(see also P-28.3.1)

When assemblies of otherwise identical rings contain both mancude and saturated rings, substitutive names lead to preferred IUPAC names and when the requirements for the formation of phane names are met, phane names are the preferred IUPAC names.

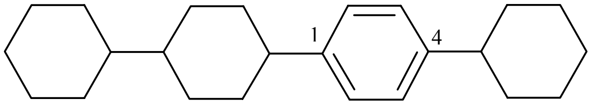
Examples:



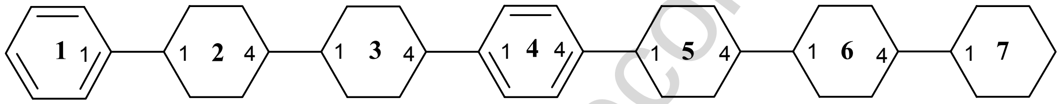
cyclohexylbenzene (PIN)



2-(piperidin-2-yl)pyridine (PIN)



4-(cyclohexylphenyl)-1,1′ -bicyclohexane (PIN)



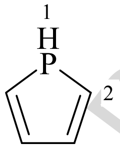
1(1), 4(1,4)-dibenzena-2,3,5,6(1,4),7(1)-pentacyclohexanaheptaphane (PIN)
1-[4-(4′-phenyl-[1,1′-bicyclohexan]-1-yl)phenyl]-1^1,2^1:2^4,3^1-tercyclohexane

P-53.2 Names modified by 'hydro' prefixes

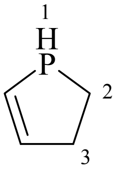
P-53.2.1 Monoheterocycles having Hantzsch-Widman names

Preferred IUPAC names for Hantzsch-Widman rings correspond to either fully unsaturated or fully saturated compounds (see P-22.2.2.1.1). 'Hydro' prefixes added to names of fully unsaturated Hantzsch-Widman rings lead to preferred IUPAC names for partially unsaturated rings.

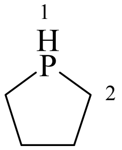
Examples:



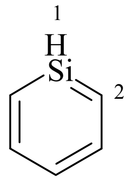
1*H*-phosphole (PIN)



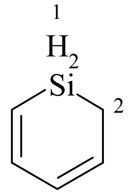
2,3-dihydro-1*H*-phosphole (PIN)



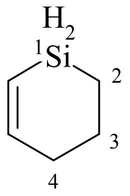
phospholane (PIN)



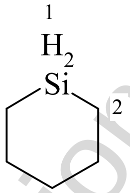
silinine (PIN)



1,2-dihydrosilinine (PIN)



1,2,3,4-tetrahydrosilinine (PIN)



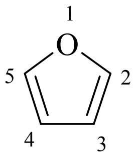
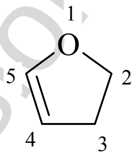
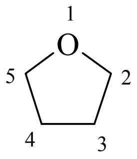
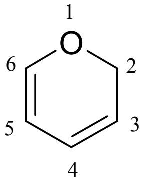
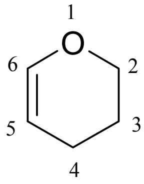
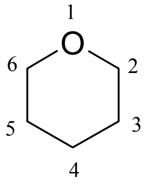
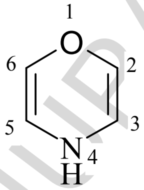
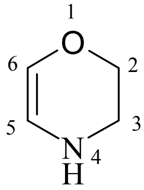
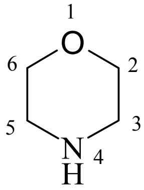
silinane (PIN)

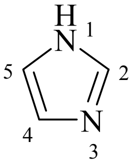
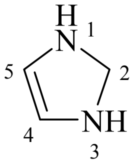
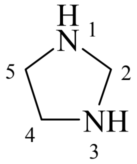
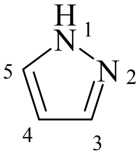
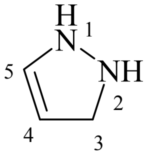
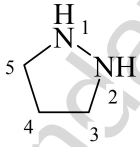
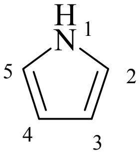
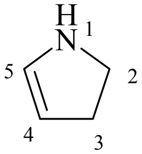
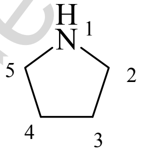
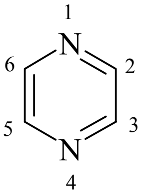
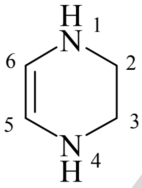
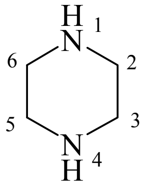
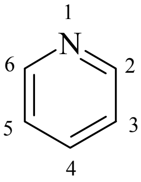
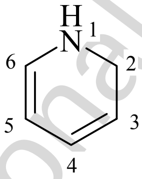
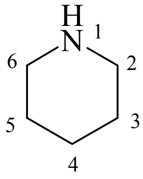
P-53.2.2 Heteromonocylic compounds with retained names

Retained names are used for unsaturated and saturated heteromonocyclic compounds before modification with ‘hydro’ prefixes and for saturated compounds after modification by ‘hydro’ prefixes, in accordance with Table 5.1. Hantzsch-Widman names are described in P-22.2.2; retained names are listed in P-22.2.1 and in Tables 2.2 and 2.3.

Names of fully saturated compounds can also be formed by adding the maximum number of ‘hydro’ prefixes, for example ‘hexahydropyridine’; these names are not preferred IUPAC names but are acceptable in general nomenclature.

Table 5.1 Retained heteromonocyclic names modified by ‘hydro’ prefixes

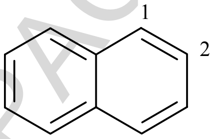
Structure	Name before modification by ‘hydro’ prefixes	Structure	Name after partial modification by ‘hydro’ prefixes	Structure	Name after full modification by ‘hydro’ prefixes
	furan (PIN)		2,3-dihydrofuran (PIN)		oxolane (PIN) tetrahydrofuran
	2*H*-pyran (PIN)		2,3-dihydro-2*H*-pyran (PIN)		oxane (PIN)
	4*H*-oxazine(PIN)		2*H*-3,4-dihydro-oxazine (PIN)		morpholine (PIN) tetrahydro-2*H*-oxazine

	1*H*-imidazole (PIN)		2,3-dihydro-1*H*-imidazole (PIN)		imidazolidine (PIN)
	1*H*-pyrazole (PIN)		2,3-dihydro-1*H*-pyrazole (PIN)		pyrazolidine (PIN)
	1*H*-pyrrole (PIN)		2,3-dihydro-1*H*-pyrrole (PIN)		pyrrolidine (PIN)
	pyrazine (PIN)		1,2,3,4-tetrahydro pyrazine (PIN)		piperazine (PIN)
	pyridine (PIN)		1,2-dihydro pyridine (PIN)		piperidine (PIN)

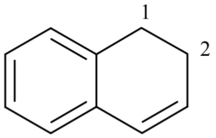
P-53.2.3 Fused ring systems and mancude ring assemblies

P-53.2.3.1 Retained fusion names are used for the fully unsaturated compounds (see P-25); they are the preferred IUPAC names. Preferred IUPAC names for the partially saturated and fully saturated compounds are formed by using 'hydro' prefixes. Preferred IUPAC names for partially saturated and mancude ring assemblies are formed in the same way.

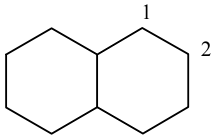
Examples:



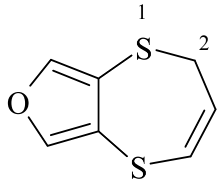
naphthalene (PIN)



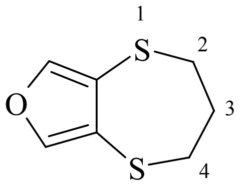
1,2-dihydronaphthalene (PIN)



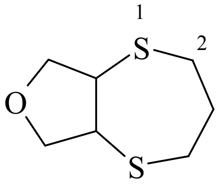
decahydronaphthalene (PIN)
bicyclo[4,4,0]decane



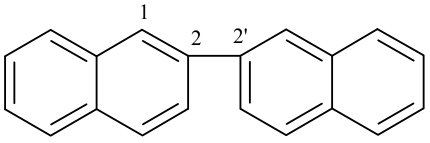
2*H*-thiepino[1,3-*c*]furan (PIN)



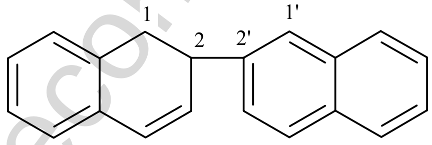
3,4-dihydro-2*H*-thiepino[1,3-*c*]furan (PIN)



hexahydro-2*H*-thiepino[1,3-*c*]furan (PIN)



2,2′-binaphthalene (PIN)
2,2′-binaphthyl



1,2-dihydro-2,2′-binaphthalene (PIN)
1,2-dihydro-2,2′-binaphthyl

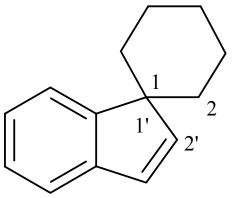
P-53.2.3.2 The retained names for the partially saturated heterocycles, ‘indane’, ‘indoline’, ‘isoindoline’, ‘chromane’, and ‘isochromane’ are not used as preferred IUPAC names, but are acceptable for use in general nomenclature (see P-31.2.3.3.1).

P-53.3 Names modified by ‘ene’ and ‘yne’ endings and ‘hydro’ prefixes

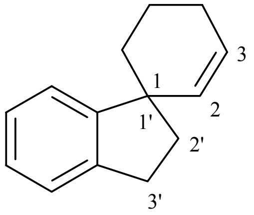
P-53.3.1 Spiro compounds

Saturated and mancude components, when present in a spiro compound, are modified individually in accordance with the rule applicable to the component.

Example:



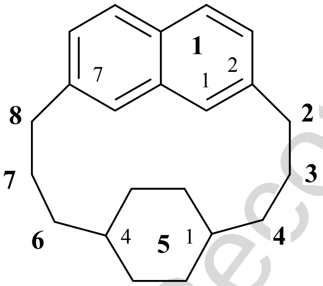
spiro[cyclohexane-1,1′-indene] (PIN)



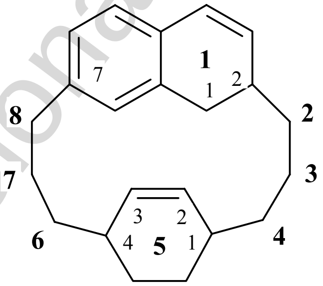
2′,3′-dihydrospiro[cyclohexane-1,1′-indene]-2-ene (PIN)

P-53.3.2 Mancude and saturated amplificants, when present in a phane system, are each modified in accordance with the rules applicable to each individual amplificant.

Eample:



1(2,7)-naphthalena-5(1,4)-cyclohexanacyclooctaphane (PIN)

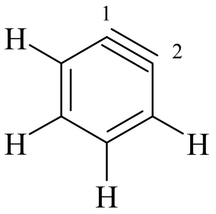


1^1,1^2-dihydro-1(2,7)-naphthalena-5(1,4)-cyclohexanacyclooctaphan-5^2-ene (PIN)

P-53.4 Names modified by ‘dehydro’ prefixes

‘Dehydro’ prefixes are used to generate preferred IUPAC names of dehydrogenated mancude compounds. They may be used in general nomenclature to introduce double and triple bonds in saturated parent hydrides.

Example:



1,2-dehydrobenzene (PIN)
cyclohexa-1,3-dien-5-yne
(not benzyne)

P-54 Selecting suffixes

Suffixes have always been described as unique elements of the formation of names. In the past, some suffixes have been discarded and replaced by new ones.

P-54.1 The suffixes ‘amidine’ and ‘carboxamidine’ for $-C(=NH)-NH_2$, are no longer recommended; the new suffixes ‘imidamide’ and ‘carboximidamide’ (see P-66.4.1) are used in preferred IUPAC names.

Examples:

$CH_3-C(=NH)-NH_2$	$C_6H_{11}-C(=NH)-NH_2$
ethanimidamide (PIN) (no longer acetamidine)	cyclohexanecarboximidamide (PIN) (no longer cyclohexanecarboxamidine)

P-54.2 The suffix ‘sulfenic acid’ for $-S-OH$ was discarded in the 1993 recommendations (ref 2); in these recommendations, it is replaced by the new suffix, ‘*SO*-thioperoxol’ (see P-63.3.2).

Example:

CH_3-S-OH

methane-*SO*-thioperoxol (PIN)
(no longer methanesulfenic acid)

P-54.3 The suffix ‘ylene’ was used to describe divalent substituent groups in which the free valences do not form a double bond, i.e., –E– or E<, in contrast to substituent groups in which the free valences form a double bond, i.e., E=. The suffix ‘ylene’ has been replaced by the suffixes ‘diyl’ to express the –E– or E< type, and ‘ylidene’ for E=, for example, methanediyl for $H_2C<$ and methylidene for $H_2C=$, respectively. However, the name ‘methylene’ is retained to describe the substituent group $H_2C<$; it is used in preferred IUPAC names rather than methanediyl. In these recommendations, preferred names are expressed as follows:

$-CH_2-$	$H_2C=$
methylene (PIN, retained name) methanediyl	methylidene (PIN) (formerly methylene)

$-CH_2-CH_2-$	$CH_3-CH=$
ethane-1,2-diyl (PIN)) ethylene	ethylidene (PIN)
$-SiH_2-$	$H_2Ge=$
silanediyl (preselected name) (not silylene, a name still used by CAS)	germylidene (preselected name) (not germylene, a name still used by CAS)
$-BH-$	$HB=$
boranediyl (preselected name) (not borylene, a name still used by CAS)	boranylidene (preselected name) (not borylene, a name still used by CAS)
$-SbH-$	$HSb=$
stibanediyl (preselected name) stibinediyl (not stibylene, a name still used by CAS)	stibanylidene (preselected name) stibinylidene (not stibylene, a name still used by CAS)

$-NH-CO-NH-$

carbonylbis(azanediyl) (PIN, a name used in multiplicative nomenclature)
(carbonyldiimino, a name still used by CAS)
(not ureylene)

P-55 Preferred retained names

Trivial names (names having no part used in a systematic sense) and semisystematic names retained for use in naming organic compounds are given in this Section. Some of them are used as preferred IUPAC names; all of them may be used in general nomenclature. References to rules established in Chapters 2 and 3 are given.

Trivial or semisystematic names retained for naming organic compounds are known as 'retained names'. Their number was sharply reduced in the 1979 Rules, and reduced still further in the 1993 Recommendations. The following list gives the recommendations for 2005 and is to be considered limiting, unless specified otherwise; see, for example, fusion nomenclature in P-25, and phane nomenclature in P-26. Substituent groups names not derived from a systematic transformation are given in Section P-56. All the names in the list can be used in general nomenclature.

Retained names are classified into three types based on their substitutability (see also P-29.6, P-35, P-35, and P-46).

Type 1. Unlimited substitution by substituent groups cited as suffixes or prefixes;

Type 2. Limited substitution classified as follows:

Type 2a. Substitution limited to substituent groups cited as prefixes in recognition of functional groups explicitly expressed or implied in the functional parent compound name;

Type 2b. Substitution limited to substituent groups cited as compulsory prefixes;

Type 2c. Substitution for parent structures not covered by Type 2a or 2b.

Type 3. Substitution of any kind not allowed.

P-55.1 Acyclic, alicyclic, monocyclic, and partially saturated hydrocarbons

The preferred IUPAC names for acyclic, alicyclic and monocyclic hydrocarbons, with the exception of toluene and xylene, have no restriction as to their ability to be substituted by substituent groups and by characteristic groups cited as suffixes and/or prefixes.

IUPAC preferred retained names			Retained names only for general nomenclature		
acetylene	Type 3	P-34.3.1	allene	Type 2b	P-34.3.1
adamantane	Type 1	P-23.7	[*n*]annulene	Type 1	P-22.1.2
benzene	Type 1	P-22.1.2	cubane	Type 1	P-23.7
butane	Type 1	P-21.1.1	indane	Type 1	P-31.3.2.1
ethane	Type 1	P-21.1.1	isoprene	Type 3	P-34.3.1
methane	Type 1	P-21.1.1	mesitylene	Type 3	P-22.1.3
propane	Type 1	P-21.1.1	styrene	Type 3	P-34.3.1
toluene	Type 2c	P-22.1.3			
xylene	Type 3	P-22.1.3			

P-55.1.2 Polycyclic fully unsaturated (mancude) hydrocarbons

The retained names for fully unsaturated (mancude) hydrocarbons given below are all IUPAC preferred names, fully substitutable, and are listed in Table 2.5, P-25.1.1.

anthracene
fluoranthene
indene
phenalene
pyrene

azulene
fluorene
naphthalene
phenanthrene
pyranthrene

chrysene
as-indacene
ovalene
picene
rubicene

coronene
s-indacene
perylene
pleiadene

P-55.2 Heterocycles

P-55.2.1 Fully unsaturated (mancude) heteromonocycles

P-55.2.1.1 The retained names for fully unsaturated (mancude) heteromonocycles given below are all IUPAC preferred names, fully substitutable, and are listed in Table 2.2, P-22.2.1.

furan
imidazole
pyran
pyrazine
pyrazole
pyridazine
pyridine
pyrimidine
pyrrole
selenophene
tellurophene
thiophene

P-55.2.1.2.

The retained names for fully unsaturated (mancude) heteromonocycles given below are not preferred IUPAC preferred names, but are acceptable in general nomenclature. They are fully substitutable, and are listed in Table 2.2, P-22.2.1.

isothiazole
1,2-thiazole (PIN)

isoxazole
1,2-oxazole (PIN)

oxazole
1,3-oxazole (PIN)

thiazole
1,3-thiazole (PIN)

P-55.2.2 Saturated heterocycles

P-55.2.1.1 The retained names for the saturated heteromonocycles given below are all IUPAC preferred names, fully substitutable, and are listed in Table 2.3, P-22.2.1.

imidazolidine
morpholine
piperazine
piperidine
pyrazolidine
pyrrolidine

P-55.2.1.2 The retained names for the saturated or partially saturated heteropolycycles given below are not preferred IUPAC names, but are acceptable for general nomenclature, are fully substitutable, and, except for quinuclidine, are listed in P-31.3.2.

quinuclidine (see P-23.7)
1-azabicyclo[2.2.2]octane (PIN)

indoline
2,3-dihydro-1*H*-indole (PIN)

isoindoline
2,3-dihydro-1*H*-isoindole (PIN)

chromane
3,4-dihydro-2*H*-1-benzopyran (PIN)

thiochromane
3,4-dihydro-2*H*-1-benzothiopyran (PIN)

selenochromane
3,4-dihydro-2*H*-1-benzoselenopyran (PIN)

tellurochromane
3,4-dihydro-2*H*-1-benzotelluropyran (PIN)

isochromane
3,4-dihydro-1*H*-2-benzopyran (PIN)

isothiochromane
3,4-dihydro-1*H*-2-benzothiopyran (PIN)

isoselenochromane
3,4-dihydro-1*H*-2-benzoselenopyran (PIN)

isotellurochromane
3,4-dihydro-1*H*-2-benzotelluropyran (PIN)

P-55.2.3 Fully unsaturated (mancude) heteropolycycles

P-55.2.3.1 The retained names for the fully unsaturated (mancude) heteropolycycles given below are all IUPAC preferred names, fully substitutable, and are listed in Tables 2.6 and 2.7, P-25.1.

acridarsine
acridine
acridophosphine
arsanthridine
arsindole
arsinoline
carbazole
chromene
cinnoline
imidazole
indazole
indole
indolizine
isoarsindole
isoarsinoline
isochromene
isoindole
isophosphindole
isophosphinoline
isoquinoline
naphthyridine
perimidine
phenanthridine
phenanthroline
phenazine
phosphindole
phosphinoline
phthalazine
pteridine
purine
pyrazine
pyrrolizine
quinazoline
quinoline
quinolizine
quinoxaline
xanthene

P-55.2.3.2 The retained names for the fully unsaturated (mancude) heteropolycycles given below are not preferred IUPAC names, but are acceptable in general nomenclature. They are fully substitutable and are included in Tables 2.6 and 2.7, P-25.1.

β-carboline
9*H*-pyrido[3,4-*b*]indole (PIN)

isobenzofuran
1*H*-2-benzofuran (PIN)

isobenzothiopyran
1*H*-2-benzothiofuran (PIN)

isobenzoselenopyran
1*H*-2-benzoselenofuran (PIN)

isobenzotelluropyran
1*H*-2-benzotellurofuran (PIN)

P-55.3 Retained names for nitrogen parent hydrides. The following are the preferred IUPAC names for the fully substitutable structures given in P-34.3.8.

hydrazine (preselected name, see P-12)

formazan (PIN)

P-55.4 Retained functional parent names

The following retained names for functional parent compounds are used as preferred names and are used in general nomenclature. Substitution of the corresponding structures follows the general types as given in P-55.0, except that substitution by groups corresponding to the same or higher functional class is not allowed.

P-55.4.1 Hydroxy compounds and ethers

IUPAC preferred retained names			Retained names only for general nomenclature		
anisole	Type 3	P-34.3.2	anisole	Type 2c	P-34.3.3
phenol	Type 1	P-34.3.2	ethylene glycol	Type 3	P-34.3.3
			glycerol	Type 3	P-34.3.3
			p-cresol (also *o*- and *m*- isomers)	Type 3	P-34.3.3
			picric acid	Type 3	P-34.3.3

P-55.4.2 Carbonyl compounds. The following retained names are not preferred IUPAC names but are acceptable in general nomenclature (all compounds are given in P-34.3.2)

acetone	Type 2a
ketene	Type 2b
acetophenone	Type 3
benzophenone	Type 3
1,4-benzoquinone (also 1,2- isomer)	Type 2a
9,10-anthraquinone (also 1,2-, 1,4-and 2,3- isomers)	Type 2a
1,4-naphthoquinone (also 1,2- and 2,3- isomers	Type 2a

P-55.4.3 Carboxylic acids

P-55.4.3.1 The retained names for the carboxylic acids given below are IUPAC preferred names, fully substitutable (Type 2a), except for formic acid which is Type 2c, and are listed in Tables 2.6 and 2.7, P-34.3.4.

acetic acid
benzoic acid
formic acid (Type 2c)
phthalic acid
terephthalic acid

P-55.4.3.2 The retained names for the carboxylic acids given below are not preferred IUPAC names but are acceptable in general use; they are not substitutable (Type 3), and are listed in P-34.3.4.

acrylic acid
adipic acid
butyric acid
cinnamic acid
citric acid
furoic acid
glutaric acid
isonicotinic acid
isophthalic acid
lactic acid
malonic acid
methacrylic acid
naphthoic acid
nicotinic acid
oleic acid
palmitic acid
propionic acid
pyruvic acid
stearic acid
succinic acid
tartaric acid

P-55.4.4 Retained names for other 'carbon acids' (carbonic acid and oxalic acid) and related acids given below are IUPAC preferred names, and are fully substitutable where the possiblility of substitution exists. They are listed in P-34.3.5.

carbonic acid
carbamic acid
cyanic acid
oxalic acid
oxamic acid
oxaldehydic acid

P-55.4.5 Nitrogen functional parent structures

Preferred IUPAC retained names			Retained names only for general nomenclature		
aniline	Type 2a	P-34.3.6	benzidine	Type 3	P-34.3.4
formazan	Type 2b	P-34.3.4	semicarbazide	Type 2b	P-34.3.4
urea	Type 2b	P-34.3.4	biuret	Type 2b	P-34.3.4
guanidine	Type 2b	P-34.3.4	biguanide	Type 2b	P-34.3.4
hydroxylamine	Type 2c	P-34.3.4			

P-55.4.6 Preferred IUPAC names for natural products

P-55.4.6.1 Names of alkaloids, steroids, terpenes and other natural product parent hydrides are retained because they carry implied stereochemical configuration, have widespread usage, and may have a complex structure. Preferred IUPAC names and names for use only in general nomenclature are listed in Table 10.1 in Chapter 10. The list is nonlimiting. Some structures are also given in Chapter 10; all are listed in the Appendix in ref 9.

P-55.4.6.2 Preferred IUPAC names for functional parent structures, such as carbohydrates and α-amino acids, follow the nomenclature procedures for these compound classes as given in P-102 through P-107.

P-56 Names of substituent groups derived from parent structures

P-56.1 Substituent groups derived from parent structures with retained names.

This Section describes preferred IUPAC names that are retained names of substituent groups derived from parent structures described in P-55 as well as names for use in general nomenclature. Names of substituent groups derived from the parent structures in P-33 that are formed by a systematic procedure given in P-29 and P-32 are NOT included. References to rules established in Chapters 2 and 3 are given. The substitutability of each structure is indicated in the same manner as for the parent structures in P-55.

Type 1. Unlimited substitution by substituent groups cited as suffixes or prefixes;

Type 2. Limited substitution classified as follows:

Type 2a. Substitution limited to substituent groups cited as prefixes in recognition of functional groups explicitly expressed or implied in the functional parent compound name;

Type 2b. Substitution limited to substituent groups cited as compulsory prefixes;

Type 2c. Substitution for parent structures not covered by Type 2a or 2b.

Type 3. Substitution of any kind not allowed

To facilitate the choice of a preferred prefix, all usual prefixes, including those described below, are listed in Appendix 2, with clear indications as to their preferred status in the nomenclature of organic compounds

P-56.1.1 Substituent groups derived from parent hydrides.

Preferred IUPAC retained names			Retained names only for general nomenclature		
adamantyl 1- and 2-isomers	Type 2a	P-29.6	allyl	Type 2b	P-32.3

benzyl	Type 2c	P-29.6	allylidene	Type 2b	P-32.3
benzylidene	Type 2c	P-29.6	anthryl 1-, 2-, and 9- isomers	Type 2a	P-29.6.1
benzylidyne	Type 2a	P-29.6	ethylene	Type 2a	P-29.6.1
tert-butyl	Type 3	P-29.6	furyl 2- and 3- isomers	Type 2a	P-29.6.1
hydrazinyl	Type 2a	P-29.6	isopropyl	Type 3	P-29.6.3
hydrazinylidene	Type 2a	P-29.6	isopropylidene	Type 3	P-29.6.3
methylene	Type 2a	P-29.6	isoquinolyl 1-, 2-, 3-, 4-, 5-, 6-, 7-, and 8- isomers	Type 2a	P-29.6.1
phenyl	Type 2a	P-29.6	naphthyl 1-, and 2- isomers	Type 2a	P-29.6.1
phenylene 1,2-, 1,3-, and 1,4- isomers	Type 2a	P-29.6.1	phenanthryl 1-, 2-, 3-, 4-, and 9- isomers	Type 2a	P-29.6.1
trityl	Type 3	P-29.6.3	piperidyl 1-, 2-, 3-, and 4- isomers	Type 2a	P-29.6.1
			pyridyl 2-, 3-, and 4- isomers	Type 2a	P-29.6.1
			quinolyl 2-, 3-, 4-, 5-, 6-, 7-, and 8- isomers	Type 2a	P-29.6.1
			styryl	Type 3	P-29.6.3
			thienyl		

			1-, 2- and 3- isomers	Type 2a	P-29.6.1
			tolyl *o*-,*m*-, and *p*- isomers)	Type 2a	P-29.6.3
			vinyl	Type 2a	P-32.3
			vinylidene	Type 2a	P-32.3

P-56.1.2 Substituent groups derived from functional parents

IUPAC preferred retained names			Retained names only for general nomenclature		
acetyl	Type 2a	P-34.4.1	acetonyl	Type 3	P-34.3.3
butoxy	Type 2a	P-34.4.2	*sec*-butoxy	Type 3	P-34.4.2
tert-butoxy	Type 3	P-34.4.2	*tert*-butoxy	Type 3	P-34.4.2
carbonyl	NA	P-35.2.3	butyryl	Type 3	P-34.4.1
ethoxy	Type 2a	P-34.4.2	cyano	NA	P-35.2.1
formyl	Type 2c	P-34.4.1	glutaryl	Type 3	P-34.4.1
methoxy	Type 2a	P-34.4.2	isopropoxy	Type 3	P-34.3.1
oxalo	NA	P-65.2.3	malonyl	Type 3	P-34.4.1
oxalyl	NA	P-34.4.1	propionyl	Type 3	P-34.4.1
oxamoyl	Type 2a	P-34.4.1	succinyl	Type 3	P-34.4.1
oxaldehydoyl	Type 2c	P-65.2.3			
phenoxy	Type 2a	P-34.4.2			
propoxy	Type 2a	P-34.4.2			
seleninyl	NA	P-35.2.3			

selenonyl	NA	P-35.2.3
sulfinyl	NA	P-35.2.3
sulfonyl	NA	P-35.2.3
tellurinyl	NA	P-35.2.3
telluronyl	NA	P-35.2.3

P-56.1.3 Amido, imido, amino, and other nitrogeneous groups

Retained names for amide and imido prefixes derived from the acids given in P-34.3.1 are formed by changing the name of the ....amide or ....imide' ending to ...amido or ...imido, respectively, for example, acetamido, phthalamido, succinimido. These names follow the same rules for selection of preferred IUPAC names and the same substitution rules as the corresponding acid given above.

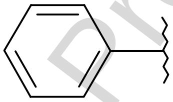
The retained names anilino, formazan-1-yl, formazan-3-yl, and formazan-5-yl are preferred IUPAC names, are used in general nomenclature, and are classified as Type 2 for the purposes of substitution.

P-56.2 Selection of preferred substituent group names between retained names and systematic names for which two methods of formation are recommended according to P-29 and P-32. The following rules are recommended for the selection of preferred IUPAC names. Names of substituent groups are listed in Appendix 2, with indications concerning their use as preferred names or for general nomenclature only.

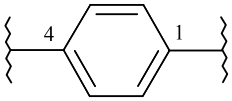
P-56.2.1 Methylene and phenylene

$-CH_2-$

methylene (PIN; not used to indicate a double bond)
methanediyl



phenyl (PIN)



1,4-phenylene (PIN)
(also, the 1,2- and 1,3-isomers are preferred IUPAC names)
p-phenylene

P-56.2.2 Selecting preferred IUPAC names for acyclic hydrocarbon substituent groups

P-56.2.2.1 When the free valence(s) are at the end of the longest chain of an alkane, alkyl substituent prefixes are preferred IUPAC names, not alkanyl substituent prefixes.

Examples:

CH_3-

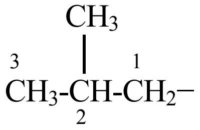
methyl (PIN)
methanyl

$\overset{2}{CH_3}-\overset{1}{CH}=$

ethylidene (PIN)
ethanylidene

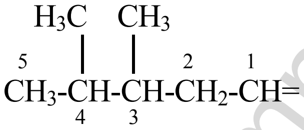
$\overset{3}{CH_3}-\overset{2}{CH_2}-\overset{1}{C}\equiv$

propylidyne (PIN)
propanylidyne



$$\overset{3}{CH_3}-\underset{2}{\overset{\overset{CH_3}{|}}{C}}H-\overset{1}{CH_2}-$$

2-methylpropyl (PIN)



$$\overset{5}{CH_3}-\underset{4}{\overset{\overset{H_3C}{|}}{C}}H-\underset{3}{\overset{\overset{CH_3}{|}}{C}}H-\overset{2}{CH_2}-\overset{1}{CH}=$$

3,4-dimethylpentylidene (PIN)

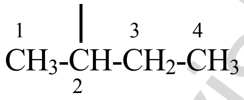
$\overset{3}{CH_2}=\overset{2}{CH}-\overset{1}{CH_2}-$

prop-2-en-1-yl (PIN)

$\overset{4}{CH_2}=\overset{3}{CH}-\overset{2}{CH_2}-\overset{1}{CH_2}-$

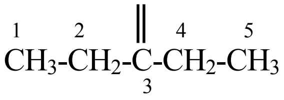
but-2-en-1-yl (PIN)

P-56.2.2.2 Alkanyl substituent prefixes are preferred IUPAC names when the free valence(s) is (are) located on a nonterminal atom of the longest continuous chain. These names are preferred to those formed by substituting alkyl groups.
Examples:



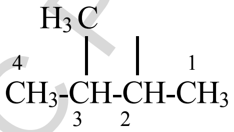
$$\overset{1}{CH_3}-\underset{2}{\overset{|}{C}}H-\overset{3}{CH_2}-\overset{4}{CH_3}$$

butan-2-yl (PIN)
1-methylpropyl



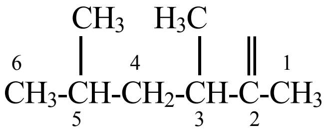
$$\overset{1}{CH_3}-\overset{2}{CH_2}-\underset{3}{\overset{\|}{C}}-\overset{4}{CH_2}-\overset{5}{CH_3}$$

pentan-3-ylidene (PIN)
1-ethylpropylidene



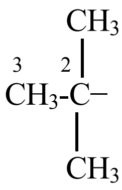
$$\overset{4}{CH_3}-\underset{3}{\overset{\overset{H_3C}{|}}{C}}H-\underset{2}{\overset{|}{C}}H-\overset{1}{CH_3}$$

3-methylbutan-2-yl (PIN)
1,2-dimethylpropyl



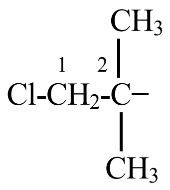
$$\overset{6}{CH_3}-\underset{5}{\overset{\overset{CH_3}{|}}{C}}H-\overset{4}{CH_2}-\underset{3}{\overset{\overset{H_3C}{|}}{C}}H-\underset{2}{\overset{\|}{C}}-\overset{1}{CH_3}$$

3,5-dimethylbutan-2-ylidene (PIN)
1,2,4-trimethylpentylidene



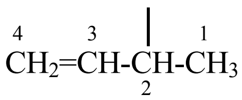
$$CH_3\text{-}C(CH_3)_2\text{–}$$

tert-butyl (PIN)
2-methylpropan-2-yl
1,1-dimethylethyl



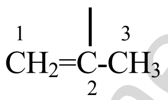
$$Cl\text{-}CH_2\text{-}C(CH_3)_2\text{–}$$

1-chloro-2-methylpropan-2-yl (PIN)
2-chloro-1,2-dimethylethyl



$$CH_2{=}CH\text{-}CH(\text{–})\text{-}CH_3$$

but-3-en-2-yl (PIN)
1-methylprop-2-en-1-yl

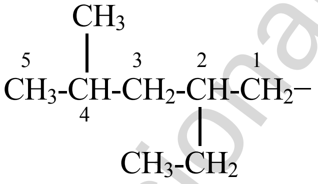


$$CH_2{=}C(\text{–})\text{-}CH_3$$

prop-1-en-2-yl (PIN)
1-methylethenyl

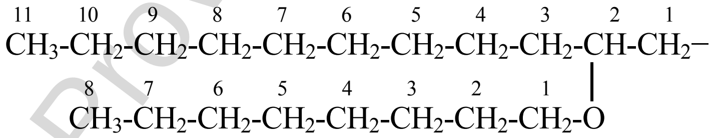
P-56.2.2.3 For compound substituent groups (substituted substituent groups), P-56.1.2.1 or P-56.1.2.2 is applied according to the requirements for each chain. When the longest chain of the parent substituent or of each substituent chain terminates at the free valence, it is named as an alkyl substituent. When the free valence is not at the end of the longest chain of the parent substituent or of each substituent chain, it is named as an alkanyl group.

Examples:



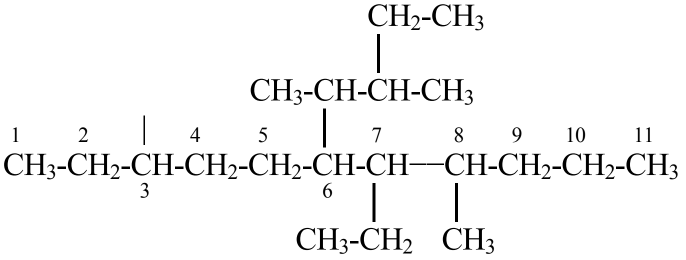
$$CH_3\text{-}CH(CH_3)\text{-}CH_2\text{-}CH(CH_2\text{-}CH_3)\text{-}CH_2\text{–}$$

2-ethyl-4-methylpentyl (PIN)



$$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH(O\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3)\text{-}CH_2\text{–}$$

2-(octyloxy)undecyl (PIN)



$$\overset{1}{C}H_3-\overset{2}{C}H_2-\underset{3}{\overset{|}{C}}H-\overset{4}{C}H_2-\overset{5}{C}H_2-\underset{6}{\overset{\overset{CH_2-CH_3}{\overset{|}{CH_3-CH-CH-CH_3}}}{\overset{|}{C}}}H-\underset{\underset{CH_3-CH_2}{|}}{\overset{7}{C}}H-\underset{\underset{CH_3}{|}}{\overset{8}{C}}H-\overset{9}{C}H_2-\overset{10}{C}H_2-\overset{11}{C}H_3$$

7-ethyl-8-methyl-6-(3-methylpentan-2-yl)undecan-3-yl (PIN)
(not 7-ethyl-6-(1,2-dimethylbutyl)-8-methylundecan-3-yl

P-56.2.3 Systematic vs. retained names

When there is a choice between a systematic name and a retained name other than those cited in P-56.1.1 and P-56.1.2, a systematic name is preferred, respecting the substitution rules for the retained name.

Examples:

$-\overset{2}{C}H_2-\overset{1}{C}H_2-$

ethane-1,2-diyl (PIN)
ethylene

$\overset{2}{C}H_2=\overset{1}{C}H-$

ethenyl (PIN)
vinyl

$\overset{2}{C}H_2=\overset{1}{C}=$

ethenylidene (PIN)
vinylidene

$\overset{3}{C}H_2=\overset{2}{C}H-\overset{1}{C}H_2-$

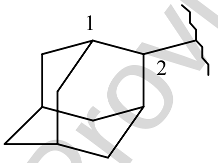
prop-2-en-1-yl (PIN)
allyl

$\overset{3}{C}H_2=\overset{2}{C}H-\overset{1}{C}H=$

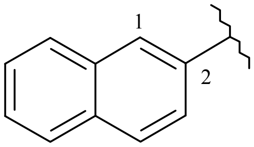
prop-2-en-1-ylidene (PIN)
allylidene

$\overset{3}{C}H_2=\overset{2}{C}H-\overset{1}{C}\equiv$

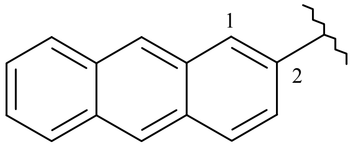
prop-2-en-1-ylidyne (PIN)
allylidyne



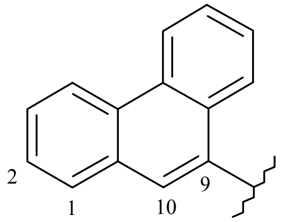
adamantan-2-yl (PIN)
2-adamantyl



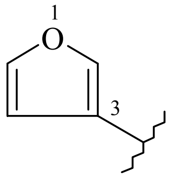
naphthalen-2-yl (PIN)
2-naphthyl



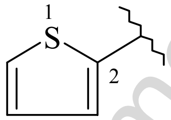
anthracen-2-yl (PIN)
2-anthryl



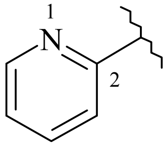
phenanthren-9-yl (PIN)
9-phenanthryl



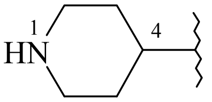
furan-3-yl (PIN)
3-furyl



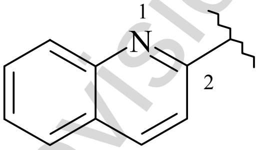
thiophen-2-yl (PIN)
2-thienyl



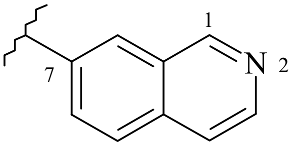
pyridin-2-yl (PIN)
2-pyridyl



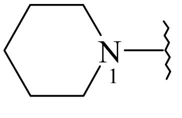
piperidin-4-yl (PIN)
4-piperidyl



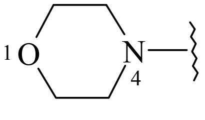
quinolin-2-yl (PIN)
2-quinolyl



isoquinolin-7-yl (PIN)
7-isoquinolyl



piperidin-1-yl (PIN)
1-piperidyl
(not piperidino)



morpholin-4-yl (PIN)
(not morpholino)

P-56.3 Retained names for characteristic groups expressed as prefixes

Prefixes denoting characteristic groups that are derived from parent structures are classified into four categories.

- P-56.3.1 Retained names for simple characteristic groups
- P-56.3.2 Names derived from retained names rather than systematic names of parent structures.
- P-56.3.3 Systematic names preferred to traditional retained names
- P-56.3.4 Systematic names used to replace traditional prefixes

Prefixes denoting characteristic groups are listed in Appendix 2; preferred prefixes are indicated when one or two alternative prefixes are recommended.. In this section, retained and systematically formed prefixes are listed. They are simple prefixes; their multiplicity is denoted by the basic multiplying prefixes ‘di’, ‘tri’, etc.

P-56.3.1 Retained names for simple characteristic groups

The following names are retained as preselected IUPAC names. The corresponding systematic names, with the exception of azanylidyne, are not recommended as preselected IUPAC names, but may be used in general nomenclature, for example ‘amino’ is a predelected IUPAC name but ‘azanyl’ is not.

H_2N-	$HN=$	$-\overset{\vert}{N}-$
amino (preselected name) azanyl	imino (preselected name) azanylidene	nitrilo (preselected name) azanetriyl
$HO-$	$-O-$	$O=$
hydroxy (preselected name) (not oxidanyl)	oxy (preselected name) (not (oxidanediyl)	oxo (preselected name) (not oxidanylidene)

$HOO-$	$-OO-$
hydroperoxy (preselected name) (not dioxidanyl)	peroxy (preselected name) (not dioxidanediyl) (not dioxy)
$F-$	$Cl-$
fluoro (preselected name) (not fluoranyl)	chloro (preselected name) (not chloranyl)

Br–

bromo (preselected name))
(not bromanyl)

I–

iodo (preselected name)
(not iodanyl)

P-56.3.2 Names derived from retained names rather than systematic names of parent structures.

Names derived from hydrazine and formazan are preferred to those derived from diazane and (hydrazinylidenemethyl)diazene, respectively. In turn, the traditional prefixes ending with the letter ‘o’ are no longer recommended.

Examples:

$–NHNH_2$

hydrazinyl (preselected name)
diazanyl
(not hydrazino)

$=NNH_2$

hydrazinylidene (preselected name)
diazanylidene
(not hydrazono)

=N-N=

hydrazinediylidene (preselected name)
diazanediylidene
(not azino)

–NH-NH–

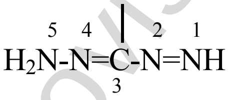
hydrazine-1,2-diyl (preselected name)
diazane-1,2-diyl
(not hydrazo nor hydrazi)

$\overset{5}{H_2N}\text{-}\overset{4}{N}\text{=}\overset{3}{CH}\text{-}\overset{2}{N}\text{=}\overset{1}{N}\text{–}$

formazan-1-yl (PIN)
(hydrazinylidenemethyl)diazenyl

$\overset{1}{HN}\text{=}\overset{2}{N}\text{-}\overset{3}{CH}\text{=}\overset{4}{N}\text{-}\overset{5}{NH}\text{–}$

formazan-5-yl (PIN)
(diazenylmethylidene)hydrazinyl

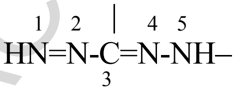


$\overset{5}{H_2N}\text{-}\overset{4}{N}\text{=}\underset{3}{\overset{|}{C}}\text{-}\overset{2}{N}\text{=}\overset{1}{NH}$

formazan-3-yl (PIN)
(hydrazinylhydrazinylidene)methyl

$\text{–}\overset{5}{NH}\text{-}\overset{4}{N}\text{=}\overset{3}{CH}\text{-}\overset{2}{N}\text{=}\overset{1}{N}\text{–}$

formazan-1,5-diyl (PIN)

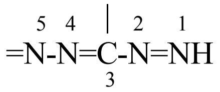


$\overset{1}{HN}\text{=}\overset{2}{N}\text{-}\underset{3}{\overset{|}{C}}\text{=}\overset{4}{N}\text{-}\overset{5}{NH}\text{–}$

formazan-3,5-diyl (PIN)

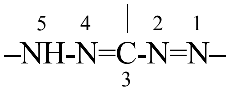
$=\overset{5}{N}\text{-}\overset{4}{N}\text{=}\overset{3}{CH}\text{-}\overset{2}{N}\text{=}\overset{1}{N}\text{–}$

formazan-1-yl-5-ylidene (PIN)



$=\overset{5}{N}-\overset{4}{N}=\underset{3}{\overset{|}{C}}-\overset{2}{N}=\overset{1}{N}H$

formazan-3-yl-5-ylidene (PIN)



$-\overset{5}{N}H-\overset{4}{N}=\underset{3}{\overset{|}{C}}-\overset{2}{N}=\overset{1}{N}-$

formazan-1,3,5-triyl (PIN)

P-56.3.3 Systematic names that are preselected IUPAC names; traditional retained names may be used in general nomenclature

S= sulfanylidene (preselected name)
thioxo

Se= selanylidene (preselected name)
selenoxo

Te= tellanylidene (preselected name)
telluroxo

P-56.3.4 Systematic names that are preselected IUPAC names rather than traditional prefix names.

–S–
sulfanediyl (preselected name)
thio

–SS–
disulfanediyl (preselected name)
dithio

–Se–
selanediyl (preselected name)
(not seleno)

–SeSe–
diselanediyl (preselected name)
(not diseleno)

–Te–
tellanediyl (preselected name)
(not telluro)

–TeTe–
ditellanediyl (preselected name)
(not ditelluro)

–NH–
azanediyl (preselected name)
(not imino)

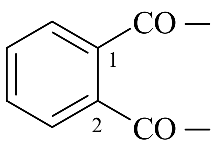
–N=
azanylylidene (preselected name)
(not nitrilo)

N≡
azanylidyne (PIN)
(not nitrilo)

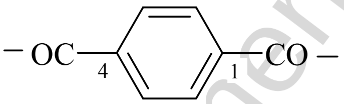
P-56.3.5 Acyl groups

P-56.3.5.1 The following names are retained as preferred names for acyl groups derived from the carboxylic acids listed in Section P-34.4.5, and the sulfur acids in P-34.7.

HCO–	CH_3-CO–	C_6H_5-CO–
formyl (PIN)	acetyl (PIN)	benzoyl (PIN)



phthaloyl (PIN)



terephthaloyl (PIN)

H_2N-CO–	H_2N-C(=NH)–	H_2N-SO_2–
carbamoyl (PIN) aminocarbonyl	carbamimidoyl (PIN) aminoiminomethyl	sulfamoyl (preselected name) aminosulfonyl

P-56.3.5.2 Preferred IUPAC names for acyl group prefixes

When acyl groups derived from carboxylic acids described in P-56.2.3 are attached to a carbon chain, preferred IUPAC names are formed by making the carbon atom of the acyl group part of the principal chain and appropriate prefixes are used. Note, however, that the –COOH group is never fragmented.

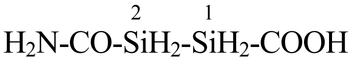
Examples:

$H_2N\text{-}\overset{4}{C}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

4-amino-4-oxobutanoic acid (PIN)
3-carbamoylpropanoic acid
3-(aminocarbonyl)propanoic acid
[not (aminoformyl)propanoic acid]
succinamic acid

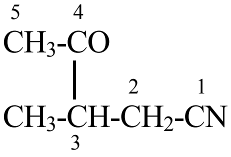
$Cl\text{-}\overset{3}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

3-chloro-3-oxopropanoic acid (PIN)
2-(carbonochloridoyl)acetic acid
2-(chlorocarbonyl)acetic acid
[not (chloroformyl)acetic acid]



$H_2N\text{-}CO\text{-}\overset{2}{Si}H_2\text{-}\overset{1}{Si}H_2\text{-}COOH$

2-carbamoyldisilane-1-carboxylic acid (PIN)
2-(aminocarbonyl)disilane-1-carboxylic acid
[not 2-(aminoformyl)disilane-1-carboxylic acid]



$$\begin{array}{l} \overset{5}{C}H_3\text{-}\overset{4}{C}O \\ \qquad | \\ CH_3\text{-}\underset{3}{C}H\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}N \end{array}$$

3-methyl-4-oxopentanenitrile (PIN)
(not 3-acetylbutanenitrile)

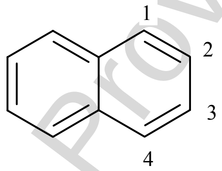
P-56.4 Substitution in compounds having the maximum number of noncumulative double bonds (mancude compounds) at positions where there is an insufficient number of hydrogen atoms for the substitutive operation.

P-56.4.1. Compounds without indicated hydrogen atoms

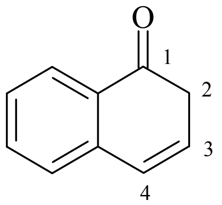
After introduction of free valences, radical or ionic centers, or principal characteristic groups, the maximum number of noncumulative double bonds is inserted and any hydrogen atoms needed to achieve tetravalency are denoted as ‘added hydrogen’ (see P-14.6). Lowest permissible locants are assigned first to suffixes and then to any ‘added hydrogen atoms’.

In names, each ‘added hydrogen’ is expressed by the letter *H* preceded by the appropriate locant. The ‘added hydrogen’ expression is enclosed in parentheses and inserted into the name after the locant or locants denoting the free valence(s), radical or ionic center(s), or principal characteristic group(s).

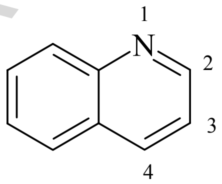
Examples:



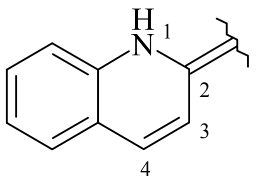
naphthalene (PIN, parent hydride)



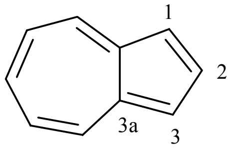
naphthalene-1(2*H*)-one (PIN)



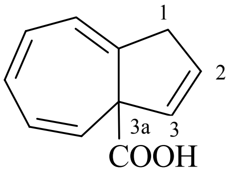
quinoline (PIN, parent hydride)



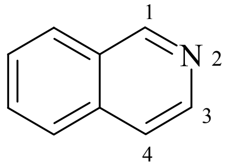
quinolin-2(1*H*)-ylidene (PIN)



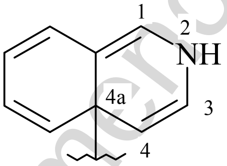
azulene (PIN, parent hydride)



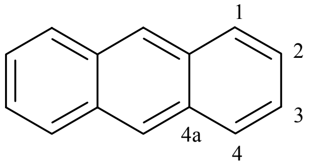
azulene-3a(1*H*)-carboxylic acid (PIN)



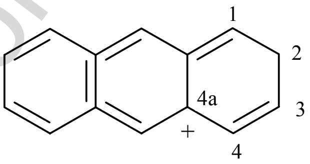
isoquinoline (PIN, parent hydride)



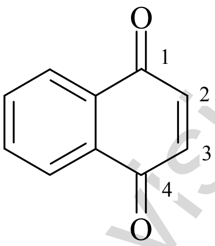
isoquinolin-4a(2*H*)-yl (PIN)



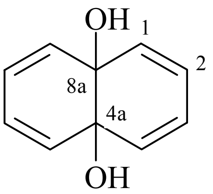
anthracene (PIN, parent hydride)



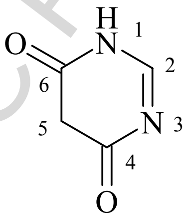
anthracen-4a(2*H*)-ylium (PIN)



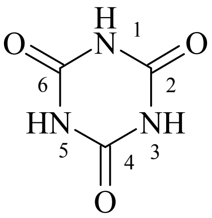
naphthalene-1,4-dione (PIN)



naphthalene-4a,8a-diol (PIN)



pyrimidine-4,6(1*H*,5*H*)-dione (PIN)

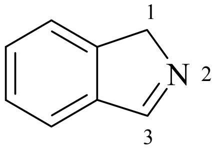


1,3,5-triazine-2,4,6(1*H*,3*H*,5*H*)-trione (PIN)

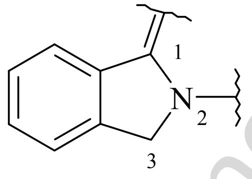
P-56.4.2 Substitution in compounds with indicated hydrogen atoms

Indicated hydrogen atoms are assigned the lowest locants permitted by the structure unless they can accommodate structural features elsewhere in the structure. Then, lowest possible locants are assigned to the nomenclatural feature cited as suffix and finally to added hydrogen atom(s), as noted in P-56.4.1.

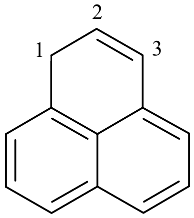
Examples:



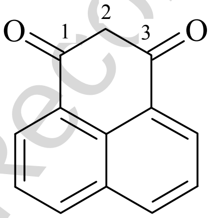
1*H*-isoindole (PIN)



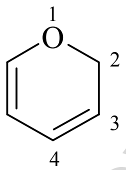
1*H*-isoindol-2(3*H*)-yl-1-ylidene (PIN)
(not 2*H*-isoindol-2-yl-1(3*H*)-ylidene)



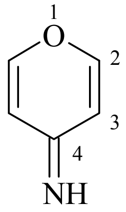
1*H*-phenalene (PIN)



1*H*-phenalen-1,3(2*H*)-dione (PIN)



2*H*-pyran (PIN)



4*H*-pyran-4-imine (PIN)

P-56.4.3 Compounds with indicated and/or added hydrogen atoms and additional saturation

Hydro prefixes are used to indicate additional saturation of double bonds in compounds already containing indicated and/or added hydrogen atoms. Lowest locants are assigned in the following order:

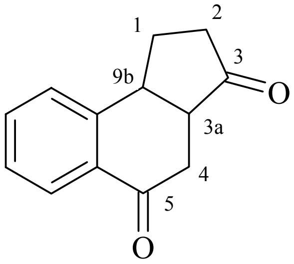
(a) indicated hydrogen atoms

(b) suffixes and associated added hydrogen atoms

(c) hydro prefixes

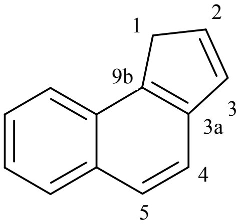
In names, hydro prefixes, indicated hydrogen, parent hydride, and suffixes appear in that order.

Examples:

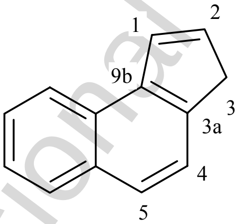


1,3a,4,9b-tetrahydro-3*H*-cyclopenta[*a*]naphthalene-3,5(2*H*)-dione (PIN)

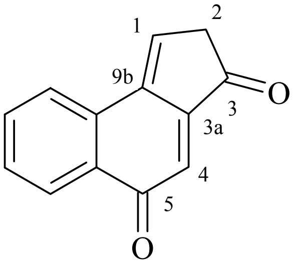
Guide to name construction.



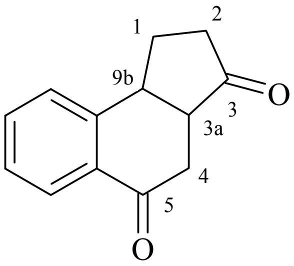
Step 1: Parent structure: 1*H*-cyclopenta[*a*]naphthalene (PIN, parent hydride)
(indicated hydrogen atom at the lowest possible position)



Step 2: 3*H*-cyclopenta[*a*]naphthalene (PIN, parent hydride; indicated hydrogen atom moved from position 1 to position 3 to accommodate further substitution by the ketone suffix 'one')



Step 3: 3*H*-cyclopenta[*a*]naphthalene-3,5(2*H*)-dione (PIN, at position 3, the ketone suffix 'one' introduced by direct substitution; at position 5, the introduction of the one suffix requires an added hydrogen atom at position 2, the position with the lowest locant possible)

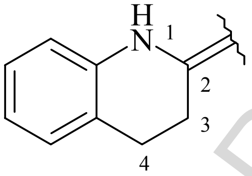


Step 4: 1,3a,4,9a-tetrahydro-3*H*-cyclopenta[*a*]naphthalene-3,5(2*H*)-dione (PIN)
(the prefix tetrahydro is added to saturate double bonds
at 1-9a and 3a-4)

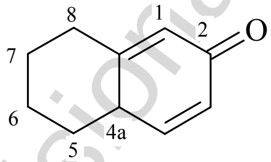
These four steps lead to the preferred IUPAC name:

1,3a,4,9b-tetrahydro-3*H*-cyclopenta[*a*]naphthalene-3,5(2*H*)-dione (PIN)

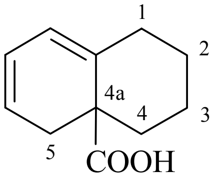
Further examples:



3,4-dihydroquinolin-2(1*H*)-ylidene (PIN)



5,6,7,8-tetrahydronaphthalen-2(4a*H*)-one (PIN)

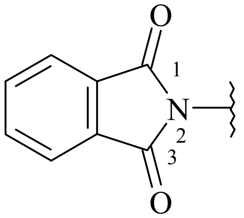


1,3,4,5-tetrahydronaphthalene-4a(2*H*)-carboxylic acid (PIN)

P-56.4.4 Compounds with detachable prefixes

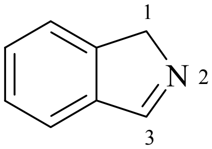
Substituent groups denoted by detachable (alphabetized) prefixes are introduced, as required, as the last step in the name construction. The addition of the necessary amount of hydrogen atoms to saturate double bonds is a prerequisite to the introduction of detachable substituents. In names, detachable prefixes denoting substituent groups are placed at the front of the name, before hydro prefixes.

Examples:

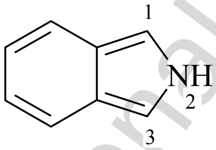


1,3-dioxo-1,3-dihydro-2*H*-isoindol-2-yl (PIN)

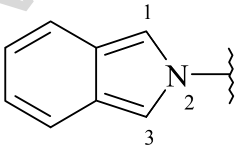
Guidelines for name construction:



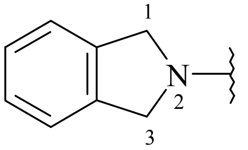
Step 1:. 1*H*-isoindole (PIN, parent hydride)
('indicated hydrogen' atom at the lowest possible position)



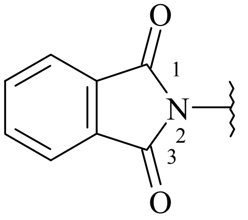
Step 2. 2*H*-isoindole (PIN, parent hydride)
('indicated hydrogen' atom moved to position 2 to
accommodate the introduction of the free valence)



Step 3. 2*H*-isoindol-2-yl (PIN)
(the suffix 'yl' indicates the presence of a free valence
in position 2; no 'added hydrogen' is necessary)



Step 4. 1,3-dihydro-2*H*-isoindol-2-yl (PIN)
(hydro prefixes are necessary to introduce the number of hydrogen atoms required for the introduction of the divalent ‘ylidene’ suffix)



Step 5. 1,3-dioxo-1,3-dihydro-2*H*-isoindol-2-yl (PIN)
(two ketonic substituent groups introduced denoted by the detachable prefix ‘oxo’)

These five steps lead to the preferred IUPAC name:

1,3-dioxo-1,3-dihydro-2*H*-isoindol-2-yl (PIN)

.

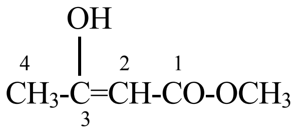
P-57 Selecting names for tautomeric structures

Naming tautomers is not a major problem for preferred IUPAC nomenclature, because each tautomer can be named individually. It is traditional to denote a mixture of tautomers by naming the component belonging to the highest class. A preferred IUPAC name for a tautomeric structure is given in accordance with the indicated structure chosen by the authors that selected a preferred structure.

Examples:

$\overset{4}{CH_3}\text{-}\overset{3}{CO}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{COOCH_3}$

methyl 3-oxobutanoate (PIN)

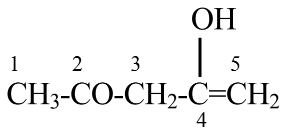


$\overset{4}{CH_3}\text{-}\underset{3}{\overset{OH}{C}}\text{=}\overset{2}{CH}\text{-}\overset{1}{CO}\text{-}OCH_3$

methyl 3-hydroxybut-2-enoate (PIN)

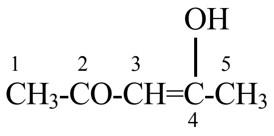
$\overset{5}{CH_3}\text{-}\overset{4}{CO}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CO}\text{-}\overset{1}{CH_3}$

pentane-2,4-dione (PIN)



$\overset{1}{CH_3}\text{-}\overset{2}{CO}\text{-}\overset{3}{CH_2}\text{-}\underset{4}{\overset{OH}{C}}\text{=}\overset{5}{CH_2}$

4-hydroxypent-4-en-2-one (PIN)

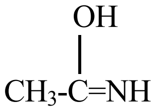


$\overset{1}{CH_3}\text{-}\overset{2}{CO}\text{-}\overset{3}{CH}\text{=}\underset{4}{\overset{OH}{C}}\text{-}\overset{5}{CH_3}$

4-hydroxypent-3-en-2-one (PIN)

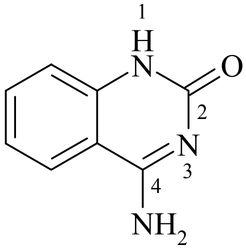
CH_3-CO-NH_2

acetamide (PIN)

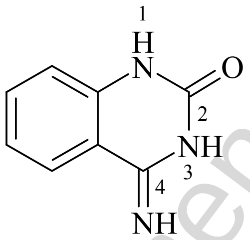


$CH_3-\overset{\displaystyle OH}{\overset{|}{C}}=NH$

acetimidic acid (PIN)



4-aminoquinazolin-2(1*H*)-one (PIN)



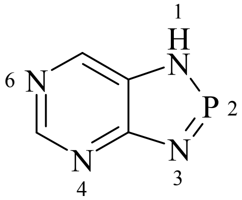
4-imino-3,4-dihydroquinazolin-2(1*H*)-one (PIN)

CH_3-C(=NNH_2)-NH_2

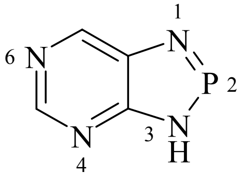
acetohydrazonamide (PIN)

CH_3-C(=NH)-$NHNH_2$

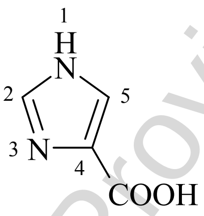
acetimidohydrazide (PIN)



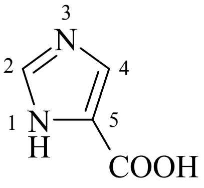
1*H*-1,3,2-diazaphospholo[4,5-*d*]pyrimidine (PIN)



3*H*-1,3,2-diazaphospholo[4,5-*d*]pyrimidine (PIN)



1*H*-imidazole-4-carboxylic acid (PIN)



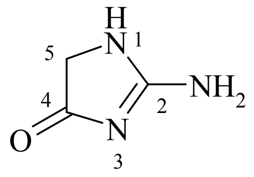
1*H*-imidazole-5-carboxylic acid (PIN)

C_6H_5-NH-N=N-CH_2-COOH

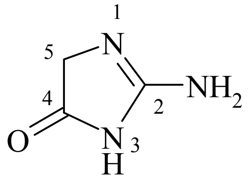
(3-phenyltriaz-1-en-1-yl)acetic acid (PIN)

C_6H_5-N=N-NH-CH_2-COOH

(3-phenyltriaz-2-en-1-yl)acetic acid (PIN)

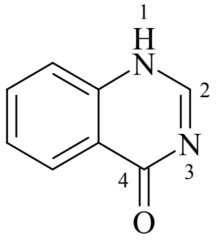


2-amino-1,5-dihydro-4*H*-imidazol-4-one (PIN)

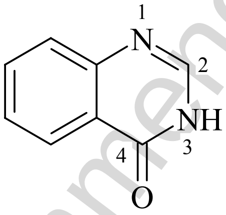


2-amino-3,5-dihydro-4*H*-imidazol-4-one (PIN)

:



quinazolin-4(1*H*)-one (PIN)



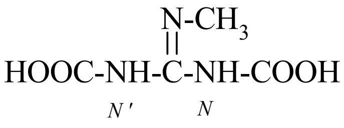
quinazolin-4(3*H*)-one (PIN)

$C_6H_5\text{-}C(=\overset{N'}{N}\text{-}CH_3)\text{-}\overset{N}{N}H\text{-}CH_2\text{-}CH_3$

N-ethyl-*N*′-methylbenzenecarboximidamide (PIN)

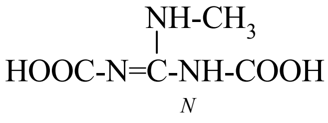
$C_6H_5\text{-}C(=\overset{N'}{N}\text{-}CH_2\text{-}CH_3)\text{-}\overset{N}{N}H\text{-}CH_3$

N′-ethyl-*N*-methylbenzenecarboximidamide (PIN)



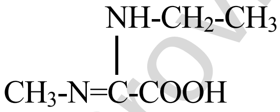
$HOOC\text{-}\underset{N'}{NH}\text{-}\overset{\overset{N\text{-}CH_3}{\|}}{C}\text{-}\underset{N}{NH}\text{-}COOH$

N,*N*′-(methylcarbonimidoyl)di-
(carbamic acid) (PIN)



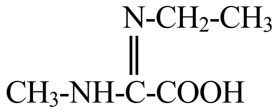
$HOOC\text{-}N{=}\overset{\overset{NH\text{-}CH_3}{|}}{C}\text{-}\underset{N}{NH}\text{-}COOH$

[*N*′-carboxy-*N*-methylcarbamimidoyl]-
carbamic acid (PIN)



$CH_3\text{-}N{=}\overset{\overset{NH\text{-}CH_2\text{-}CH_3}{|}}{C}\text{-}COOH$

(ethylamino)(methylimino)acetic acid (PIN)



$CH_3\text{-}NH\text{-}\overset{\overset{N\text{-}CH_2\text{-}CH_3}{\|}}{C}\text{-}COOH$

(ethylimino)(methylamino)acetic acid (PIN)

P-58 Name construction

P-58.0 Introduction

This Section describes the procedure for the systematic formation of a preferred IUPAC name for an organic compound. This procedure can also be followed for generation of names for general nomenclature.

P-58.1 General methodology

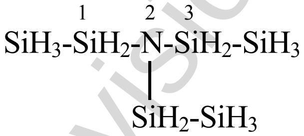
The procedure for formation of a preferred systematic name for an organic compound involves a number of steps outlined in this and in the following subsections, to be taken as far as they are applicable in the following order.

P-58.1.1 From the nature of the compound, determine the type(s) of nomenclature (see P-15) and operations (see P-13) to be used. Although the so-called 'substitutive nomenclature' is the preferred type of nomenclature, other nomenclature types must be used when specified by strict rules, for instance 'skeletal replacement ('a') nomenclature, and 'functional class nomenclature' for compounds such as esters, and acid halides.

P-58.1.2 Determine the class to which the compound belongs and the characteristic group to be cited as the suffix (if any) in accord with the seniority order of classes as indicated in P-41 or as a functional class name (see P-15.2). Only one kind of characteristic group (known as the principal group) can be cited as suffix or functional class name. All atoms or groups not so cited must be specified as substituent prefixes. Radicals and ions are named using suffixes that have the unique property of being cumulative, both among themselves and in conjunction with certain suffixes that express characteristic groups.

P-58.1.3 Determine the senior parent hydride, including any appropriate nondetachable prefixes as described in Chapter 2 and in P-52 for preferred names, or functional parent compound as described in P-34 and P-55 for preferred names.

Example:



$$\begin{array}{c}\mathrm{SiH_3{-}\overset{1}{Si}H_2{-}\overset{2}{N}{-}\overset{3}{Si}H_2{-}SiH_3}\\ |\\ \mathrm{SiH_2{-}SiH_3}\end{array}$$

2-disilanyl-1,3-bis(silyl)disilazane (preselected name)
[disilazane is a parent hydride, not a functional parent compound (see P-21.2.3.1) and since N containing parent hydrides > Si containing parent hydrides, disilazane must be chosen over disilane]

P-58.1.4 Name the parent hydride and the principal characteristic group, if any, or the functional parent compound, using rules indicated in P-58 in order to take functional modifications into consideration.

P-58.1.5 Determine affixes and/or prefixes, in accordance with P-15.5 and Appendix 2, and appropriate multiplying prefixes (see P-14.2) and number the parent structure as far as possible using the general rule P-14.4.

P-58.1.6 Name the detachable substitutive prefixes in accordance with P-56 and P-57 for preferred prefixes and complete the numbering of the structure, if necessary.

P-58.1.7 Assemble the components into a complete name, using alphanumerical order described in P-14.4 and P-14.5 for all substitutive detachable prefixes.

P-58.1.8 Complete the name with all required descriptors for indicating changes from standard valences, isotopic modifications, and stereochemical features.

P-58.2 Suffixes and prefixes

In substitutive nomenclature, some characteristic groups can be denoted either as suffixes or prefixes (see P-33 and P-36), but others only as prefixes (see Table 5.2). Functional class names differ in that a separate word (or a suffix in some languages) designating the name of a functional class is associated with a substituent group name describing the reminder of the structure.

Characteristic groups that can be cited as suffixes in substitutive nomenclature are not necessarily identical with groups designated by the name of a corresponding functional class when functional class names are formed (e.g., butanone and ethyl methyl ketone, where 'one' denotes =O and 'ketone' denotes –CO–).

The characteristic groups listed in Table 5.2 are always cited as prefixes to the name of the parent structure described in Chapter 2. Multiplying prefixes (see P-14.2) and locants are added as necessary (see P-14.3)

.

Table 5.2 Characteristic groups always cited as prefixes in substitutive nomenclature

Characteristic group	Prefix	Characteristic group	Prefix
–Br	bromo	$=N_2$	diazo
–Cl	chloro	$-N_3$	azido
–ClO	chlorosyl	–NO	nitroso
$-ClO_2$	chloryl	$-NO_2$	nitro
$-ClO_3$	perchloryl-	–PO	phosphoroso
–F	fluoro	$-PO_2$	phospho
–I	iodo	–NCO	isocyanato
–IO	iodosyl	–NC	isocyano
$-IO_2$	iodyl	–OR	(R)-oxy

* R designates an 'organic' substituent group.

Examples:

$Cl\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}Cl$

1,3-dichloropropane (PIN)

$C_6H_5\text{-}NO$

nitrosobenzene (PIN)

Characteristic groups other than those listed in Table 5.2 may be cited as either suffixes or prefixes to the name of the parent hydride.

If characteristic groups other than those given in Table 5.2 are present, one (and only one) kind must be cited as suffix (the principal characteristic group) for classes other than radicals and ions.

When a compound contains more than one kind of characteristic group not given in Table 5.2, the principal characteristic group is the one that characterizes the class occurring earliest (i.e., nearest to the top) in the seniority order of classes (see P-41.2, and P-42 and P-43, if necessary). All other characteristic groups are cited as prefixes.

If, and only if, the complete suffix (that is, the suffix plus its multiplying prefixes, if any, as described in Appendix 1) begins with a vowel, a terminal letter ‘e’ (if any) of the preceding parent hydride name is elided. Elision or retention of the terminal letter ‘e’ is independent of the presence of numerals between it and the following letter.

When a substituent is itself substituted (compound substituent, see P-35, P-36, and P-46), all the subsidiary substituents are named as prefixes. The substituent bearing the subsidiary substituent is regarded as a parent substituent (analogous to a parent hydride). The nomenclature of the whole substituent is subject to all the procedures adopted for compounds, with two exceptions, which are:

(a) that no characteristic group is expressed as a suffix (instead, a suffix such as ‘yl’, ‘ylidene’, etc., is used); and

(b) that the point of attachment of the substituent has the lowest permissible locant.

When the parent hydride (principal chain, ring system), principal group and substituents have been selected and named, the numbering of the complete compound is allocated using the rule of lowest locants. General rules for locants and numbering are described in P-14.4. They do apply each and every time a name is constructed, not only for substitutive and functional class nomenclature, but for all types of nomenclature.

The list of seniority of structural features that receive lowest possible locants has been refined by reallocating the placement of ‘a’ prefixes for skeletal replacement in chains and by giving a special status of detachable prefix to hydro/dehydro prefixes.

Insofar as the preceding rules leave a choice, the starting point and direction of numbering of a compound are chosen so as to give lowest locants to the structural features (if present) considered successively in the order given until a decision is reached.

(a) fixed numbering, as for naphthalene, bicyclo[2.2.2]octane, etc.

(b) heteroatoms in heterocycles and in acyclic parent structures

(c) indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with structural feature (d)].

(d) principal group named as suffix

(e) added hydrogen (consistent with the structure of the compound and in accordance with further substitution)

(f) saturation (‘hydro’/‘dehydro’ prefixes) or unsaturation (‘ene’/‘yne’ endings)

(g) substituents named as prefixes (low locants are allocated for substituents regardless of kind; then, if necessary, in the order of citation in the name).

The various components having been selected, named and numbered, any necessary additive or subtractive modifications are made, and the complete name is assembled, prefixes being arranged in alphanumerical order. Notifications for changes in standard valences, isotopic modifiers and stereodescriptors are added, as required.

P-58.3 Examples illustrating the methodology described above

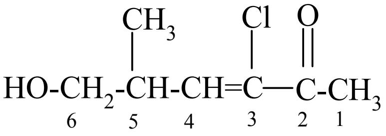
P-58.3.1 Selection of parent compounds
P-58.3.2 Seniority of heteroatoms over suffixes
P-58.3.3 Seniority of suffixes over unsaturation
P-58.3.4 Seniority of hydro/dehydro prefixes over detachable substituent prefixes
P-58.3.5 Treatment of detachable prefixes

P-58.3.1 Selection of parent compounds

After the principal group has been chosen and named, the parent compound is chosen by one of the following methods. For details of numbering, see Chapter 2 describing the numbering of the various parent hydrides and the general rule of lowest locants as formulated in P-14.3. For the arrangement of prefixes, see the general rule on alphanumerical order described in P-14.5.

P-58.3.1.1 If the compound is purely acyclic, the principal chain is chosen as parent by the method described in P-44.

Example:



$$HO\text{-}\underset{6}{CH_2}\text{-}\underset{5}{\overset{\overset{CH_3}{|}}{C}H}\text{-}\underset{4}{CH}{=}\underset{3}{\overset{\overset{Cl}{|}}{C}}\text{—}\underset{2}{\overset{\overset{O}{\|}}{C}}\text{-}\underset{1}{CH_3}$$

Analysis:

Principal group:	=CO	one
Principal chain:	CH_3-CH_2-CH_2-CH_2-CH_2-CH_3	hexane
Principal chain including principal group	CH_3-CH_2-CH_2-CH_2-CO-CH_3	hexan-2-one
Subtractive modification	CH_2-CH_2-CH=CH-CO-CH_3	hex-3-en-2-one
Prefixes:	Cl–	chloro
	HO–	hydroxy
	CH_3–	methyl

Together with other rules, this analysis leads to the name:

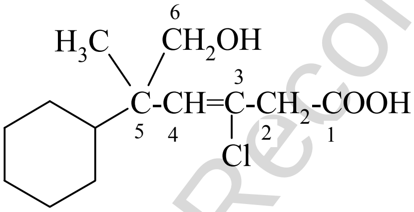
3-chloro-6-hydroxy-5-methylhex-3-en-2-one (PIN)

Guide to construction of this name.

> The suffix 'one' receives the lowest possible locant, 2, thus determining the direction of numbering of the chain. Two hexane chains are possible; the principal chain, in accord with the criteria for selecting the principal chain, is the one that is most substituted (3 substituents compared to 2). Unsaturation is denoted by the ending 'ene'. The three prefixes are arranged in alphanumerical order to complete the name.

P-58.3.1.2 If the principal group occurs only in a chain that carries a cyclic substituent, the compound is named as an acyclic compound into which the cyclic component is expressed by a substituent prefix.

Example:



Analysis:

Principal group:	–(C)OOH	oic acid
Principal chain:	CH_3-CH_2-CH_2-CH_2-CH_2-CH_3	hexane
Principal chain including principal group	CH_3-CH_2-CH_2-CH_2-CH_2-COOH	hexanoic acid
Subtractive modification	CH_3-CH_2-CH=CH_2-CH_2-COOH	hex-3-enoic acid
Prefixes:	Cl–	chloro
	C_6H_{11}–	cyclohexyl
	HO–	hydroxy
	CH_3–	methyl

Together with other rules, this analysis leads to the name:

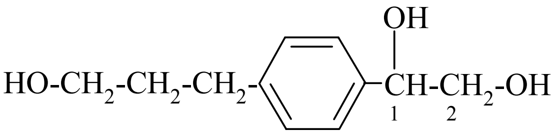
3-chloro-5-cyclohexyl-6-hydroxy-5-methylhex-3-enoic acid (PIN)

Guide to the construction of this name.

> The presence of a carboxylic acid group at the end of the chain determines the direction of numbering of that chain. The 'ene' ending and the prefixes, in alphanumerical order, are located on the chain in accord with the determined numbering.

P-58.3.1.3 If the principal group occurs in two or more carbon chains that are not attached to one another (that is, do not together form a continuous or branched chain but are separated by, for instance, a ring or a heteroatom), and when multiplicative nomenclature is not possible, then that chain carrying the largest number of the principal groups is chosen as parent for nomenclature; if the numbers of these groups in two or more chains are the same, choice is made by the principles for selection of the principal chain.

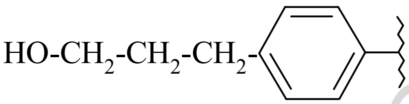
Example 1:



Analysis:

Principal group:	–OH	ol
Principal chain, carrying two OH groups:	HO-CH$_2$-CH$_2$-OH	ethanediol

Prefix:



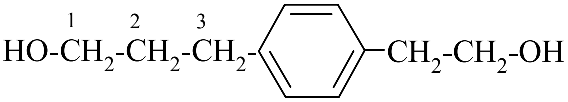
Prefix components:	–OH	hydroxy
	–CH$_2$-CH$_2$-CH$_3$	propyl
	–C$_6$H$_5$	phenyl

Prefix name: 4-(3-hydroxypropyl)phenyl

Together with other rules, this analysis leads to the name:

1-[4-(3-hydroxypropyl)phenyl]ethane-1,2-diol (PIN)

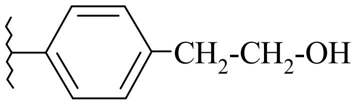
Example 2: In the following example, the longest chain is chosen as parent hydride, in accord with the criteria for selecting the principal chain. This compound can also be named by conjunctive nomenclature (see P-13.5)



Analysis:

Principal group:	–OH	ol
Parent hydride:	CH$_3$-CH$_2$-CH$_3$	propane
Parent hydride + principal group	CH$_3$-CH$_2$-CH$_2$-OH	propan-1-ol

Prefix:



Prefix components:	$-OH$	hydroxy
	$-CH_2\text{-}CH_3$	ethyl
	$-C_6H_5$	phenyl

Prefix name: 4-(2-hydroxyethyl)phenyl

Together with other rules, this analysis leads to the substitutive name:

3-[4-(2-hydroxyethyl)phenyl]propan-1-ol (PIN)

Example 3: A multiplicative name is formed when identical parent structures are attached symmetrically to a central component (the parent structures may be unsymmetrically substituted). The numbering of the multiplied unit (including the characteristic group) is retained. This compound can also be named by conjunctive nomenclature; this procedure is illustrated in P-46.3.1.7.

Analysis:

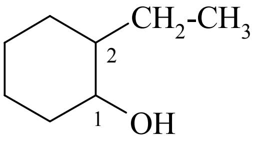
Principal group:	$-OH$	ol
Parent hydride:	$CH_3\text{-}CH_2\text{-}CH_3$	propane
Parent hydride + principal group	$\overset{3}{CH_3}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CH_2}\text{-}OH$	propanol
Multiplicative connecting group:	$-C_6H_4-$	1,4-phenylene

This, together with other rules, leads to the name:

3,3′-(1,4-phenylene)di(propan-1-ol) (PIN)

P-58.3.1.4 If the principal group occurs only in one cyclic system, that cyclic system forms the parent for nomenclature.

Example:



Analysis:

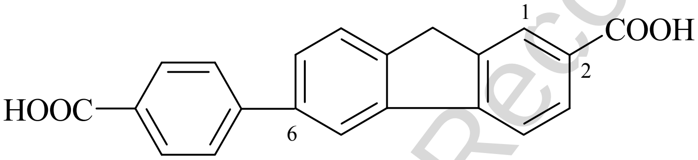
Principal group:	–OH	ol
Parent hydride:	C_6H_{12}	cyclohexane
Prefix:	$–CH_2\text{-}CH_3$	ethyl

Together with other rules, this analysis leads to the name:

2-ethylcyclohexan-1-ol (PIN)

P-58.3.1.5 If the principal group occurs in more than one cyclic system, the system chosen as parent for nomenclature is in accordance with the criteria for choosing a senior ring or ring system.

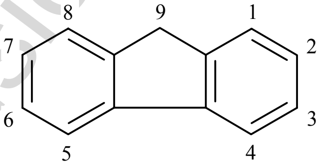
Example:

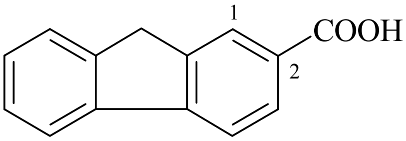


Analysis:

Principal group:	–COOH	carboxylic acid

Senior ring system for parent: fluorene





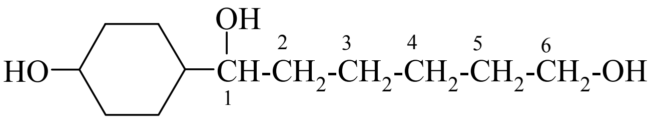
Name of parent including principal group:		fluorene-2-carboxylic acid
Prefixes	$-C_6H_5$	phenyl
	−COOH	carboxy

Together with other rules, this analysis leads to the name:

6-(4-carboxyphenyl)fluorene-2-carboxylic acid (PIN)

P-58.3.1.6 If the principal group occurs both in a chain and in a cyclic system, the parent for nomenclature is that portion in which the principal group occurs in the greater number; if the number of occurrences of the principal group is the same in two or more portions, the ring or ring system is chosen as parent for nomenclature.

Example 1:



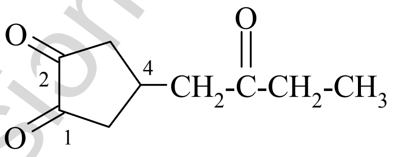
Analysis:

Principal group:	$-OH$	ol
Component with the greater number of the principal group:	$HO-CH_2-CH_2-CH_2-CH_2-CH_2-CH_2-OH$	
Name of parent including suffix:		hexane-1,6-diol
Prefixes:	$-C_6H_{11}$	cyclohexyl
	$-OH$	hydroxy

Together with other rules this analysis leads to the name:

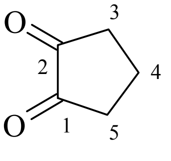
1-(4-hydroxycyclohexyl)hexane-1,6-diol (PIN)

Example 2:



Analysis:

Principal group:	=O	one
Component with the greater number of the principal group:		



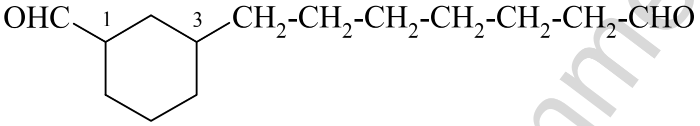
Name of parent including suffix:		cyclopentane-1,2-dione
Prefixes:	=O	oxo
	$CH_3-CH_2-CH_2-CH_2-$	butyl

Together with other rules, this analysis leads to the name:

4-(2-oxobutyl)cyclopentane-1,2-dione (PIN)

P-58.3.1.7 If the number of occurrences of the principal group is the same in two or more nomenclaturally significant parts of the compound, preferred IUPAC names are formed by choosing the ring or ring system as parent for nomenclature. In general nomenclature, a ring or ring system or a chain may be chosen as parent, depending on the importance given to a specific portion (Rule P-44.1.2.2). When the principal group identified by this suffix is not attached directly to a ring or ring system, a principal chain must be chosen.

Example:



Analysis:

Principal group:	–CHO	carbaldehyde or al
Parent:	ring	cyclohexane
	chain	heptane
Parent including suffix:	ring	cyclohexane-1-carbaldehyde
	chain	heptanal
Prefixes:	$-CH_2[CH_2]_5$-CHO	7-oxoheptyl
	$-C_6H_4$-CHO(3)	3-formylcyclohexyl

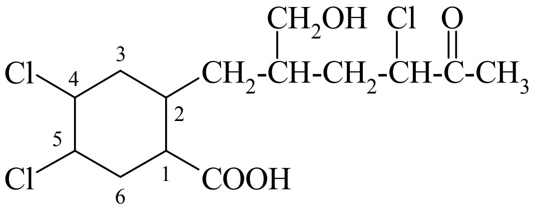
Together with other rules, this analysis leads to the names:

3-(7-oxoheptyl)cyclohexane-1-carbaldehyde (PIN)

7-(3-formylcyclohexyl)heptanal

P-58.3.1.8 When a substituent is itself substituted, all the subsidiary substituents are named as prefixes. The substituent bearing the subsidiary substituents is regarded as a ‘parent substituent’ (analogous to a parent compound). The nomenclature of the whole substituent is subject to all the procedures adopted for compounds (for instance, choice of principal chain), with two exceptions, namely: (a) that no suffix is used, and (b) that the point of attachment of the substituent bears the lowest permissible locant number depending on the nomenclature of the substituent group, alkyl or alkanyl.

Example:



Analysis:

Principal group:	–COOH	carboxylic acid
Parent:		cyclohexane
Primary substituents to be named as prefixes:	–Cl	chloro
	$-CH_2$-CH-CH_2-CHCl-CO-CH_3	
Parent substituent chain:	$-CH_2$-CH_2-CH_2-CH_2-CH_2-CH_3	hexyl

Secondary prefixes:	–Cl	chloro
	=O	oxo
	$-CH_2$-OH	

Secondary compound prefix name composed of:

$-CH_3$	methyl
–OH	hydroxy

Name of secondary compound prefix: hydroxymethyl

Name of substituted primary prefix: 4-chloro-2-(hydroxymethyl)-5-oxohexyl

Together with other rules, this analysis leads to the name:

4,5-dichloro-2-[4-chloro-2-(hydroxymethyl)-5-oxohexyl]cyclohexane-1-carboxylic acid (PIN)

P-58.3.2 Seniority of heteroatoms over suffixes

Heterocyclic compounds and chains modified by skeletal replacement (‘a’) nomenclature are treated similarly. They are considered as parent compounds with a fixed numbering. As a consequence, heteroatoms have seniority for low locants and suffixes are assigned the next lowest possible locants. For chains, this order is a major change from the 1979 organic nomenclature recommendations in which suffixes had seniority over heteroatoms.

P-58.3.2.1 For chains the replacement operation is applied to the hydrocarbon parent to create a new parent hydride with a fixed numbering. Suffixes receive the lowest possible locants in accordance with the resulting numbering.

Example:

$$\overset{1}{\mathrm{CH_3}}\text{-}\mathrm{CH_2}\text{-}\overset{3}{\mathrm{O}}\text{-}\mathrm{CH_2}\text{-}\mathrm{CH_2}\text{-}\overset{6}{\mathrm{O}}\text{-}\mathrm{CH_2}\text{-}\mathrm{CH_2}\text{-}\overset{9}{\mathrm{O}}\text{-}\mathrm{CH_2}\text{-}\mathrm{CH_2}\text{-}\overset{12}{\mathrm{O}}\text{-}\mathrm{CH_2}\text{-}\mathrm{CH_2}\text{-}\overset{15}{\mathrm{COOH}}$$

Principal group:	–(C)OOH	oic acid
Parent hydrocarbon	$CH_3\text{-}[CH_2]_{13}\text{-}CH_3$	pentadecane
‘a’ Prefix	–O–	oxa
Heteroacyclic parent		

$$\overset{1}{\mathrm{CH_3}}\text{-}\mathrm{CH_2}\text{-}\overset{3}{\mathrm{O}}\text{-}\mathrm{CH_2}\text{-}\mathrm{CH_2}\text{-}\overset{6}{\mathrm{O}}\text{-}\mathrm{CH_2}\text{-}\mathrm{CH_2}\text{-}\overset{9}{\mathrm{O}}\text{-}\mathrm{CH_2}\text{-}\mathrm{CH_2}\text{-}\overset{12}{\mathrm{O}}\text{-}\mathrm{CH_2}\text{-}\mathrm{CH_2}\text{-}\overset{15}{\mathrm{CH_3}}$$

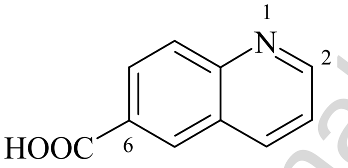
Name of heteroacyclic parent 3,6,9,12-tetraoxapentadecane

Together with other rules, this analysis leads to the name:

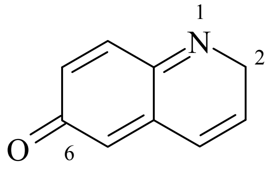
3,6,9,12-tetraoxapentadecan-15-oic acid (PIN)

P-58.3.2.2 Heterocyclic compounds having retained and systematic names are considered as parent compounds. Thus, suffixes are added and assigned lowest possible locants in accordance with the fixed numbering of the heterocyclic ring or ring system. Added hydrogen atoms, if needed, are assigned next lowest possible locants.

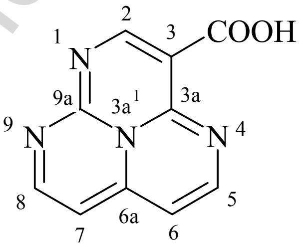
Examples:



quinoline-6-carboxylic acid (PIN)



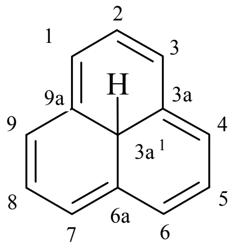
quinolin-6(2*H*)-one (PIN)



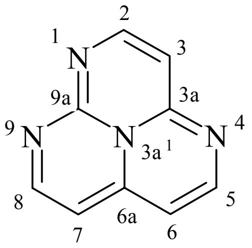
Analysis:

Principal group:	–COOH	carboxylic acid
Parent hydrocarbon:		$3a^1$*H*-phenalene

[Note the new system of numbering for internal atoms in fused systems, $3a^1$ in place of 9b; see P-25.3.3.3.]



Skeletal replacement ('a') prefix: –N< aza



Name of parent heterocycle: 1,3a^1,4,9-tetraazaphenalene

Together with other rules, this analysis leads to the name:

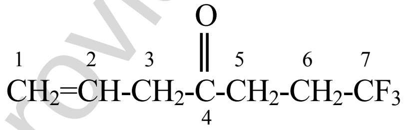
1,3a^1,4,9-tetraazaphenalene-3-carboxylic acid (PIN)

[Note: The indicated hydrogen, 3a^1*H*, of the parent hydrocarbon does not appear in the name of the heterocycle.]

P-58.3.3. Seniority of suffixes over unsaturation

P-58.3.3.1 After suffixes, if there is a choice, low locants are assigned to 'ene' and 'yne' endings, and then to detachable prefixes, if applicable.

Example:



$$\overset{1}{C}H_2{=}\overset{2}{C}H{-}\overset{3}{C}H_2{-}\underset{4}{\overset{\overset{O}{\|}}{C}}{-}\overset{5}{C}H_2{-}\overset{6}{C}H_2{-}\overset{7}{C}F_3$$

Analysis:

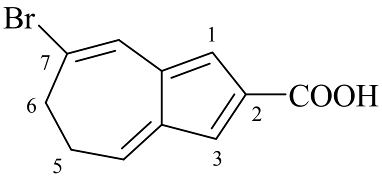
Principal group:	=O	one
Parent hydride:	CH_3-$[CH_2]_5$-CH_3	heptane
Parent hydride + principal group	CH_3-$[CH_2]_2$-CO-$[CH_2]_2$-CH_3	heptan-4-one
Subtractive modification	>C=C<	ene
Substituent prefix	–F	fluoro

Together with other rules, this analysis leads to the name:

7,7,7-trifluorohept-1-en-4-one (PIN)

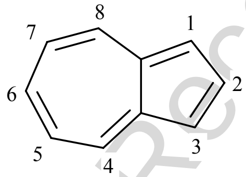
P-58.3.3.2 Hydro and dehydro prefixes are used to express a change in the degree of hydrogenation of the parent hydride. In these recommendations, these prefixes are considered detachable but only in the context of numbering; they are not included among the detachable substituent prefixes. In names, they are cited immediately before the name of the parent compound, after those of detachable substituent prefixes arranged in alphanumerical order.

Example:

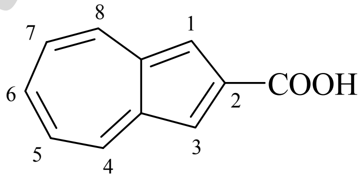


Analysis:

Principal group:	–COOH	carboxylic acid
Parent hydride:		azulene



Parent hydride + principal group:



azulene-2-carboxylic acid

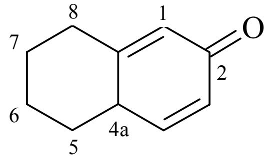
Saturation prefix	–H	hydro
Prefix	–Br	bromo

Together with other rules, this analysis leads to the name:

7-bromo-5,6-dihydroazulene-2-carboxylic acid (PIN)

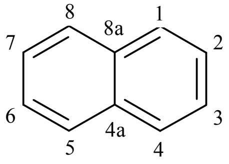
P-58.3.3.3 Mancude ketones, imines and 'ylidene' substituent groups are named by the 'added hydrogen' method. If there is a choice, 'indicated hydrogen' atoms have priority for low locants, then suffixes, 'added hydrogen' atoms and finally hydro prefixes, in that order.

Example 1:

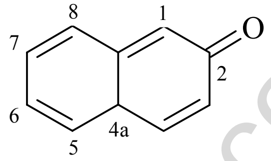


Analysis:

Principal group:	=O	one
Parent hydride:		naphthalene



Parent hydride + principal group:



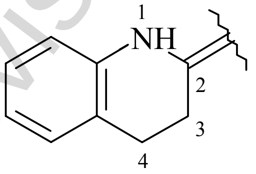
naphthalen-2(4a*H*)-one

Saturation Prefix	–H	hydro

Together with other rules, this analysis leads to the name:

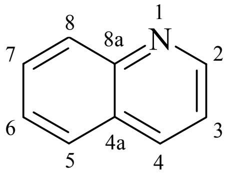
5,6,7,8-tetrahydronaphthalen-2(4a*H*)-one (PIN)

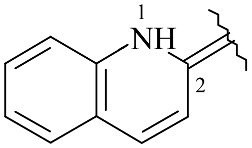
Example 2:



Analysis:

Free valences:	X=	ylidene
Parent hydride:		quinoline





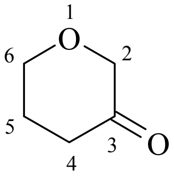
Parent hydride + free valences: uinolin-2(1*H*)-ylidene

Saturation prefix: –H hydro

Together with other rules, this analysis leads to the name:

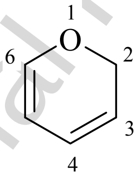
3,4-dihydroquinolin-2(1*H*)-ylidene (PIN)

Example 3:

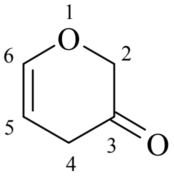


Analysis:

Principal group: =O one
Parent hydride: 2*H*-pyran



Parent hydride + principal group:



2*H*-pyran-3(4*H*)-one

Saturation prefix: –H hydro

Together with other rules, this analysis leads to the name:

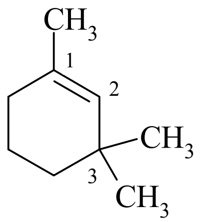
dihydro-2*H*-pyran-3(4*H*)-one (PIN)

(Note: no locants are required when the cyclic system becomes fully saturated using hydro prefixes; see P-14.3.3)

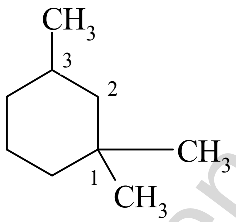
P-58.3.4. Seniority of hydro prefixes over detachable substituent prefixes

If there is a choice, low locants are assigned to 'ene' and 'yne' endings and 'hydro/dehydro' prefixes.

Examples:

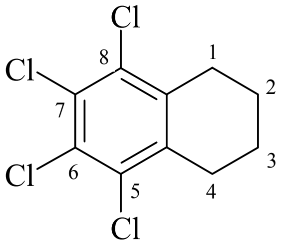


compare with

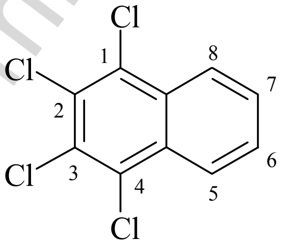


1,3,3-trimethylcyclohex-1-ene (PIN)

1,1,3-trimethylcyclohexane (PIN)



compare with



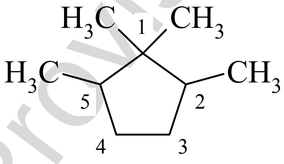
5,6,7,8-tetrachloro-1,2,3,4-tetrahydronaphthalene (PIN)

1,2,3,4-tetrachloronaphthalene (PIN)

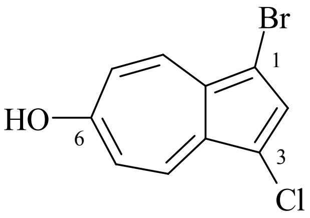
P-58.3.5 Treatment of detachable prefixes

If there is a choice, low locants are assigned to detachable prefixes considered together, and, if there is a further choice, in alphanumerical order.

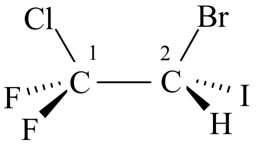
Examples:



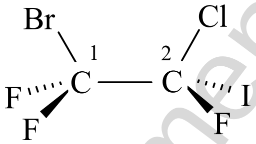
1,1,2,5-tetramethylcyclopentane (PIN)
(not 1,2,2,3-tetramethylcyclopentane; the set of locants 1,1,2,5 is lower than 1,2,2,3)



1-bromo-3-chloroazulen-6-ol (PIN)



2-bromo-1-chloro-1,1-difluoro-
2-iodoethane (PIN)



1-bromo-2-chloro-1,1,2-trifluoro-
2-iodoethane (PIN)

CHAPTER 6 APPLICATIONS TO SPECIFIC CLASSES OF COMPOUNDS

P-60 Introduction

P-60.1 The recommendations in this chapter illustrate how the general principles and specific rules set out in the preceding sections are applied to various types of compounds.

Section 61 describes compounds that are named substitutively only by the prefix mode. It includes and exemplifies binary compounds formed by substituting parent hydrides by substituents derived from other parent hydrides and by characteristic groups that are always used as prefixes.

Sections 62 to 66 include compounds that are named, in substitutive nomenclature, by suffixes and prefixes, and by means of other types of nomenclature. The traditional classes from acids to imines are described (see P-41).

Section 67 describes nomenclature of organic derivatives of noncarbon acids and their functional replacement analogs.

Section P-68 covers the nomenclature of organic compounds of the Groups 13, 14, 15, 16, and 17 elements not included in Sections 62-67.

Section 69 describes the nomenclature of organometallic compounds.

P-60.2 Presentation of names.

Names described in this Chapter are presented in a systematic way. General methods recommended to generate IUPAC preferred names are all described in a simplified way with reference to the following full descriptions.

(a) Names formed substitutively using suffixes follow the general method described in Section 15.1. Substitutive names are formed by adding a suffix such as ‘al’, ‘ol’, ‘yl’, ‘carbaldehyde’, ‘carboxylic acid’, etc., to the name of a parent hydride, with elision of the final letter ‘e’ of the parent hydride, if any, before ‘a’, ‘i’, ‘o’, ‘u’, and ‘y’.

(b) Names formed substitutively by using prefixes follow the general method. Substitutive names are formed by adding a prefix such as amino, hydroxy, etc., to the name of the parent hydride or parent compound; in order to preserve their formal identity, there is no elision of the last letter of these prefixes

(c) Names formed by functional class nomenclature follow the general method described in Section 15.2. Functional class names are formed by citing the name of the class, such as alcohol, oxide, ketone, etc., preceded by the name of the substituent groups cited in alphabetical order and separated by a space, if required.

(d) Names formed by skeletal replacement (‘a’) nomenclature follow the methodology described in Section 15.4.

(e) Functional parents are discussed in terms of preferred names and names that can be used in general nomenclature.

The method to generate preferred IUPAC names is indicated by a phrase such as ‘This method generates preferred IUPAC names’ or ‘Method (1) leads to preferred IUPAC names. The abbreviation ‘PIN’ is placed after preferred IUPAC names. Names that were recommended in the past but are not included in these recommendations are described parenthetically by the phrase ‘no longer recommended’. For example, the prefix ‘methylene’ is ‘no longer recommended’ in IUPAC nomenclature to designate the $=CH_2$ group.

Names preceded by ‘not’ are names that are not constructed in accordance with the rule described in this section. Thus, they are ‘incorrect’ names.’ As they are not alternatives to preferred IUPAC names, they must not be used. For example, the name ‘ethanolamine’, which is still widely used, is badly constructed because of the presence of two suffixes; it is not an alternative to the preferred IUPAC name, ‘2-aminoethanol’.

P-61 Substitutive nomenclature: prefix mode

P-61.0 Introduction

This subsection describes the names of compounds formed by substitutive nomenclature that includes only prefixes denoting substituent groups and/or characteristic groups. These prefixes are detachable and cited in a name in alphabetical order.

Hydrocarbyl groups and their corresponding polyvalent groups (substituent groups derived from hydrocarbon parent hydrides) are included in this subsection because they occupy the penultimate rank in the seniority order of classes (see P-41) and thus are treated as prefixes in presence of a higher class. A similar situation prevails for halogen compounds in their standard bonding number, which are last in the order of seniority of classes.

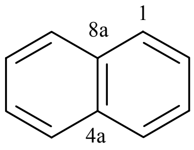
Nitro and nitroso compounds, azides, isocyanates, isocyanides, and fulminates/isofulminates are also included in this Section. Ethers, peroxides, and acetals are not considered in this Section, but are treated at length in association with hydroxy compounds and aldehydes (see P-63.2, P-63.5 and P-66.6.5, respectively).

The characteristic groups described here (see Table 4.6) are referred to as 'characteristic groups denoted, in substitutive nomenclature, only as prefixes' (see R-4.1, ref. 2). This statement must not be interpreted as a must for always using these characteristic groups as prefixes. Substitutive nomenclature is based on a seniority system based on classes. The senior class must be determined first (see for example, P-62.4).

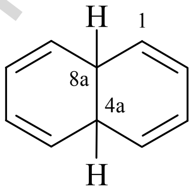
P-61.1 General methodology

Substitutive nomenclature is based on the substitutive operation involving the exchange of one or more hydrogen atoms of a parent hydride or parent compound for another atom or group. This process is expressed by either a prefix or suffix denoting the atom or group being introduced. Substitution is not possible when no hydrogen atoms are present. However, if hydrogen atoms are added to a structure by an additive operation (to a double bond, for example), substitution then becomes possible. The formal addition of hydrogen atoms must precede the substitution operation when atoms or groups denoted by prefixes are involved; thus, they are cited after the alphabetized prefixes.

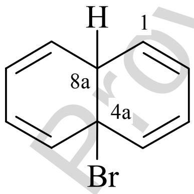
Examples:



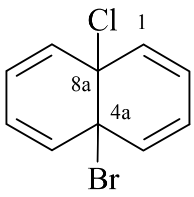
naphthalene (PIN)



4a,8a-dihydronapththalene (PIN)



4a-bromo-4a,8a-dihydronaphthalene (PIN)



4a-bromo-8a-chloro-4a,8a-dihydronaphthalene (PIN)

The seniority order of parent structures, the principal chain, and the senior ring system are chosen in accordance with Rule P-44.

When there is a choice for numbering, the general rule described in P-14.4 is applied. The starting point and the direction of numbering of a compound are chosen so as to give lowest locants to the following structural features (if present) considered successively in the order given until a decision is reached.

(a) fixed numbering, as for naphthalene, bicyclo[2.2.2]octane, etc.

(b) heteroatoms in heterocycles and in acyclic parent structures

(c) indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with structural feature (d)].

(d) principal group named as suffix

(e) added hydrogen (consistent with the structure of the compound and in accordance with further substitution)

(f) saturation (‘hydro’/‘dehydro’ prefixes) or unsaturation (‘ene’/‘yne’ endings)

(g) substituents named as prefixes (low locants are allocated for substituents regardless of kind; then, if necessary, in the order of citation in the name).

P-61.2 Hydrocarbyl groups and corresponding di- and polyvalent groups

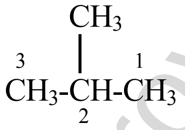
Only substituted hydrocarbons are discussed here. For substitution on other parent hydrides see P-68.1 for Group 13, P-68.2 for Group 14, P-68.3 for Group 15, and P-68.4 for Group 16.

Substituted hydrocarbons for which a parent hydride name is not available (see Chapter 2) have a name that consists of a parent hydride name and appropriate substitutive prefixes derived from other parent hydrides.

P-61.2.1 Aliphatic hydrocarbons

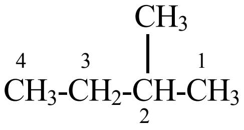
Names of substituted acyclic hydrocarbons are formed substitutively by selecting the principal chain in accordance with rule P-44. This rule has been modified from previous rules; seniority is now given to the length of the chain rather than to unsaturation. The name ‘isoprene’ is retained, but no substitution is allowed. (see P-55.1)

Examples:



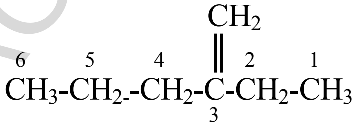
$$\overset{3}{C}H_3\text{-}\overset{\overset{CH_3}{|}}{\underset{2}{C}}H\text{-}\overset{1}{C}H_3$$

2-methylpropane (PIN)
isobutane (no longer recommended)



$$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{\overset{CH_3}{|}}{\underset{2}{C}}H\text{-}\overset{1}{C}H_3$$

2-methylbutane (PIN)
isopentane (no longer recommended)



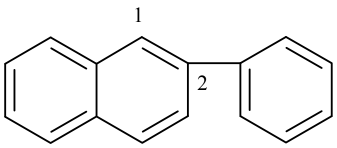
$$\overset{6}{C}H_3\text{-}\overset{5}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{\overset{CH_2}{\|}}{\underset{3}{C}}\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_3$$

3-methylidenehexane (PIN)
2-ethylpent-1-ene (the longest chain now supersedes a shorter unsaturated chain; see P-44.3)

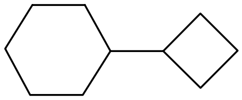
P-61.2.2 Cyclic hydrocarbons

Names of rings or cyclic systems substituted by rings or ring systems are formed in accordance with the seniority order of rings and ring systems (see P-44.2).

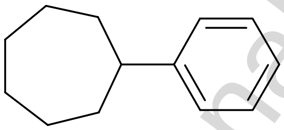
Examples:



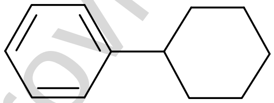
2-phenylnaphthalene (PIN)
(naphthalene, having two rings, is senior to benzene, which has only one ring; see P-44.2.1)



cyclobutylcyclohexane (PIN)
(cyclohexane has more ring atoms than cyclobutane; see P-44.2.1)



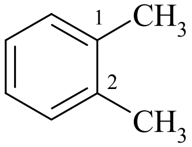
phenylcycloheptane (PIN)
(cycloheptane has more ring atoms than benzene; see P-44.2.1)



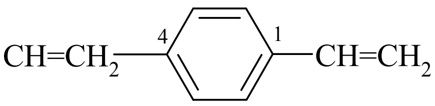
cyclohexylbenzene (PIN)
(benzene has more multiple bonds; see P-44.2.3)

P-61.2.3 Names of cyclic hydrocarbons substituted by chains are formed by substituting chains, saturated or unsaturated, into rings (see P-44.1.2.2). This rule must be strictly applied in the context of preferred IUPAC names. The name ‘toluene’ is retained with no substitution allowed for preferred IUPAC names, but substitution is allowed on both the ring and side chain with certain restrictions (see P-46.3.1) for general nomenclature; the names ‘xylene, ‘mesitylene’ and ‘styrene’ are retained, but no substitution is allowed even for general nomenclature (see P-22.1.3).

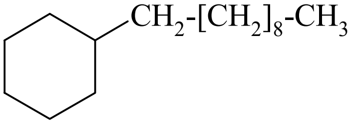
Examples:



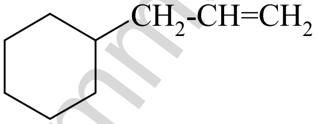
o-xylene (PIN)
1,2-dimethylbenzene
(not *o*-methyltoluene, substitution of toluene by additional methyl groups not allowed; see P-46.3.1.2)



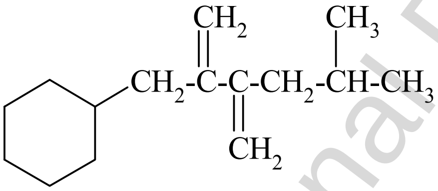
1,4-diethenylbenzene (PIN)
p-divinylbenzene
(not *p*-vinylstyrene; substitution of styrene not allowed: see P-22.1.3)



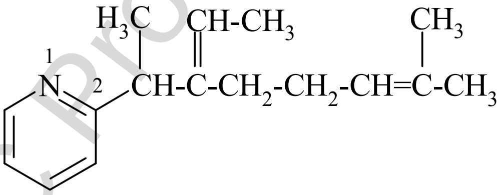
decylcyclohexane (PIN)
(ring preferred to chain, see P-58.3.1.6)
1-cyclohexyldecane



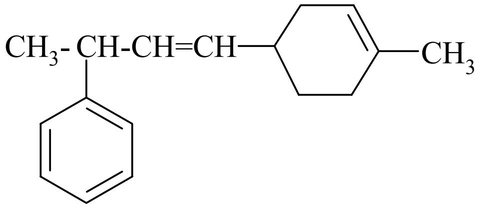
prop-2-en-1-ylcyclohexane (PIN)
(ring preferred to chain, see P-58.3.1.6)
allylcyclohexane



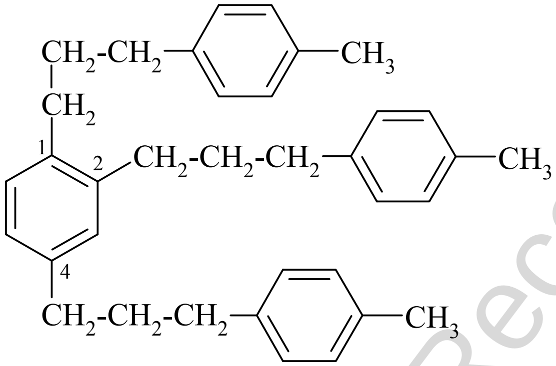
(5-methyl-2,3-dimethylidenehexyl)cyclohexane (PIN);
(the longest chain is preferred to the shorter unsaturated chain, see P-44.3)
[2-methylidene-3-(2-methylpropyl)but-3-en-1-yl]cyclohexane



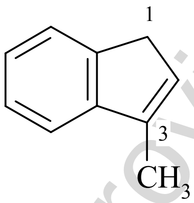
2-(3-ethylidene-7-methyloct-6-en-2-yl)pyridine (PIN)
(preferred parent substituent prefix, see P-45.1)
2-(2-ethylidene-1,6-dimethylhept-5-en-1-yl)pyridine



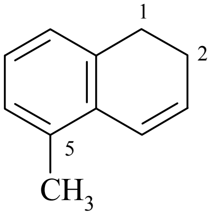
[4-(4-methylcyclohex-3-en-1-yl)but-3-en-2-yl]benzene (PIN; see P-56.1.1)
[1-methyl-3-(4-methylcyclohex-3-en-1-yl)allyl]benzene



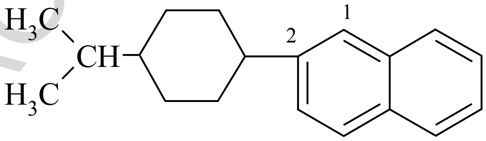
1,1′,1″-(benzene-1,2,4-triyltripropane-1,3-diyl)tris(4-methylbenzene) (PIN)
(multiplicative name, see P-51.2)
1,2,4-tris[3-(4-methylphenyl)propyl]benzene
1,2,4-tris(3-*p*-tolylpropyl)benzene



3-methyl-1*H*-indene (PIN)



5-methyl-1,2-dihydronaphthalene (PIN)



2-[4-(propan-2-yl)cyclohexyl]naphthalene (PIN)
2-(4-isopropylcyclohexyl)naphthalene

P-61.3 Halogen compounds

Halogen compounds are always expressed by prefixes in substitutive nomenclature or, as the principal characteristic group, expressed as a separate word in functional class nomenclature.

P-61.3.1 Halogen compounds are named in two ways:

(1) by substitutive nomenclature, using the prefixes ‘bromo’, ‘chloro’, ‘fluoro’, and ‘iodo’ and appropriate multiplicative prefixes, as required; or

(2) by functional class nomenclature, in which names are formed by citing the name of the organic ‘groups’ followed by the class name ‘fluoride’, ‘chloride’, ‘bromide’, and ‘iodide’, as a separate word, preceded, if necessary, by a multiplicative prefix. Functional class names usually are used to denote simple structures, having one kind of halogen, and are not used to name more complex structures. Additive names, such as stilbene dibromide, are not recommended.

Method (1) leads to preferred IUPAC names.

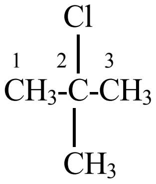
Examples:

CH_3-I

iodomethane (PIN)
methyl iodide

C_6H_5-CH_2-Br

(bromomethyl)benzene (PIN)
(no substitution on toluene)
α-bromotoluene (see P-46.3 for toluene substitution rules)
benzyl bromide



$$\overset{1}{CH_3}\text{-}\overset{2}{C}(Cl)(CH_3)\text{-}\overset{3}{CH_3}$$

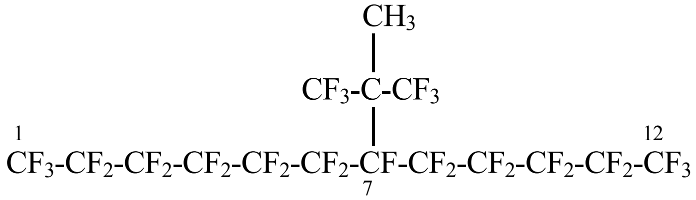
2-chloro-2-methylpropane (PIN)
tert-butyl chloride

$$\text{Br-}\overset{1}{CH_2}\text{-}\overset{2}{CH_2}\text{-Br}$$

1,2-dibromoethane (PIN)
ethylene dibromide

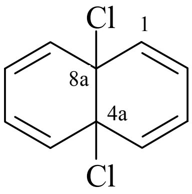
$$C_6H_5\text{-}\overset{1}{C}HBr\text{-}\overset{2}{C}HBr\text{-}C_6H_5$$

1,1′-(1,2-dibromoethane-1,2-diyl)dibenzene ((PIN)
(multiplicative name, see P-51.2)
1,2-dibromo-1,2-diphenylethane (substitutive name)
stilbene dibromide (additive name, not recommended)

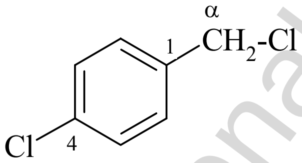


7-(1,1,1,3,3,3-hexafluoro-2-methylpropan-2-yl)-1,1,1,2,2,3,3,4,4,5,5,6,6,7,8,8,9,9,-10,10,11,11,12,12,12-pentacosafluorododecane (PIN)
(preferred substituent prefix; see P-45.1)

7-[1-(trifluoromethyl)-1-methyl-2,2,2-trifluoroethyl]-1,1,1,2,2,3,3,4,4,5,5,6,6,7,8,8,9,9,-10,10,11,11,12,12,12-pentacosafluorododecane

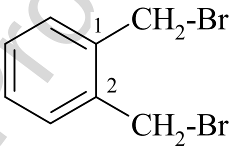


4a,8a-dichloro-4a,8a-dihydronaphthalene (PIN)



1-chloro-4-(chloromethyl)benzene (PIN)
(no substitution on toluene)

α,4-dichlorotoluene (see P-46.3 for toluene substitution rules)



1,2-bis(bromomethyl)benzene (PIN)

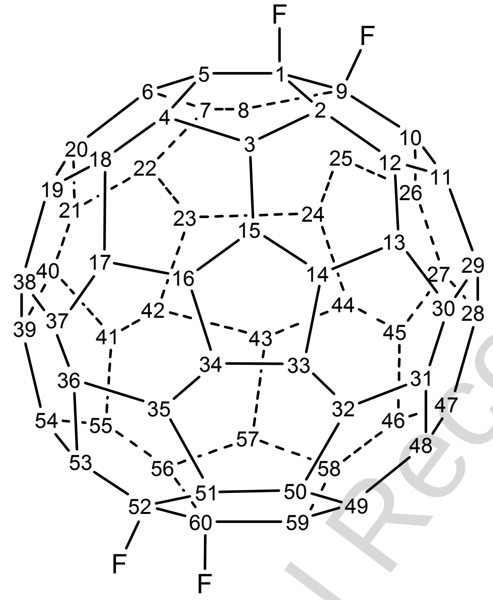
2-(bromomethyl)-α-bromotoluene (see P-46.3 for toluene substitution rules)
[not α,α′-dibromo-*o*-xylene (no substitution on xylene, see P-34.3.1.1)

$\overset{6}{CH_3}\text{-}\overset{5}{CH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CHCl}\text{-}\overset{1}{CH_3}$

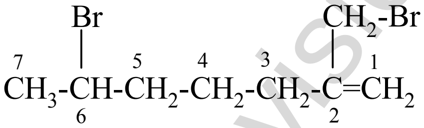
2-chlorohexane (PIN)
hexan-2-yl chloride
1-methylpentyl chloride

$F_2N\text{-}CO\text{-}NF_2$

tetrafluorourea (PIN)
tetrafluorocarbonic diamide

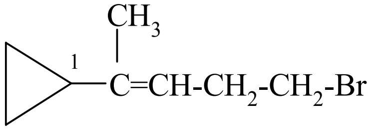


1,9,52,60-tetrafluoro-1,9,52,60-tetrahydro($C_{60}I_h$)[5,6]fullerene (PIN)
($C_{60}I_h$)[5,6]fullerene-1,9,52,60-tetrayl tetrafluoride

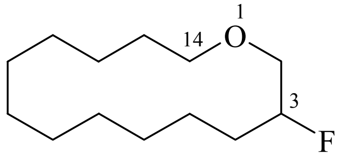


$$\overset{7}{CH_3}\text{-}\underset{6}{\overset{Br}{CH}}\text{-}\overset{5}{CH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{CH_2}\text{-}\underset{2}{\overset{CH_2\text{-}Br}{C}}=\overset{1}{CH_2}$$

6-bromo-2-(bromomethyl)hept-1-ene (PIN)
2-methyleneheptan-1,6-diyl dibromide



1-(5-bromopent-2-en-2-yl)cyclopropane (PIN)
(ring preferred to chain, see P-58.3.1.6;
preferred substituent prefix, see P-45.1)
1-(4-bromo-1-methylbut-1-en-1-yl)cyclopropane
5-bromo-2-cyclopropylpent-2-ene



3-fluoro-1-oxacyclotetradecane (PIN)
1-oxacyclotetradecan-3-yl fluoride

$\overset{1}{C}H_3-\overset{2}{Si}H_2-CH_2-\overset{4}{Si}H_2-CH_2-\overset{6}{Si}H_2-CH_2-\overset{8}{Si}H_2-CH_2-\overset{10}{C}H_2-Cl$

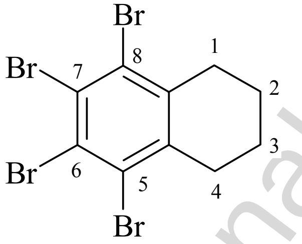
10-chloro-2,4,6,8-tetrasiladecane (PIN)
2,4,6,8-tetrasiladecan-1-yl chloride

$\overset{1}{C}H_2=CH-CH_2-CH_2-\overset{5}{C}H_2-I$

5-iodopent-1-ene (PIN)
pent-4-en-1-yl iodide

$Br-\overset{1}{C}H_2-CH_2-\overset{3}{C}H=CH-CH_2-\overset{6}{C}H_3$

1-bromohex-3-ene (PIN)
hex-3-en-1-yl bromide



5,6,7,8-tetrabromo-1,2,3,4-tetrahydronaphthalene (PIN)
5,6,7,8,-tetrahydronaphthalene-1,2,3,4-tetrayl tetrabromide

$Cl-Si(CH_3)_3$

chlorotrimethylsilane (PIN; silane is a preselected name; see P-12)
trimethylsilyl chloride

Cl_3Si-CH_2I

trichloro(iodomethyl)silane (PIN; silane is a preselected name; see P-12)

$F_2Si=CH_2$

difluoro(methylidene)silane (PIN; silane is a preselected name; see P-12)

P-61.3.2 Compounds containing the groups $-XO$, $-XO_2$ or XO_3 (X = halogen) are expressed by the following prefixes in substitutive nomenclature:

$-XO$	chlorosyl (no longer chloroso), bromosyl, iodosyl, fluorosyl
$-XO_2$	chloryl (no longer chloroxy), bromyl, iodyl, fluoryl
$-XO_3$	perchloryl, perbromyl, periodyl, perfluoryl

Examples:

$C_6H_5\text{-}ClO_3$	$C_6H_5\text{-}IO$
perchlorylbenzene (PIN)	iodosylbenzene (PIN)

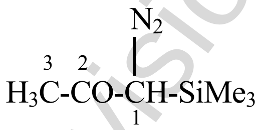
P-61.3.3 Compounds containing the group $-I(OH)_2$ or similar groups are named substitutively by using prefixes based on the preselected parent hydride name λ^3-iodane, as indicated in P-21.1 2.

P-61.4 Diazo compounds

Compounds containing a group $=N_2$ attached to a single carbon atom are named by adding the prefix 'diazo-' to the name of the parent hydride or functional parent hydride.

Examples:

CH_2N_2	$N_2CH\text{-}CO\text{-}O\text{-}C_2H_5$
diazomethane (PIN)	ethyl diazoacetate (PIN)



$\overset{3}{H_3C}\text{-}\overset{2}{C}O\text{-}\underset{1}{\overset{N_2}{C}}H\text{-}SiMe_3$

1-diazo-1-(trimethylsilyl)propan-2-one (PIN)
1-diazo-1-(trimethylsilyl)acetone

P-61.5 Nitro, nitroso and related compounds

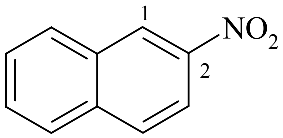
P-61.5.1 Nitro and nitroso compounds

Compounds containing the $-NO_2$ or the $-NO$ group are named by means of the prefixes 'nitro' and 'nitroso', respectively, unless these groups are to be named on the basis of the parent structures nitric and nitrous acids, $NO_2\text{-}OH$ and $NO\text{-}OH$, respectively, or their corresponding esters, anhydrides, amides and hydrazides.

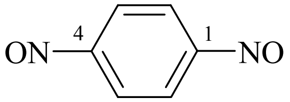
Examples:

$CH_3\text{-}NO_2$

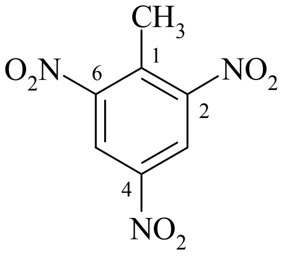
nitromethane (PIN)



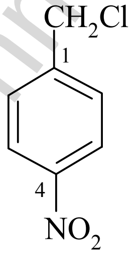
2-nitronaphthalene (PIN)



1,4-dinitrosobenzene (PIN)
p-dinitrosobenzene



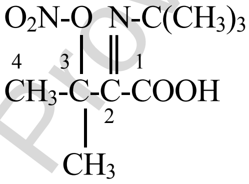
1-methyl-2,4,6-trinitrobenzene (PIN)
2,4,6-trinitrotoluene (see P-46.3 for toluene substitution rules)



1-(chloromethyl)-4-nitrobenzene (PIN)
α-chloro-4-nitrotoluene (see P-46.3 for toluene substitution rules)
4-nitrobenzyl chloride

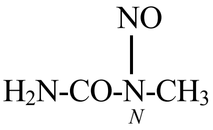
P-61.5.2 In the presence of a characteristic group having seniority to be named as suffix or parent structure, nitro and nitroso groups can be attached to any atom. When linked to another nitrogen atom they are not considered to lengthen the nitrogen chain.

Examples:



$$\begin{array}{l} O_2N\text{-}O\ \ N\text{-}C(CH_3)_3 \\ \quad\ \ \vert\quad \Vert \\ \overset{4}{C}H_3\text{-}\overset{3}{C}\text{-}\overset{1}{\underset{2}{C}}\text{-}COOH \\ \quad\ \ \vert \\ \quad\ CH_3 \end{array}$$

2-(*tert*-butylimino)-3-methyl-3-(nitrooxy)butanoic acid (PIN)



$$\begin{array}{l} \qquad\qquad\ NO \\ \qquad\qquad\ \ \vert \\ H_2N\text{-}CO\text{-}\underset{N}{N}\text{-}CH_3 \end{array}$$

N-methyl-*N*-nitrosourea (PIN)

P-61.5.3 Amides and hydrazides of nitric and nitrous acids

Nitramines are amides of nitric acid (see ref. 17). The class is composed of ‘nitramide’ (a shortened form of nitric amide), $NO_2\text{-}NH_2$, and its derivatives formed by substitution and named as such. Nitrosamines are amides of nitrous acid (see ref. 17); they are named as derivatives of this amide. Nitric acid and nitrous acid are preferred preselected names, see P-12.

> Formerly, nitramines and nitrosamines were named as nitro and nitroso amines. This former method can be used in general nomenclature, but preferred IUPAC names are those of substituted amides, in accordance with the seniority order of classes.

Similarly, nitric hydrazide (I) and nitrous hydrazide (II) are preferred preselected names used as parent structures for generation of preferred IUPAC names.

$O_2N\text{-}\overset{N}{NH}\text{-}\overset{N'}{NH_2}$

(I)

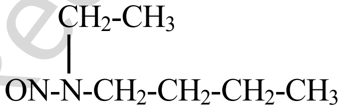
$ON\text{-}\overset{N}{NH}\text{-}\overset{N'}{NH_2}$

(II)

Examples:

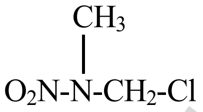
$ON\text{-}N(CH_2\text{-}CH_2\text{-}CH_3)_2$

N,*N*-dipropylnitrous amide (PIN)
N-nitroso-*N*-propylpropan-1-amine



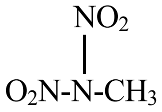
$ON\text{-}\overset{CH_2\text{-}CH_3}{\overset{|}{N}}\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3$

N-butyl-*N*-ethylnitrous amide (PIN)
N-ethyl-*N*-nitrosobutan-1-amine



$O_2N\text{-}\overset{CH_3}{\overset{|}{N}}\text{-}CH_2\text{-}Cl$

N-(chloromethyl)-*N*-methylnitramide (PIN)
1-chloro-*N*-methyl-*N*-nitromethanamine



$O_2N\text{-}\overset{NO_2}{\overset{|}{N}}\text{-}CH_3$

N-methyl-*N*-nitronitramide (PIN)
N,*N*-dinitromethanamine

$ON\text{-}\overset{N}{NH}\text{-}\overset{N'}{N}{=}CH\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3$

N′-hexylidenenitrous hydrazide (PIN)

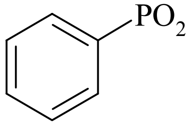
P-61.5.4 *aci*-Nitro compounds

Compounds containing the group $=N(O)OH$ are named as derivatives of azinic acid, $H_2N(O)\text{-}OH$, a preferred preselected name, and by using the prefix name hydroxy(oxo)-λ^5-azanylidene, when a characteristic group having priority for citation as a suffix is present. The use of the prefix ‘*aci*-nitro’ is no longer recommended (see P-67.1.6).

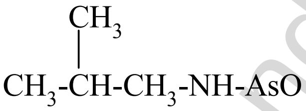
P-61.5.5 Compounds containing the $–PO_2$, $–PO$, $–AsO_2$, or $–AsO$ groups are described by the compulsory prefix names phospho, phosphoroso, arso, and arsoroso.

> Note: The term 'phospho' is widely used in biochemical nomenclature in place of phosphono for designating the $–P(O)(OH)_2$ group linked to a heteroatom, as in phosphocholine and 6-phospho-D-glucose; and as an infix to describe phosphoric diesters, as in glycerophosphocholine.

Examples:



phosphobenzene (PIN)
dioxo(phenyl)-λ^5-phosphane



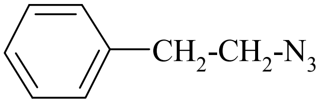
$CH_3\text{-}\overset{\displaystyle CH_3}{\overset{|}{C}H}\text{-}CH_3\text{-}NH\text{-}AsO$

N-arsoroso-2-methylpropanamine(PIN)
N-(2-methylpropyl)oxoarsanamine

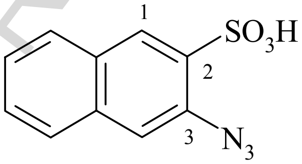
P-61.6 Azides

Compounds containing a $−N_3$ ($−N{=}N^+{=}N^−$) group attached to a parent hydride, are named using substitutive nomenclature and the prefix 'azido'. This method gives preferred IUPAC names rather than names based on the class name 'azide' in functional class nomenclature.

Examples:



(2-azidoethyl)benzene (PIN)
phenethyl azide



3-azidonaphthalene-2-sulfonic acid (PIN)

P-61.7 Isocyanates

> In these Recommendations, preferred IUPAC names are generated by using the prefix 'isocyanato' as a compulsory prefix, i.e., it is attached directly to a parent hydride in substitutive nomenclature. Previously, functional class names were recommended for this class.

Compounds containing the −N=C=O group attached to a parent hydride structure, are named by using substitutive nomenclature and the prefix 'isocyanato'. This method leads to preferred IUPAC names rather than names based on functional class nomenclature and the functional class name 'isocyanate'. Chalcogen analogues are named by inserting the appropriate functional replacement prefix 'thio', 'seleno', or 'telluro' into the names 'isocyanate' or 'isocyanato' just after 'iso'.

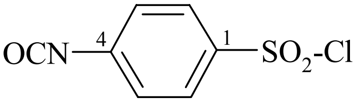
Examples:

C_6H_{11}-NCO

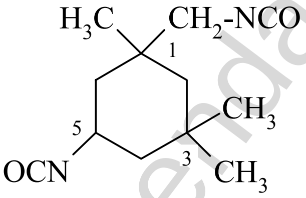
isocyanatocyclohexane (PIN)
cyclohexyl isocyanate

C_6H_5-NCS

isothiocyanatobenzene (PIN)
phenyl isothiocyanate



4-isocyanatobenzenesulfonyl chloride (PIN)



5-isocyanato-1-(isocyanatomethyl)-1,3,3-trimethylcyclohexane (PIN)
3-(isocyanatomethyl)-3,5,5-trimethylcyclohexyl isocyanate

H_3Si-NCS

isothiocyanatosilane (PIN; silane is a preselected name; see P-12)

P-61.8 Isocyanides

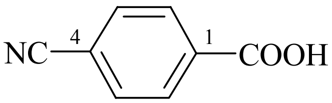
> In these Recommendations, preferred IUPAC names are formed by using the prefix ‘isocyano’ as a compulsory prefix, i.e., it is attached directly to a parent hydride in substitutive nomenclature. Previously, functional class names were recommended for this class.

Compounds containing the −NC group attached to a parent hydride structure, are named by substitutive nomenclature and the prefix ‘isocyano’. This method leads to preferred IUPAC names rather than names based on functional class nomenclature and the functional class name ‘isocyanide’.

Examples:

C_6H_6-NC

isocyanobenzene (PIN)
phenyl isocyanide



4-isocyanobenzoic acid (PIN)

P-61.9 Fulminates and isofulminates

The structure of fulminic acid was indicated in the 1979 Recommendations (Rule C-833.1, ref. 1) and in the 1993 Recommendations (Rule R-5.7.9.2, ref. 2) as HO-N≡C by the class name fulminate and the compulsory prefix fulminato. Although consistent with the pseudohalogen cyanate, the structure of this acid in the literature is claimed to be HCNO. Accordingly, the name fulminic acid and of its substituent group fulminato must be deprecated; and the names isofulminic acid and isofulminate must also be deprecated. The IUPAC preferred name for the structure HCNO is formonitrile oxide (see P-66.5.3) and the IUPAC preferred name for its isomer, HO-N=C, is based on hydroxylamine (see P-68.3.1.1).

Examples:

H-C≡NO

formonitrile oxide (PIN)

–C≡N=O

(oxo-λ^5-azanylidyne)methyl (PIN)

HO-N=C

λ^2-methylidenehydroxylamine (PIN)

–O-N=C

(λ^2-methylideneamino)oxy (PIN)
(not fulminato)

P-61.10 Polyfunctional compounds

In substitutive names, detachable prefixes in names are cited in alphanumerical order. Low locants are assigned to:

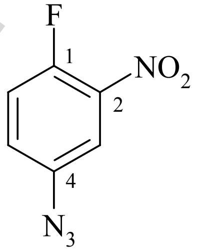
(1) the prefixes as a set, and if there is a choice,

(2) to the prefix that is cited first in a name.

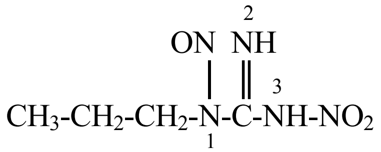
In functional class nomenclature, names are formed by using the order of classes (see P-41) and the order of seniority of halides and pseudohalides (see P-41 and P-65.5.2.1) to choose the principal function. Names formed substitutively rather than functional class names are preferred IUPAC names.

P-61.10.1 Low locants are assigned as a set, without regard to kind.

Examples:



4-azido-1-fluoro-2-nitrobenzene (PIN)
4-azido-2-nitrophenyl fluoride



$$CH_3\text{-}CH_2\text{-}CH_2\text{-}\underset{1}{N}(ON)\text{-}C(=\overset{2}{N}H)\text{-}\overset{3}{N}H\text{-}NO_2$$

3-nitro-1-nitroso-1-propylguanidine (PIN)

P-61.10.2 Low locants are assigned to the prefix cited first in a name

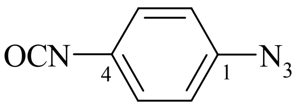
Examples:

$$Cl_3\overset{1}{Si}\text{-}\overset{2}{Si}H_2\text{-}\overset{3}{Si}H_2\text{-}\overset{4}{Si}H_2\text{-}\overset{5}{Si}(CH_3)_3$$

1,1,1-trichloro-5,5,5-trimethylpentasilane (PIN)
(pentasilane is a preferred preselected
name, see P-12)

$$Br\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}Cl$$

1-bromo-2-chloroethane (PIN)



1-azido-4-isocyanatobenzene (PIN)
4-azidophenyl isocyanate

P-62 Amines and imines

P-62.0 Introduction

The nomenclature of amines and imines is rich in traditions and a variety of methods have been used for constructing their names (see refs. 1 and 2). The rationalization necessary to define preferred IUPAC names is a good opportunity to establish proper names for amines and imines and retain clear and unambiguous methods for choosing the appropriate parent and naming individual compounds.

Rules C-11.4 and C-811-C-815 in the 1979 Recommendations (ref. 1) are superceded, as well as are Rules R-5.4.1-R-5.4.3 in the 1993 Recommendations (ref. 2).

P-62.1 General methodology

The general methodology is based on the following principles:

(a) Definitions, as given in the Glossary of Class Names Based on Structure (ref. 17), classify amines and imines unambiguously as follows:

(1) amines are compounds formally derived from ammonia by replacing one, two, or three of its hydrogen atoms by hydrocarbyl groups, and having the general structures $R\text{-}NH_2$ (primary amines), R_2NH (secondary amines), R_3N (tertiary amines).

(2) imines are compounds having the structure $R\text{-}N{=}CR_2$ (R = H, hydrocarbyl), corresponding either to ketimines, $RR'C{=}NR''$ or to aldimines, $RCH{=}NR'$.

(b) amines are senior to imines in the seniority order of classes.

(c) methods for naming amines and imines will be restricted to a minimum, preference being given to the substitutive method using the suffix ‘amine’.

(d) a minimum of traditional names will be retained.

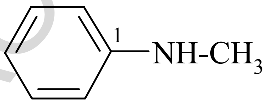
P-62.2 Amines

P-62.2.1 Amines derived from parent hydrides

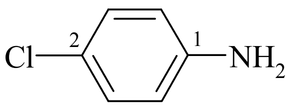
P-62.2.1.1 Primary amines

P-62.2.1.1.1 One trivial name only for a primary amine is retained as a preferred name, i.e., aniline, for $C_6H_5\text{-}NH_2$, with full substitution permitted on the ring and on the nitrogen atom. Rules for substituting aniline are described in P-46.2.

Examples:



N-methylaniline (PIN)
N-methylbenzenamine



4-chloroaniline (PIN)
4-chlorobenzenamine

P-62.2.1.1.2 Primary amines, R-NH_2, are systematically named in two ways:

(1) by adding the suffix ‘amine’ to the name of the parent hydride;
(2) by adding the name of the substituent group R− to the term ‘amine’ used as a parent hydride name.

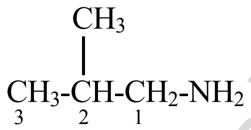
Two or more ‘amine’ suffixes are indicated by an appropriate multiplying numerical prefix ‘di’, tri’, ‘tetra’, etc. The terminal letter ‘a’ of a numerical prefix is elided before the suffix amine, i. e., ‘tetramine’, not ‘tetraamine’, but not before the parent name amine. Numerical locants, including ‘1’ in the case of amines derived from mononuclear parent hydrides, are used to denote substitution on atoms of the parent hydride and ‘*N* ’ locants for substitution on the nitrogen atom for amines named by method (1).

Method (1) leads to preferred IUPAC names.

Examples:

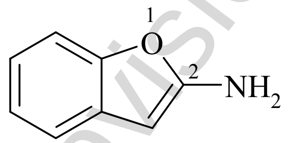
$\overset{1}{C}H_3\text{-}\overset{N}{N}H_2$

(1) methanamine (PIN)
(2) methylamine

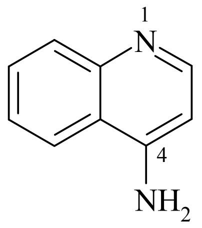


$\underset{3}{C}H_3\text{-}\underset{2}{\overset{CH_3}{C}}H\text{-}\underset{1}{C}H_2\text{-}NH_2$

(1) 2-methylpropan-1-amine (PIN)
(2) (2-methylpropyl)amine



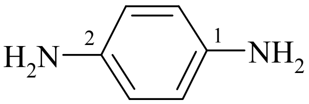
1-benzofuran-2-amine (PIN)
1-benzofuran-2-ylamine



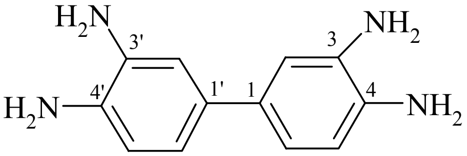
quinolin-4-amine (PIN)
(quinolin-4-yl)amine
4-quinolylamine

$H_2N\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}NH_2$

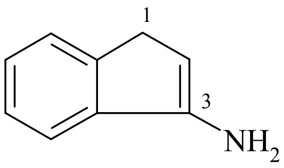
ethane-1,2-diamine (PIN)
ethylenediamine



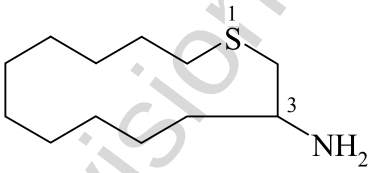
benzene-1,4-diamine (PIN)
1,4-phenylenediamine
p-phenylenediamine



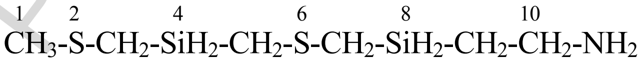
[1,1′-biphenyl]-3,3′,4,4′-tetramine (PIN; note elision of ‘a’ from ‘tetra’ in ‘tetramine’)
[1,1′-biphenyl-3,3′,4,4′-tetrayl]tetraamine (note no elision of ‘a’ from ‘tetra’ in ‘tetraamine’)



1*H*-inden-3-amine (PIN)
1*H*-inden-3-ylamine

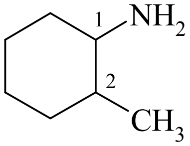


1-thiacyclotridecan-3-amine (PIN)
(1-thiacyclotridecan-3-yl)amine

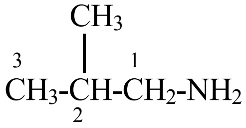


$$\overset{1}{\mathrm{C}}\mathrm{H_3}\text{-}\overset{2}{\mathrm{S}}\text{-}\mathrm{CH_2}\text{-}\overset{4}{\mathrm{Si}}\mathrm{H_2}\text{-}\mathrm{CH_2}\text{-}\overset{6}{\mathrm{S}}\text{-}\mathrm{CH_2}\text{-}\overset{8}{\mathrm{Si}}\mathrm{H_2}\text{-}\mathrm{CH_2}\text{-}\overset{10}{\mathrm{C}}\mathrm{H_2}\text{-}\mathrm{NH_2}$$

2,6-dithia-4,8-disiladecan-10-amine (PIN)
(2,6-dithia-4,8-disiladecan-10-yl)amine



2-methylcyclohexan-1-amine (PIN)
(2-methylcyclohexyl)amine



$\overset{3}{C}H_3\text{-}\underset{2}{\overset{\overset{CH_3}{|}}{C}}H\text{-}\overset{1}{C}H_2\text{-}NH_2$

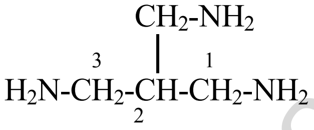
2-methylpropan-1-amine (PIN)
isobutylamine
(2-methylpropyl)amine

$Cl\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}NH_2$

2-chloroethanamine (PIN)
(2-chloroethyl)amine

P-62.2.1.1.3 When all amino groups cannot be expressed as suffixes, or when the $-NH_2$ group is not the principal characteristic group, the prefix 'amino', not azanyl, is used in preferred IUPAC names. Azanyl may be used in general nomenclature. The substituent prefix name anilino is no longer recommended.

Examples:

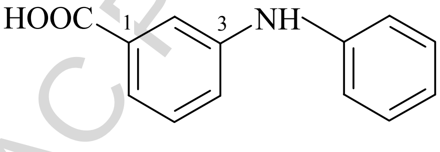


$H_2N\text{-}\overset{3}{C}H_2\text{-}\underset{2}{\overset{\overset{CH_2\text{-}NH_2}{|}}{C}}H\text{-}\overset{1}{C}H_2\text{-}NH_2$

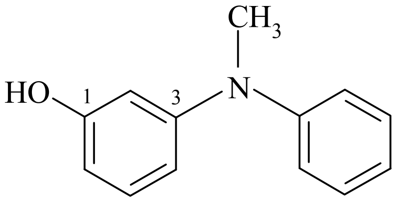
2-(aminomethyl)propane-1,3-diamine (PIN)
2-(azanylmethyl)propane-1,3-diamine
[2-(aminomethyl)propane-1,3-diyl]diamine

$H_2N\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

3-aminopropanoic acid (PIN)
3-azanylpropanoic acid



3-anilinobenzoic acid (PIN))
3-(phenylamino)benzoic acid

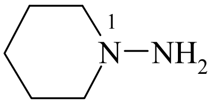


3-(*N*-methylanilino)phenol (PIN)
3-[methyl(phenyl)amino]phenol

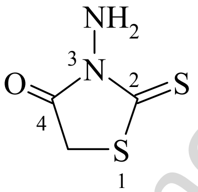
P-62.2.1.1.4 Amino groups attached to heteroatoms

When attached to heteroatoms, amino groups are expressed as suffixes when representing the principal characteristic group and by the amino prefix in presence of a characteristic group having seniority over amines.

Examples:



piperidin-1-amine (PIN)
1-aminopiperidine



3-amino-2-sulfanylidene-1,3-thiazolidin-4-one (PIN)
(not 3-amino-2-thioxo-1,3-thiazolidin-4-one)

P-62.2.1.2 Secondary and tertiary amines

P-62.2.1.2.1 Symmetrical and unsymmetrical secondary and tertiary amines are named by the same two methods.

(1) substitutively using the retained name aniline or the suffix 'amine' with further *N*-substitution;

(2) substitutively, by prefixing, in alphabetical order when required, the name(s) of the substituent group(s) R, R′ or R″ to the parent hydride name 'amine'. In order to avoid ambiguity, the second prefix in secondary amines, and the second and the third prefixes in tertiary amines must be enclosed in parentheses when these prefixes denote simple substituents.

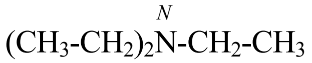
Method (1) generates preferred IUPAC names. Names like diethylamine and triethylamine are deprecated.

Preferred IUPAC names for prefixes corresponding to −NHR or −NRR′ or $-NR_2$ are formed by prefixing the names of the groups R and R′ to the prefix 'amino', for example 'methylamino', for $-NH\text{-}CH_3$. Prefixes such as azanyl and azanylidene may be used in general nomenclature.

Examples:

$\mathrm{C_6H_5\text{-}\overset{\mathit{N}}{N}H\text{-}C_6H_5}$

N-phenylaniline (PIN)
diphenylamine
(not azanediyldibenzene; the retained name 'aniline' must be used for all *N* derivatives)



$\mathrm{(CH_3\text{-}CH_2)_2\overset{\mathit{N}}{N}\text{-}CH_2\text{-}CH_3}$

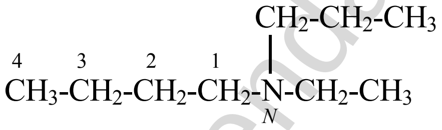
N,*N*-diethylethanamine (PIN)
triethylamine

$$Cl\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CH_2}\text{-}\overset{N}{NH}\text{-}CH_2\text{-}CH_2\text{-}Cl$$

2-chloro-*N*-(2-chloroethyl)ethanamine (PIN)
bis(2-chloroethyl)amine
(not 2,2′-dichlorodiethylamine)

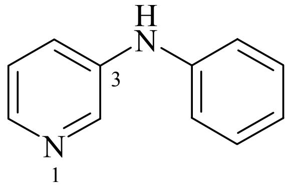
$$\overset{3}{CH_3}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CH_2}\text{-}\overset{N}{NH}\text{-}CH_2\text{-}CH_2\text{-}Cl$$

N-(2-chloroethyl)propan-1-amine (PIN)
(2-chloroethyl)(propyl)amine



$$\overset{4}{CH_3}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CH_2}\text{-}\underset{N}{\overset{\overset{CH_2\text{-}CH_2\text{-}CH_3}{|}}{N}}\text{-}CH_2\text{-}CH_3$$

N-ethyl-*N*-propylbutan-l-amine (PIN)
butyl(ethyl)(propyl)amine
(no longer *N*-ethyl-*N*-propylbutylamine)



N-phenylpyridin-3-amine (PIN)

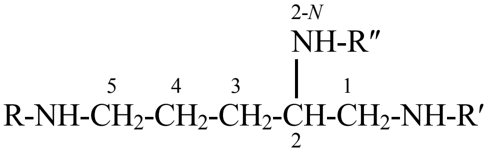
P-62.2.1.2.2 Di-, triamines, etc., are named in a similar way. The locants *N* and *N* ′ are used with symmetrical diamines. When unsymmetrically substituted, the locant of the parent hydride to which the nitrogen atom is attached is placed in front of the symbol *N, N* ′*,* etc.

> This is a change in format. The locant of the parent hydride to which the nitrogen atom is attached was formerly cited as a superscript to the *N, N*′*,* etc.

Examples:

$$CH_3\text{-}\overset{N'}{NH}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CH_2}\text{-}\overset{N}{NH}\text{-}CH_2\text{-}CH_3$$

(1) *N*-ethyl-*N*′-methylpropane-1,3-diamine (PIN)
(2) *N*-ethyl-*N*′-methyl(propane-1,3-diyldiamine)

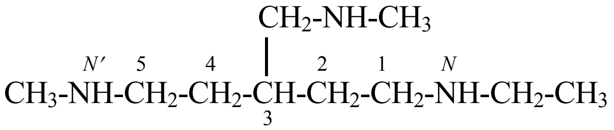


$$R\text{-}NH\text{-}\overset{5}{CH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{CH_2}\text{-}\underset{2}{\overset{\overset{\overset{2\text{-}N}{NH\text{-}R''}}{|}}{CH}}\text{-}\overset{1}{CH_2}\text{-}NH\text{-}R'$$

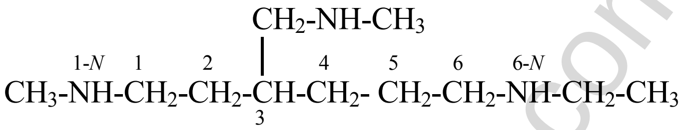
R = R′ = R″ = H (1) pentane-1,2,5-triamine (PIN)
(2) pentane-1,2,5-triyltriamine

R = R′ = H; (1) 2-*N*-methylpentane-1,2,5-triamine (PIN)
R″ = −CH_3 (2) 2-*N*-methyl(pentane-1,2,5-triyltriamine)

R = H; R′ = −CH_3; (1) 2-*N*-ethyl-1-*N*-methylpentane-1,2,5-triamine (PIN)
R″ = −C_2H_5 (2) 2-*N*-ethyl-1-*N*-methyl(pentane-1,2,5-triyltriamine)


$$CH_3\text{-}\overset{N'}{NH}\text{-}\overset{5}{CH_2}\text{-}\overset{4}{CH_2}\text{-}\underset{3}{\overset{\overset{CH_2\text{-}NH\text{-}CH_3}{|}}{CH}}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CH_2}\text{-}\overset{N}{NH}\text{-}CH_2\text{-}CH_3$$

(1) *N*-ethyl-*N*′-methyl-3-[(methylamino)methyl]pentane-1,5-diamine (PIN)
(2) *N*-ethyl-*N*′-methyl-3-[(methylamino)methyl](pentane1,5-diyldiamine)

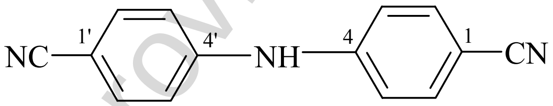

$$CH_3\text{-}\overset{1\text{-}N}{NH}\text{-}\overset{1}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\underset{3}{\overset{\overset{CH_2\text{-}NH\text{-}CH_3}{|}}{CH}}\text{-}\overset{4}{CH_2}\text{-}\ \overset{5}{CH_2}\text{-}\overset{6}{CH_2}\text{-}\overset{6\text{-}N}{NH}\text{-}CH_2\text{-}CH_3$$

(1) 6-*N*-ethyl-1-*N*-methyl-3-[(methylamino)methyl]hexane-1,6-diamine (PIN)
(2) 6-*N*-ethyl-1-*N*-methyl-3-[(methylamino)methyl](hexane-1,6-diyldiamine)

P-62.2.1.2.3 Multiplicative nomenclature

The prefixes ‘nitrilo’ for −N< and ‘azanediyl’ for −NH− (also written HN<) are recommended for use in multiplicative nomenclature (see P-15.3). The prefix ‘imino’ is reserved to denote only the divalent substituent group =NH. Names formed by multiplicative nomenclature are preferred to those formed by substitutive nomenclature (see P-51.2).

Examples:



4,4′-azanediyldibenzonitrile (PIN)
4-[(4-cyanophenyl)amino]benzonitrile

$\overset{2,2',2''}{N}(CH_2\text{-}COOH)_3$

N,*N*-bis(carboxymethyl)glycine (PIN)
2,2′,2″-nitrilotriacetic acid

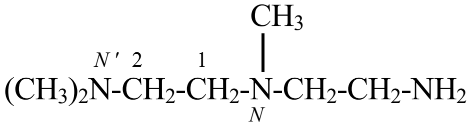
P-62.2.1.3 Polyamine systems

Polyamine systems are composed of two or more amines, identical or different. They are named by *N*-substitution of the senior amine. The senior amine is chosen in accordance with the choice of a principal chain or a senior ring or ring system. Alphanumerical order is applied when a choice is to be made. Multiplicative nomenclature, skeletal replacement (‘a’) nomenclature, or phane names are used when the conditions required by these types of nomenclature are fulfilled.

Examples:

$\mathrm{H_2N\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}\overset{\mathit{N}}{N}H\text{-}CH_2\text{-}NH_2}$

N-(aminomethyl)ethane-1,2-diamine (PIN)
(regular substitutive nomenclature;the diamine having the longest carbon chain is chosen as parent structure)



$\mathrm{(CH_3)_2\overset{\mathit{N'}}{N}\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}\underset{\mathit{N}}{\overset{CH_3}{N}}\text{-}CH_2\text{-}CH_2\text{-}NH_2}$

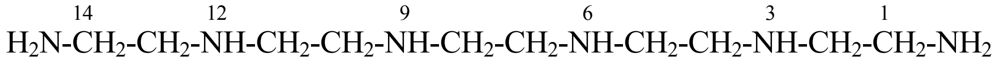
N-(2-aminoethyl)-*N*,*N′*,*N′* -trimethylethane-1,2-diamine (PIN; numbering shown)
(the most substituted diamine is chosen as parent structure)
(not *N*,*N*-dimethyl-2,2′-(methylazanediyl)diethanamine; the preferred IUPAC name must be a diamine)

$\mathrm{H_2N\text{-}CH_2\text{-}CH_2\text{-}\overset{\mathit{N}}{N}H\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}NH\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}\overset{\mathit{N'''}}{N}H\text{-}CH_2\text{-}CH_2\text{-}NH_2}$

N,*N″*-(azanediyldiethane-2,1-diyl)bis(ethane-1,2-diamine) (PIN; numbering shown)
N-(2-aminoethyl)-*N′*-{2-[(2-aminoethyl)amino]ethyl}ethane-1,2-diamine
(not 2,2′-azanediylbis[*N*-(2-aminoethyl)ethanamine]; the preferred IUPAC name must be a diamine)

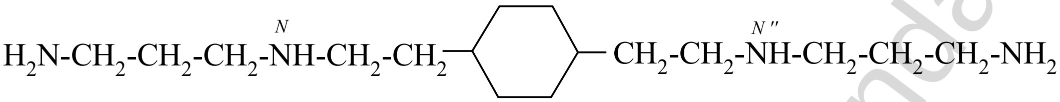
$\mathrm{H_2N\text{-}CH_2\text{-}\overset{\mathit{N'}}{N}H\text{-}CH_2\text{-}CH_2\text{-}\overset{\mathit{N}}{N}H\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}NH_2}$

N-{2-[(2-aminoethyl)amino]ethyl}-*N′*-(2-aminomethyl)ethane-1,2-diamine (PIN)
(not *N*-(2-aminomethyl)-*N′*-{2-[(2-aminoethyl)amino]ethyl}ethane-1,2-diamine; ‘aminoethyl’ precedes ‘aminomethyl’ in alphanumerical order)
(not *N*-(aminoethyl)-*N* ′-(aminomethyl)-2,2′-azanediyldiethaneamine; the preferred IUPAC name must be a diamine)

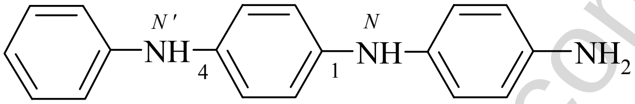


$H_2\overset{14}{N}\text{-}CH_2\text{-}CH_2\text{-}\overset{12}{N}H\text{-}CH_2\text{-}CH_2\text{-}\overset{9}{N}H\text{-}CH_2\text{-}CH_2\text{-}\overset{6}{N}H\text{-}CH_2\text{-}CH_2\text{-}\overset{3}{N}H\text{-}CH_2\text{-}\overset{1}{C}H_2\text{-}NH_2$

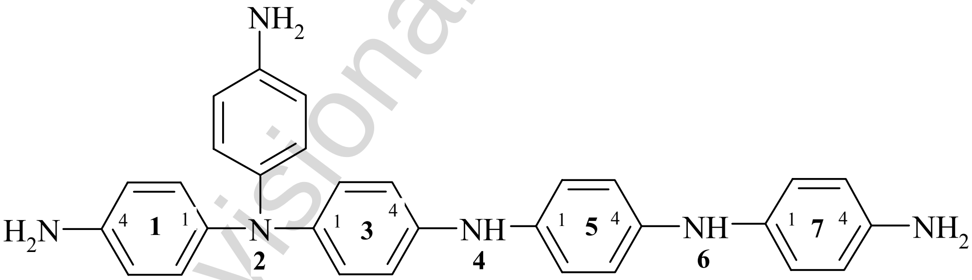
3,6,9,12-tetraazatetradecane-1,14-diamine (PIN)
(skeletal replacement (‘a’) name; see P-51.3.2)



N,*N″* -(cyclohexane-1,4-diydiethane-2,1-diyl)bis(propane-1,3-diamine) (PIN)
(multiplicative nomenclature allows four amine characteristic groups to be included in the parent structure)



N-(4-aminophenyl)-*N′*-phenylbenzene-1,4-diamine (PIN)
[maximum number of substituents cited as prefixes; see P-44.2.3(g) and P-44.3(k)]



2-(4-aminophenyl)-2,4,6-triaza-1,7(1),3,5(1,4)-tetrabenzenaheptaphane-1^4,7^4-diamine (PIN)
(four benzene rings and a total of seven phane nodes justify a phane name; see P-51.4)

P-62.2.2.2 Modification of the degree of saturation/unsaturation of amines

P-62.2.2.2.1 General methodology

When there is a choice for numbering, the starting point and the direction of numbering of a compound are chosen so as to give lowest locants to the following structural features (if present) considered successively in the order given until a decision is reached.

(a) fixed numbering (naphthalene, bicyclo[2.2.2]octane, etc.)

(b) heteroatoms in heterocycles and in acyclic parent structures

(c) indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with the structural feature (d)].

(d) principal group named as suffix

(e) added hydrogen (consistent with the structure of the compound and in accordance with further substitution)

(f) saturation (‘hydro’/‘dehydro’ prefixes) or unsaturation (‘ene’, ‘yne’ endings)

(g) substituents named as prefixes (low locants are allocated for substituents regardless of kind; then, if necessary, in the order of citation)

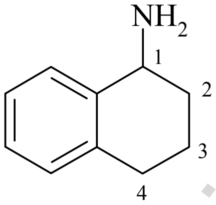
P-62.2.2.2.2 Modification of the degree of saturation/unsaturation of primary amines

Criteria (d), (e) and (f) described in the general methodology (P-62.2.2.2.1) are used.

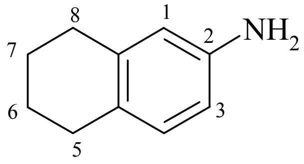
Examples:

$\overset{3}{C}H_2=\overset{2}{C}H-\overset{1}{C}H_2-NH_2$

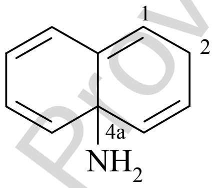
prop-2-en-1-amine (PIN)
allylamine



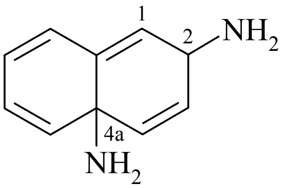
1,2,3,4-tetrahydronaphthalen-1-amine (PIN)



5,6,7,8-tetrahydronaphthalen-2-amine (PIN)



naphthalen-4a(2*H*)-amine (PIN)
2,4a-dihydronaphthalen-4a-amine
(see P-53.1)

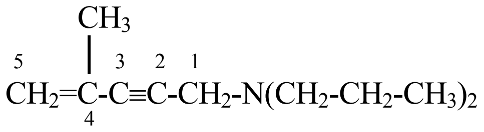


naphthalene-2,4a(2*H*)-diamine (PIN)
2,4a-dihydronaphthalene-2,4a-diamine
(see P-53.1)

P-62.2.2.3 Selection of the principal chain or senior ring system in secondary and tertiary amines

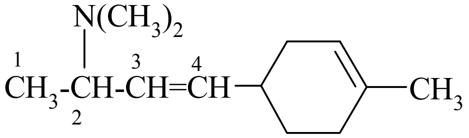
Names of amines formed substitutively by using the retained name aniline or the suffix ‘amine’ are based on a principal chain and a senior ring system (see P-44.1). When a choice for parent hydride is possible between a ring and a chain, the ring is preferred. In names using amine as a parent structure, substituent groups expressed as prefixes are cited in alphanumerical order; the prefix(es) immediately preceding the term ‘amine’ is placed in parentheses.

Examples:

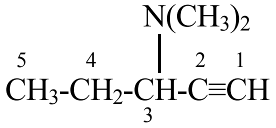


$$\overset{5}{CH_2}=\underset{4}{\overset{CH_3}{C}}-\overset{3}{C}\equiv\overset{2}{C}-\overset{1}{CH_2}-N(CH_2-CH_2-CH_3)_2$$

4-methyl-*N*,*N*-dipropylpent-4-en-2-yn-1-amine (PIN)
[not (4-methylpent-4-en-2-yn-1-yl)dipropylamine]



N,*N*-dimethyl-4-(4-methylcyclohex-3-en-1-yl)but-3-en-2-amine (PIN)

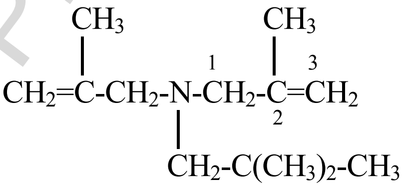


$$\overset{5}{CH_3}-\overset{4}{CH_2}-\underset{3}{\overset{N(CH_3)_2}{C}}H-\overset{2}{C}\equiv\overset{1}{C}H$$

N,*N*-dimethylpent-1-yn-3-amine (PIN)
dimethyl(pent-1-yn-3-yl)amine

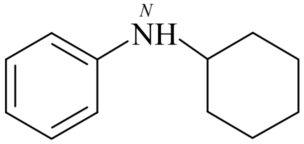
$$\overset{4}{CH_3}-\overset{3}{CH_2}-\overset{2}{CH_2}-\overset{1}{CH_2}-NH-CH=CH_2$$

N-ethenylbutan-1-amine (PIN)
butyl(ethenyl)amine

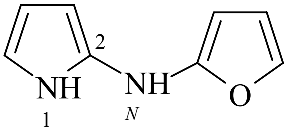


$$CH_2=\overset{CH_3}{C}-CH_2-\underset{CH_2-C(CH_3)_2-CH_3}{N}-\overset{1}{CH_2}-\underset{2}{\overset{CH_3}{C}}=\overset{3}{CH_2}$$

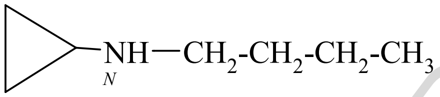
N-(2,2-dimethylpropyl)-2-methyl-*N*-(2-methylprop-2-en-1-yl)prop-2-en-1-amine (PIN)
(2,2-dimethylpropyl)bis(2-methylprop-2-en-1-yl)amine
(not 2,2′-dimethyl-*N*-(2,2-dimethylpropyl)di(prop-2-en-1-amine)



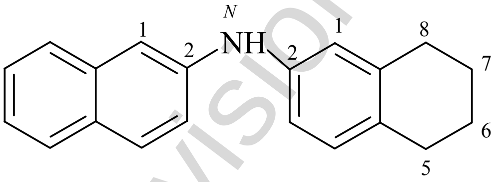
N-cyclohexylaniline (PIN)
cyclohexyl(phenyl)amine



N-(furan-2-yl)pyrrol-2-amine (PIN)
(furan-2-yl)(pyrrol-2-yl)amine
2-furyl(1*H*-pyrrol-2-yl)amine



N-butylcyclopropanamine (PIN)
N-cyclopropylbutan-1-amine
cyclopropyl(butyl)amine



N-(5,6,7,8-tetrahydronaphthalen-2-yl)naphthalen-2-amine (PIN)
2-naphthyl(5,6,7,8-tetrahydro-2-naphthyl)amine
(not 5,6,7,8-tetrahydrodi-2-naphthylamine)

P-62.3 Imines

Compounds having the general structure R-CH=NR′ or R(R′)C=NR″ are called generically ‘aldimines’ and ‘ketimines’, respectively. Imines are characterized by a double bond between a carbon atom and a nitrogen atom. Thus, *N*-substituted imines, R-CH=N-R′ or R(R′)C=N-R″, must be classified as imines and not as amines in spite of the fact that there is a single bond between a carbon atom and the nitrogen atom; amines must have three single bonds linked to carbon atoms (see P-62.0).

P-62.3.1 Substitutive names of imines

P-62.3.1.1 All imines are named substitutively using the suffix ‘imine’; the presence of several ‘imine’ characteristic groups is denoted by the numerical multiplying prefixes ‘di’, ‘tri’, etc. When there is a choice for numbering, the starting point and the direction of numbering of a compound are chosen so as to give lowest locants to the following structural features (if present) considered successively in the order given until a decision is reached.

(a) fixed numbering (naphthalene, bicyclo[2.2.2]octane, etc.)

(b) heteroatoms in heterocycles and in acyclic parent structures

(c) indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with the structural feature (d)]

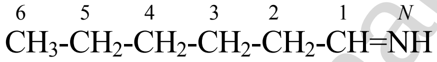
(d) principal group named as suffix

(e) added hydrogen (consistent with the structure of the compound and in accordance with further substitution)

(f) saturation (‘hydro’/‘dehydro’ prefixes) or unsaturation (‘ene’, ‘yne’ endings)

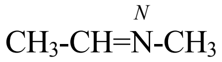
(g) substituents named as prefixes (low locants are allocated for substituents regradless of kind; then, if necessary, in the order of citation)

Examples:



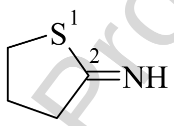
$\overset{6}{CH_3}\text{-}\overset{5}{CH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CH}{=}\overset{N}{NH}$

hexan-1-imine (PIN)

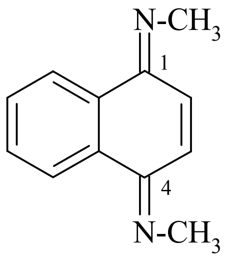


$CH_3\text{-}CH{=}\overset{N}{N}\text{-}CH_3$

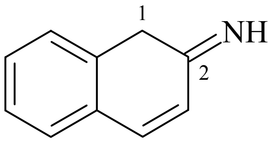
N-methylethanimine (PIN)
(not *N*-ethylidenemethanamine)
[not *N*-ethylidene(methyl)amine]



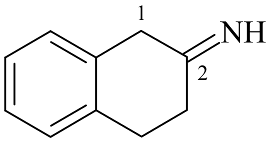
thiolan-2-imine (PIN)



N,N ′-dimethylnaphthalene-1,4-diimine (PIN; see also P-53.1)
N,N ′-dimethyl-1,4-dihydronaphthalene-1,4-diimine
(not *N,N* ′-dimethyl-1,4-naphthoquinone diimine; two suffixes of different kinds are incompatible)
[not *N*,*N*′-naphthalene-1,4-iylidenebis(methanamine)]
[not *N*,*N*′-naphthalene-1,4-diylidenebis(methylamine)]
[not dimethyl(napththalene-1,4-diylidene)bis(amine)]



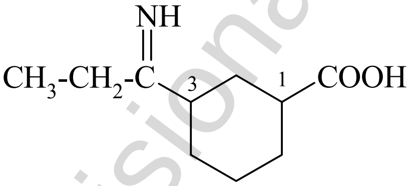
naphthalen-2(1*H*)-imine (PIN; see also P-53.1)
1,2-dihydronaphthalen-2-imine



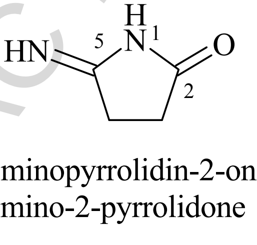
3,4-dihydronaphthalen-2(1*H*)-imine (PIN; see also P-53.1)
1,2,3,4-tetrahydronaphthalen-2-imine

P-62.3.1.2 The prefix ‘imino’ for =NH is used in presence of characteristic groups having seniority over imines. In multiplicative nomenclature, the prefix ‘azanylylidene’ for −N= is used. Substituent groups attached to rings, ring systems or heteroatoms of the type R-(C=NH)−, where R− is a ring or a chain, are named as acyl groups (see imidic acids, P-65.1.3.1 and acyl groups P-65.2).

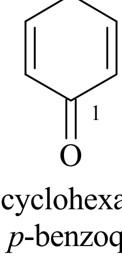
Examples:



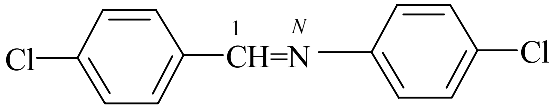
3-propanimidoylcyclohexane-1-carboxylic acid (PIN)



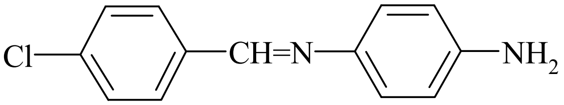
5-iminopyrrolidin-2-one (PIN)
5-imino-2-pyrrolidone



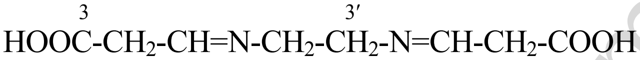
4-iminocyclohexa-2,5-dien-1-one (PIN)
(not *p*-benzoquinone monoimine)



N,1-bis(4-chlorophenyl)methanimine (PIN) (see following example)

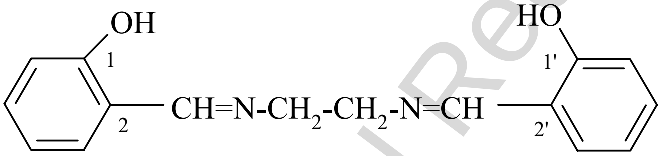


4-{[(4-chlorophenyl)methylidene]amino}aniline (PIN)



$\overset{3}{\mathrm{HOOC}}\text{-}CH_2\text{-}CH=N\text{-}CH_2\text{-}\overset{3'}{CH_2}\text{-}N=CH\text{-}CH_2\text{-}COOH$

3,3′-[ethane-1,2-diylbis(azanylylidene)]dipropanoic acid (PIN)



2,2′-[ethane-1,2-diylbis(azanylylidenemethanylylidene)]diphenol (PIN)

P-62.3.1.3 Imino groups attached to heteroatoms (pseudoimines)

Compounds containing the group X=NH, where X is a heteroatom and =NH the principal characteristic group, are named as imines; the prefix ‘imino’ is used to express the =NH group when another characteristic groups has seniority over imines.

Examples:

$CH_3\text{-}P=NH$	$(CH_3)_3Si=N\text{-}C_6H_5$
methylphosphanimine (PIN)	trimethyl-*N*-phenylsilanimine (PIN) (silane is a preferred preselected parent name, see P-12)

$CH_3\text{-}N=SiH\text{-}CH_2\text{-}COO\text{-}CH_3$

methyl [(methylimino)silyl]acetate (PIN)
(silyl is a preferred preselected prefix name, see P-12)

P-62.3.1.4 Carbodiimides

The hypothetical compound HN=C=NH is named systematically ‘methanediimine’. Its derivatives are named as substitution products thereof. These names are preferred to those based on the retained name ‘carbodiimide’, which now should be used only as a class name.

Example:

$C_6H_{11}\text{-}N{=}C{=}N\text{-}C_6H_{11}$

dicyclohexylmethanediimine (PIN)
(formerly dicyclohexylcarbodiimide)

P-62.4 *N*-Substitution of amines and imines

Traditionally, substitution on the nitrogen atom of amines and imines was allowed for substituents always cited as prefixes (see P-46.1), such as −Cl and other halogen atoms, −NO, $-NO_2$, −O-R and even −OH groups, and chalcogen analogues.

> In accordance with the seniority of classes (see P-41), compounds such as R-NH-Cl, R-NH-NO, and $R\text{-}NH\text{-}NO_2$ are named as derivatives of amides (see P-67.1.2.3). Compounds such as R-NH-OH are named as *N*-derivatives of hydroxylamine, $NH_2\text{-}OH$ (see P- 68.3.1.1.1). Names based on *N*-substitution of amines are not recommended in these cases.

Substitution of amines is permitted by −OR , −SR, −SeR, and −TeR groups, where R is an alkyl or aryl substituent group.

Examples:

$CH_3\text{-}CH_2\text{-}NH\text{-}O\text{-}CH_3$

N-methoxyethan-1-amine (PIN, see P-68.3.1.1.3)

$CH_3\text{-}CH_2\text{-}NH\text{-}OH$

N-ethylhydroxylamine (PIN)

$CH_3\text{-}CH_2\text{-}\overset{N}{N}H\text{-}Cl$

N-ethylhypochlorous amide (PIN)
(not *N*-chloroethan-1-amine)

$CH_3\text{-}\overset{N}{N}H\text{-}NO$

N-methylnitrous amide (PIN)
(not *N*-nitrosomethanamine)

$CH_3\text{-}N(NO_2)_2$

N-methyl-*N*-nitronitric amide (PIN)
(not *N*,*N*-dinitromethanamine)

P-62.5 Amine oxides and imine oxides

Amine oxides and imine oxides are named:

(1) by functional class nomenclature using the class name 'oxide';

(2) by use of prefixes derived from the parent name λ^5-azane;

(3) as zwitterions (see P-74.2.1.2)

Method (1) is used when the oxide is located on a nitrogen atom of the parent structure so that, if a locant is necessary, it can be used to unambiguously locate the oxide. Because of the zwitterionic nature of a nitrogen oxide, amine and imine oxides are placed with zwitterions in the order of compound classes (see P-41). Method (2) is used when the oxide is on a nitrogen atom of a substituent to the parent structure. Methods (1) and (2) lead to preferred IUPAC names. When method (3) is used, the zwitterion is the parent structure.

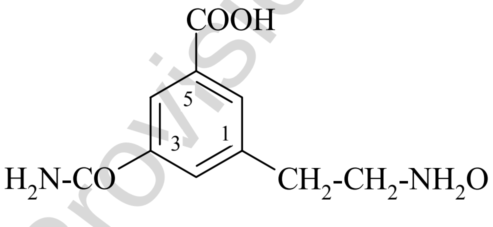
Examples:

$(CH_3)_3NO$ or $(CH_3)_3N^+\text{-}O^-$

(1) *N*,*N*-dimethylmethanamine oxide (PIN)
trimethylamine oxide
(3) (trimethylazaniumyl)oxidanide

$CH_2{=}N(O)Cl$

(1) *N*-chloromethanimine oxide (PIN)
(3) [chloro(methylidene)azaniumyl]oxidanide (see also P-74.2.1.2)



(1) 2-(3-carbamoyl-5-carboxyphenyl)ethanamine oxide (PIN)
(3) {[2-(3-carbamoyl-5-carboxyphenyl)ethyl]azaniumyl}oxidanide (see also P-74.2.1.2)

$\bullet CH_2\text{-}CH_2\text{-}NH_2O$

2-(oxo-λ^5-azanyl)ethyl (PIN)

P-63 Hydroxy compounds, ethers, peroxols, peroxides and chalcogen analogues

P-63.0 Introduction

Traditionally, hydroxy compounds are compounds having one or more hydroxy groups attached to carbon atoms. Alcohols, phenols, enols and ynols are recognized as hydroxy compounds. The category is extended so as to include compounds having one or more hydroxy groups attached to atoms other than carbon without being classifed as acids as defined in the seniority of classes. For instance, H_2Si-OH is classified and named as a hydroxy compound, silanol, but $Si(OH)_4$ is classified and named as an acid, orthosilicic acid.

Several changes are recommended in naming of characteristic groups having two contiguous chalcogen atoms. The suffix ‘peroxol’ is now introduced to name the group –OOH, formerly named by functional class nomenclature as ‘hydroperoxide’. ☐

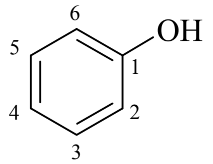
P-63.1 Hydroxy compounds and chalcogen analogues

Names generated substitutively are preferred IUPAC names rather than functional class names or retained names, with the exception of the retained name ‘phenol’ that can be fully substituted. Functional class names are traditional names that are restricted today to alcohols, R-OH, where the R– group is a simple aliphatic or alicyclic group.

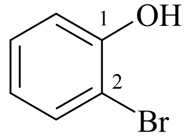
P-63.1.1 Retained names

Only one name is retained, phenol, for C_6H_5-OH, both as a preferred name and for general nomenclature. The structure is substitutable at any position. Locants 2, 3, and 4 are preferred to the prefixes *o*, *m*, and *p*. Naphthol (both isomers) and anthrol (all isomers) are retained names for general nomenclature only; they are substitutable at any position.

Examples:



phenol (PIN; retained name)



2-bromophenol (PIN)
o-bromophenol

P-63.1.2 Systematic names of alcohols, phenols, enols, and ynols

Hydroxy compounds are named in four ways.

(1) substitutively, using the suffix ‘ol’ and the prefix ‘hydroxy’. The presence of several ‘ol’ characteristic groups is denoted by the numerical multiplying prefixes ‘di’, ‘tri’, etc.; the final letter ‘a’ in a multiplying prefix is elided before the suffix ‘ol’. Rule P-44 is applied when a principal chain or a senior ring system must be chosen. When there is a choice for numbering, the starting point and the direction of numbering of a compound are chosen so as to give lowest locants to the following structural features (if present) considered successively in the order given until a decision is reached.

- (a) fixed numbering (naphthalene, bicyclo[2.2.2]octane, etc.)
- (b) heteroatoms in heterocycles and in acyclic parent structures
- (c) indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with the structural feature (d)].
- (d) principal group named as suffix
- (e) added hydrogen (consistent with the structure of the compound and in accordance with further substitution)
- (f) saturation (‘hydro’/‘dehydro’ prefixes) or unsaturation (‘ene’, ‘yne)
- (g) substituents named as prefixes (low locants are allocated for substituents regardless of kind; then, if necessary, in the order of citation)

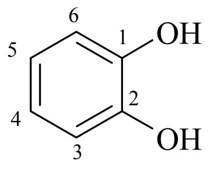
(2) by using functional nomenclature and the functional class term ‘alcohol’

(3) as assemblies of identical units when the conditions of symmetry are fulfilled

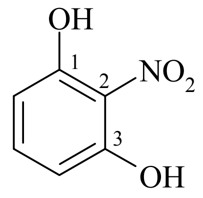
(4) retained names for general nomenclature only

Method (1) generates preferred IUPAC names rather than functional class names and names of assemblies of identical units are preferred to those that are formed by normal substitution.

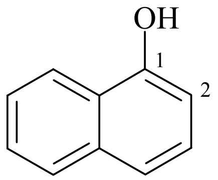
Examples:



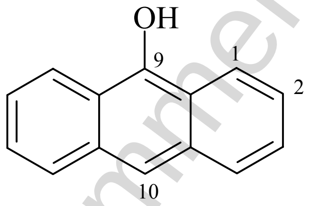
(1) benzene-1,2-diol (PIN)
(not pyrocatechol)



(1) 2-nitrobenzene-1,3-diol (PIN)



(1) naphthalen-1-ol (PIN)
(4) 1-naphthol



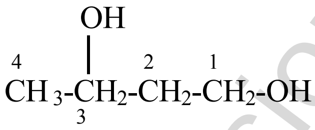
(1) anthracen-9-ol (PIN)
(4) 9-anthrol

CH_3-OH

(1) methanol (PIN)
(2) methyl alcohol

$(CH_3)_3C$-OH

(1) 2-methylpropan-2-ol (PIN)
(2) *tert*-butyl alcohol

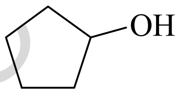


$\overset{4}{CH_3}-\underset{3}{\overset{OH}{CH}}-\overset{2}{CH_2}-\overset{1}{CH_2}-OH$

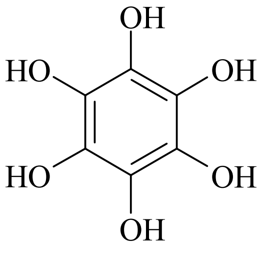
(1) butane-1,3-diol (PIN)

$HO-\overset{5}{CH_2}-\overset{4}{CH_2}-\overset{3}{CH}=\overset{2}{CH}-\overset{1}{CH_2}-OH$

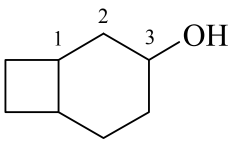
(1) pent-2-ene-1,5-diol (PIN)



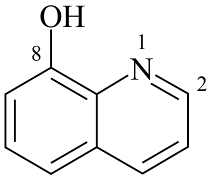
(1) cyclopentanol (PIN)



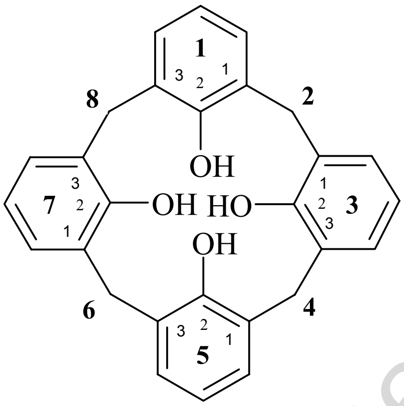
(1) benzenehexol (PIN)



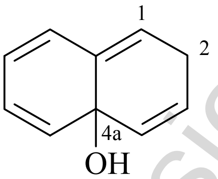
(1) bicyclo[4.2.0]octan-3-ol (PIN)



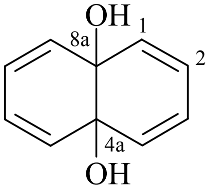
(1) quinolin-8-ol (PIN)



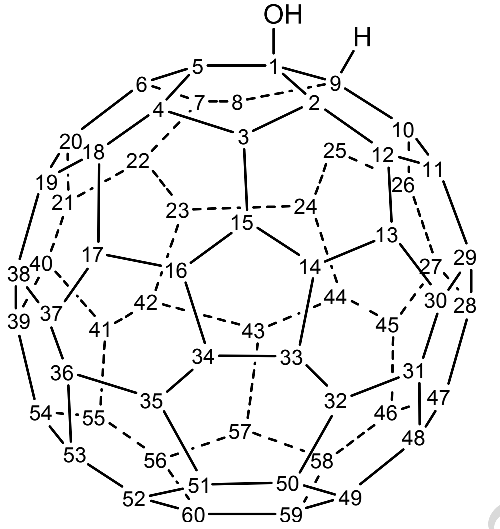
1,3,5,7(1,3)-tetrabenzenacyclooctaphane-1^2,3^2,5^2,7^2-tetrol (PIN)



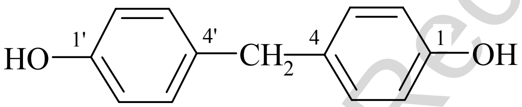
(1) naphthalen-4a(2*H*)-ol (PIN)
2,4a-dihydronaphthalen-4a-ol
(see P-53.1)



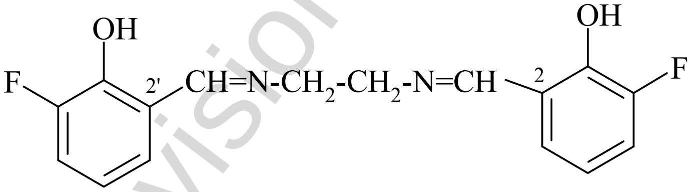
(1) naphthalene-4a,8a-diol (PIN)
4a,8a-dihydronaphthalene-4a,8a-diol
(see P-53.1)



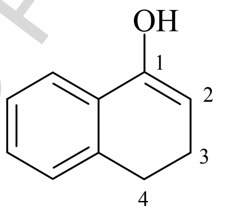
(1) (C_{60}-I_h)[5,6]fulleren-1(9*H*)-ol (see P-53.1) (PIN)
1,9-dihydro(C_{60}-I_h)[5,6]fulleren-1-ol (see P-53.1)

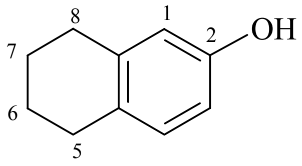


(3) 4,4′-methylenediphenol (PIN)
(1) 4-[(4-hydroxyphenyl)methyl]phenol

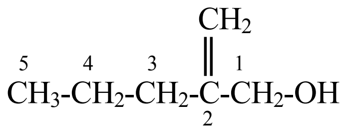


(3) 2,2′-[ethane-1,2-diylbis(azanylylidenemethanylylidene)]bis(6-fluorophenol) (PIN)



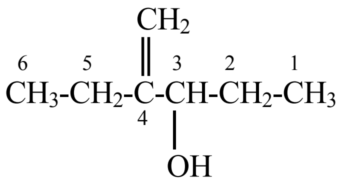


(1) 3,4-dihydronaphthalen-1-ol (PIN) (1) 5,6,7,8-tetrahydronaphthalen-2-ol (PIN)



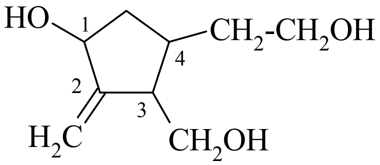
$$\overset{5}{CH_3}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{CH_2}\text{-}\underset{2}{\overset{\overset{CH_2}{\|}}{C}}\text{-}\overset{1}{CH_2}\text{-}OH$$

(1) 2-methylidenepentan-1-ol (PIN)

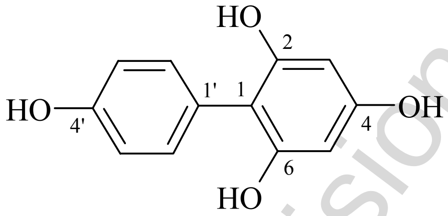


$$\overset{6}{CH_3}\text{-}\overset{5}{CH_2}\text{-}\underset{4}{\overset{\overset{CH_2}{\|}}{C}}\text{-}\overset{3}{\underset{\underset{OH}{|}}{CH}}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CH_3}$$

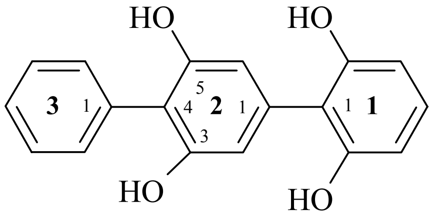
(1) 4-methylidenehexan-3-ol (PIN)



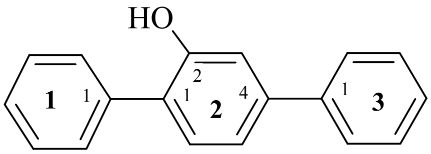
(1) 4-(2-hydroxyethyl)-3-(hydroxymethyl)-2-methylidenecyclopentan-1-ol (PIN)



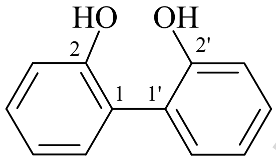
(1) [1,1′-biphenyl]-2,4,4′,6-tetrol (PIN)
biphenyl-2,4,4′,6-tetrol



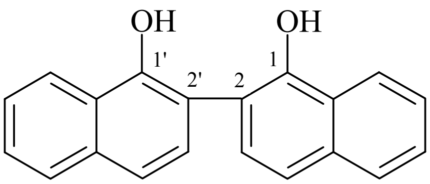
(1) [1^1,2^1:2^4,3^1-terphenyl]-1^2,1^6,2^3,2^5-tetrol (PIN)
[in the preferred name brackets enclose the name of an assembly requiring locants when suffixes are present; for numbering, see P-28.3.1(a)]
1,1′:4′,1″-terphenyl-2,3′,5′,6-tetrol
[see P-28.3.1(b)]



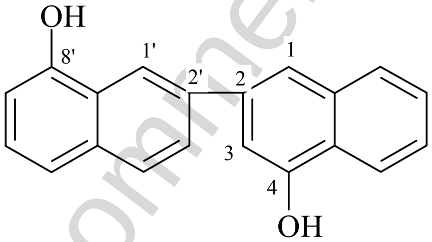
$[1^{1},2^{1}:2^{4},3^{1}$-terphenyl]-2^{2}-ol (PIN;
see P-28.3.1(a)]
1,1′:4′,1″-terphenyl-2′-ol [P-28.3.1(b)]



[1,1′-biphenyl]-2,2′-diol (PIN)
(not 2,2′-biphenol)



[2,2′-binaphthalene]-1,1′-diol (PIN)
(not 2,2′-bi-1-naphthol)



[2,2′-binaphthalene]-4,8′-diol (PIN)
(not 3,7′-bi-1-naphthol)

P-63.1.3 Heterols

When the hydroxy group is attached to an atom other than carbon, hydroxy compounds belong to a class called heterols. They are classified as hydroxy compounds and named using the suffix ‘ol’, unless they are classified as acids and denoted by a retained name. Names formed using a suffix are preferred to those formed by means of the prefix ‘hydroxy’.

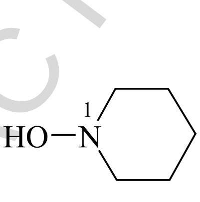
Examples:

$(CH_3)_3Si-OH$

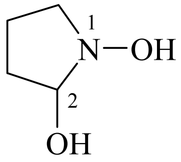
trimethylsilanol (PIN)
hydroxy(trimethyl)silane
(silane is a preferred preselected name; see P-12)

$(CH_3-CH_2)_2Al-OH$

diethylalumanol (PIN)
diethyl(hydroxy)alumane
(alumane is a preferred preselected name; see P-12)



piperidin-1-ol (PIN)
1-hydroxypiperidine
N-hydroxypiperidine



pyrrolidine-1,2-diol (PIN)
1-hydroxypyrrolidin-2-ol
N-hydroxypyrrolidin-2-ol

$P(OH)_3$ $H_2As\text{-}OH$

phosphorous acid (retained preselected name) (not phosphanetriol)

arsinous acid (retained preselected name) (not arsanol)

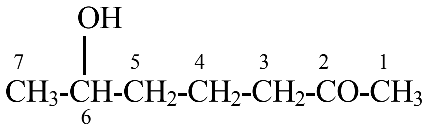
P-63.1.4 Substitutive nomenclature, prefix mode

Hydroxy groups are indicated by the prefix ‘hydroxy’ when:

(1) a group having priority for citation as the principal characteristic group is present; or

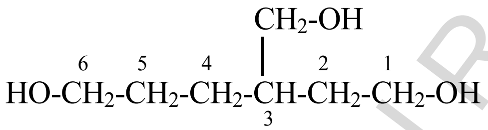
(2) a hydroxy group cannot be denoted by a suffix.

Examples:



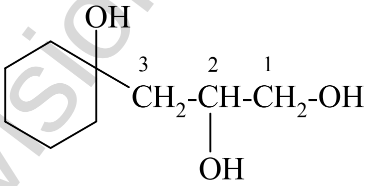
$$\overset{7}{C}H_3\text{-}\underset{6}{\overset{OH}{C}}H\text{-}\overset{5}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}O\text{-}\overset{1}{C}H_3$$

(1) 6-hydroxyheptan-2-one (PIN)

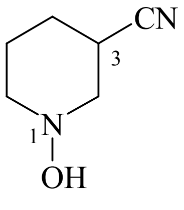


$$HO\text{-}\overset{6}{C}H_2\text{-}\overset{5}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\underset{3}{\overset{CH_2\text{-}OH}{C}}H\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}OH$$

(2) 3-(hydroxymethyl)hexane-1,6-diol (PIN)



(2) 3-(1-hydroxycyclohexyl)propane-1,2-diol (PIN)



(1) 1-hydroxypiperidine-3-carbonitrile (PIN)

$$\text{HO-PH-}\overset{3}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{1}{\text{C}}\text{OOH}$$

(1) 3-(hydroxyphosphanyl)propanoic acid (PIN)
3-(hydroxyphosphanyl)propionic acid

P-63.1.5 Sulfur, selenium, and tellurium analogues of hydroxy compounds

Sulfur, selenium, and tellurium analogues of hydroxy compounds are named substitutively using the suffixes ‘thiol’, ‘selenol’, and ‘tellurol’, and the prefixes ‘sulfanyl’, ‘selanyl’, and ‘tellanyl’, respectively; the presence of several of the same kind of ‘ol’ characteristic groups is denoted by the numerical multiplying prefixes ‘di’, ‘tri’, etc. The prefixes ‘mercapto’ (−SH), and ‘hydroseleno’ (−SeH) are no longer recommended.

Functional class nomenclature is not used.

Names of assemblies of identical units are formed by the general method described in P-15.3 and are preferred to those formed substitutively.

The seniority order of sulfur, selenium, and tellurium analogues of hydroxy compounds is:
O > S > Se > Te.

Examples:

$$\overset{3}{\text{C}}\text{H}_3\text{-}\overset{2}{\text{C}}\text{H(SH)-}\overset{1}{\text{C}}\text{H}_3$$

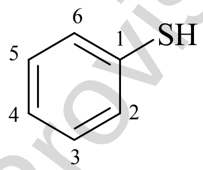
propane-2-thiol (PIN)

$\text{CH}_3\text{-CH}_2\text{-SeH}$

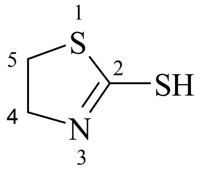
ethaneselenol (PIN)

$$\text{HS-}\overset{4}{\text{C}}\text{H}_2\text{-}\overset{3}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{1}{\text{C}}\text{H}_2\text{-SH}$$

butane-1,4-dithiol (PIN)



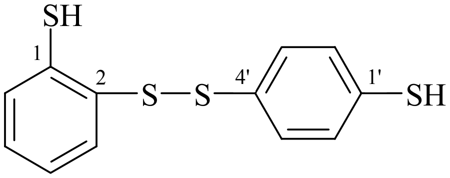
benzenethiol (PIN)
(not thiophenol)



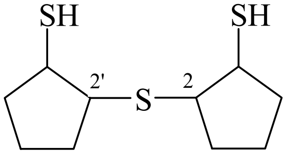
4,5-dihydrothiazole-2-thiol (PIN)

$$\text{HS-}\overset{3}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{1}{\text{C}}\text{OOH}$$

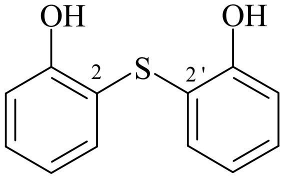
3-sulfanylpropanoic acid (PIN)



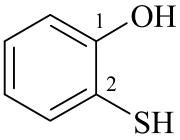
2,4′-disulfanediyldi(benzene-1-thiol) (PIN)



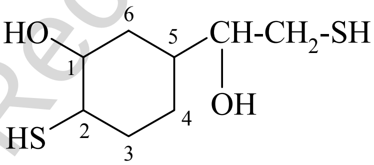
2,2′-sulfanediyldi(cyclopentane-1-thiol) (PIN)



2,2′-sulfanediyldiphenol (PIN)
2-[(2-hydroxyphenyl)sulfanyl]phenol



2-sulfanylphenol (PIN)



5-(1-hydroxy-2-sulfanylethyl)-2-sulfanylcyclohexan-1-ol (PIN)
(ring preferred to chain, see P-58.3.1.6)
1-(3-hydroxy-4-sulfanylcyclohexyl)-2-sulfanylethan-1-ol

P-63.2 Ethers and chalcogen analogs

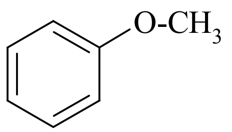
P-63.2.1 Definitions and general methodology
P-63.2.2 Names of substituent groups R′-O –, R′-S –, R′-Se –, and R′-Te –
P-63.2.3 Retained names
P-63.2.4 Systematic names of ethers
P-63.2.5 Chalcogen analogs of ethers: sulfides, selenides and tellurides

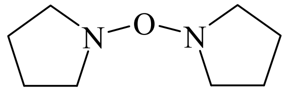
P-63.2.1 Definitions and general methodology

Ethers have the general formula R-O-R′, in which R = R′ or R ≠ R′; R and R′ can be any substituent group, aliphatic or cyclic, organyl (the free valence attached to a carbon atom) or organoheteryl (the free valence attached to an atom other than carbon), derived from the parent hydrides described in P-28.

Examples:

CH_3-O-CH_3 $(CH_3)_3$Si-O-CH_3 H_3Ge-O-GeH_3.





Chalcogen analogues are generically called sulfides, R-S-R′ , selenides, R-Se-R′ , and tellurides, R-Te-R′.

Names for ethers and their chalcogen analogues are formed by different methods in accordance with the principles of substitutive nomenclature, multiplicative nomenclature, skeletal replacement (‘a’) nomenclature, phane nomenclature, and functional class nomenclature. However, some ethers and chalcogen analogues are classified as parent hydrides and named as such, for example H_3Ge-O-GeH_3, digermoxane, and similar compounds described in Section P-21.2.3.1. These compounds are thus not named by the methods described in this Section, because their names are subject to selection rules with regard to heteroatom content.

In substitutive nomenclature, when R is different from R′, R is chosen as parent hydride and R′-O- is cited as a substituent to it. Names of these substituent groups are described in Section P-63.4.2. In functional class nomenclature, R and R′ are used as substituent groups.

P-63.2.2 Names of substituent groups R′-O –, R′-S –, R′-Se –, and R′-Te –

P-63.2.2.1 Systematic names

P-63.2.2.1.1 Substituent prefix names for R′-O– groups are formed by concatenation, i.e., by adding the prefix ‘oxy’ to the substituent prefix name for the group R′. These compound prefixes require the numerical multiplying prefixes ‘bis’, ‘tris’, etc.

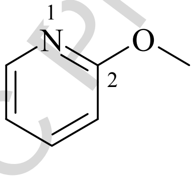
Examples:

CH_3-CH_2-CH_2-CH_2-CH_2-O–

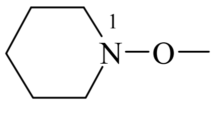
pentyloxy (PIN)

$\overset{4}{C}H_3$-$\overset{3}{C}H_2$-$\overset{2}{C}H(CH_3)$-O–

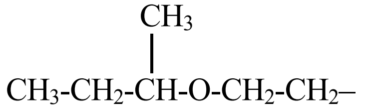
butan-2-yloxy (PIN)
(1-methylpropyl)oxy
sec-butoxy



pyridin-2-yloxy (PIN)
2-pyridyloxy



piperidin-1-yloxy (PIN)
piperidinooxy



$$CH_3\text{-}CH_2\text{-}\overset{\overset{\displaystyle CH_3}{|}}{C}H\text{-}O\text{-}CH_2\text{-}CH_2\text{–}$$

2-(butan-2-yloxy)ethyl (PIN)

P-63.2.2.1.2 Substituent prefixes for R′S–, R′Se–, and R′Te–, are substituents whose names are formed by substitution of the groups HS–, sulfanyl; HSe–, selanyl; and HTe–, tellanyl. The prefixes thus formed are preferred to compound prefixes formed by adding the name of the appropriate substituent to the prefix names thio, –S–; seleno, –Se–; or telluro, –Te–. The latter require the multiplicative prefixes 'bis', 'tris', etc.

Examples:

$CH_3\text{-}S\text{–}$
methylsulfanyl (PIN)
(not methylthio)

$C_6H_5\text{-}Se\text{–}$
phenylselanyl (PIN)
(not phenylseleno)

P-63.2.2.1.3 Divalent groups, such as –O-Y-O– or –S-Y-S–, are named by adding the prefixes oxy, sulfanediyl, etc. to the name of the divalent group Y. The multiplying prefix 'bis' is used in preferred names instead of 'di' to avoid ambiguity. Parentheses are used after the multiplying prefix 'bis', 'tris' etc., even around simple prefixes.

Examples:

$\text{–}O\text{-}CH_2\text{-}O\text{–}$
methylenebis(oxy) (PIN)
methylenedioxy

$\text{–}S\text{-}CH_2\text{-}S\text{–}$
methylenebis(sulfanediyl) (PIN)

$\text{–}CH_2\text{-}S\text{-}CH_2\text{–}$
sulfanediylbis(methylene) (PIN)
sulfanediyldimethylene

P-63.2.2.2 Retained names

Some contracted names are retained for R-O– substituent groups. They are used both as preferred IUPAC names and in general nomenclature; they are fully substitutable (with the exception of *tert*-butoxy), are compulsory prefixes, and are considered as simple prefixes requiring the numerical prefixes 'di', 'tri', etc. They are:

$CH_3\text{-}O\text{–}$
methoxy (PIN)

$CH_3\text{-}CH_2\text{-}O\text{–}$
ethoxy (PIN)

$CH_3\text{-}[CH_2]_2\text{-}O\text{–}$
propoxy (PIN)

$CH_3\text{-}[CH_2]_3\text{-}O\text{–}$
butoxy (PIN)

C_6H_5-O–	$(CH_3)_3$C-O–
phenoxy (PIN)	*tert*-butoxy (PIN) (no substitution)

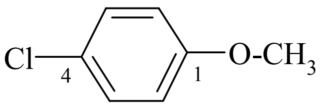
The following names are retained for use in general nomenclature only; no substitution is allowed:

$(CH_3)_2$CH-O–	CH_3-CH_2-CH(CH_3)-O–
isopropoxy propan-2-yloxy (PIN)	*sec*-butoxy butan-2-yloxy (PIN)

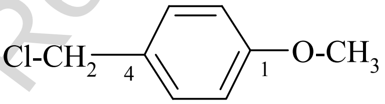
P-63.2.3 Retained names of ethers

Anisole, C_6H_5-O-CH_3, is the only name in the class of ethers which is retained both as a preferred IUPAC name and for use in general nomenclature. For preferred IUPAC names, no substitution is allowed; for general nomenclature substitution is allowed on the ring and on the side chain under certain conditions (see P-34.3.2, and P-46.3).

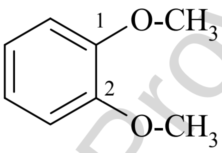
Examples:



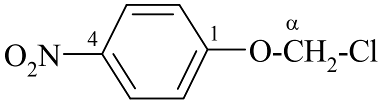
1-chloro-4-methoxybenzene (PIN)
(no substitution on anisole)
4-chloroanisole



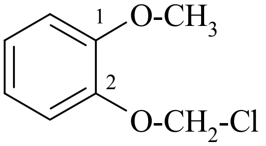
1-(chloromethyl)-4-methoxybenzene (PIN)
(no substitution on anisole)
4-(chloromethyl)anisole
(not 4-methoxybenzyl chloride; no substitution on benzyl)



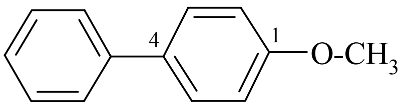
1,2-dimethoxybenzene (PIN)
(no substitution on anisole)
(not 2-methoxyanisole; see P-46.3 for substitution rules for anisole)



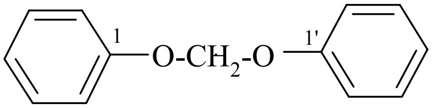
1-(chloromethoxy)-4-nitrobenzene (PIN)
(no substitution on anisole)
α-chloro-4-nitroanisole (see P-46.3 for substitution rules for anisole)



1-(chloromethoxy)-2-methoxybenzene (PIN)
(no substitution on anisole)
α-chloro-2-methoxyanisole
(not 2-(chloromethoxy)anisole)



4-methoxy-1,1′-biphenyl (PIN)
(not 4-phenylanisole nor 1-methoxy-4-phenylbenzene; the biphenyl ring system is senior to a single benzene ring)



1,1′-[methylenebis(oxy)]dibenzene (PIN)
α-phenoxyanisole

P-63.2.4 Systematic names of ethers

Ethers having the general structure R-O-R′ (R=R′, or R≠R′) have the class names ‘ethers’ and are named by one of the five following methods:

(1) substitutively by prefixing the name of the R′-O – group to that of the parent hydride;

(2) by functional class nomenclature, using the term ‘ether’ and, when the groups are different, citing the two substituent groups in alphanumerical order;

(3) by multiplicative nomenclature, when R and R′ are cyclic components;

(4) by skeletal replacement (‘a’) nomenclature;

(5) by phane nomenclature.

P-63.2.4.1 Names of ethers, when R and R′ are both aliphatic groups or when one is cyclic, are formed by methods (1), (2), or (4). Methods (1) and (5) lead to preferred IUPAC names.

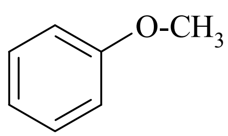
Examples:

CH_3-O-CH_3

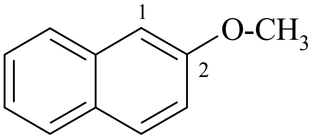
(1) methoxymethane (PIN)
(2) dimethyl ether

CH_3-CH_2-O-CH_3

(1) methoxyethane (PIN)
(2) ethyl methyl ether



(1) anisole (PIN; retained name)
methoxybenzene
(2) methyl phenyl ether



(1) 2-methoxynaphthalene (PIN)
(2) methyl naphthalen-2-yl ether
methyl 2-naphthyl ether

$Cl\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}O\text{-}CH_2\text{-}CH_3$

(1) 1-chloro-2-ethoxyethane (PIN)
(2) 2-chloroethyl ethyl ether
(not 2-chloroethyl ethyl oxide)

$CH_3\text{-}O\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}O\text{-}CH_3$

(1) 1,2-dimethoxyethane (PIN)
(2) ethane-1,2-diyl dimethyl ether

$CH_3\text{-}O\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_3$

(1) 1-methoxy-2-(2-methoxyethoxy)ethane (PIN)

Skeletal replacement (‘a’) nomenclature [method (4)] generates preferred IUPAC names, when the conditions for using this type of nomenclature are met; otherwise substitutive nomenclature must be used.

Examples:

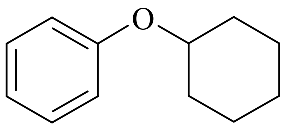
$\overset{1}{C}H_3\text{-}\overset{2}{O}\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{5}{O}\text{-}\overset{6}{C}H_2\text{-}\overset{7}{C}H_2\text{-}\overset{8}{O}\text{-}\overset{9}{C}H_2\text{-}\overset{10}{C}H_2\text{-}\overset{11}{O}\text{-}\overset{12}{C}H_3$

(4) 2,5,8,11-tetraoxadodecane (PIN)
(1) 1-methoxy-2-[2-(2-methoxyethoxy)ethoxy]ethane

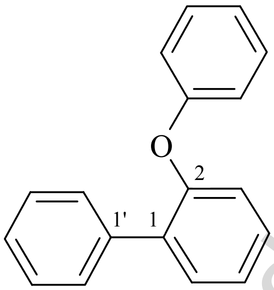
P-63.2.4.2 The names of ethers when both R and R′ groups are cyclic are formed by methods (1), (2), (3), and (5). Methods (1), (2), and (5) lead to preferred IUPAC names.

When method (1), substitutive nomenclature, is used, the senior ring or ring system must be chosen as the parent hydride (see P-44).

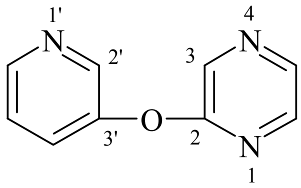
Examples:



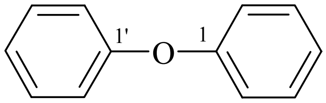
(1) (cyclohexyloxy)benzene (PIN)
(2) cyclohexyl phenyl ether



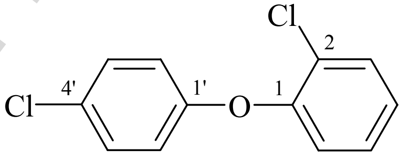
(1) 2-phenoxybiphenyl (PIN)
(2) biphenyl-2-yl phenyl ether



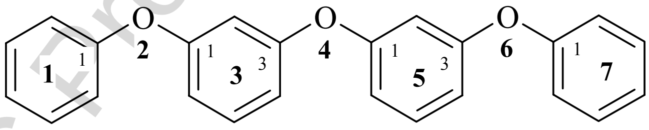
(1) 2-(pyridin-3-yloxy)pyrazine (PIN)
(2) pyrazin-2-yl 3-pyridyl ether



(2) 1,1′-oxydibenzene (PIN)
(1) phenoxybenzene
(3) diphenyl ether



(2) 2,4′-dichloro-1,1′-oxydibenzene (PIN)
(1) 1-chloro-2-(4-chlorophenoxy)benzene
(3) 2-chlorophenyl 4-chlorophenyl ether



(5) 2,4,6-trioxa-1,7(1),3,5(1,3)-tetrabenzenaheptaphane (PIN)

P-63.2.5 Names of chalcogen analogs of ethers: sulfides, selenides and tellurides

P-63.2.5.1 General methodology

Sulfides, R-S-R′, selenides R-Se-R′, and tellurides R-Te-R′, are named by the following methods:

(1) by prefixing the names of the substituent groups R′-S –, R′-Se –, or R′-Te –, i.e., R′-sulfanyl, R′-selanyl, and R′-tellanyl, respectively, to that of the appropriate parent hydride; the names R′-thio, R′-seleno, and R′-telluro are no longer recommended. The prefixes R′-sulfanyl, R′-selanyl, and R′-tellanyl are compulsory prefixes and can be attached to any atom of any parent hydride;

(2) by functional class nomenclature using the terms sulfides, selenides and tellurides for –S–, –Se –, and –Te –, respectively;

(3) by multiplicative nomenclature in the case of cyclic parent hydrides, using the prefixes sulfanediyl, –S– (not thio); selanediyl –Se – (not seleno); and tellanediyl –Te – (not telluro), respectively;

(4) by skeletal replacement (‘a’) nomenclature;

(5) by phane nomenclature;

Names formed by substituting the parent hydrides oxidane, sulfane, selane, and tellane for H_2O, H_2S, H_2Se, and H_2Te, respectively, by the appropriate substituent groups are not recommended.

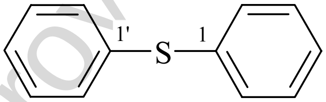
Names formed by functional replacement nomenclature of the retained name anisole are no longer recommended. Class names such as thiooxide are not recommended.

Method (1), substitutive nomenclature, is preferred to method (2), functional class nomenclature, for the formation of preferred IUPAC names; methods (3), (4), and (5) are applied in place of method (1) when the conditions for their use are satisfied.

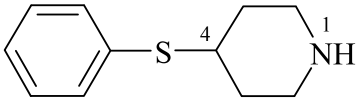
Examples:

CH_3-S-CH_3

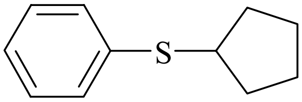
(1) (methylsulfanyl)methane (PIN)
(2) dimethyl sulfide



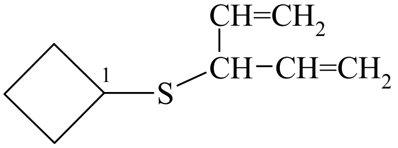
(3) 1,1′-sulfanediyldibenzene (PIN)
(not 1,1′-thiodibenzene)
(1) (phenylsulfanyl)benzene
(2) diphenyl sulfide



(a) 4-(phenylsulfanyl)piperidine (PIN)
[not 4-(phenylthio)piperidine]
(b) phenyl piperidin-2-yl sulfide



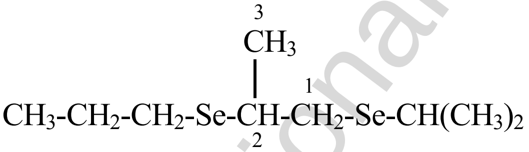
(a) (cyclopentylselanyl)benzene (PIN)
[not (cyclopentylseleno)benzene]
(b) cyclopentyl phenyl selenide



(1) 1-[(penta-1,4-dien-3-yl)sulfanyl)]cyclobutane (PIN)
(ring preferred to chain, see P-58.3.1.6)
(2) cyclobutyl penta-1,4-dien-3-yl sulfide

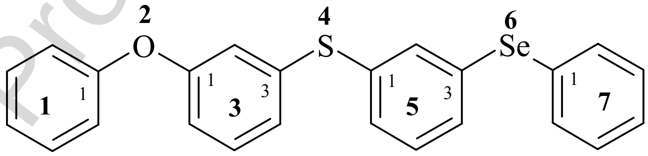
$$\overset{1}{CH_3}\text{-}\overset{2}{S}\text{-}\overset{3}{CH_2}\text{-}\overset{4}{S}\text{-}\overset{5}{CH_2}\text{-}\overset{6}{S}\text{-}\overset{7}{CH_2}\text{-}\overset{8}{CH}(CH_3)\text{-}\overset{9}{S}\text{-}\overset{10}{CH_2}\text{-}\overset{11}{S}\text{-}\overset{12}{CH_3}$$

(4) 8-methyl-2,4,6,9,11-pentathiadodecane (PIN)

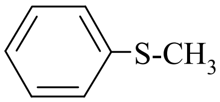


$$CH_3\text{-}CH_2\text{-}CH_2\text{-}Se\text{-}\underset{2}{\overset{\overset{3}{CH_3}}{CH}}\text{-}\overset{1}{CH_2}\text{-}Se\text{-}CH(CH_3)_2$$

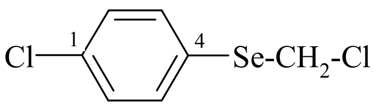
(1) 1-(propan-2-ylselanyl)-2-(propylselanyl)propane (PIN)
(not 2,5-dimethyl-3,6-diselenanonane; skeletal replacement (‘a’) nomenclature requires four heterounits)



(5) 2-oxa-4-thia-6-selena-1,7(1),3,5(1,3)-tetrabenzenaheptaphane (PIN)



(1) (methylsulfanyl)benzene (PIN)
(not thioanisole)



(1) 1-chloro-4-chloromethyl)selanyl]benzene (PIN)
(not α,4-dichloroselenoanisole)

P-63.3 Peroxides and chalcogen analogues

P-63.3.1 Peroxides, disulfides, diselenides, and ditellurides

Compounds with the general structures R-OO-R′ , R-SS-R′ , R-SeSe-R′ , and R-TeTe-R′ are named in the following ways:

(1) substitutively by combining the prefix name for R′ additively with ‘peroxy’ giving the names ‘R′-peroxy’, ‘R′-disulfanyl’, R′-diselanyl’ or R′-ditellanyl’ prefixed to the name of the parent hydride corresponding to R;

(2) by functional class nomenclature by citing the names of the groups R and R′, in alphanumerical order if two different groups are present, and the class name, peroxide, disulfide, diselenide, and ditelluride, respectively, as a separate word (class names such as dithioperoxide are not recommended);

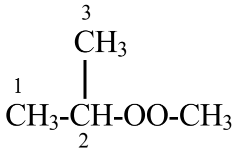
(3) by ring assembly nomenclature, multiplicative nomenclature, skeletal replacement (‘a’) nomenclature, or phane nomenclature, when the conditions for their application are fulfilled.

Method (1) leads to preferred IUPAC names.

Examples:

CH_3-CH_2-OO-CH_3

(1) (methylperoxy)ethane (PIN)
(2) ethyl methyl peroxide

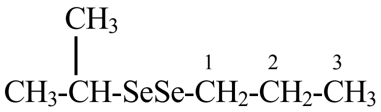


$\overset{1}{CH_3}\text{-}\underset{2}{CH}(\overset{3}{CH_3})\text{-OO-}CH_3$

(1) 2-(methylperoxy)propane (PIN)
(2) isopropyl methyl peroxide

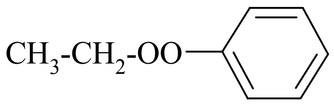
CH_3-SS-CH_3

(1) (methyldisulfanyl)methane (PIN)
(2) dimethyl disulfide



$CH_3\text{-}CH(CH_3)\text{-SeSe-}\overset{1}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{3}{CH_3}$

(1) 1-(propan-2-yldiselanyl)propane (PIN)
(2) isopropyl propyl diselenide



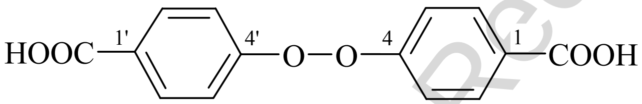
(1) (ethylperoxy)benzene (PIN)
(2) ethyl phenyl peroxide

$CH_3\text{-}SS\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}SeSe\text{-}CH_3$

(1) 1-(methyldiselanyl)-2-(methyldisulfanyl)ethane (PIN)

$CH_3\text{-}SeSe\text{-}\overset{1}{Si}H_2\text{-}\overset{2}{Si}H_2\text{-}TeTe\text{-}CH_3$

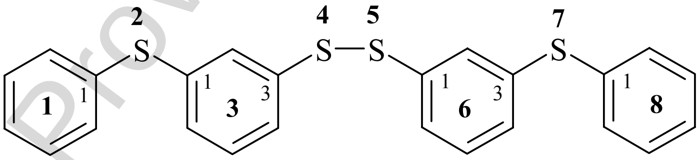
(1) 1-(methyldiselanyl)-2-(methylditellanyl)disilane (PIN)
(disilane is a preferred preselected name, see P-12)



(3) 4,4′-peroxydibenzoic acid (PIN)
[4-(4-carboxyphenyl)peroxy]benzoic acid

$\overset{1}{C}H_3\text{-}\overset{2}{S}\text{-}\overset{3}{C}H_2\text{-}\overset{4}{S}\text{-}\overset{5}{S}\text{-}\overset{6}{C}H_2\text{-}\overset{7}{C}H_2\text{-}\overset{8}{S}\text{-}\overset{9}{C}H_2\text{-}\overset{10}{C}H_2\text{-}\overset{11}{S}\text{-}\overset{12}{C}H_3$

(3) 2,4,5,8,11-pentathiadodecane (PIN)



(3) 2,4,5,7-tetrathia-1,8(1),3,6(1,3)-tetrabenzenaoctaphane (PIN)

P-63.3.2 Mixed chalcogen analogs of peroxides

Mixed chalcogen structures such as R-XY-R′ in which X and Y are O, S, Se, or Te atoms are named by two methods:

(1) by prefixing the names of the substituent groups R′-S –, R′-Se –, or R′-Te –, i.e., R′-sulfanyl, R′-selanyl, and R′-tellanyl, respectively, to that of the appropriate parent

hydride. The prefixes R′-sulfanyl, R′-selanyl, and R′-tellanyl are compulsory prefixes and can be attached to any atom of any parent hydride; multiplicative nomenclature is used when the conditions for its use are fulfilled;

(2) by citing the prefix names of the groups R and R′, in alphanumerical order, followed by an appropriate class name 'thioperoxide', 'diselenoperoxide', 'selenothioperoxide', etc. Each prefix R and R′ is preceded by a capital italicized letter locant, as appropriate;

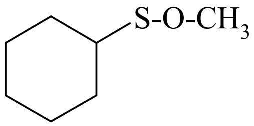
(3) by skeletal replacement ('a') nomenclature or phane nomenclature, when the conditions for its use are fulfilled.

Method (1) leads to preferred IUPAC names.

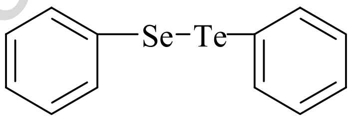
Examples:

CH_3-CH_2-OS-CH_3

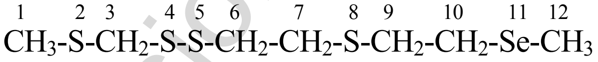
(1) [(methylsulfanyl)oxy]ethane (PIN)
(2) *O*-ethyl *S*-methyl thioperoxide



(1) (methoxysulfanyl)cyclohexane (PIN)
(2) *S*-cyclohexyl *O*-methyl thioperoxide

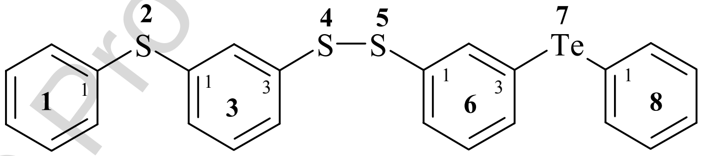


(1) (selanediyltellanediyl)dibenzene (PIN)
(2) diphenyl selenothioperoxide



$$\overset{1}{CH_3}\text{-}\overset{2}{S}\text{-}\overset{3}{CH_2}\text{-}\overset{4}{S}\text{-}\overset{5}{S}\text{-}\overset{6}{CH_2}\text{-}\overset{7}{CH_2}\text{-}\overset{8}{S}\text{-}\overset{9}{CH_2}\text{-}\overset{10}{CH_2}\text{-}\overset{11}{Se}\text{-}\overset{12}{CH_3}$$

(3) 2,4,5,8-tetrathia-11-selenadodecane (PIN)



(3) 2,4,5-trithia-7-tellura-1,8(1),3,6(1,3)-tetrabenzenaoctaphane (PIN)

P-63.4 Hydroperoxides (peroxols) and chalcogen analogues

P-63.4.1 Hydroperoxides

The suffix 'peroxol' is recommended for the characteristic group –OOH.

Compounds with the general structure R-OOH are called generically ‘hydroperoxides’. The class name ‘peroxols’ could be more appropriate. They are named in two ways when the –OOH group is the principal function.

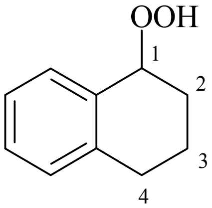
(1) substitutively using the suffix ‘peroxol’**;**

(2) by functional class nomenclature using the class name ‘hydroperoxide’.

The prefix ‘peroxy, not ‘dioxy’, is retained for the group –OO– (see P-63.4). The prefix ‘hydroperoxy’ is formed by concatenation to describe the group –OOH as a substituent in the presence of a characteristic group having priority for citation as a suffix.

Method (1) leads to preferred IUPAC names.

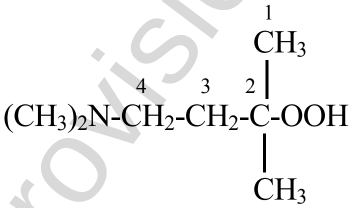
Examples:



(1) 1,2,3,4-tetrahydronaphthalene-1-peroxol (PIN)
(2) 1,2,3,4-tetrahydronaphthalen-1-yl hydroperoxide

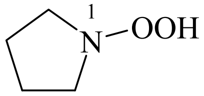
$HOO\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}C_6H_5$

2-hydroperoxy-1-phenylethan-1-one (PIN)



$$(CH_3)_2N\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\underset{\underset{CH_3}{|}}{\overset{\overset{\overset{1}{CH_3}}{|}}{\overset{2}{C}}}\text{-}OOH$$

(1) 4-(dimethylamino)-2-methylbutane-2-peroxol (PIN)
(2) [3-(dimethylamino)-1,1-dimethylpropyl] hydroperoxide
[3-(dimethylamino)-2-methylbutan-2-yl] hydroperoxide



(1) pyrrolidine-1-peroxol (PIN)
(2) pyrrolidin-1-yl hydroperoxide

P-63.4.2 Chalcogen analogues of hydroperoxides.

P-63.4.2.1 Compounds having the general structure R-SOH or R-OSH are called generically 'thiohydroperoxides' or 'thioperoxols'. Similarly, compounds R-SeOH or R-OSeH and R-TeOH or R-OTeH, are called 'selenohydroperoxides' or 'selenoperoxols' and tellurohydroperoxides' or 'telluroperoxols', respectively. When representing the principal function, they are named by two methods.

(1) by substitutive nomenclature and the appropriate suffix listed in Table 6.1, formed by functional replacement, to denote a principal function;

(2) by functional class nomenclature using the name of the class 'thiohydroperoxide', 'selenohydroperoxide' and 'tellurohydroperoxide'; when required, the prefixes, 'thio', 'seleno' and 'telluro' are placed in alphabetical order, for example, 'selenothiohydroperoxide', etc.; the locants *O, S, Se,* or *Te* designate the bonding of the R− group; when the same element is present the class names 'disulfide', 'diselenide', or 'ditelluride' are used.

Compounds of the type R-SOH, R-SeOH and R-TeOH and their chalcogen analogswere previously named sulfenic, selenenic and tellurenic acids, using the suffixes'sulfenic acid', 'selenenic acid', and 'tellurenic acid', respectively; this method is no longer recommended.

Method (1) generates preferred IUPAC names.

Table 6.1 Suffixes to denote peroxols (hydroperoxides) modified by functional replacement nomenclature (in decreasing order of seniority as principal group)

–S-OH	-*SO*-thioperoxol	–Se-SH	-*SeS*-selenothioperoxol
–Se-OH	-*SeO*-selenoperoxol	–Te-SH	-*TeS*-tellurothioperoxol
–Te-OH	-*TeO*-telluroperoxol	–S-SeH	-*SSe*-selenothioperoxol
–O-SH	-*OS*-thioperoxol	–S-TeH	-*STe*-tellurothioperoxol
–O-SeH	-*OSe*-selenoperoxol	–Se-SeH	-diselenoperoxol
–O-TeH	-*OTe*-telluroperoxol	–Te-SeH	-*TeSe*-selenotelluroperoxol
–S-SH	-dithioperoxol	–Se-TeH	-*SeTe*-selenotelluroperoxol
		–Te-TeH	-ditelluroperoxol

Examples:

CH_3-SOH

(1) methane-*SO*-thioperoxol (PIN)
(2) *S*-methyl thiohydroperoxide
(no longer methanesulfenic acid)

$\overset{3}{CH_3}-\overset{2}{CH_2}-\overset{1}{CH_2}-OSH$

(1) propane-1-*OS*-thioperoxol (PIN)
(2) *O*-propyl thiohydroperoxide

CH_3-CH_2-SSH

(1) ethanedithioperoxol (PIN)
(2) ethyl hydrodisulfide
ethyl dithiohydroperoxide

CH_3-SSeH

(1) methane-*SSe*-selenothioperoxol (PIN)
(2) *S*-methyl selenothiohydroperoxide

P-63.4.2.2 Prefixes corresponding to the suffixes described in P-63.4.2.1 are formed:

(1) by using prefixes such as ‘hydroperoxy’, –OOH; ‘disulfanyl’, –SSH, or by combining simple prefixes, ‘hydroxy’ –OH; ‘oxy-’, –O–; ‘sulfanyl’, –SH; etc.; or

(2) by using prefixes such as dithiohydroperoxy, −SSH; *SO*-thiohydroperoxy, −OSH; *SeS*-selenothiohydroperoxy, −SSeH; etc.

Method (1) leads to preferred IUPAC names.

Examples:

HOO-CH_2-CH_2-OH

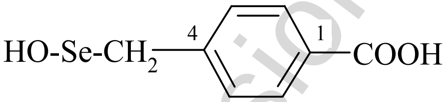
2-hydroperoxyethanol (PIN)

HSS-CH_2-COOH

(1) 2-disulfanylacetic acid (PIN)
(2) (dithiohydroperoxy)acetic acid

HS-O-CH_2-CH_2-CN

3-(sulfanyloxy)propanenitrile (PIN)
3-(*SO*-thiohydroperoxy)propanenitrile



4-[(hydroxyselanyl)methyl]benzoic acid (PIN)
4-(*OSe*-selenohydroperoxymethyl)benzoic acid

P-63.5 Cyclic ethers, sulfides, selenides, and tellurides

Cyclic ethers, sulfides, selenides and tellurides are heterocycles named by the following methods:

(1) preferred retained names described in P-55 are chosen first;

(2) for monocycles, by the extended Hantzsch-Widman system or by replacement nomenclature when the Hantzsch-Widman system is not applicable;

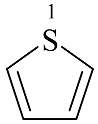
(3) by bridged fused nomenclature;

(4) by detachable prefixes ‘epoxy’, epithio’, ‘episeleno’, or ‘epitelluro’ in substitutive nomenclature;

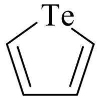
(5) by additive names formed by the addition of the terms 'oxide' , 'sulfide', selenide', or 'telluride' to the name of an unsaturated compound to the term.

As a general rule, names of heterocyclic compounds are preferred IUPAC names.

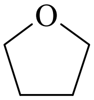
Examples:



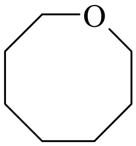
(1) thiophene (PIN)



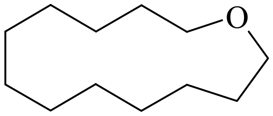
(1) tellurophene (PIN)



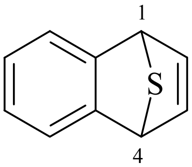
(1) oxolane (PIN)
tetrahydrofuran



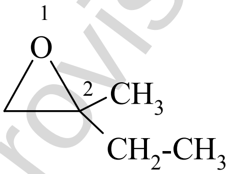
(1) thiocane (PIN)



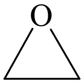
(2) oxacyclotridecane (PIN)



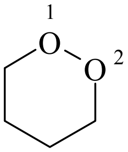
(3) 1,4-dihydro-1,4-sulfanonaphthalene (PIN)



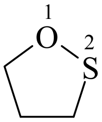
(2) 2-ethyl-2-methyloxirane (PIN)
(4) 1,2-epoxy-2-methylbutane



(2) oxirane (PIN)
(3) ethylene oxide



1,2-dioxane (PIN)



1,2-oxathiolane (PIN)

P-63.6 Sulfoxides and sulfones

Compounds with the general structures R-SO-R′ and R-SO$_2$-R′ are called generically ‘sulfoxides’ and ‘sulfones’, respectively, when R and R′ are hydrocarbyl groups. They are named in three ways as follows;

(1) substitutively, by prefixing the name of the acyl group R′-SO– or R′-SO$_2$– to the name of the parent hydride corresponding to R as described in P-65.3.2.2.2;

(2) by functional class nomenclature, using the class names ‘sulfoxide’ and ‘sulfone’, respectively;

(3) by multiplicative nomenclature,, except where R and R′ are alkyl groups.

Method (1) generates preferred names.

Selenium and tellurium analogues are named in the same way using acyl groups derived from the appropriate seleninic, selenonic, tellurenic, and telluronic acids, and the class names ‘selenoxide’, ‘selenone’, ‘telluroxide’, ‘tellurone’.

Prefix names such as ‘alkylsulfinyl’ or ‘arylsulfonyl’ are no longer recommended.

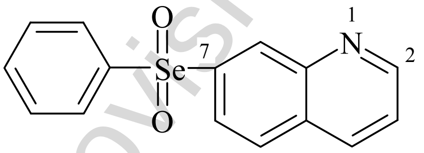
Examples:

$CH_3\text{-}CH_2\text{-}S(=O)\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_3$

(1) 1-(ethanesulfinyl)butane (PIN)
[not 1-(ethylsulfinyl)butane]
(2) butyl ethyl sulfoxide

$C_6H_5\text{-}Se(=O)\text{-}CH_2\text{-}CH_3$

(1) (ethaneseleninyl)benzene (PIN)
[not (ethylseleninyl)benzene]
(2) ethyl phenyl selenoxide



(1) 7-(benzeneselenonyl)quinoline (PIN)
[not 7-(phenylselenonyl)quinoline]
(2) phenyl quinolin-7-yl selenone
phenyl 7-quinolyl selenone

$C_6H_5\text{-}S(=O)\text{-}C_6H_5$

(3) sulfinyldibenzene (PIN)
(2) diphenyl sulfoxide
(1) benzenesulfinylbenzene
[not (phenylsulfinyl)benzene]

$C_6H_5\text{-}Se(=O)_2\text{-}C_6H_5$

(3) selenonyldibenzene (PIN)
(2) diphenyl selenone
(1) (ethaneselenonyl)ethane
[not (phenylselenonyl)benzene]

$CH_3\text{-}CH_2\text{-}S(=O)_2\text{-}CH_2\text{-}CH_3$

(1) (ethanesulfonyl)ethane (PIN)
[not (ethylsulfonyl)ethane]
(2) diethyl sulfone
(3) multiplication of acyclic hydrocarbons is not permitted)

P-63.7 Polyfunctional compounds

In the order of seniority of classes, hydroxy compounds and hydroperoxides are ranked in descending order after aldehydes and ketones, but before amines and imines. Chalcogen analogues are ranked after each class, according to the maximum number of O, S, Se, and Te atoms. In descending order, they are as follows.

(1) hydroxy compounds –OH, then their chalcogen analogues –SH > –SeH > –TeH

(2) hydroperoxides –OOH, then their chalcogen analogues –SOH > –SeOH > –TeOH, etc. (see Table 63.1)

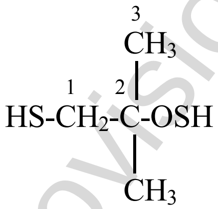
(3) amines > imines

(4) ethers –O–, then their chalcogen analogues –S– > –Se– > –Te–

(5) peroxides –OO–, then their chalcogen analogues –OS– > –OSe– > –OTe–, etc.

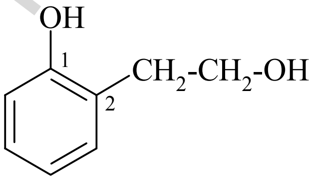
There is no seniority order between phenols and hydroxy compounds. The choice for parent hydride is decided by the maximum number of hydroxy groups cited as suffixes; and a ring is preferred to a chain when there is a choice (see P-58.3.1.6).

Examples:

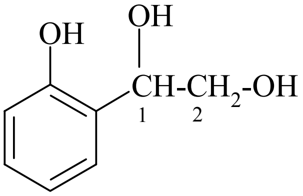


$$HS\text{-}\overset{1}{C}H_2\text{-}\underset{CH_3}{\overset{\overset{3}{CH_3}}{\overset{2}{C}}}\text{-}OSH$$

2-methyl-2-(sulfanyloxy)propane-1-thiol (PIN)



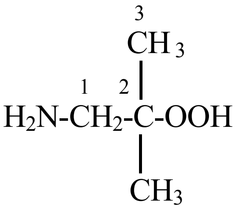
2-(2-hydroxyethyl)phenol (PIN)
2-(2-hydroxyphenyl)ethan-1-ol
(the ring is senior to the chain in the preferred name, see P-58.3.1.6)



1-(2-hydroxyphenyl)ethane-1,2-diol (PIN)
[not 2-(1,2-dihydroxyethyl)phenol; two principal groups are senior to one]

$\mathrm{HOO\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}OSeH}$

2-(selanyloxy)ethaneperoxol (PIN)

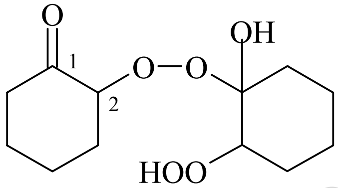


$$\mathrm{H_2N\text{-}\overset{1}{C}H_2\text{-}\underset{\underset{CH_3}{|}}{\overset{\overset{\overset{3}{CH_3}}{|}}{\overset{2}{C}}}\text{-}OOH}$$

1-amino-2-methylpropane-2-peroxol (PIN)

$\mathrm{CH_3\text{-}SO_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2OH}$

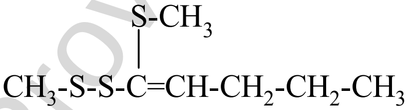
2-methanesulfonylethanol (PIN)



2-[(2-hydroperoxy-1-hydroxycyclohexyl)peroxy]cyclohexan-1-one (PIN)
(a ketone is senior to alcohols and peroxols)

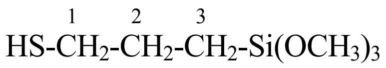
$\mathrm{H_2N\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}OH}$

2-aminoethan-1-ol (PIN)
(not ethanolamine)

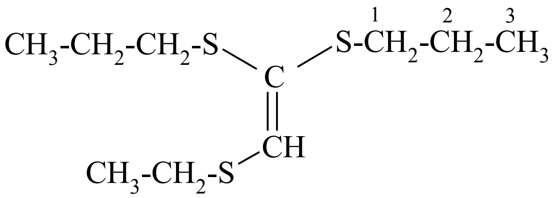


$$\mathrm{CH_3\text{-}S\text{-}S\text{-}\overset{\overset{S\text{-}CH_3}{|}}{C}{=}CH\text{-}CH_2\text{-}CH_2\text{-}CH_3}$$

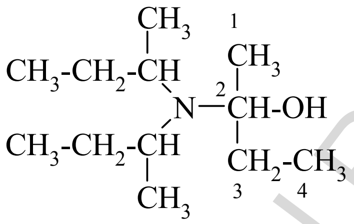
1-(methyldisulfanyl)-1-(methylsulfanyl)pent-1-ene (PIN)
1-methyl-2-[1-(methylsulfanyl)pent-1-en-1-yl]disulfane
methyl 1-(methylsulfanyl)pent-1-en-1-yl disulfide
(not 1-methyl-2-[1-(methylthio)pent-1-en-1-yl]disulfane;
nor methyl 1-(methylthio)pent-1-en-1-yl disulfide)


$HS\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}Si(OCH_3)_3$

3-(trimethoxysilyl)propane-1-thiol (PIN)
[not trimethoxy(3-sulfanylpropyl)silane; the suffix, ‘thiol’, has precedence over silane)



1-{[2-(ethylsulfanyl)-1-(propylsulfanyl)ethen-1-yl]sulfanyl}propane (PIN)
(multiplication of acyclic hydrocarbons is not permitted)



2-[di(butan-2-yl)amino]butan-2-ol (PIN)
2-(di-*sec*-butylamino)butan-2-ol

P-64 Ketones, pseudoketones, and heterones

P-64.0 Introduction

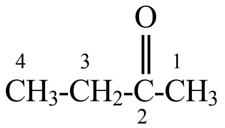
The substitutive nomenclature of ketones is well established. The suffix ‘one’ is used to denote a principal characteristic group, and the prefix ‘oxo’ is used when a characteristic group having seniority is present. The suffix ‘one’ and the prefix ‘oxo’ were indiscriminately used to name some classes compounds other than ketones. Full systematization based on the strict application of the suffix ‘one’ for denoting the principal characteristic group =O is recommended in this Section.

Traditionally, the nomenclature of ketones was described with that of aldehydes. In these recommendations, the two classes are discussed separately (for aldehydes, see P-66.6), to emphasize the similarities between carboxylic acids and aldehydes with respect to nomenclature. Finally, to avoid fragmentation, the nomenclature of acetals and ketals is discussed with that of aldehydes in Section P-66.6.

P-64.1 Definitions

P-64.1.1 Ketones are defined classically as compounds in which a carbonyl group is bonded to two carbon atoms: R_2CO (neither R may be H) (see ref. 17).

Example:



$$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\underset{2}{\overset{\overset{O}{\|}}{C}}\text{-}\overset{1}{C}H_3$$

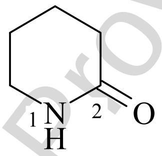
butan-2-one (PIN)

P-64.1.2 Pseudoketones are

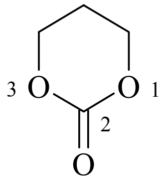
(a) cyclic compounds in which a carbonyl group in a ring is bonded to one or two skeletal heteroatoms; or

(b) compounds in which an acyclic carbonyl group is bonded to one or two acyclic skeletal heteroatoms, except nitrogen, halogen, or halogenoid atoms, or to a heteroatom of a ring or ring system. When the heteroatom of the ring is a nitrogen atom the compound has been called a ‘hidden amide’.

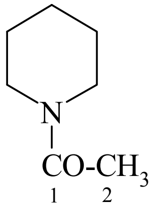
Examples:



(a) piperidin-2-one (PIN)



(a) 1,3-dioxan-2-one (PIN)



(b) 1-(piperidin-1-yl)ethan-1-one (PIN; a ‘hidden amide’)
1-acetylpiperidine

$H_3Si\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_3$

(b) 1-silylethan-1-one (PIN)
acetylsilane

$H_2P\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_3$

(b) 1-phosphanylpropan-1-one (PIN)
propanoylphosphane

$\overset{2}{C}H_3\text{-}\overset{1}{C}O\text{-}SS\text{-}O\text{-}CH_3$

(b) 1-(methoxydisulfanyl)ethan-1-one (PIN)
(see also P-58.4.2)

$\overset{3}{C}H_3\text{-}\overset{2}{C}H_3\text{-}\overset{1}{C}O\text{-}O\text{-}S\text{-}O\text{-}CH_3$

(b)1-[(methoxysulfanyl)oxy]propan-1-one (PIN)
(see also P-58.4.2)

P-64.1.3 Heterones

Heterones are compounds having an oxygen atom formally doubly bonded to a heteroatom (see P-62.3.1.3 and P-63.1.3; see also P-68).

This systematization, the adjunction of two new subclasses to the general class of ketones, clarifies the general use of suffixes and prefixes in substitutive nomenclature by always giving precedence to suffixes that designate a principal characteristic group.

P-64.2 Ketones

P-64.2.1 Retained names

For use in general nomenclature only, the names acetone, 1,4-benzoquinone, naphthoquinone, and anthraquinone are retained with full substitution on the corresponding structures. Also, the name ketene is retained for general nomenclature only, with substitution restricted to compulsory prefixes, and the names acetophenone and benzophenone are retained only for general nomenclature, but no substitution is allowed. (see P-34.3). Substitutive names, systematically constructed, are the preferred IUPAC names for ketones

P-64.2.2 Systematic construction of names for ketones.

P-64.2.2.1 Acyclic ketones

Unsubstituted acyclic ketones are systematically named in two ways:

(1) substitutively, using the suffix ‘one’ and the prefix ‘oxo’; the presence of several ‘one’ characteristic groups is denoted by the numerical multiplying prefixes ‘di’, ‘tri’, etc.; the final letter ‘a’ of a numerical multiplying prefix is elided before the suffix ‘-one’, for example, ‘tetrone’;

(2) by functional class nomenclature using the class names ‘ketone’, diketone’ etc.; substituent groups are placed, as separate words, in alphanumerical order before the class name.

Method (1) generates preferred IUPAC names.

Examples:

3 2 1
CH_3-CO-CH_3

propan-2-one (PIN)
propanone
acetone

4 3 2 1
CH_3-CH_2-CO-CH_3

butan-2-one (PIN)
ethyl methyl ketone
(not methyl ethyl ketone; groups must be cited in alphanumerical order)

7 6 5 4 3 2 1
CH_3-CH_2-CH_2-CH_2-CO-CH_2-CH_3

heptan-3-one (PIN)
butyl ethyl ketone

25 19 17 9 7 1
CH_3-$[CH_2]_5$-CO-CH_2-CO-$[CH_2]_7$-CO-CH_2-CO-$[CH_2]_5$-CH_3

pentacosane-7,9,17,19-tetrone (PIN)

6 5 4 3 2 1
CH_3-CH(CH_3)-CH_2-CH_2-CO-CH_3

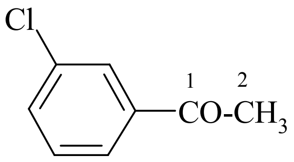
5-methylhexan-2-one (PIN)
isopentyl methyl ketone

1 2 3
C_6H_5-CH_2-CO-CH_3

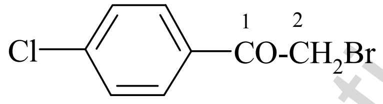
1-phenylpropan-2-one (PIN)
benzyl methyl ketone

1 2
C_6H_5-CO-CH_3

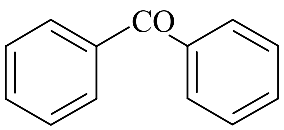
1-phenylethan-1-one (PIN)
acetophenone (no substitution)



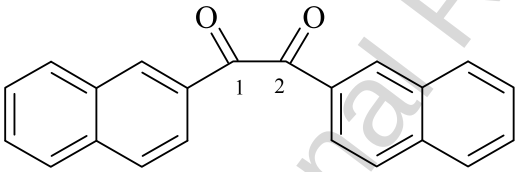
1-(3-chlorophenyl)ethan-1-one (PIN)
(not 3′-chloroacetophenone;
no substitution allowed for
acetophenone)



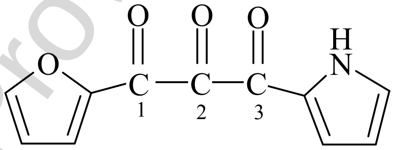
2-bromo-1-(4-chlorophenyl)ethan-1-one (PIN)
(not 4-chlorophenacyl bromide)
(not 2-bromo-4′-chloroacetophenone; no
substitution allowed for acetophenone)



diphenylmethanone (PIN)
benzophenone
diphenyl ketone



1,2-di(naphthalen-2-yl)ethane-1,2-dione (PIN)
di-2-naphthylethanedione
di-2-naphthyl diketone



1-(furan-2-yl)-3-(1*H*-pyrrol-2-yl)propane-1,2,3-trione (PIN)
1-(2-furyl)-3-(2-pyrrolyl)propanetrione
2-furyl-2-pyrrolyl triketone

P-64.2.2.2 Cyclic ketones

Names of cyclic ketones are formed substitutively by using the suffix ‘one’. As the formation of ketones is achieved by the conversion of a methylene, $>CH_2$, group into a $>C=O$ group, the suffix ‘one’ with appropriate locants can be added to the name of parent hydrides having such groups.

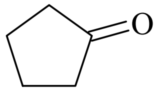
Methylene groups occur in saturated rings and ring systems and in mancude compounds having indicated hydrogen atoms.

Mancude compounds not having suitably located indicated hydrogen atoms or composed only of =CH– groups, must be hydrogenated in order to create >CH_2 groups; when the hydrogenation operation occurs simultaneously with substitution by the >C=O, it is called ‘added hydrogen’.(see P-14.6). The added hydrogen method generates preferred IUPAC names.

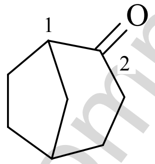
P-64.2.2.2.1 Alicyclic ketones

Ketones resulting from the substitution of >CH_2 groups are named substitutively using the suffix ‘one’ to designate the principal characteristic group.

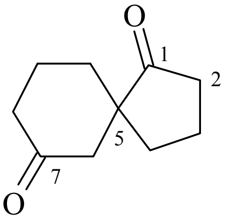
Examples:



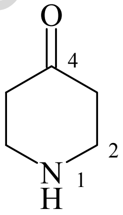
cyclopentanone (PIN)



bicyclo[3.2.1]octan-2-one (PIN)



spiro[5.6]decane-1,7-dione (PIN)

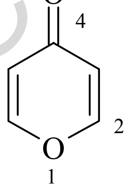


piperidin-4-one (PIN)

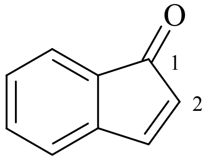
P-64.2.2.2.2 Ketones derived from mancude parent hydrides

Ketones derived from mancude parent hydrides having indicated hydrogen atoms are named by direct substitution of a >CH_2 group as indicated in P-64.2.2.2.1. When no indicated hydrogen is present, the methodology of ‘added hydrogen’ is applied (see P-14.6).

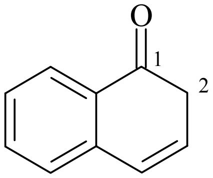
Examples:



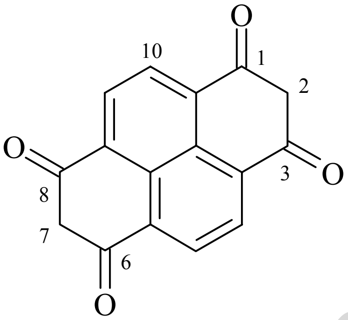
4*H*-pyran-4-one (PIN)
pyran-4-one



1*H*-inden-1-one (PIN)
inden-1-one



naphthalen-1(2*H*)-one (PIN)
1,2-dihydronaphthalen-1-one

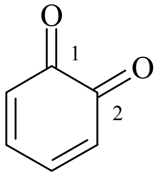


chrysene-1,3,6,8(2*H*,7*H*)-tetrone (PIN)
1,2,3,6,7,8-hexahydrochrysene-1,3,6,8-tetrone

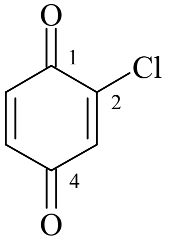
P-64.2.2.2.3 Quinones

No retained quinone names are used as preferred IUPAC names. 1,4-benzoquinone, naphthoquinone, and anthraquinone are retained for use in general nomenclature with full substitution. All other quinones are named systematically. Diketones derived from mancude compounds without indicated hydrogen atoms by conversion of two or four =CH− groups into >C=O groups with any rearrangement of double bonds to a quinonoid structure are named systematically (see P-64.2.2.2.2).

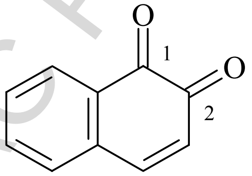
Examples:



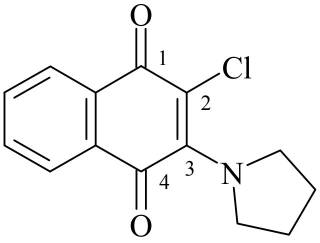
cyclohexa-3,5-diene-1,2-dione (PIN)
(not 1,2-benzoquinone)
(not *o*-benzoquinone)



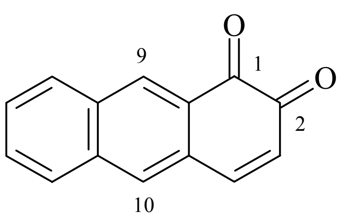
2-chlorocyclohexa-2,5-diene-1,4-dione (PIN)
2-chloro-1,4-benzoquinone
(not 2-chloro-*p*-benzoquinone)



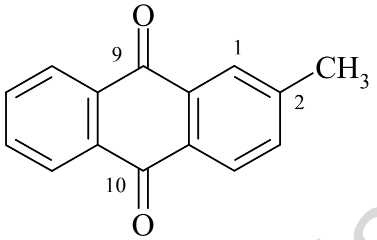
naphthalene-1,2-dione(PIN)
naphthalene-1,2-quinone



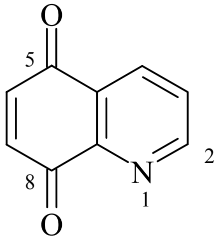
2-chloro-3-(pyrrolidin-1-yl)naphthalene-1,4-dione (PIN)
2-chloro-3-(pyrrolidin-1-yl)-1,4-naphthoquinone



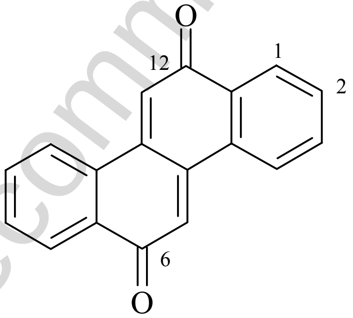
anthracene-1,2-dione (PIN)
anthracene-1,2-quinone



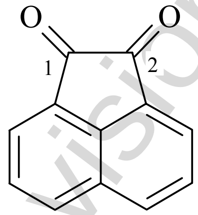
2-methylanthracene-9,10-dione (PIN)
2-methylanthracene-9,10-dione
2-methylanthracene-9,10-quinone



quinoline-5,8-dione (PIN)
(not quinoline-5,8-quinone)



chrysene-6,12-dione (PIN)
(not chrysene-6,12-quinone);



acenaphthylene-1,2-dione (PIN)
acenaphthylene-1,2-quinone)

P-64.2.2.3 Seniority order for numbering

When there is a choice for numbering, the starting point and the direction of numbering of a compound are chosen so as to give lowest locants to the following structural features (if present) considered successively in the order given until a decision is reached.

(a) fixed numbering (naphthalene, bicyclo[2.2.2]octane, etc.)

(b) heteroatoms in heterocycles and in acyclic parent structures

(c) indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with structural feature (d)]

(d) principal group named as suffix

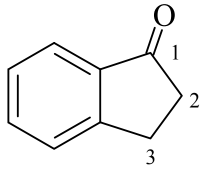
(e) added hydrogen (consistent with the structure of the compound and in accordance with further substitution)

(f) saturation (‘hydro’/‘dehydro’ prefixes) or unsaturation (‘ene’, ‘yne’ endings)

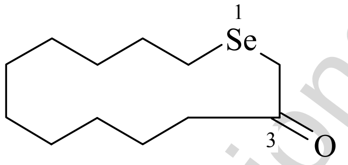
(g) substituents named as prefixes (low locants are allocated for substituents regardless of kind; then, if necessary, in the order of citation).

Rule P-44 is applied when a choice for the principal chain or senior ring system is required.

Examples:



2,3-dihydro-1*H*-inden-1-one (PIN; see P-53.1)
indan-1-one



1-selenacyclotridecan-3-one (PIN)

$\overset{1}{CH_3}\text{-}\overset{2}{SiH_2}\text{-}CH_2\text{-}\overset{4}{SiH_2}\text{-}CH_2\text{-}\overset{6}{SiH_2}\text{-}CH_2\text{-}\overset{8}{SiH_2}\text{-}CH_2\text{-}\overset{10}{CO}\text{-}\overset{11}{CH_3}$

2,4,6,8-tetrasilaundecan-10-one (PIN)

$\overset{4}{CH_2}=\overset{3}{CH}\text{-}\overset{2}{CO}\text{-}\overset{1}{CH_3}$

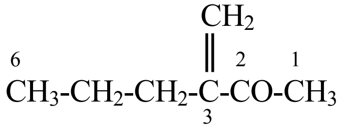
but-3-en-2-one (PIN)

$\overset{5}{CH_3}\text{-}\overset{4}{C}\equiv\overset{3}{C}\text{-}\overset{2}{CO}\text{-}\overset{1}{CH_3}$

pent-3-yn-2-one (PIN)

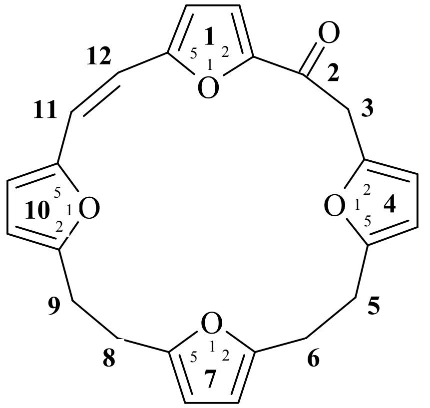
$\overset{1}{CH_2}=\overset{2}{CH}\text{-}\overset{3}{CO}\text{-}\overset{4}{C}\equiv\overset{5}{CH}$

pent-1-en-4-yn-3-one (PIN)

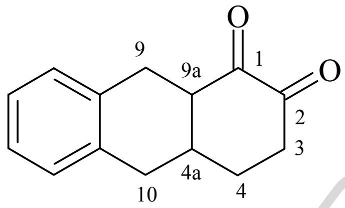


$\overset{6}{CH_3}\text{-}CH_2\text{-}CH_2\text{-}\underset{3}{\overset{\overset{\displaystyle CH_2}{\|}}{C}}\text{-}\overset{2}{CO}\text{-}\overset{1}{CH_3}$

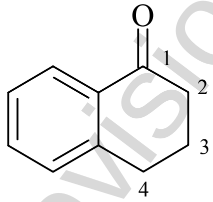
3-methylidenehexane-2-one (PIN)



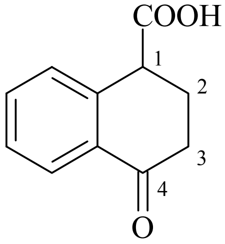
1,3,6,8(2,5)-tetrafuranacyclodecaphane-11-en-2-one (PIN)



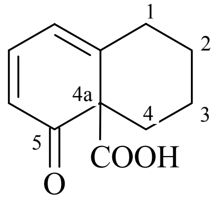
3,4,4a,9,9a,10-hexahydroanthracene-1,2-dione (PIN)
(not 3,4,4a,9,9a,10-hexahydroanthraquinone)
(not 1,2,3,4,4a,9,9a,10-octahydroanthracene-1,2-dione)



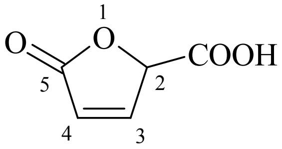
3,4-dihydronaphthalen-1(2*H*)-one (PIN; see P-53.1)
1,2,3,4-tetrahydronaphthalen-1-one



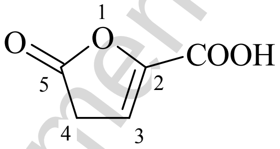
4-oxo-1,2,3,4-tetrahydronaphthalene-1-carboxylic acid (PIN)



5-oxo-1,3,4,5-tetrahydronaphthalene-4a(2*H*)-carboxylic acid (PIN)



5-oxo-2,5-dihydrofuran-2-carboxylic acid (PIN)

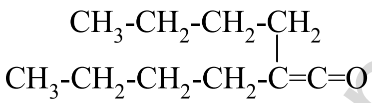


5-oxo-4,5-dihydrofuran-2-carboxylic acid (PIN)

P-64.2.2.4 Ketenes

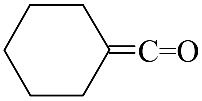
Ketene is the class name for $H_2C{=}C{=}O$ and its derivatives; the name ketene can be used in general nomenclature to name the unsubstituted structure and derivatives named by compulsory prefixes. Other derivatives are named by using the principles for naming ketones.

Examples:



$$\begin{array}{r} CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2 \\ | \\ CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}C{=}C{=}O \end{array}$$

2-butylhex-1-en-1-one (PIN)
(not dibutylketene)



cyclohexylidenemethanone (PIN)

$Br_2C{=}C{=}O$

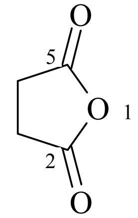
2,2-dibromoethen-1-one (PIN)
dibromoketene

P-64.3 Pseudoketones.

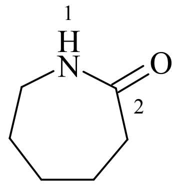
Pseudoketones are compounds having a carbonyl group joined to a carbon atom and a heteroatom, −C-CO-X−, or to two heteroatoms, −X-CO-X−, where X ≠ F, Cl, Br, I, pseudohalogen, or acyclic N. These compounds are named substitutively using the suffix ‘one’, in accordance with rules expressed for ketones, when required.

P-64.3.1 Cyclic anhydrides, esters and amides are named as pseudoketones; the resulting names are preferred IUPAC names.

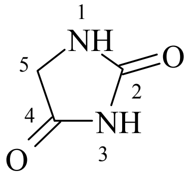
Examples:



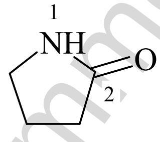
oxolane-2,5-dione (PIN)
succinic anhydride (see P-65.7.3)



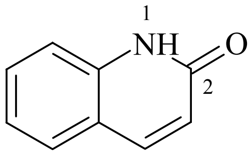
azepan-2-one ((PIN)
hexano-6-lactam (see P-66.1.4.1)



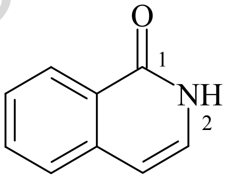
imidazolidine-2,4-dione (PIN)



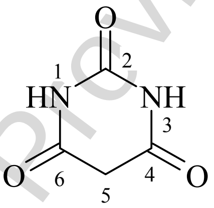
pyrrolidin-2-one (PIN)
2-pyrrolidone



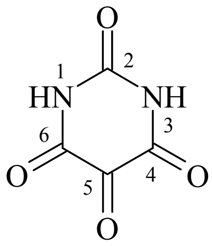
quinolin-2(1*H*)-one (PIN)
1,2-dihydroquinolin-2-one



isoquinolin-1(2*H*)-one (PIN)
1,2-dihydroisoquinolin-1-one



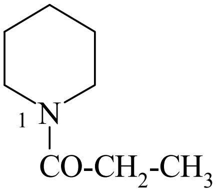
pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (PIN)



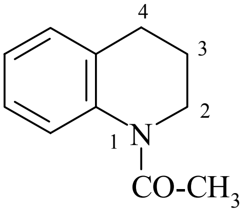
1,3,5-triazine-2,4,6(1*H*,3*H*,5*H*)-trione (PIN)

P-64.3.2 Acyclic pseudoketones, including those in which the carbonyl group is linked to a heteroatom of a heterocycle (hidden amides, for instance), are named substitutively by using the suffix 'one' to indicate the principal function. This method is preferred to that using acyl groups, when present, to denote the –CO-R group.

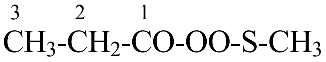
Examples:



1-(piperidin-1-yl)propan-1-one (PIN)
1-propanoylpiperidine

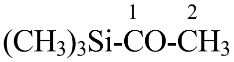


1-(1,2,3,4-tetrahydroquinolin-1-yl)ethan-1-one (PIN)
1-acetyl-1,2,3,4-tetrahydroquinoline



$\overset{3}{CH_3}$-$\overset{2}{CH_2}$-$\overset{1}{CO}$-OO-S-CH_3

1-[(methylsulfanyl)peroxy]propan-1-one (PIN)
(see also P-68.4.2)



$(CH_3)_3Si$-$\overset{1}{CO}$-$\overset{2}{CH_3}$

1-(trimethylsilyl)ethan-1-one (PIN)
acetyl(trimethyl)silane

P-64.4 Heterones

Heterones are compounds having an oxygen atom formally doubly bonded to a heteroatom (see P-664,1,3, P-62.3.1.3, and P-63.1.3; see also P-68).

P-64.4.1 Acyclic heterones
P-64.4.2 Thioketone and thioaldehyde oxides

P-64.4.1 Acyclic heterones are compounds having an oxygen atom doubly bonded to a heteroatom. They may be named in two ways.

(1) by the suffix 'one';

(2) by functional class names using the class name 'oxide' when the oxygen atom is bonded to a S, Se, Te, P, As, Sb, or Bi atom.

Method (1) leads to preferred IUPAC names.

The distinction between ketones, 'C-CO-C', and aldehydes, 'C-CHO', is not retained for naming compounds having the oxygen atom linked to a heteroatom. Sulfones, sulfoxides, and related chalcogen compounds are exceptions (see P-63.6)

Examples:

$HP{=}O$

(1) phosphanone (PIN)
(2) phosphane oxide
(not phosphine oxide)

$(CH_3)_2Si{=}O$

dimethylsilanone (PIN)

$(C_6H_5)_3PO$

(1) triphenyl-λ^5-phosphanone (PIN)
(2) triphenylphosphane oxide
(not triphenylphosphine oxide)

$CH_3\text{-}SO\text{-}CH_2CH_3$

methanesulfonylethane (PIN; see P-63.6)
(2) ethyl methyl sulfoxide
(1) ethyl(methyl)-λ^4-sulfanone

Thioketone oxides are named by two methods.

(1) substitutively, as heterones, using the suffix ‘one’;

(2) by functional class nomenclature, using the class name ‘oxide’, and ‘dioxide’, if required.

Method (1) leads to preferred IUPAC names.

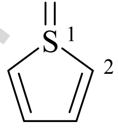
Example:

$CH_3\text{-}CH_2\text{-}CH{=}S{=}O$

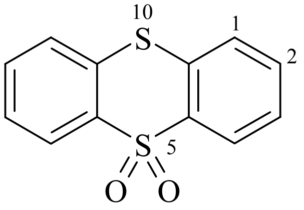
(1) propylidene-λ^4-sulfanone (PIN)
(2) propanethial oxide

When a group –SO– or –SO_2– is part of a ring system, oxygen atom(s) are expressed substitutively by the suffix ‘-one’ added to the name of the heterocycle in which the sulfur atoms are designated as λ^4 or λ^6 atoms (see P-14.10). This method generates preferred IUPAC names rather than those based on functional class nomenclature, in which the class name ‘oxide’ follows the name of the heterocycle.

Examples:



1λ^4-thiophen-1-one (PIN)
thiophene oxide



5λ^6-thianthrene-5,5-dione (PIN)
thianthrene 5,5-dioxide

P-64.5 Expressing carbonyl groups as prefixes

When a carbonyl group is not the principal characteristic group expressed as a suffix, it is denoted by a prefix. Three types of prefixes are used:

(1) the prefix ‘oxo’ when the doubly bonded oxygen atom (ketone, pseudoketone, or heterone group) is not in position 1 of a side chain. Lowest possible locants are assigned to suffixes, and then to prefixes;

(2) carbonyl groups in position 1 of a side chain, i.e., –CO-R, are described by the appropriate acyl group name (see P-65.2 for names of acyl groups);

(3) the group –CO– is named substitutively as the acyl group ‘carbonyl’; the group =C=O is named substitutively as ‘oxomethylidene’; the substituent group –CHO is named substitutively as the acyl group ‘formyl’, .

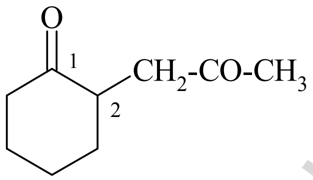
P-64.5.1 Ketones

The prefix ‘oxo’ and/or acyl prefixes are used to denote carbonyl groups when:

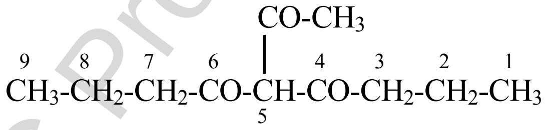
(a) all carbonyl or oxo groups cannot be cited as suffixes; or

(b) in the presence of a characteristic group having priority to be cited as suffix.

Examples:



2-(2-oxopropyl)cyclohexan-1-one (PIN)
(ring preferred to chain; see P-58.3.1.6)
2-acetonylcyclohexan-1-one
2-(2-oxocyclohexyl)propan-2-one

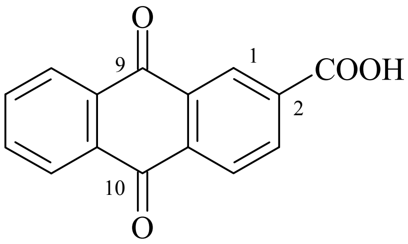


$$\overset{9}{\mathrm{CH_3}}\text{-}\overset{8}{\mathrm{CH_2}}\text{-}\overset{7}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{CO}}\text{-}\underset{5}{\overset{\overset{\mathrm{CO\text{-}CH_3}}{|}}{\mathrm{C}}}\mathrm{H}\text{-}\overset{4}{\mathrm{CO}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{CH_3}}$$

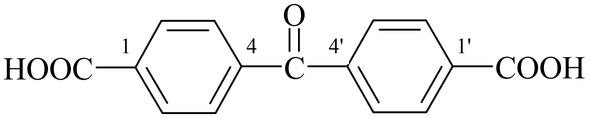
5-acetylnonane-4,6-dione (PIN)
[not 5-(1-oxoethyl)nonane-4,6-dione]

$$\overset{4}{\mathrm{CH_3}}\text{-}\overset{3}{\mathrm{CO}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{COOH}}$$

3-oxopropanoic acid (PIN)
(not 3-oxopropionic acid)



9,10-dioxo-9,10-dihydroanthracene-2-carboxylic acid (PIN)
(not 9,10-anthraquinone-2-carboxylic acid)



4,4′-carbonyldibenzoic acid (PIN)
4,4′-(oxomethylene)dibenzoic acid
4-(4-carboxybenzoyl)benzoic acid (substitutive name)

P-64.5.2 Pseudoketones

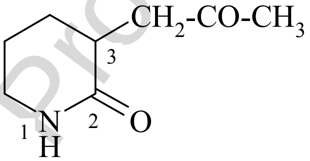
P-64.5.2.1 In cyclic pseudoketones, the prefix ‘oxo’ and/or acyl group prefixes are used to denote a carbonyl group:

(a) when all carbonyl groups cannot be cited as suffixes; or

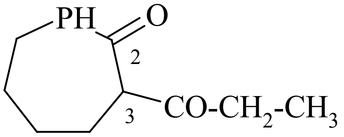
(b) in the presence of a characteristic group having priority to be cited as suffix;

Formerly, acyl groups were used to name pseudoketones in so-called ‘hidden amides’ having the structure R-CO-N<, where the nitrogen atom is part of a ring or ring system.

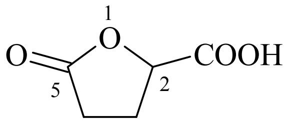
Examples:



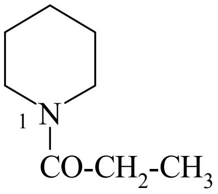
3-(2-oxopropyl)piperidin-2-one (PIN)
(ring preferred to chain, see
P-58.3.1.6)
3-acetonylpiperidin-2-one
3-(2-oxopiperidin-3-yl)propan-2-one



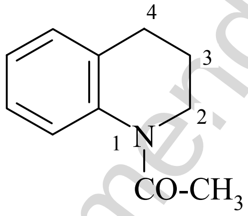
3-propanoylphosphepan-2-one (PIN)
3-propionylphosphepan-2-one



5-oxooxolane-2-carboxylic acid (PIN)



1-(piperidin-1-yl)propan-1-one (PIN)
1-propanoylpiperidine
. 1-propionylpiperidine
(a ‘hidden amide’)



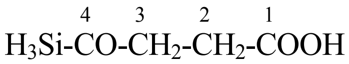
(1,2,3,4-tetrahydroquinolin-1-yl)ethan-1-one (PIN)
1-acetyl-1,2,3,4-tetrahydroquinoline
(a ‘hidden amide’)

P-64.5.2.2 Acyclic pseudoketones are named in the same way; traditionally they have been named using acyl groups.

Examples:

$H_2P\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CH_3$

1-phosphanylbutan-1-one (PIN)
butanoylphosphane



$H_3Si\text{-}\overset{4}{C}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

4-oxo-4-silylbutanoic acid (PIN)
3-silanecarbonylpropanoic acid

P-64.6 Chalcogen analogs of ketones, pseudoketones and heterones

P-64.6.1 Chalcogen analogs of ketones, pseudoketones and heterones are named by using the following suffixes and prefixes:

=S ‘-thione’ and ‘sulfanylidene’ (preferred to ‘thioxo’)

=Se ‘-selone’ and ‘selanylidene‘ (preferred to ‘selenoxo’)

=Te ‘-tellone’ and ‘tellanylidene’ (preferred to ‘telluroxo’)

Acyl group prefixes are named by functional replacement of O by S, Se, and Te using infixes (see P-65.2). The use of functional replacement prefixes ‘thio’ or ‘seleno’ with retained names is no longer recommended; all preferred IUPAC names are systematically constructed.

Examples:

4 3 2 1
$CH_3\text{-}CH_2\text{-}CS\text{-}CH_3$

butane-2-thione (PIN)

1 2 3 4 5 6
$CH_3\text{-}CH_2\text{-}CSe\text{-}CH_2\text{-}CH_2\text{-}CH_3$

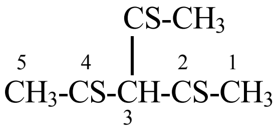
hexane-3-selone (PIN)

5 4 3 2 1
$CH_3\text{-}CS\text{-}CH_2\text{-}CS\text{-}CH_3$

pentane-2,4-dithione (PIN)

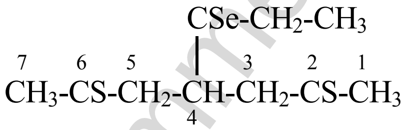
3 2 1
$CH_3\text{-}CS\text{-}CH_3$

propane-2-thione (PIN)
(not thioacetone)



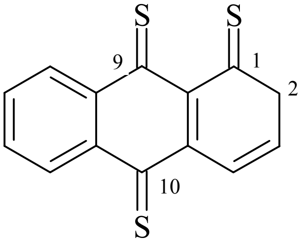
$\overset{5}{CH_3}\text{-}\overset{4}{CS}\text{-}\underset{3}{\overset{CS\text{-}CH_3}{|}{CH}}\text{-}\overset{2}{CS}\text{-}\overset{1}{CH_3}$

3-(thioacetyl)pentane-2,4-dithione (PIN)
3-(ethanethioyl)pentane-2,4-dithione

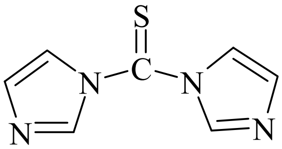


$\overset{7}{CH_3}\text{-}\overset{6}{CS}\text{-}\overset{5}{CH_2}\text{-}\underset{4}{\overset{CSe\text{-}CH_2\text{-}CH_3}{|}{CH}}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CS}\text{-}\overset{1}{CH_3}$

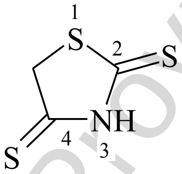
4-(propaneselenoyl)heptane-2,5-dithione (PIN)



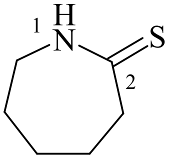
anthracene-1,9,10(2*H*)-trithione (PIN)



di(1*H*-imidazol-1-yl)methanethione (PIN)



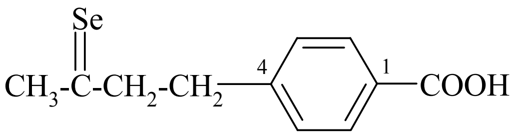
1,3-thiazolidine-2,4-dithione (PIN)



azepane-2-thione (PIN)

4 3 2 1
$CH_3\text{-}CS\text{-}CH_2\text{-}COOH$

3-sulfanylidenebutanoic acid (PIN)
3-thioxobutanoic acid



4-(3-selanylidenebutyl)benzoic acid (PIN)
4-(3-selenoxobutyl)benzoic acid

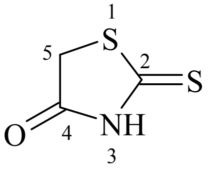
64.6.2 Seniority order of suffixes

The order of seniority of suffixes is C=O > C=S > C=Se > C=Te. Lowest locants are assigned in accordance with that order.

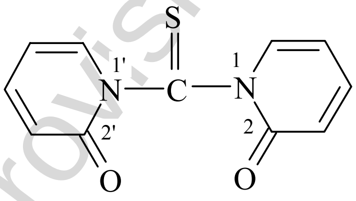
Examples:

$\overset{5}{\mathrm{CH_3}}\text{-}\overset{4}{\mathrm{C}}\mathrm{S}\text{-}\overset{3}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{2}{\mathrm{C}}\mathrm{O}\text{-}\overset{1}{\mathrm{C}}\mathrm{H_3}$

4-sulfanylidenepentan-2-one (PIN)
4-thioxopentan-2-one



2-sulfanylidene-1,3-thiazolidin-4-one (PIN)
2-thioxo-1,3-thazolidin-4-one

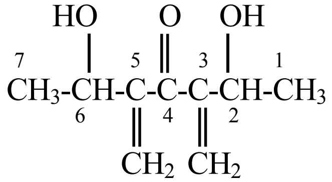


1,1′-carbonothioyldi[pyridine-2(1*H*)-one] (PIN)
1,1′-thiocarbonyldi[pyridine-2(1*H*)-one]

P-64.7 Polyfunctional ketones, pseudoketones, and heterones

P-64.7.1 Ketones, pseudoketones and heterones, and their chalcogen analogs in the order =O > =S > =Se > =Te, are senior to hydroxy compounds and their chalcogen analogs, amines, and imines in the seniority order of classes. In the presence of a characteristic group having priority to be cited as suffix as described in P-64.4 and P-64, they are cited as prefixes (see P-41).

Examples:

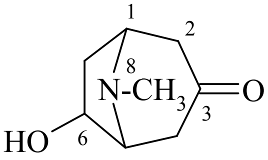


$CH_3\text{-}\overset{HO}{\overset{|}{CH}}\text{-}\underset{CH_2}{\underset{\|}{C}}\text{-}\overset{O}{\overset{\|}{C}}\text{-}\underset{CH_2}{\underset{\|}{C}}\text{-}\overset{OH}{\overset{|}{CH}}\text{-}CH_3$

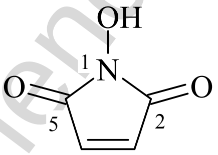
2,6-dihydroxy-3,5-dimethylideneheptan-3-one (PIN)

$\overset{4}{CH_3}\text{-}\overset{3}{CO}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{COOH}$

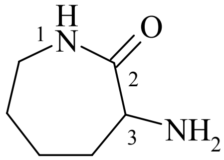
3-oxobutanoic acid (PIN)



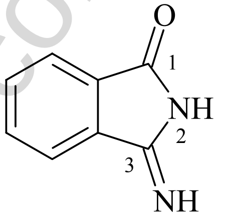
6-hydroxy-8-methyl-8-azabicyclo[3.2.1]octan-3-one (PIN)



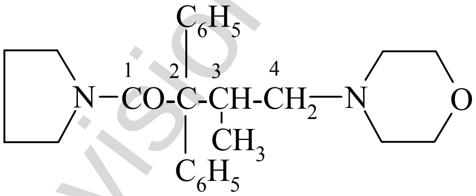
1-hydroxypyrrole-2,5-dione (PIN)



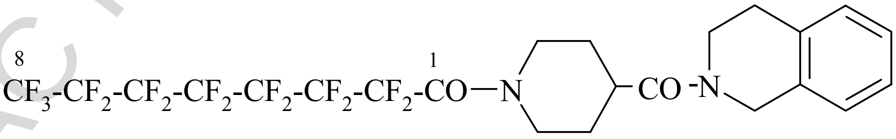
3-aminoazepan-2-one (PIN)



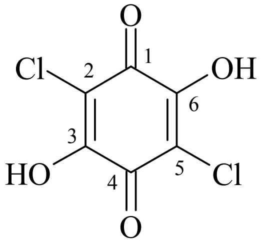
3-imino-2,3-dihydro-1*H*-isoindol-1-one (PIN)



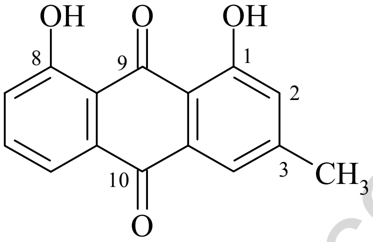
3-methyl-4-(morpholin-4-yl)-2,2-diphenyl-1-(pyrrolidin-1-yl)butan-1-one (PIN)



pentadecafluoro-1-[4-(1,2,3,4-tetrahydroisoquinolin-2-yl-
carbonyl)piperidin-1-yl]octan-1-one (PIN)



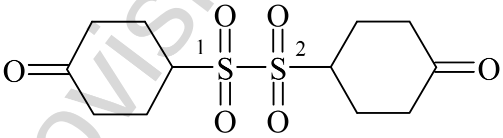
2,5-dichloro-3,6-dihydroxycyclohexadiene-1,4-dione (PIN)
2,5-dichloro-3,6-dihydroxy-1,4-benzoquinone



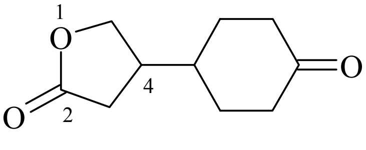
1,8-dihydroxy-3-methylanthracene-9,10-dione (PIN)
1,8-dihydroxy-3-methyl-9,10-anthraquinone

P-64.7.2 There is no seniority order between ketones and pseudoketones. When necessary, the maximum number of carbonyl groups, the seniority order between chains and rings, and between rings and ring systems, are considered, as appropriate. Heterones follow the seniority order of the corresponding acyclic parent hydride.

Examples:



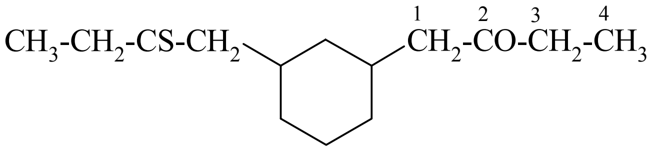
1,2-bis(4-oxocyclohexyl)-1λ^6,2λ^6-disulfane-1,1,2,2-tetrone (PIN)
(in the seniority order of classes, 1λ^6,2λ^6-disulfanes
are senior to carbon compounds, see P-41)



4-(4-oxocyclohexyl)oxolan-2-one (PIN)
[not 4-(2-oxooxolan-4-yl)cyclohexanone; a heterocyclic
ring is senior to a carbocyclic ring, see P-44.2.1)

P-64.7.3 After functional replacement, the seniority order of ketones, pseudoketones, and heterones is O > S > Se > Te.

Example:



1-[3-(2-sulfanylidenebutyl)cyclohexyl]butan-2-one (PIN)
(not 1-[3-(2-thioxobutyl)cyclohexyl]butan-2-one)

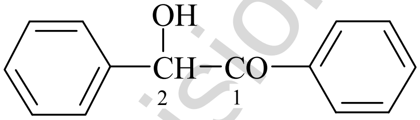
P-64.8 Acyloins

α-Hydroxy ketones, RCH(OH)-CO-R, in which R is an alkyl, aryl, or a heterocyclic group, have the class name ‘acyloins’ and are named by substitutive nomenclature as substituted ketones, in accordance with the seniority order: ketones > hydroxy compounds (see P-41). Names ending in ‘oin’ are not recommended.

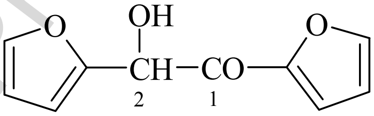
Examples:

$\overset{4}{\mathrm{C}}\mathrm{H_3}\text{-}\overset{3}{\mathrm{C}}\mathrm{H(OH)}\text{-}\overset{2}{\mathrm{C}}\mathrm{O}\text{-}\overset{1}{\mathrm{C}}\mathrm{H_3}$

3-hydroxybutan-2-one (PIN)
(not acetoin)



2-hydroxy-1,2-diphenylethan-1-one (PIN)



1,2-di(furan-2-yl)-2-hydroxyethan-1-one (PIN)
1,2-di(2-furyl)-2-hydroxyethan-1-one

P-65 Acids, acyl halides and pseudohalides, salts, esters, and anhydrides

P-65.0 Introduction

This Chapter includes acids named substitutively by means of suffixes, that is, carboxylic acids, sulfonic, sulfinic, and analogous selenium and tellurium acids. Their derivatives, such as esters, acyl halides and anhydrides, are described. Salts are included in this Section although anions are formally treated in Chapter 7. Carbon acids not named substitutively, i.e., carbonic acid, formic acid, cyanic acid, oxalic acid, and the bi- and polynuclear carbon acids are also included here. Mononuclear and polynuclear noncarbon (inorganic) acids used as parent structures for organic derivatives are discussed in Section P-67.

The hydrogen atom of an acid group is not substitutable for the purposes of substitutive nomenclature; replacement of acid hydrogen atoms by specific atoms or groups is called ‘functionalization’, as other classes are generated, for example esters. Substitution takes place when other hydrogen atoms in the structure are exchanged with other atoms or groups, as illustrated by the name ‘chloroacetic acid’.

P-65.1 Carboxylic acids and nitrogenous analogues

Carboxylic acids are ‘oxoacids’ having the structure R-C(=O)-OH, where R can be a hydrogen atom. Nitrogenous analogues are carboxylic acids in which =O has been replaced by =NH, =NNH_2, =N-OH, or in which –OH has been replaced by –NH-OH.

Names of α-amino acids, as well as carboxylic acids derived from carbohydrates, are not covered extensively in this Chapter. Traditional names are maintained, as recommended in specialized publications (ref. 23), and listed in Chapter 10 devoted to preferred IUPAC names for natural products.

P-65.1.1 Retained names

Carboxylic acids derived from natural sources were often given trivial names reminiscent of their animal or vegetable origin. In both 1979 and 1993, the list of these trivial names was significantly reduced, systematic names being recommended.

P-65.1.1.1 Retained names as preferred IUPAC names

Only the following three retained names are preferred IUPAC names. All can be functionalized, but only acetic acid and benzoic acid can be fully substituted; for substitution rules regarding formic acid, see P-65.1.8. Systematic substitutive names are used to generate acids modified by functional replacement.

HCOOH	CH_3-COOH	C_6H_5-COOH
formic acid (PIN) methanoic acid	acetic acid (PIN) ethanoic acid	benzoic acid (PIN) benzenecarboxylic acid

P-65.1.1.2 Retained names for general nomenclature

For general nomenclature, the following names are retained with full substitution allowed (see P-34).

furoic acid

isophthalic acid

phthalic acid

terephthalic acid

The following names are retained for general nomenclature with functionalization but no substitution allowed. Functionalization leads to anhydrides, salts and esters, for example, the formation of esters leads to names such as methyl butyrate.

acrylic acid

adipic acid

butyric acid

cinnamic acid

fumaric acid

glutaric acid

isonicotinic acid

maleic acid

malonic acid

methacrylic acid

naphthoic acid

nicotinic acid

oleic acid

palmitic acid

propionic acid

stearic acid

succinic acid

The names citric acid, lactic acid, glyceric acid, pyruvic acid, and tartaric acid, related to natural products, are also retained; no substitution is recommended, but the formation of salts and esters is allowed.

Names of α-amino acids related to peptides and proteins are also retained and used as preferred IUPAC names (see P-103). In particular, the name ‘glycine’ for H_2N-CH_2-COOH is used to form systematic substitutive preferred IUPAC names.

P-65.1.2 Systematic names

Carboxylic acids are named substitutively using the suffix ‘oic acid’ or ‘carboxylic acid’ and the prefix ‘carboxy’.

P-65.1.2.1 Carboxylic acid groups, $-COOH$, that conceptually replace a $-CH_3$ group of methane or terminating an unbranched hydrocarbon chain are named by replacing the final ‘e’ of the name of the corresponding hydrocarbon by the suffix ‘oic acid’. No locants are necessary to denote the positions of the carboxylic acid groups in a hydrocarbon chain; locants are used when hydrocarbon chains are modified by skeletal replacement, as shown in P-15.4.3.1.2. Except for formic acid (see P-65.1.8.1) and acetic acid (see P-65.1.1.1), systematically formed names are preferred IUPAC names; the names given in P-65.1.1.2 are retained names for use in general nomenclature.

Examples:

$$\overset{4}{CH_3}-\overset{3}{CH_2}-\overset{2}{CH_2}-\overset{1}{COOH}$$

butanoic acid (PIN)
butyric acid

$$\overset{10}{CH_3}-[CH_2]_8-\overset{1}{COOH}$$

decanoic acid (PIN)

$$\overset{12}{HOOC}-[CH_2]_{10}-\overset{1}{COOH}$$

dodecanedioic acid (PIN)

$$\overset{15}{CH_3}-CH_2-CH_2-\overset{12}{O}-CH_2-CH_2-\overset{9}{O}-CH_2-CH_2-\overset{6}{O}-CH_2-CH_2-\overset{3}{O}-CH_2-\overset{1}{COOH}$$

3,6,9,12-tetraoxapentadecan-1-oic acid (PIN)

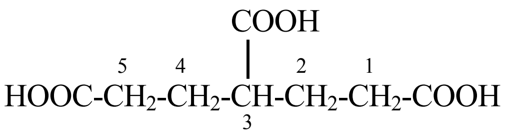
$$\overset{15}{HOOC}-CH_2-CH_2-\overset{12}{O}-CH_2-CH_2-\overset{9}{O}-CH_2-CH_2-\overset{6}{O}-CH_2-CH_2-\overset{3}{O}-CH_2-\overset{1}{CH_3}$$

3,6,9,12-tetraoxapentadecan-15-oic acid (PIN)

P-65.1.2.2 The suffix ‘carboxylic acid’ is used for all carboxylic acids not covered by P-65.1.2.1, except for benzoic acid (see P-65.1.1.1). The carboxy group can be attached to any atom, carbon or heteroatom, of any parent hydride; the proper methodology must be applied in the case of mancude parent hydrides as exemplified in P-65.1.2.3.

P-65.1.2.2.1 If an unbranched chain is linked to more than two carboxy groups, all carboxy groups are named from the parent hydride by substitutive use of the suffix 'carboxylic acid', preceded by the appropriate numerical prefix 'tri', 'tetra' etc. and appropriate locants.

Examples:



$HOOC-\overset{5}{C}H_2-\overset{4}{C}H_2-\underset{3}{\overset{COOH}{\overset{|}{C}}}H-\overset{2}{C}H_2-\overset{1}{C}H_2-COOH$

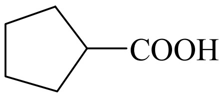
pentane-1,3,5-tricarboxylic acid (PIN)

$(HOOC)_2\overset{1}{C}H-\overset{2}{C}H(COOH)_2$

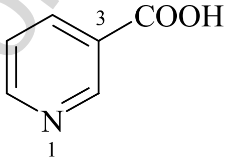
ethane-1,1,2,2-tetracarboxylic acid (PIN)

P-65.1.2.2.2 Carboxy groups attached to cyclic parent hydrides or heteroacyclic parent hydrides are always named by using the suffix 'carboxylic acid'.

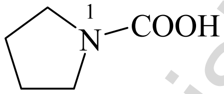
Examples:



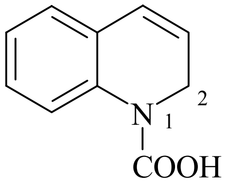
cyclopentanecarboxylic acid (PIN)



pyridine-3-carboxylic acid (PIN)
nicotinic acid



pyrrolidine-1-carboxylic acid (PIN)



quinoline-1(2*H*)-carboxylic acid (PIN)

$H_3Si-O-SiH_2-COOH$

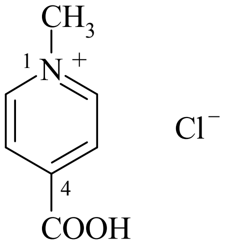
disiloxanecarboxylic acid (PIN)

$H_2N-NH-COOH$

hydrazinecarboxylic acid (PIN)
(not carbazic acid)
carbonohydrazidic acid (see P-65.2.1.4)

P-65.1.2.2.3 When another group is present that has priority for citation as suffix, for example, a radical anion or cation, or when all carboxylic acid groups cannot be described by a suffix, carboxylic acid groups are indicated by the prefix 'carboxy'.

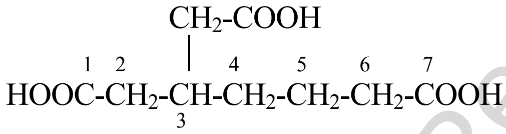
Examples:



4-carboxy-1-methylpyridinium chloride (PIN)

$^{\bullet}CH_2\text{-}CH_2\text{-}COOH$ or $-CH_2\text{-}CH_2\text{-}COOH$

2-carboxyethyl (PIN)
(radicals and substituent prefixes often have identical names; see P-31.2.1)



$$\overset{1}{\mathrm{HOOC}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\underset{3}{\overset{\overset{\displaystyle \mathrm{CH_2\text{-}COOH}}{|}}{\mathrm{C}}}\mathrm{H}\text{-}\overset{4}{\mathrm{CH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{6}{\mathrm{CH_2}}\text{-}\overset{7}{\mathrm{COOH}}$$

3-(carboxymethyl)heptanedioic acid (PIN)

P-65.1.2.3 Seniority order for numbering

When required, numbering is based on the following seniority order:

(a) fixed numbering of parent hydride (e.g. naphthalene, bicyclo[2.2.2]octane, etc.)

(b) heteroatoms in rings and chains

(c) indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with the structural feature (d)].

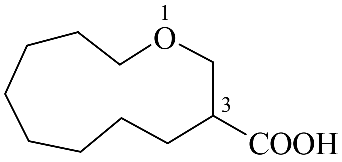
(d) principal group named as suffix

(e) added hydrogen (consistent with the structure of the compound and in accordance with further substitution)

(f) unsaturation/saturation (ene/yne endings or hydro/dehydro prefixes)

(g) detachable (alphabetized) prefixes

Examples:

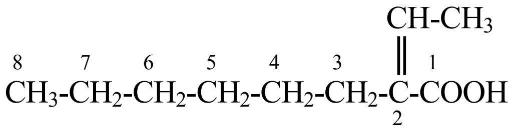


1-oxacycloundecane-3-carboxylic acid (PIN)

1 2 5 8 11 14

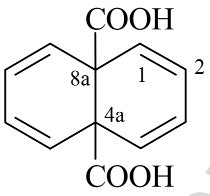
$CH_3\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}S\text{-}CH_2\text{-}CH_2\text{-}COOH$

2,5,8-trioxa-11-thiatetradecan-14-oic acid (PIN)

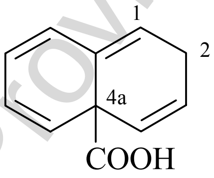


$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}\overset{\overset{\displaystyle CH\text{-}CH_3}{\|}}{C}\text{-}COOH$

2-ethylideneoctanoic acid (PIN)
[not 2-hexylbut-2-enoic acid; see P-44.3, criterion (b)]



naphthalene-4a,8a-dicarboxylic acid (PIN; see P-53.1)
4a,8a-dihydronaphthalene-4a,8a-dicarboxylic acid



naphthalene-4a(2*H*)-carboxylic acid (PIN; see P-53.1)
2,4a-dihydronaphthalene-4a-carboxylic acid

P-65.1.2.4 Polyfunctional carboxylic acids

Systematic names of substituted carboxylic acids are formed by adding appropriate prefixes, such as ‘oxo’, ‘hydroxy’, ‘amino’, ‘imino’, ‘halo’, ‘nitro’, etc., to the name of the acid. Prefixes are not ranked as functional entities; they are cited in a name in alphabetical order, which is also used to assign lowest locants when required.

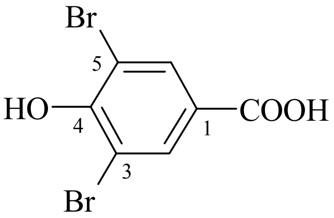
Examples:

$\overset{6}{CH_3}\text{-}\overset{5}{CO}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{COOH}$

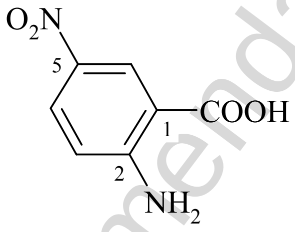
5-oxohexanoic acid (PIN)

$H_2N\text{-}\overset{5}{CH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{COOH}$

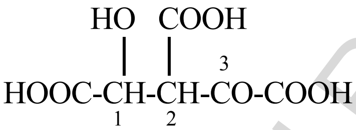
5-aminopentanoic acid (PIN)



3,5-dibromo-4-hydroxybenzoic acid (PIN)



2-amino-5-nitrobenzoic acid (PIN)
(not 5-nitroanthranilic acid;
anthranilic acid is not a
retained name)

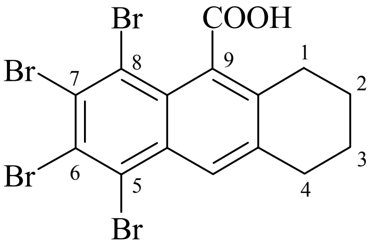


$\mathrm{HOOC\text{-}\underset{1}{\overset{HO}{CH}}\text{-}\underset{2}{\overset{COOH}{CH}}\text{-}\overset{3}{CO}\text{-}COOH}$

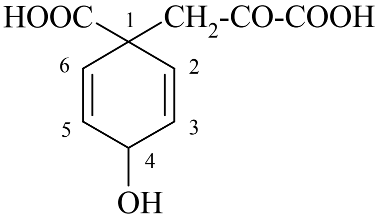
1-hydroxy-3-oxopropane-1,2,3-tricarboxylic acid (PIN)
[not 3-hydroxy-1-oxopropane-1,2,3-tricarboxylic acid; lowest
locants are attributed to prefixes that are cited first, see P-44.3(m)]

$H_3C\text{-}S\text{-}\overset{4}{CH_2}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CO}\text{-}\overset{1}{COOH}$

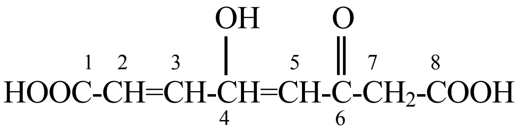
4-(methylsulfanyl)-2-oxobutanoic acid (PIN)
[not 4-(methylthio)-2-oxobutyric acid]



5,6,7,8-tetrabromo-1,2,3,4-tetrahydroanthracene-9-carboxylic acid (PIN)
(not 1,2,3,4-tetrabromo-5,6,7,8-tetrahydroanthracene-9-carboxylic acid
hydro/dehydro prefixes are given lowest possible locants before
detachable prefixes)

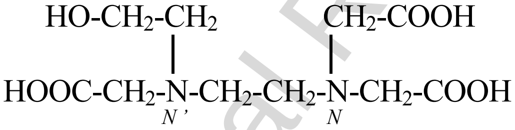


1-(2-carboxy-2-oxoethyl)-4-hydroxycyclohexa-2,5-diene-1-carboxylic acid (PIN)
1-carboxy-4-hydroxy-β-oxocyclohexa-2,5-dienepropanoic acid (a conjunctive name; see P-13.5.2)



$HOOC\text{-}\overset{1}{C}\overset{2}{H}{=}\overset{3}{C}H\text{-}\underset{4}{\overset{OH}{C}}H{=}\overset{5}{C}H\text{-}\underset{6}{\overset{O}{\overset{\|}{C}}}\text{-}\overset{7}{C}H_2\text{-}\overset{8}{C}OOH$

4-hydroxy-6-oxoocta-2,4-dienedioic acid (PIN)
(not 5-hydroxy-3-oxoocta-4,6-dienedioic acid; unsaturation is senior to detachable prefixes)



$HOOC\text{-}CH_2\text{-}\underset{N'}{\overset{HO\text{-}CH_2\text{-}CH_2}{N}}\text{-}CH_2\text{-}CH_2\text{-}\underset{N}{\overset{CH_2\text{-}COOH}{N}}\text{-}CH_2\text{-}COOH$

N-(carboxymethyl)-*N*′-(2-hydroxyethyl)-*N*,*N*′-ethane-1,2-diyldiglycine (PIN)
2,2′-({2-[(carboxymethyl)(2-hydroxyethyl)amino]ethyl}azanediyl)diacetic acid

P-65.1.3 Carboximidic, carbohydrazonic, carbohydroximic and carbohydroxamic acids

P-65.1.3.1 Carboximidic acids

P-65.1.3.1.1 Substitutive nomenclature; suffix mode

The name of an acid in which the carbonyl oxygen atom of a carboxylic acid group has been replaced by =NH is formed by functional replacement nomenclature and the infix ‘imid(o)’ to modify the ‘ic acid’ or ‘oic acid’ ending of the retained name of an acid; or the ‘oic acid’ or ‘carboxylic acid’ suffix of a systematic name of an acid, to ‘imidic acid’ or ‘carboximidic acid’. Preferred names of imidic acids are those derived from systematic substitutive preferred IUPAC names of carboxylic acids.

This is a change in the case of formic acid, acetic acid, benzoic acid.

Examples:

$HC(=NH)\text{-}OH$

methanimidic acid (PIN)
formimidic acid

$CH_3\text{-}C(=NH)\text{-}OH$

ethanimidic acid (PIN)
acetimidic acid

$C_6H_5\text{-}C(=NH)\text{-}OH$

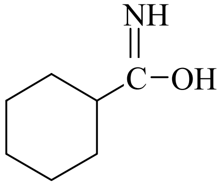
benzenecarboximidic acid (PIN)
benzimidic acid

$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}(=NH)\text{-}OH$

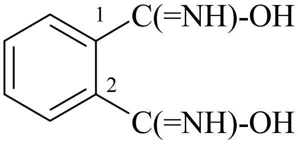
butanimidic acid (PIN)
butyrimidic acid

$HO\text{-}\overset{4}{C}(=NH)\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}(=NH)\text{-}OH$

butanediimidic acid (PIN)
succinimidic acid



cyclohexanecarboximidic acid (PIN)



benzene-1,2-dicarboximidic acid (PIN)
phthalimidic acid

P-65.1.3.1.2 Substitutive nomenclature, prefix mode

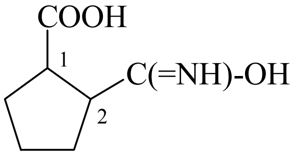
When another group is present that has seniority for citation as principal group, the following prefixes are used.

(1) the compound prefix '*C*-hydroxycarbonimidoyl' is used to denote the acyl group –C(=NH)-OH; the compound prefix name is formed by concatenation based on the simple prefix name carbonimidoyl, –C(=NH)–, derived from carbonimidic acid (see P-65.2.1.5).

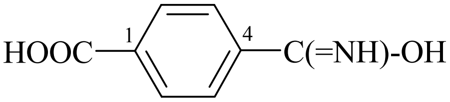
(2) the combination of the prefixes 'hydroxy' and 'imino' at the end of a carbon chain is used in preferred IUPAC names rather than the prefix '*C*-hydroxycarbonimidoyl'.

Note that the italicized letter '*C*' is used to avoid potential confusion with *N*-hydroxy substitution. The name carbonohydroximoyl is not used to generate preferred IUPAC names.

Examples:



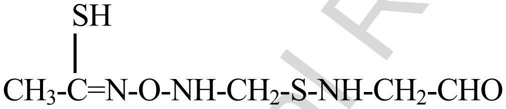
(1) 2-(*C*-hydroxycarbonimidoyl)cyclopentane-1-carboxylic acid (PIN)



(1) 4-(*C*-hydroxycarbonimidoyl)benzoic acid (PIN)

$$\overset{4}{\text{HO-C}}\text{(=NH)-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$$

(2) 4-hydroxy-4-iminobutanoic acid (PIN)
(1) 3-(*C*-hydroxycarbonimidoyl)propanoic acid



$$CH_3\text{-}\overset{\overset{\displaystyle SH}{|}}{C}\text{=N-O-NH-}CH_2\text{-S-NH-}CH_2\text{-CHO}$$

N-{[({[(2-oxoethyl)amino]sulfanyl}methyl)amino]oxy}ethanimidothioic acid (PIN)
(see P-65.1.3.1.1; P-65.1.5.2)

P-65.1.3.2 Carbohydrazonic acids

P-65.1.3.2.1 Substitutive nomenclature; suffix mode

The name of an acid in which the carbonyl oxygen atom of a carboxylic acid group has been replaced by $=NNH_2$ is formed by functional replacement nomenclature. The infix 'hydrazon(o)' is used to modify the 'ic acid' or 'oic acid' ending of the retained name of an acid; or the 'oic acid' or 'carboxylic acid' suffix of a systematic name of an acid is changed to 'hydrazonic acid' or 'carbohydrazonic acid'.

Preferred IUPAC names of hydrazonic acids are those derived from systematic substitutive preferred IUPAC names of carboxylic acids.

This is a change in the case of formic, acetic, and benzoic acids

Examples:

$\mathrm{CH_3-C(=N-NH_2)-OH}$

methanehydrazonic acid (PIN)
formohydrazonic acid

$\mathrm{CH_3-C(=N-NH_2)-OH}$

ethanehydrazonic acid (PIN)
acetohydrazonic acid

$\mathrm{C_6H_5-C(=N-NH_2)-OH}$

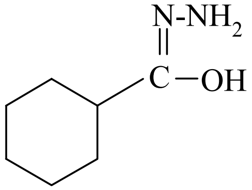
benzenecarbohydrazonic acid (PIN)
benzohydrazonic acid

$\overset{4}{\mathrm{C}}\mathrm{H_3}-\overset{3}{\mathrm{C}}\mathrm{H_2}-\overset{2}{\mathrm{C}}\mathrm{H_2}-\overset{1}{\mathrm{C}}\mathrm{(=N-NH_2)-OH}$

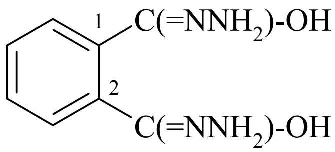
butanehydrazonic acid (PIN)
butyrohydrazonic acid

$\mathrm{HO-}\overset{4}{\mathrm{C}}\mathrm{(=N-NH_2)-}\overset{3}{\mathrm{C}}\mathrm{H_2}-\overset{2}{\mathrm{C}}\mathrm{H_2}-\overset{1}{\mathrm{C}}\mathrm{(=N-NH_2)-OH}$

butanedihydrazonic acid (PIN)
succinohydrazonic acid



cyclohexanecarbohydrazonic acid (PIN)



benzene-1,2- dicarbohydrazonic acid (PIN)
phthalohydrazonic acid

P-65.1.3.2.2 Substitutive nomenclature, prefix mode

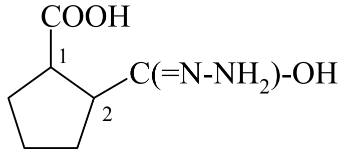
When another group is present that has seniority for citation as principal group, the following prefixes are used:

(1) the compound prefix '*C*-hydroxycarbonohydrazonoyl' is used to denote the acyl group $\mathrm{-C(=N-NH_2)-OH}$; the compound prefix name is formed by concatenation based on the simple prefix name carbonohydrazonoyl, $\mathrm{-C(=NNH_2)-}$, derived from carbonohydrazonic acid (see P-65.2.1.5)]

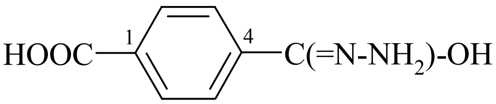
(2) the combination of prefixes 'hydroxy' and 'hydrazono' at the end of a carbon chain is used in preferred IUPAC names rather than the prefix '*C*-hydroxycarbonohydrazonoyl'.

Note that the italicized letter '*C*' is used to avoid potential confusion with *N*-hydroxy substitution.

Examples:



(1) 2-(*C*-hydroxycarbonohydrazonoyl)cyclopentane-1-carboxylic acid (PIN)



(1) 4-(*C*-hydroxycarbonohydrazonoyl)benzoic acid (PIN)

$HO\text{-}\overset{5}{C}(=N\text{-}NH_2)\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

(2) 5-hydrazono-5-hydroxypentanoic acid (PIN)
(1) 4-(*C*-hydroxycarbonohydrazonoyl)butanoic acid

P-65.1.3.3 Carbohydroximic acids

P-65.1.3.3.1 Substitutive nomenclature; suffix mode

Acids in which the carbonyl oxygen atom of a carboxylic acid group has been replaced by =N-OH are named:

(1) as *N*-hydroxy derivatives of imidic acids named in P-65.1.3.1

(2) by modifying the ‘ic acid’ or ‘oic acid’ ending of the retained name of an acid to ‘hydroximic acid’. The letter ‘o’ is added for euphony between ‘h’ and a preceding consonant;

(3) by using the suffixes ‘hydroximic acid’ and ‘carbohydroximic acid’ that are attached to the name of a parent hydride.

Method (1) generates preferred IUPAC names.

Examples:

$CH_3\text{-}C(=N\text{-}OH)\text{-}OH$

(1) *N*-hydroxyethanimidic acid (PIN)
(2) acetohydroximic acid

$C_6H_5\text{-C(=N-OH)-OH}$

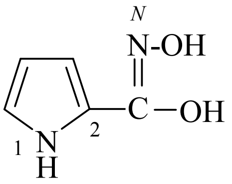
(1) *N*-hydroxybenzenecarboximidic acid (PIN)
(2) benzohydroximic acid

$\overset{4}{\text{C}}\text{H}_3\text{-}\overset{3}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{1}{\text{C}}\text{(=N-OH)-OH}$

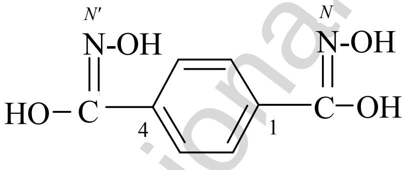
(1) *N*-hydroxybutanimidic acid (PIN)
(2) butyrohydroximic acid
(3) butanehydroximic acid

$\text{HO-}\overset{4}{\text{C}}\text{(=N-OH)-}\overset{3}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{1}{\text{C}}\text{(=N-OH)-OH}$

(1) *N*,*N*′-dihydroxybutanediimidic acid (PIN)
(2) succinohydroximic acid
(3) butanedihydroximic acid



(1) 2-*N*-hydroxy-1*H*-pyrrole-2-carboximidic acid (PIN)
(3) pyrrole-2-carbohydroximic acid



(1) *N*,*N*′-dihydroxybenzene-1,4-dicarboximidic acid (PIN)
(2) terephthalohydroximic acid

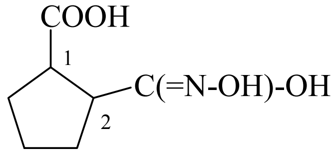
P-65.1.3.3.2 Substitutive nomenclature, prefix mode

When another group is present that has seniority for citation as principal group, the following prefixes are used:

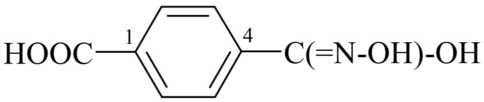
(1) ‘dihydroxycarbonimidoyl’ to denote the group –C(=N-OH)-OH;

(2) the combination of the prefixes ‘hydroxy’ and ‘hydroxyimino’ at the end of a carbon chain is used in preferred IUPAC names rather than the prefix ‘dihydroxycarbonimidoyl’.

Examples:



(1) 2-(dihydroxycarbonimidoyl)cyclopentane-1-carboxylic acid (PIN)



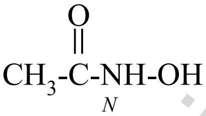
(1) 4-(dihydroxycarbonimidoyl)benzoic acid (PIN)

$\overset{5}{\text{HO-C}}\text{(=N-OH)-}\overset{4}{\text{C}}\text{H}_2\text{-}\overset{3}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{1}{\text{C}}\text{OOH}$

(2) 5-hydroxy-5-(hydroxyimino)pentanoic acid (PIN)
(1) 4-(dihydroxycarbonimidoyl)butanoic acid

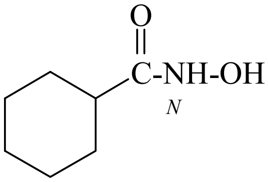
P-65.1.3.4 Hydroxamic acids have the generic structure R-CO-NH-OH and are named as *N*-hydroxy amides (see P-66.1.1.3.3). The suffixes ‘hydroxamic acid’ and ‘carbohydroxamic acid’ are no longer recommended.

Examples:



$\text{CH}_3\text{-}\overset{\text{O}}{\overset{\|}{\text{C}}}\text{-}\underset{N}{\text{N}}\text{H-OH}$

N-hydroxyacetamide (PIN)
(no longer acetohydroxamic acid)



N-hydroxycyclohexanecarboxamide (PIN)
(no longer cyclohexanecarbohydroxamic acid)

P-65.1.4 Peroxycarboxylic acids

The general methodology for modifying acids expressed by suffixes by functional replacement nomenclature is to use modified suffixes in the same way as for unmodified acids. A major change and simplification, i.e., that suffixes are always modified by infixes, is recommended.

P-65.1.4.1 Peroxycarboxylic acids are named systematically using the following suffixes:

–(C)O-OOH	peroxoic acid
–CO-OOH	carboperoxoic acid

Retained names of peroxy carboxylic acids are modified by the prefix ‘peroxy’. Preferred IUPAC names are formed by functional replacement of systematic substitutive names.

This is a change in the case of formic, acetic, and benzoic acids

Examples:

HCO-OOH

methaneperoxoic acid (PIN)
peroxyformic acid
(not performic acid)

CH_3-CO-OOH

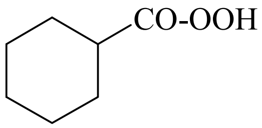
ethaneperoxoic acid (PIN)
peroxyacetic acid
(not peracetic acid)

$\overset{6}{\mathrm{C}}\mathrm{H_3\text{-}[CH_2]_4\text{-}}\overset{1}{\mathrm{C}}\mathrm{O\text{-}OOH}$

hexaneperoxoic acid (PIN)

C_6H_5-CO-OOH

benzenecarboperoxoic acid (PIN)
peroxybenzoic acid
(not perbenzoic acid)



cyclohexanecarboperoxoic acid (PIN)

P-65.1.4.2 When another group is present that has priority for citation as a suffix (see seniority of classes, P-41), the following prefixes are used:

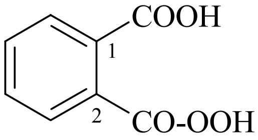
(1) the functional replacement prefix ‘carbonoperoxoyl-’ or the compound prefix ‘hydroperoxycarbonyl-’ is used to denote the acyl group –C(O)-OOH; the compound prefix ‘hydroperoxycarbonyl-’ is formed by concatenation, on the basis of the simple acyl group ‘carbonyl’, for >C=O (see P-65.2.1.5); the prefix ‘carbonoperoxoyl’ is used in preferred IUPAC names, except as noted in (2) below.

(2) the combination of the prefixes ‘hydroperoxy and oxo’ at the end of a carbon chain is used in preferred IUPAC names rather than the prefix ‘hydroperoxycarbonyl-’ or the prefix ‘carbonoperoxoyl-’.

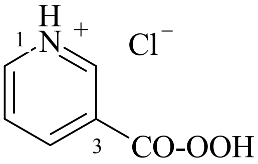
Examples:

$\mathrm{HOO\text{-}}\overset{6}{\mathrm{C}}\mathrm{O\text{-}[CH_2]_4\text{-}}\overset{1}{\mathrm{C}}\mathrm{OOH}$

(2) 6-hydroperoxy-6-oxohexanoic acid (PIN)
(1) 5-carbonoperoxoylpentanoic acid
5-(hydroperoxycarbonyl)pentanoic acid



(1) 2-carbonoperoxoylbenzoic acid (PIN)
2-(hydroperoxycarbonyl)benzoic acid
(2) monoperoxyphthalic acid (see P-65.1.4.1)

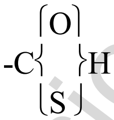


(1) 3-carbonoperoxoylpyridin-1-ium chloride (PIN)
3-(hydroperoxycarbonyl)pyridin-1-ium chloride

P-65.1.5 Chalcogen analogues of carboxylic acids

P-65.1.5.1 Functional replacement in systematic names of carboxylic acids.

Replacement of oxygen atom(s) of a carboxylic acid group by another chalcogen is indicated by the affixes ‘thio’, ‘seleno’, and ‘telluro’. These names do not differentiate between tautomeric forms of mixed chalcogen acids; such nonspecificity may be shown in a structure such as:



$$-C\left\{\begin{matrix}O\\S\end{matrix}\right\}H \qquad \text{or} \qquad -C\{O/S\}H$$

In names, tautomeric groups in mixed chalcocarboxylic acids, such as –CO-SH or –CS-OH, –S(O)-SH or –S(S)-OH, are distinguished by prefixing italic element symbols, such as *O* or *S*, respectively, to the term ‘acid ’, for example, thioic *S*-acid for –(C)O-SH and carbothioic *O*-acid for –CS-OH. Normally, these locants are omitted, because the exact position of chalcogen atoms is not known in acids; such letter locants are principally used in naming esters.

When the position of chalcogen atoms is undetermined, the prefix for the unmodified acid, i.e. ‘carboxy’ for –COOH, is used and modified by functional replacement using prefixes, as in ‘thiocarboxy’ for –C{O/S}H, and is enclosed in parentheses to avoid the possibility of ambiguity. The order of seniority of these suffixes is fully described in Section P-43.

When the position of chalcogen atoms is known, combinations of prefixes such as ‘hydroxy- and sulfanylidene-’ and ‘sulfanyl- and oxo-’ are used in acyclic compounds; compound prefixes such as ‘[hydroxy(carbonothioyl)]-’ and ‘(sulfanylcarbonyl)-’ are used in cyclic compounds, as appropriate (see P-64.6.1). The compound prefixes are formed by concatenation using simple acyl prefixes derived from carbonic acids (see P-65.2.1.5)

The seniority order between acids and acids modified by functional replacement is discussed in P-43 and expressed in Tables 4.3 and 4.4. In presence of unmodified acids cited as suffix, modified acids are cited as prefixes.

Examples:

$CH_3-CH_2-CH_2-CH_2-CH_2-CS-OH$

hexanethioic *O*-acid (PIN)

$CH_3-CH_2-CH_2-CH_2-CH_2-C\{S/Se\}H$

hexaneselenothioic acid (PIN)

$CH_3-CH_2-CH_2-CH_2-CH_2-CSe-SH$

hexaneselenothioic *S*-acid (PIN)

$H\{S,O\}C-CH_2-CH_2-CH_2-CH_2-C\{O/S\}H$

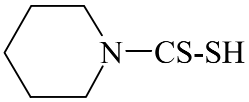
hexanebis(thioic) acid (PIN)

$HSSC-CH_2-CH_2-CH_2-CH_2-CS-SH$

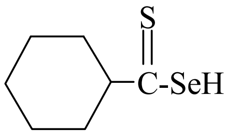
hexanebis(dithioic) acid (PIN)

$CH_3-CH_2-CH_2-CH_2-CH_2-C\{O/Se\}H$

hexaneselenoic acid (PIN)



piperidine-1-carbodithioic acid (PIN)



cyclohexanecarboselenothioic *Se*-acid (PIN)

$H\{S/O\}\overset{5}{C}-\overset{4}{C}H_2-\overset{3}{C}H_2-\overset{2}{C}H_2-\overset{1}{C}H_2-COOH$

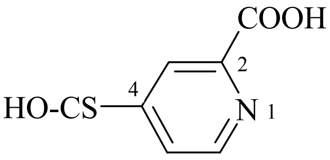
5-(thiocarboxy)pentanoic acid (PIN)

$HS-\overset{4}{C}O-\overset{3}{C}H_2-\overset{2}{C}H_2-\overset{1}{C}OOH$

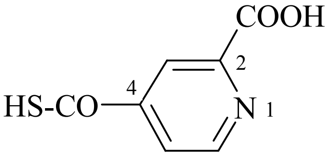
4-oxo-4-sulfanylbutanoic acid (PIN)
4-(sulfanylcarbonyl)propanoic acid

$HO-C(=S)-CH_2-CH_2-COOH$

4-hydroxy-4-sulfanylidenebutanoic acid (PIN)



4-[hydroxy(carbonothioyl)]pyridine-2-carboxylic acid (PIN)



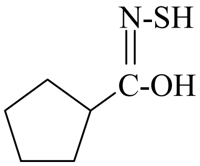
4-(sulfanylcarbonyl)pyridine-2-carboxylic acid (PIN)

$CH_3\text{-}CH_2\text{-}C(\text{=}NH)\text{-}SH$

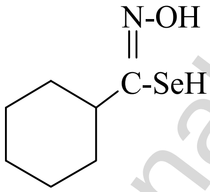
propanimidothioic acid (PIN)

$CH_3\text{-}CH_2\text{-}CH_2\text{-}C(\text{=}NNH_2)\text{-}SeH$

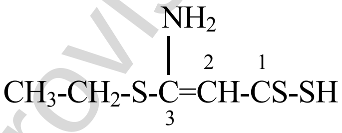
butanehydrazonoselenoic acid (PIN)



N-sulfanylcyclopentanecarboximidic acid (PIN)



N-hydroxycyclohexanecarboximidoselenoic acid (PIN)



$$CH_3\text{-}CH_2\text{-}S\text{-}\overset{NH_2}{\underset{3}{C}}\text{=}\overset{2}{C}H\text{-}\overset{1}{C}S\text{-}SH$$

3-amino-3-(ethylsulfanyl)prop-2-enedithioic acid (PIN)

P-65.1.5.2 Functional replacement in retained names of carboxylic acids

Preferred names of chalcogen analogues of monocarboxylic acids are formed using the suffixes ‘thioic acid’, ‘selenoic acid’, ‘telluroic acid’ or ‘carbothioic acid’, ‘carboselenoic acid’, ‘carbotelluroic acid’ and names of appropriate parent hydrides, even in the case of formic acid, acetic acid and benzoic acid.

This is a change in the case of formic, acetic, and benzoic

Chalcogen analogues of monocarboxylic acids with retained names may also be named by placing the prefix ‘thio’, ‘seleno’ or ‘telluro’ in front of the name of the acid.

Chalcogen analogues of dicarboxylic acids are named systematically; retained names are not used to name chalcogen analogues of dicarboxylic acids.

The symbols *O*, *S*, *Se* and *T*e are used to specify the structure of the acid, as indicated in P-65.1.5.1).

Examples:

$CH_3\text{-CS-OH}$

ethanethioic *O*-acid (PIN)
thioacetic *O*-acid

$C_6H_5\text{-C}\{\text{O,Se}\}\text{H}$

benzenecarboselenoic acid (PIN)
selenobenzoic acid

HCO-SH

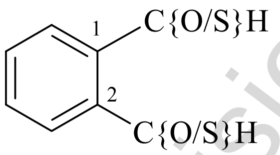
methanethioic *S*-acid (PIN)
thioformic *S*-acid

$\text{H}\{\text{S,O}\}\text{C-}\overset{4}{\text{CH}_2}\text{-}\overset{3}{\text{CH}_2}\text{-}\overset{2}{\text{CH}_2}\text{-}\overset{1}{\text{COOH}}$

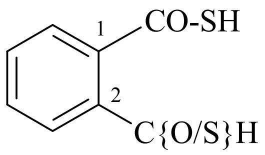
3-(thiocarboxy)butanoic acid (PIN)
(not thioglutaric acid)

$\text{HS-}\overset{4}{\text{CO}}\text{-}\overset{3}{\text{CH}_2}\text{-}\overset{2}{\text{CH}_2}\text{-}\overset{1}{\text{COOH}}$

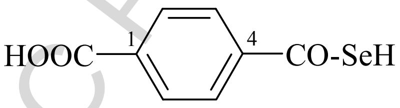
4-oxo-4-sulfanylbutanoic acid (PIN)
(not thiosuccinic acid)



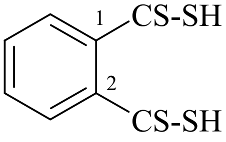
benzene-1,2-dicarbothioic acid (PIN)
(not 1,2-dithiophthalic acid)



2-(thiocarboxy)benzenecarbothioic *S*-acid (PIN)
(not 1,2-dithiophthalic *S*-acid)



4-(selanylcarbonyl)benzoic acid (PIN)
(not 1-selenophthalic *Se*-acid)



benzene-1,2-dicarbodithioic acid (PIN)
(not tetrathiophthalic acid)

P-65.1.5.3 Functional replacement in peroxycarboxylic acids.

Peroxy acid suffixes can be modified by S , Se, and Te using functional replacement nomenclature. Italic prefixes in front of the term ‘acid’ are used for specificity, where necessary (see Table 4.3; for more suffixes modified by functional replacement and their seniority order). Preferred names are all formed by using appropriate suffixes and parent hydrides, even in the case of derivatives of formic acid, acetic acid, and benzoic acid.

This is a change in the case of formic, acetic, and benzoic acids

Examples:

–(C)O-OSH	(thioperoxoic) *OS*-acid
–(C)Se-SSH	(dithioperoxo)selenoic acid
–CO-SOH	carbo(thioperoxoic) *SO*-acid
–CS-OOH	carboperoxothioic acid
$-COS_2H$	dithiocarboperoxic acid (location of sulfur atom unknown)

The recommended suffixes, and their seniority order, are fully discussed in Section P-43.

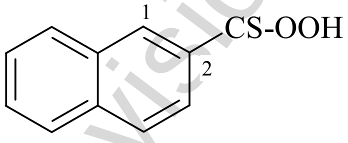
Examples:

CH_3-CO-OSH

ethane(thioperoxoic) *OS*-acid (PIN)
(not peroxythioacetic *OS*-acid)

C_6H_5-CO-SOH

benzenecarbo(thioperoxoic acid) *SO*-acid (PIN)
(not peroxothiobenzoic *SO*-acid)



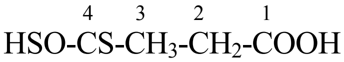
naphthalene-2-carboperoxothioic acid (PIN)
(not peroxythio-2-naphthoic acid)

Compound prefixes, such as ‘sulfanyloxy’ and ‘oxo’ and ‘hydroxysulfanyl’ and ‘sulfanylidene’ at the end of acyclic chains are used to generate preferred IUPAC names.

Appropriate prefixes constructed by concatenation based on simple acyl groups derived from carbonic and related acids (see P-65.2.1.5) are also used in preferred IUPAC names. Letter locants such as *SO* and *OS* are required to specify the structures of thioperoxy groups (see also P-63.3.2.1).

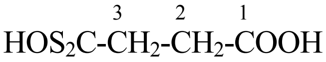
Prefixes derived by functional replacement nomenclature have only limited use because there is no accepted method to unambiguously describe precise structures of thioperoxy groups.

Examples:



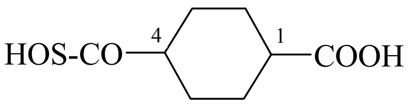
$HSO\text{-}\overset{4}{C}S\text{-}\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

4-sulfanylidene-4-(sulfanyloxy)butanoic acid (PIN)
3-[(*SO*-thiohydroperoxy)carbonothioyl]propanoic acid (see P-63.3.2.1)
(not 3-carbono(thioperoxo)thioylpropanoic acid; ambiguous name)



$HOS_2C\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

3-(dithiocarboperoxoyl)acetic acid (PIN)
(location of sulfur atoms unknown)



4-[(hydroxysulfanyl)carbonyl]cyclohexanecarboxylic acid] (PIN)
4-[(*OS*-thiohydroperoxy)carbonyl]cyclohexanecarboxylic acid

P-65.1.6 Amic, anilic and aldehydic acids

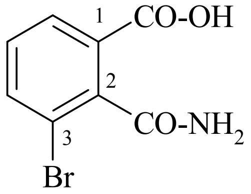
Amic acids are compounds containing a carboxy (−COOH) and a carboxamide (−$CONH_2$) group; similarly, anilic and aldehydic acids include a carboxy group and a carboxanilide (−CO-NH-C_6H_5) or formyl (−CHO) group, respectively. The endings ‘amic acid’, ‘anilic acid’ and ‘aldehydic acid’ can only be used in general nomenclature to name modified dicarboxylic acids having retained names. Preferred IUPAC names are all formed systematically using preferred names of acids and appropriate prefixes.

P-65.1.6.1 Amic acids

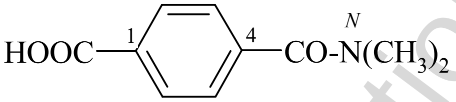
P-65.1.6.1.1 When a dicarboxylic acid has a retained name (see P-34.4.1) and when one of its carboxy groups is replaced by a carboxamide group −CO-NH_2, the resulting structure is called an amic acid and, in general nomenclature, may be named by replacing the ending ‘ic acid’ of the name of the dicarboxylic acid by the ending ‘amic acid’. Although substitution may not be allowed on the parent acid, it is allowed on nitrogen atoms of the corresponding amic acid and is denoted in names by a *N* locant.

The prefix ‘carbamoyl’ is preferred to ‘aminocarbonyl’ to name amic acids systematically. The combination of the prefixes ‘amino’ and ‘oxo’ is used for describing the −CO-NH_2 at the end of an acyclic chain resulting in preferred IUPAC names

Examples:



3-bromo-2-carbamoylbenzoic acid (PIN)
2-(aminocarbonyl)-3-bromo-benzoic acid



4-(dimethylcarbamoyl)benzoic acid (PIN)
4-[(dimethylamino)carbonyl]benzoic acid
N,*N*-dimethylterephthalamic acid

$H_2N\text{-}\overset{4}{C}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

4-amino-4-oxobutanoic acid (PIN)
3-carbamoylpropanoic acid
3-(aminocarbonyl)propanoic acid
succinamic acid

P-65.1.6.2 Anilic acids

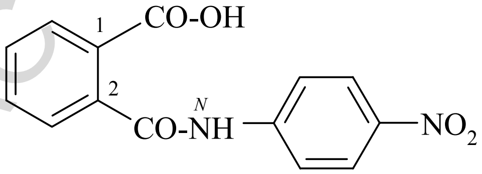
N-Phenyl derivatives of amic acids are called ‘anilic acids’ and are named by changing the ‘amic acid’ ending to ‘anilic acid’. Substitution on the nitrogen atom is indicated by the locant *N,* even if no substitution is allowed on the parent acid. Anilic acids may also be named as *N*-substituted amic acids.

The combination of the prefixes ‘anilino’ or ‘phenylamino’ and ‘oxo’ is used for describing −CO-NH-C_6H_5 at the end of an acyclic chain resulting in preferred IUPAC names

Examples:

$C_6H_5\text{-}NH\text{-}\overset{5}{C}O\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

5-anilino-5-oxopentanoic acid (PIN)
5-(phenylamino)-5-oxopentanoic acid
4-(phenylcarbamoyl)butanoic acid
N-phenylglutaramic acid
glutaranilic acid

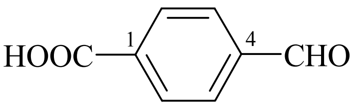


2-[(4-nitrophenyl)carbamoyl]benzoic acid (PIN)
N-(4-nitrophenyl)phthalamic acid
(not 4′-nitrophthalanilic acid; substitution of phthalanilic acid not allowed, except on the nitrogen atom)

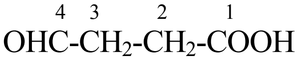
P-65.1.6.3 Aldehydic acids

When a dicarboxylic acid has a retained name (see P-34.4.1) and when one of its carboxy groups is replaced by a formyl group, −CHO (see P-65.2.2.5), the resulting structure is called an aldehydic acid and, in general nomenclature, may be named by replacing the ending ‘ic acid’ of the name of the dicarboxylic acid by the ending ‘aldehydic acid’. Systematically constructed names are preferred IUPAC names for aldehydic acids derived from all dicarboxylic acids. The prefix ‘formyl’ is used in preferred IUPAC names, except for a −CHO group at the end of an acyclic chain, which is designated by the prefix ‘oxo’.

Examples:



4-formylbenzoic acid (PIN)
terephthalaldehydic acid



$\overset{4}{O}H\overset{3}{C}\text{-}CH_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

4-oxobutanoic acid (PIN)
3-formylpropanoic acid
succinaldehydic acid

P-65.1.7 Acyl groups derived from carboxylic and related acids

P-65.1.7.1 Definitions and name construction

P-65.1.7.1.1 Definition.

Carboacyl groups are R-CO–, –OC-R-CO–, or –OC-R-[R′-CO–]$_x$-R″-CO– groups and their functional replacement analogues, where R, R′ and R″ are chains, rings, or ring systems, derived from carboxylic acids by the removal of the hydroxy group from each carboxylic acid group that is expressed by the suffix, and x = 1,2,3, etc..

P-65.1.7.1.2. Carboacyl groups.

The name of a monovalent or divalent carboacyl groups derived by removal of the –OH group from each carboxy group of a carboxylic acid or functional replacement analogue denoted by an ‘oic acid’ or ‘ic acid suffix or having a trivial name is derived from the name of the corresponding acid by changing the ‘oic acid’ or ‘ic acid’ ending to ‘oyl’ or ‘yl’. The general rule that the ending of all acyl group prefixes be ‘oyl’, proposed years ago, has not been regularly followed. This rule is fully implemented in these recommendations, but some traditional exceptions are maintained.

Carboacyl groups derived from acids named by means of the suffix ‘carboxylic acid’ are named by changing the suffix ‘carboxylic acid’ to ‘carbonyl’. Acyl groups derived from functional replacement analogues are named by changing the suffixes ‘carbothioic acid’ to ‘carbothioyl’ (and likewise for the selenium and tellurium analogues); ‘carboximidic acid’ to ‘carboximidoyl’; ‘carbohydrazononic acid’ to ‘carbohydrazonoyl’l; and ‘carbohydroximic acid’ to ‘carbohydroximidoyl’.

P-65.1.7.2 Acyl groups derived from carboxylic acids having retained names used as preferred names (see P-55.4.3.1)

P-65.1.7.2.1 Acyl groups from the carboxylic acids described in P-65.1.1.1.

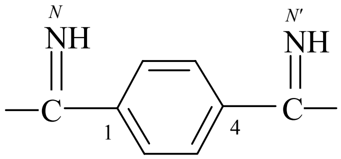
Examples:

CH_3-CO–	acetyl (PIN) ethanoyl	HCO–	formyl (PIN) methanoyl
C_6H_5-CO–	benzoyl (PIN) benzenecarbonyl		

P-65.1.7.2.2 Acyl groups corresponding to the imidic, hydrazonic, and hydroximic, and hydroxamic acids described in P-65.1.3.

Examples:

CH_3-C(=NH)–	ethanimidoyl (PIN) acetimidoyl	HC(=NH)–	methanimidoyl (PIN) formimidoyl
C_6H_5-C(=NH)–	benzenecarboximidoyl (PIN) benzimidoyl		
CH_3-C(=NNH_2)–	methanehydrazonoyl (PIN) formohydraznoyl		
CH_3-C(=NNH_2)–	ethanehydrazonoyl (PIN) acetohydrazonoyl		
C_6H_5-C(=N-OH)–	*N*-hydroxybenzenecarboximidoyl (PIN) *N*-hydroxybenzimidoyl benzenecarbohydroximoyl		



benzene-1,4-dicarboximidoyl (PIN)
terephthalimidoyl

P-65.1.7.2.3 Chalcogen analogues of acyl groups corresponding to carboxylic acids with retained names are named systematically by the infixes of functional replacement nomenclature; these names are preferred IUPAC names.

Examples:

CH_3-CSe–	ethaneselenoyl (PIN) selenoacetyl	HCS–	methanethioyl (PIN) thioformyl
C_6H_5-CS–	benzenecarbonothioyl (PIN) thiobenzoyl		

P-65.1.7.3 Acyl groups derived from acids with names retained for use only in general nomenclature.

P-65.1.7.3.1 Traditional names are maintained for acyl groups derived from acids having retained names for use only in general nomenclature (see P-55-4.3.2); no substitution is allowed. The rule of having acyl groups ending in 'oyl' is applied, with certain exceptions that end in 'yl'. The following exceptions below are limiting. Preferred IUPAC names are systematic substitutive names.

CH_3-CH_2-CH_2-CO–	butyryl butanoyl (PIN)	CH_3-CH_2-CO–	propionyl propanoyl (PIN)
–OC-CH_2-CO–	malonyl propanedioyl (PIN)	–CO-CH_2-CH_2-CO–	succinyl butanedioyl (PIN)
–OC-$[CH_2]_3$-CO–	glutaryl pentanedioyl (PIN)		

Examples:

CH_2=CH-CO–	acryloyl prop-2-enoyl (PIN)	CH_2=C(CH_3)-CO–	methacryloyl 2-methylprop-2-enoyl (PIN)

P-65.1.7.3.2 Acyl groups derived from imidic, hydrazonic, hydroximic acids with retained names for use only in general nomenclature are named by changing the ‘ic acid’ ending of the names described in P-65.1.3 into ‘oyl’.

Examples:

CH_3-CH_2-C(=NH)–
propionimidoyl
propanimidoyl (PIN)

CH_2=CH-C(=NNH_2)–
acrylohydrazonoyl
prop-2-enehydrazonoyl (PIN)

–(HN=)C-CH_2-CH_2-C(=NH)–
succinimidoyl
butanediimidoyl (PIN)

P-65.1.7.3.3 Chalcogen acyl groups derived acids with retained names corresponding to acids used only in general nomenclature are described by prefixes expressing functional replacement

Names of acyl groups derived from monocarboxylic acids are modified by prefixes expressing functional replacement by =S, =Se, and =Te. Acyl group prefixes corresponding to dicarboxylic acids are formed systematically, in accordance with Rule P-65.1.7.4.

Examples:

CH_3-CH_2-CS–
thiopropionyl
propanethioyl (PIN)

CH_2=CH-CSe–
selenoacryloyl
prop-2-eneselenoyl (PIN)

P-65.1.7.4 Acyl groups derived from systematically named carboxylic acids

P-65.1.7.4.1 The name of a monovalent or divalent acyl group formed by removal of the -OH group from each carboxy group of a carboxylic acid denoted by an ‘oic acid’ suffix is derived from the name of the corresponding acid by changing the ending ‘oic acid’ to ‘oyl’. Names of acyl groups derived from carboxylic acids modified by functional replacement are all denoted by the ending ‘oyl’.

Examples:

$\overset{3}{\mathrm{C}}\mathrm{H_3}\text{-}\overset{2}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{1}{\mathrm{C}}\mathrm{O}–$
propanoyl (PIN)
propionyl

$–\mathrm{O}\overset{10}{\mathrm{C}}\text{-}[\mathrm{CH_2}]_8\text{-}\overset{1}{\mathrm{C}}\mathrm{O}–$
decanedioyl (PIN)

$\overset{4}{CH_3}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{C}(=NH)–$

butanimidoyl (PIN)
butyrimidoyl

$–\overset{3}{C}(=NH)\text{-}\overset{2}{CH_2}\text{-}\overset{1}{C}(=NH)–$

propanediimidoyl (PIN)
malonimidoyl

$\overset{3}{CH_3}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CS}–$

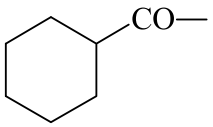
propanethioyl (PIN)
thiopropionyl

$–\overset{4}{C}S\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CS}–$

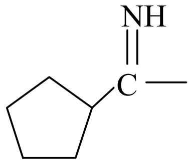
butanebis(thioyl) (PIN)
(not dithiosuccinyl)

P-65.1.7.4.2 Acyl groups derived from an acid named by means of the suffix 'carboxylic acid' are named by changing the 'carboxylic acid' suffix to the suffix 'carbonyl'. Similarly, the suffix 'carbothioic acid' is changed to 'carbothioyl'; the suffix 'carboselenoic acid' is changed to 'carboselenoyl'; the suffix 'carbotelluroic acid' is changed to 'carbotelluroyl'; the suffix 'carboximidic acid' is changed to 'carboximidoyl' and the suffix 'carbohydrazonic acid' is changed to 'carbohydrazonoyl'.

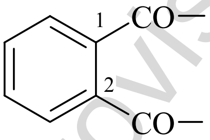
Examples:



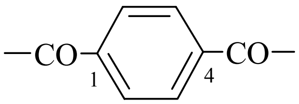
cyclohexanecarbonyl (PIN)



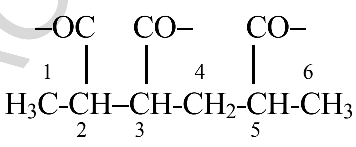
cyclopentanecarboximidoyl (PIN)



benzene-1,2-dicarbonyl (PIN)
phthaloyl

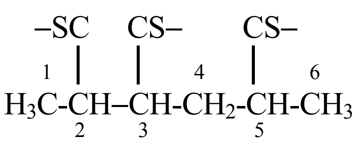


benzene-1,4-dicarbonyl (PIN)
terephthaloyl



$\overset{1}{H_3C}\text{-}\underset{2}{\overset{–OC}{CH}}–\underset{3}{\overset{CO–}{CH}}\text{-}\overset{4}{CH_2}\text{-}\underset{5}{\overset{CO–}{CH}}\text{-}\overset{6}{CH_3}$

hexane-2,3,5-tricarbonyl (PIN)



$\overset{1}{H_3C}\text{-}\underset{2}{\overset{–SC}{CH}}–\underset{3}{\overset{CS–}{CH}}\text{-}\overset{4}{CH_2}\text{-}\underset{5}{\overset{CS–}{CH}}\text{-}\overset{6}{CH_3}$

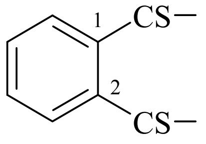
hexane-2,3,5-tricarbothioyl (PIN)

P-65.1.7.4.3 Acyl groups derived from dicarboxylic acids with retained names modified by functional replacement by =S, =Se, and =Te are formed systematically, as described in P-65.1.7.4.2.

Examples:

$$\overset{4}{-\mathrm{C}}\mathrm{S}\text{-}\overset{3}{\mathrm{C}}\mathrm{H}_2\text{-}\overset{2}{\mathrm{C}}\mathrm{H}_2\text{-}\overset{1}{\mathrm{C}}\mathrm{S}-$$

butanebis(thioyl) (PIN)
(not dithiosuccinyl)



benzenedicarbothioyl (PIN)
(not dithiophthaloyl)

P-65.1.8. Formic acid

For organic nomenclature, formic acid is considered to be a monocarboxylic acid (see P-65.1). It is a retained name and treated like acetic acid; it can be functionalized leading to salts, esters, and anhydrides, and forms an acyl group that is used as a substituent group. Functional replacement analogues are named systematically, for example, methanethioic acid and methanimidic acid. The hydrogen atom attached to carbon is substitutable under specific conditions that are described in P-65.1.8.1, P-65.1.8.2, and P-65.1.8.3

P-65.1.8.1 Substitution of the hydrogen atom of formic acid by the following atoms or groups leads to preferred IUPAC names derived from carbonic acid by functional replacement nomenclature (see P-65.2.1.4):

–OOH, –SH, –SeH, –TeH, –F, –Cl, –Br, –I, $–N_3$,
–NC, –CN, –NCO, –NCS, –NCSe, –NCTe, $–NH_2$.

Examples:

Cl-COOH	HS-COOH
carbonochloridic acid (PIN) chloroformic acid	carbonothioic acid (PIN) (not sulfanylformic acid)

P-65.1.8.2 Substitution of the hydrogen atom of formic acid by $–NHNH_2$ leads to a structure named by the suffix carboxylic acid attached to the parent hydride hydrazine (see P-68.3.1.2).

Example:

H_2N-NH-COOH

hydrazinecarboxylic acid (PIN)
carbonohydrazonic acid (see P-65.2.1.4)
(not carbazic acid)

P-65.1.8.3 Substitution of the hydrogen atom of formic acid is permitted when substituent groups are different from those cited in P-65.1.8.1.

Example:

O_2N-COOH

nitroformic acid (PIN)

65.1.8.4 Acyl groups derived from formic acid are formed as described in P-65.1.7.1 and compound prefixes are formed in accordance with the structure of the substituent group. The hydrogen atom present in the group formyl, –CHO, is substitutable under the same conditions as those described in P-65.1.8.1 to P-65.1.8.2 for formic acid.

Examples:

Cl-CO–	Br-CS–
carbonochloridoyl (PIN) (not chloroformyl)	carbonobromidothioyl (PIN) [not bromo(thioformyl)]
HCO-O–	HCO-S–
formyloxy (PIN)	formylsulfanyl (PIN)

P-65.2 Carbonic, cyanic, oxalic, and the polycarbonic acids

Carbonic acid, cyanic acid, oxalic acid, and the polycarbonic acids are a group of functional parent compounds different from carboxylic acids; these acids have no hydrogen atom(s) to be used in substitutive nomenclature.

The following acids classified as mononuclear carbon acids, have retained names that are preferred IUPAC names:

carbonic acid	HO-CO-OH (PIN)
cyanic acid	HO-CN (PIN)

The following acids are di- or polynuclear carbon acids, have retained names that are preferred IUPAC names:

polycarbonic acids	HO-[CO-O]$_n$-H	$n = 4 - 5$; higher homologues are named by skeletal replacement (‘a’) nomenclature
tricarbonic acid	HO-CO-O-CO-O-CO-OH (PIN)	
dicarbonic acid	HO-CO-O-CO-OH (PIN)	
oxalic acid	HO-OC-CO-OH (PIN)	

The decreasing order of seniority of the carbon acids as indicated in Section P-41 is: polycarbonic acids > tricarbonic acid > dicarbonic acid > oxalic acid > carbonic acid > cyanic acid

P-65.2.1 Carbonic acid
P-65.2.2 Cyanic acid
P-65.2.3 Oxalic acid
P-65.2.4 Di- and polynuclear acids

P-65.2.1 Carbonic acid

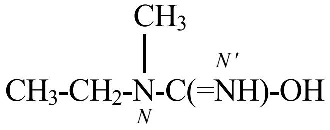
The nomenclature of chalcogen analogues and derivatives of carbonic acid is based on functional replacement of one oxygen in −OH groups or of the doubly bonded oxygen atom, =O, indicated by infixes. Substitution of formic acid is not recommended for generation of these names.

P-65.2.1.1 The contracted name ‘carbamic acid’ (from carbonamidic acid), for H_2N-CO-OH, is retained and is the preferred IUPAC name .

Examples:

$(CH_3)_2N$-COOH

dimethylcarbamic acid (PIN)



$$CH_3\text{-}CH_2\text{-}\underset{N}{\overset{\overset{CH_3}{|}}{N}}\text{-}\overset{N'}{C}(=NH)\text{-}OH$$

N-ethyl-*N*-methylcarbamimidic acid (PIN)

$H_2N\text{-}CH_2\text{-}CH_2\text{-}\overset{N}{N}H\text{-}CO\text{-}O\text{-}CH_2\text{-}\overset{2}{C}H(OH)\text{-}CH_3$

2-hydroxypropyl *N*-(2-aminoethyl)carbamate (PIN)

P-65.2.1.2 Functional replacement in carbonic acid and carbamic acid by −OO−, −S−, −Se−, and −Te− is expressed by the infixes ‘peroxo’, ‘thio’, ‘seleno’, ‘telluro’. In names, tautomeric groups in mixed chalcocarbonic acids, such as HO-CO-SH or HO-CS-OH, are distinguished by prefixing italic element symbols, such as *S* or *O*, respectively, to the term ‘acid ’; the italic symbols *OS* and *SO* are used for peroxy acids

Examples:

H_2N-CS-OH carbamothioic *O*-acid (PIN)	H_2N-CO-SeH carbamoselenoic *Se*-acid (PIN)
HO-CO-SH carbonothioic *S*-acid (PIN) (not sulfanylformic acid)	HSe-CO-SeH carbonodiselenoic *Se*,*Se*-acid (PIN)
HS-CS-SH (PIN) carbonotrithioic acid	H_2N-CO-OOH (PIN) carbamoperoxoic acid
HO-CO-OOH (PIN) carbonoperoxoic acid	HOO-CO-OOH (PIN) carbonodiperoxoic acid

HO-CO-OSH

carbono(thioperoxoic) *OS*-acid (PIN)

HOS-CO-OSH

carbonobis(thioperoxoic) *OS*,*SO*-acid (PIN)

H_2N-C(=NH)-OSH

carbamimido(thioperoxoic) *OS*-acid (PIN)

P-65.2.1.3 Functional replacement of =O in carbonic acid and carbamic acid by =NH and =N-NH_2 is expressed by the infixes 'imido' and 'hydrazono' and of oxygen in –OH groups in the resulting acids by chalcogen atoms is expressed by infixes, as in P-65.1.1.5.1.2.

Italic letter locants *N*, *N′*, etc. are used to designate substitution on nitrogen atoms.

Examples:

HO-C(=NH)-OH carbonimidic acid (PIN)	H_2N-C(=NH)-OH carbamimidic acid (PIN)
HO-C(=N-NH_2)-OH carbonohydrazonic acid (PIN)	HS-C(=NH)-OH carbonimidothioic acid (PIN)

$H_2N\text{-}C(=NH)\text{-}SH$	$HSe\text{-}C(=N\text{-}NH_2)\text{-}SeH$
carbamimidothioic acid (PIN)	carbonohydrazonodiselenoic acid (PIN)

P-65.2.1.4 Functional replacement (see P-67) of one of the −OH groups of carbonic acid by various atoms or groups is expressed by the following infixes: fluorido, −F; chlorido, −Cl; bromido, −Br; iodido, −I; azido, $-N_3$; amido, $-NH_2$; cyanido, −CN; isocyanido, −NC; isocyanatido, −NCO; isothiocyanatido, −NCS; isoselenocyanatido, −NCSe; isotellurocyanatido, −NCTe.

Italic letter locants *N*, *N*′, etc. are used to designate substitution on nitrogen atoms.

Replacement by the $-NHNH_2$ group results in hydrazinecarboxylic acid and related derivatives (see P-68.3.1.2.4).

Examples:

$H_2N\text{-}CO\text{-}OH$	$H_2N\text{-}C(=NH)\text{-}OH$
carbamic acid (PIN) (not carbonamidic acid)	carbamimidic acid (PIN) (not carbonamidimidic acid)
$H_2N\text{-}CO\text{-}SH$	$H_2N\text{-}C(=NH)\text{-}SeH$
carbamothioic *S*-acid (PIN)	carbamimidoselenoic acid (PIN)
Cl-CO-OH	NC-CO-OH
carbonochloridic acid (PIN)	carbonocyanidic acid (PIN)
$N_3\text{-}CO\text{-}OH$	SCN-CO-OH
carbonazidic acid (PIN)	carbonisothiocyanatidic acid (PIN)

$H_2N\text{-}NH\text{-}CO\text{-}OH$

hydrazinecarboxylic acid (PIN; see P-68.3.1.2.4)
(not carbonohydrazonic acid; acids expressed by suffixes are senior to carbonic acid analogues)

P-65.2.1.5 Acyl groups derived from carbonic and related acids

Acyl groups are derived from carbonic and related acids, including functional replacement analogues, by the removal of one or two hydroxy groups from the acid. They are named in accordance with the methodology described in P-65.1.7. Names are formed in two ways:

(1) Names may be formed by changing the -ic or -oic acid ending of the name of the acid to –yl or –oyl, respectively. Names of acyl groups ending in –yl are exceptions to the

general rule (see P-65.1.7). This method is the traditional method that consists in removing the two hydroxy groups from carbonic acid or its analogues; it is now recommended to be used also when only one hydroxy group is present in an acid. It is also recommended that divalent acyl groups, such as ‘carbonyl’ represent only the ‘diyl’ type of substituent prefix in which the two free valences are divergent (symbols CO< or –CO–). Substituent prefixes in which both free valences are attached to the same atom are named by substitutive nomenclature, for example, =CO is named oxomethylidene (see P-65.2.1.7)

(2) Names may be formed by a concatenation operation, i.e., by adding appropriate monovalent substituent groups to divalent acyl groups such as ‘carbonyl’, ‘carbonothioyl’, and ‘carbonimidoyl’ formed by method (1).

Names formed by method (1) are preferred IUPAC names; they are preferred to other names for acyl groups, including the use of prefixes rather than infixes or names formed by full or partial concatenation.

Examples:

HO-CO-OH
carbonic acid (PIN)

–CO–
carbonyl (PIN)

HO-CS-OH
carbonothioic *O*,*O*-acid (PIN)

–CS–
carbonothioyl (PIN)
thiocarbonyl

HO-C(=NH)-OH
carbonimidic acid (PIN)

–C(=NH)–
carbonimidoyl (PIN)

HO-C(=NH_2)-OH
carbonohydrazonic acid (PIN)

–C(=NH_2)–
carbonohydrazonoyl (PIN)

H_2N-CO-OH
carbamic acid (PIN)

H_2N-CO–
carbamoyl (PIN)
aminocarbonyl

H_2N-CS-OH
carbamothioic *O*-acid (PIN)

H_2N-CS–
carbamothioyl (PIN)
aminocarbonothioyl

$\mathrm{H_2N}$-C(=NH)-OH	$\mathrm{H_2N}$-C(=NH)–
carbamimidic acid (PIN)	carbamimidoyl (PIN) aminocarbonimidoyl
Cl-CO-OH	Cl-CO–
carbonochloridic acid (PIN)	carbonochloridoyl (PIN) chlorocarbonyl
NC-CO-OH	NC-CO–
carbonocyanidic acid (PIN)	carbonocyanidoyl (PIN) cyanocarbonyl
Br-CS-OH	Br-CS–
carbonobromidothioic *O*-acid (PIN)	carbonobromidothioyl (PIN) bromocarbonothioyl
Cl-C(=NH)-OH	Cl-C(=NH)–
carbonochloridimidic acid (PIN)	carbonochlorimidoyl (PIN) *C*-chlorocarbonimidoyl
HOO-CO-OH	HOO-CO−
carbonoperoxoic acid	carbonoperoxoyl (PIN) hydroperoxycarbonyl

P-65.2.1.6 The prefix ‘carboxy’ and related prefixes.

The prefix ‘carboxy’ for −COOH is a retained prefix. Chalcogen analogues are named by functional replacement nomenclature provided that it is not necessary to specify the location of the chalcogen atom. Specification of chalcogen atoms is accomplished by compound prefixes formed by concatenation.

Examples:

−COSH or −CSOH	HS-CO–
thiocarboxy (PIN)	sulfanylcarbonyl (PIN)

HS-CS–

dithiocarboxy (PIN)
sulfanylcarbonothioyl

HOOC-O–

carboxyoxy (PIN)

HOOC-S–

carboxysulfanyl (PIN)

HOOC-NH–

carboxyamino (PIN)

HS-CO-O−

(sulfanylcarbonyl)oxy (PIN)

P-65.2.1.7 Chalcogen analogues of the ‘carbonoperoxoyl’ prefix, −CO-OOH, are named in two ways.:

(1) by compound prefixes formed by concatenation;

(2) by thiohydroperoxy prefixes using the italic prefixes *SO*- or *OS*-, as necessary.

Method (1) leads to preferred IUPAC names.

Examples:

HOS-CSe–

(hydroxysulfanyl)carbonoselenoyl (PIN)
(*OS*-thiohydroperoxy)carboselenoyl

HOS-CO− or HSO-CO−

carbono(thioperoxoyl) (PIN)
(thiohydroperoxy)carbonyl

HS-O-CO-O–

[(sulfanyloxy)carbonyl]oxy (PIN)
[(*SO*-thiohydroperoxy)carbonyl]oxy

HSS-CO-O–

(disulfanylcarbonyl)oxy (PIN)
(dithiohydroperoxycarbonyl)oxy

P-65.2.1.8 Names of non-acyl substituent groups derived from carbonic acid

Acyl groups derived from carbonic acid and carbonic acids modified by functional replacement are divalent groups with the two free valences belonging to the ‘diyl’ type, such as CO<. When the two free valences are of the ‘ylidene’ type, =C=O for example, names of acyl groups are no longer used to designate such groups; systematic substitutive names are used instead.

Examples:

=C=O oxomethylidene (PIN)

=C=S sulfanylidenemethylidene (PIN)
thioxomethylidene

=C=NH	iminomethylidene (PIN)
$=C=N\text{-}NH_2$	hydrazinylidenemethylidene (PIN) hydrazonomethylidene

P-65.2.2 Cyanic acid

Cyanic acid is the retained name for NC-OH. The functional replacement name based on carbonic acid would be carbononitridic acid, but this name has not been used and is not recommended. Cyanic acid is classified as an acid, thus generating anhydrides (see P-65.7.2) and esters (see P-65.6.3.2).

Functional replacement by –OO–, –S–, –Se–, and –Te–, is expressed by the appropriate functional replacement prefix. This exception to the use of infixes in the functional replacement nomenclature applied to the mononuclear noncarboxylic acids carbonic acid and formic acid is necessary to maintain well entrenched traditional names and their related isocyanates, such as isothiocyanates.

Prefixes derived from cyanic acid are 'cyano' for −CN and 'cyanato' for −O-CN, 'thiocyanato ' for −S-CN, 'selenocyanato' for −Se-CN, and 'tellurocyanato' for −Te-CN.

Examples:

NC-SeH
selenocyanic acid (PIN)

NC-OOH
peroxycyanic acid (PIN)

NC-SS–
cyanodisulfanyl (PIN)
(not thiocyanatosulfanyl)

NC-SS-CN
disulfanedinitrile

$NC\text{-}CH_2\text{-}COOH$
2-cyanoacetic acid (PIN)

$NC\text{-}S\text{-}CH_2\text{-}CH_2\text{-}COOH$
3-thiocyanatopropanoic acid (PIN)

P-65.2.3 Oxalic acid, HO-CO-CO-OH

The name 'oxalic acid' is retained and is the preferred IUPAC name. This acid belongs to the group of polynuclear oxoacids having a direct link between central atoms (see P-67.2 and also Rule I-9.7.2, ref. 14).

P-65.2.3.1. Retained names for acids related to oxalic acid are as follows:

$H_2N\text{-}CO\text{-}CO\text{-}OH$	oxamic acid (PIN) (contraction of oxalamic acid) amino(oxo)acetic acid

OHC-CO-OH oxaldehydic acid (PIN)
(contraction of oxalaldehydic acid)
oxoacetic acid

P-65.2.3.2 Functional replacement nomenclature using only prefixes to designate the replacement of –OH or =O is used to name derivatives other than those in P-65.2.3.1.

P-65.2.3.2.1 General methodology
P-65.2.3.2.2 Replacement by –OOH, –S–, =S, –Se–, =Se, –Te–, =Te, =NH and $=NHNH_2$
P-65.2.3.2.3 Replacement by halides and pseudohalides
P-65.2.3.2.4 Replacement by $–NH_2$ and $–NHNH_2$

P-65.2.3.2.1 General methodology

Prefixes are used to indicate the replacement of oxygen atoms by other groups generally listed as replacing groups (see P-16). The two carbon atoms are numbered and the locants are used to indicate the position of the replacing atoms or groups cited as prefixes.

P-65.2.3.2.2 Replacement by –OO–, –S–, =S, –Se–, =Se, –Te–, =Te, =NH and $=NHNH_2$

Functional replacement of oxygen atom(s) is denoted by prefixes, i.e., peroxy, −OO−; thio, −S− or =S; seleno, −Se− or =Se; telluro, −Te− or =Te; imido, =NH, and hydrazono $=NHNH_2$ (see P-15.5). The position of each replaced oxygen atom is denoted by the appropriate numerical locant. When necessary, letter locants *O*, *S, Se*, and *Te* are used before the acid term, as appropriate, to designate the position of a chalcogen atom in the −OH group rather than the =O group. Numerical locants are used in front of the letter locants *O*, *S, Se*, and *Te*, as needed.

Italic letter locants *N*, *N*′, etc. are used to designate substitution on nitrogen atoms of imido and hydrazono groups.

Examples:

CO_3SH_2
thiooxalic acid (PIN)

$H(S/O)\overset{1}{C}\text{-}\overset{2}{C}O\text{-}OH$
1- thiooxalic acid (PIN)

$HS\text{-}\overset{1}{C}O\text{-}\overset{2}{C}O\text{-}OH$
1-thiooxalic *S*-acid (PIN)

$HS\text{-}\overset{1}{C}S\text{-}\overset{2}{C}O\text{-}OH$
1,1-dithiooxalic acid (PIN)

$HO\text{-}\overset{1}{C}S\text{-}\overset{2}{C}O\text{-}SH$
1,2-dithiooxalic *O*,*S*-acid (PIN)

$\mathrm{HS\text{-}\overset{1}{C}S\text{-}\overset{2}{C}O\text{-}SH}$

1,1,2-trithiooxalic *S*-acid (PIN)

$\mathrm{HS\text{-}\overset{1}{C}S\text{-}\overset{2}{C}S\text{-}SH}$

tetrathiooxalic acid (PIN)

$\mathrm{O\overset{2}{H}C\text{-}\overset{1}{C}O\text{-}SH}$

1-thiooxaldehydic *S*-acid (PIN)
2-oxoethanethioic *S*-acid

$\mathrm{SHC\text{-}CO\text{-}OH}$

2-thiooxaldehydic acid (PIN)
2-thioxoacetic acid

$\mathrm{HO\text{-}\overset{1}{C}(=\overset{\mathit{N}}{N}H)\text{-}\overset{2}{C}O\text{-}OH}$

imidooxalic acid (PIN)

$\mathrm{HO\text{-}\overset{1}{C}(=\overset{\mathit{N}}{N}H)\text{-}\overset{2}{C}(=\overset{\mathit{N'}}{N}H)\text{-}OH}$

diimidooxalic acid (PIN)

$\mathrm{HO\text{-}\overset{1}{C}(=N\overset{\mathit{N}}{N}H_2)\text{-}\overset{2}{C}O\text{-}OH}$

hydrazonooxalic acid (PIN)

$\mathrm{HO\text{-}\overset{1}{C}(=N\overset{\mathit{N}}{N}H_2)\text{-}\overset{2}{C}(=N\overset{\mathit{N'}}{N}H_2)\text{-}OH}$

dihydrazonooxalic acid (PIN)

$\mathrm{HO\text{-}\overset{1}{C}(=\overset{\mathit{N}}{N}H)\text{-}\overset{2}{C}(=N\overset{\mathit{N'}}{N}H_2)\text{-}OH}$

1-hydrazono-2-imidooxalic acid (PIN)

$\mathrm{HS\text{-}\overset{2}{C}O\text{-}\overset{1}{C}(=NH)\text{-}OH}$

1-imido-2-thiooxalic *S*-acid

P-65.2.3.2.3 Replacement by halides and pseudohalides

The prefixes bromo for –Br, chloro for –Cl, fluoro for –F, and iodo for –I , azido for $–N_3$, cyano for –CN, isocyano for –NC, cyanato for –NCO, isocyanato for –OCN, isothiocyanato for −SCN (and similarly for other chalcogen analogues) are used to indicate functional replacement (see P-15.5).

Examples:

$\mathrm{Br\text{-}\overset{1}{C}O\text{-}\overset{2}{C}O\text{-}OH}$

bromooxalic acid (PIN)
(not 2-bromo-2-oxoacetic acid)

$\mathrm{SCN\text{-}\overset{1}{C}O\text{-}\overset{2}{C}O\text{-}OH}$

(isothiocyanato)oxalic acid (PIN)
(not 2-isocyanato-2-oxoacetic acid)

$\mathrm{Cl\text{-}\overset{2}{C}S\text{-}\overset{1}{C}OOH}$

2-chloro-2-thiooxalic acid(PIN)
(not 2-chloro-2-thioxo-acetic acid)

$\mathrm{NC\text{-}CO\text{-}COOH}$

cyanooxalic acid (PIN)
(not 2-cyano-2-oxoacetic acid)

P-65.2.3.2.4 Replacement by $-NH_2$ and $-NHNH_2$

The prefixes amido for $-NH_2$ and hydrazido for $-NHNH_2$ are used with oxalic acid in functional replacement nomenclature. The name oxamic acid is retained for the amic acid $H_2N\text{-}CO\text{-}COOH$. Italic letter locants *N*, *N*′, etc. are used to designate substitution on nitrogen atoms. Functional replacement prefixes are used to indicate replacement of =O in oxamic acid.

Examples:

$\overset{N}{H_2N}\text{-}\overset{2}{CO}\text{-}\overset{1}{CO}\text{-}OH$

oxamic acid (PIN)
amidooxalic acid
(not 1-amino-2-oxoacetic acid)

$\overset{N'}{H_2N}\text{-}\overset{N'}{NH}\text{-}\overset{1}{CO}\text{-}\overset{2}{CO}\text{-}OH$

hydrazidooxalic acid (PIN)
(not 2-hydrazino-2-oxoacetic acid)

$\overset{N}{H_2N}\text{-}\overset{1}{C}(\overset{N'}{=NH})\text{-}\overset{2}{C}(\overset{N''}{=NH})\text{-}OH$

diimidooxamic acid (PIN)
(not 2-amino-1-iminoacetic acid)

$\overset{N'}{H_2N}\text{-}\overset{N'}{NH}\text{-}\overset{1}{CO}\text{-}\overset{2}{C}(\overset{N''}{=NH})\text{-}OH$

1-hydrazido-2-imidooxalic acid (PIN)
(not 2-hydrazino-2-iminoacetic acid)

$H_2N\text{-}\overset{2}{CO}\text{-}\overset{1}{CS}\text{-}OH$

1-thiooxamic *O*-acid (PIN)
2-amido-1-thiooxalic *O*-acid
(not 2-amino-2-oxothioacetic *O*-acid)

$H_2N\text{-}\overset{2}{CS}\text{-}\overset{1}{CO}\text{-}OH$

2-thiooxamic acid (PIN)
(not 2-amino-2-thioxoacetic acid)

P-65.2.3.3. Substituent groups cited as prefixes

The acyl groups oxalyl, oxalo, oxamoyl, and oxaldehydoyl are retained as preferred IUPAC names for use as substituent prefixes but not for naming acid halides, amides, and hydrazides, etc. (see P-65.5.1.2; P-66.1.5.5; P-66.3.5.1). Concatenation and functional replacement prefixes are used with oxalyl to form preferred IUPAC names of derivatives.

Examples:

–OC-CO–

oxalyl (PIN)
ethanedioyl
dioxoethane-1,2-diyl

HO-CO-CO–

oxalo (PIN)
carboxycarbonyl
(not carboxyformyl)
(not hydroxy(oxo)acetyl)

$\mathrm{Cl\text{-}\overset{2}{C}O\text{-}\overset{1}{C}O\text{–}}$

chlorooxalyl (PIN)
2-chloro-1,2-dioxoethyl

$\mathrm{Cl\text{-}\overset{2}{C}O\text{-}\overset{1}{C}S\text{–}}$

2-chloro-1-thiooxalyl (PIN)
2-chloro-2-oxo-1-thioxoethyl

$H_2N\text{-}CO\text{-}CO\text{–}$

oxamoyl (PIN)
(not carbamoylcarbonyl)
(not carbamoylformyl)
(not amino(oxo)acetyl)

HCO-CO–

oxaldehydoyl (PIN)
hydrooxalyl
(not formylcarbonyl)

HOOC-CS–

1-thiooxalo (PIN)
(not carboxycarbonothioyl)

H{O/S}C-CO–

2-thiooxalo (PIN)
[not (thiocarboxy)carbonyl]

HO-CS-CO–

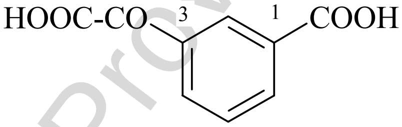
2-hydroxy-2-thiooxalyl (PIN)
[not (hydroxycarbonothioyl)carbonyl]

HS-CS-CS–

trithiooxalo (PIN)
(not dithiocarboxycarbonothioyl)

$HOOC\text{-}CO\text{-}CH_2\text{-}COOH$

2-oxaloacetic acid (PIN)
3-carboxy-3-oxopropanoic acid
(not 4-hydroxy-3,4-dioxobutanoic acid)



3-oxalobenzoic acid (PIN)
3-(carboxycarbonyl)benzoic acid

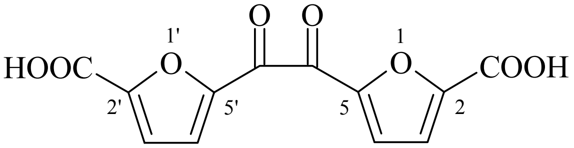
HOOC-CO-O–

oxalooxy (PIN)
(carboxycarbonyl)oxy
[not carboxyformyl)oxy]
[not [hydroxy(oxo)acetyl]oxy]

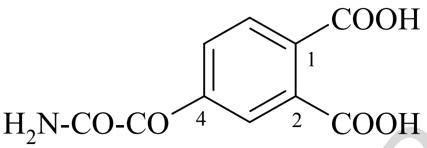
HOOC-CO-NH–

oxaloamino (PIN)
(carboxycarbonyl)amino
[not carboxyformamido]
[not [hydroxy(oxo)acetyl]amino]

HOOC-CO-S–	HOOC-CS-S–
oxalosulfanyl (PIN)	1-thiooxalylsulfanyl
(carboxycarbonyl)sulfanyl	(carboxycarbonothioyl)sulfanyl
[not (carboxyformyl)sulfanyl]	[not carboxythioformyl)sulfanyl]
[not [hydroxy(oxo)acetyl]sulfanyl]	[not [hydroxy(oxo)ethanethioyl]sulfanyl



5,5′-oxalyldi(furan-2-carboxylic acid) (PIN)
5,5′-oxalyldi-(2-furoic acid)



4-oxamoylbenzene-1,2-dicarboxylic acid (PIN)
4-oxamoylphthalic acid

P-65.2.4 Di- and polycarbonic acids

Di- and polycarbonic acids belong to the series of homopolynuclear acids, whose central atom is carbon. Their generic formula is HO-[CO-O]$_n$-H, where *n* is 2, 3, 4, etc. They are named by adding a multiplying prefix corresponding to the number of carbon atoms to the name ‘carbonic acid’. The structure is numbered consecutively from one end to the other, starting from and ending at a carbon atom:

Examples:

$\text{HO-}\overset{1}{\text{C}}\text{O-}\overset{2}{\text{O}}\text{-}\overset{3}{\text{C}}\text{O-OH}$	dicarbonic acid (PIN)
$\text{HO-}\overset{1}{\text{C}}\text{O-}\overset{2}{\text{O}}\text{-}\overset{3}{\text{C}}\text{O-}\overset{4}{\text{O}}\text{-}\overset{5}{\text{C}}\text{O-OH}$	tricarbonic acid (PIN)

P-65.2.4.1 Functional replacement for di- and polynuclear carbon acids

P-65.2.4.1.1 General methodology
P-65.2.4.1.2 Replacement by –OO–, –S–, =S, –Se–, =Se, –Te–, =Te, =NH, and =NHNH$_2$

P-65.2.4.1.3 Replacement by halides and pseudohalides
P-65.2.4.1.4 Replacement by $–NH_2$ and $–NHNH_2$ groups.

P-65.2.4.1.1 General methodology

Nomenclature for functional analogues of the polycarbonic acids follows the principles for naming polynuclear inorganic oxo acids (see P-67). Prefixes are used to indicate functional replacement and the chain is numbered consecutively from one end to the other, starting from and ending at a carbon atom. These prefixes are listed in Table 4.2; they are cited in alphabetical order in front of the retained name of the polyacid, with appropriate locants as required.

P-65.2.4.1.2 Replacement by −OO–, −S–, =S, −Se–, =Se, −Te–, =Te, −NH–, =NH, and $=NHNH_2$

Functional replacement of oxygen atom(s), -OH, =O, –O–, is denoted by prefixes, i.e., peroxy for −OO−; thio for −S− or =S; seleno for −Se− or =Se; telluro for −Te− or =Te; imido for −NH− or =NH, and hydrazono for $=NHNH_2$. The position of each replaced oxygen atom is denoted by the appropriate numerical locant.

Italic letter locants *N*, *N′*, etc. are used to designate substitution on nitrogen atoms that are not anhydride linkages.

Examples:

$\mathrm{HO}\text{-}\overset{1}{\mathrm{CO}}\text{-}\overset{2}{\mathrm{S}}\text{-}\overset{3}{\mathrm{CO}}\text{-}\mathrm{OH}$

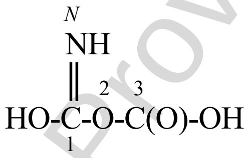
2-thiodicarbonic acid (PIN)

$\mathrm{HO}\text{-}\overset{1}{\mathrm{CO}}\text{-}\overset{2}{\mathrm{NH}}\text{-}\overset{3}{\mathrm{CO}}\text{-}\mathrm{OH}$

2-imidodicarbonic acid (PIN)

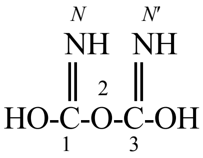
$\mathrm{HO}\text{-}\overset{1}{\mathrm{CO}}\text{-}\overset{2}{\mathrm{OO}}\text{-}\overset{3}{\mathrm{CO}}\text{-}\mathrm{OH}$

2-peroxydicarbonic acid (PIN)



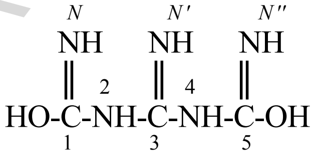
$\mathrm{HO}\text{-}\underset{1}{\overset{\overset{\mathit{N}}{\mathrm{NH}}}{\overset{\|}{\mathrm{C}}}}\text{-}\overset{2}{\mathrm{O}}\text{-}\overset{3}{\mathrm{C}}\mathrm{(O)}\text{-}\mathrm{OH}$

1-imidodicarbonic acid (PIN)



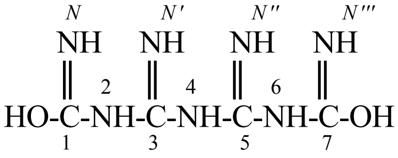
$\mathrm{HO}\text{-}\underset{1}{\overset{\overset{\mathit{N}}{\mathrm{NH}}}{\overset{\|}{\mathrm{C}}}}\text{-}\overset{2}{\mathrm{O}}\text{-}\underset{3}{\overset{\overset{\mathit{N'}}{\mathrm{NH}}}{\overset{\|}{\mathrm{C}}}}\text{-}\mathrm{OH}$

1,3-diimidodicarbonic acid (PIN)



$\mathrm{HO}\text{-}\underset{1}{\overset{\overset{\mathit{N}}{\mathrm{NH}}}{\overset{\|}{\mathrm{C}}}}\text{-}\overset{2}{\mathrm{NH}}\text{-}\underset{3}{\overset{\overset{\mathit{N'}}{\mathrm{NH}}}{\overset{\|}{\mathrm{C}}}}\text{-}\overset{4}{\mathrm{NH}}\text{-}\underset{5}{\overset{\overset{\mathit{N''}}{\mathrm{NH}}}{\overset{\|}{\mathrm{C}}}}\text{-}\mathrm{OH}$

1,2,3,4,5-pentaimidotricarbonic acid (PIN)



$\mathrm{HO}\text{-}\underset{1}{\overset{\overset{\mathit{N}}{\mathrm{NH}}}{\overset{\|}{\mathrm{C}}}}\text{-}\overset{2}{\mathrm{NH}}\text{-}\underset{3}{\overset{\overset{\mathit{N'}}{\mathrm{NH}}}{\overset{\|}{\mathrm{C}}}}\text{-}\overset{4}{\mathrm{NH}}\text{-}\underset{5}{\overset{\overset{\mathit{N''}}{\mathrm{NH}}}{\overset{\|}{\mathrm{C}}}}\text{-}\overset{6}{\mathrm{NH}}\text{-}\underset{7}{\overset{\overset{\mathit{N'''}}{\mathrm{NH}}}{\overset{\|}{\mathrm{C}}}}\text{-}\mathrm{OH}$

1,2,3,4,5,6,7-heptaimidotetracarbonic acid (PIN)

$\mathrm{HO\text{-}\overset{3}{C}O\text{-}\overset{2}{O}\text{-}\overset{1}{C}O\text{-}OOH}$

1-peroxydicarbonic acid (PIN)

$\mathrm{HOO\text{-}\overset{1}{C}O\text{-}\overset{2}{O}\text{-}\overset{3}{C}O\text{-}OOH}$

1,3-diperoxydicarbonic acid (PIN)

When necessary, letter locants *O*, *S, Se*, and *Te* are used, as appropriate, to designate the position of a chalcogen atom replacing oxygen in –OH or =O groups. Numerical locants are used in front of the letter locants *O*, *S, Se*, and *Te* placed before the term 'acid' as needed.

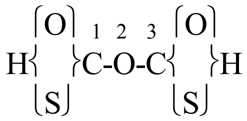
Examples:

$\mathrm{HS\text{-}\overset{3}{C}S\text{-}\overset{2}{O}\text{-}\overset{1}{C}S\text{-}SH}$

1,1,3,3-tetrathiodicarbonic acid (PIN)

$\mathrm{HS\text{-}\overset{1}{C}S\text{-}\overset{2}{S}\text{-}\overset{3}{C}S\text{-}SH}$

pentathiodicarbonic acid (PIN)



$\mathrm{H\left\{\begin{matrix}O\\S\end{matrix}\right\}\overset{1}{C}\text{-}\overset{2}{O}\text{-}\overset{3}{C}\left\{\begin{matrix}O\\S\end{matrix}\right\}H}$

or

$\mathrm{H\{O/S\}\overset{1}{C}\text{-}\overset{2}{O}\text{-}\overset{3}{C}\{O/S\}H}$

1,3-dithiodicarbonic acid (PIN; the location of the sulfur atoms is unknown)

$\mathrm{HS\text{-}\overset{1}{C}O\text{-}\overset{2}{O}\text{-}\overset{3}{C}O\text{-}SH}$

1,3-dithiodicarbonic 1-*S*,3-*S*-acid (PIN)

$\mathrm{HO\text{-}\overset{1}{C}S\text{-}\overset{2}{O}\text{-}\overset{3}{C}S\text{-}OH}$

1,3-dithiodicarbonic 1-*O*,3-*O*-acid (PIN)

Compound substituent groups may have to be used to name chalcogen analogues when the location of chalcogen atoms is not known.

Examples:

H{O/S}C-O-CO-SH

[(thiocarboxy)oxy]formothioic *S*-acid (PIN)

H{O/S}C-O-CS-OH

[(thiocarboxy)oxy]formothioic *O*-acid (PIN)

P-65.2.4.1.3 Replacement by halides and pseudohalides

Prefixes bromo for –Br, chloro for –Cl, fluoro for –F, and iodo for –I , azido for $–N_3$, isocyano for −NC, isocyanato for –NCO (and chalcogen analogues) are used to indicate functional replacement.

Examples:

$\text{Cl-}\overset{1}{\text{C}}\text{O-}\overset{2}{\text{O}}\text{-}\overset{3}{\text{C}}\text{O-OH}$

chlorodicarbonic acid (PIN)

$\text{OCN-}\overset{1}{\text{C}}\text{O-}\overset{2}{\text{N}}\text{H-}\overset{3}{\text{C}}\text{O-OH}$

1-isocyanato-2-imidodicarbonic acid
(locants are used to avoid ambiguity)

P-65.2.4.1.4 Replacement by NH_2 and $NHNH_2$ groups

The prefixes amido and hydrazido are used to indicate functional replacement by $-NH_2$ and $-NHNH_2$ groups, respectively. Italic letter locants *N*, *N′*, etc. are used to designate substitution on nitrogen atoms that are not anhydride linkages.

Examples:

$\text{H}_2\text{N-}\overset{1}{\text{C}}\text{O-}\overset{2}{\text{S}}\text{-}\overset{3}{\text{C}}\text{O-OH}$

1-amido-2-thiodicarbonic acid (PIN)

$\text{H}_2\text{N-NH-}\overset{1}{\text{C}}\text{O-}\overset{2}{\text{N}}\text{H-}\overset{3}{\text{C}}\text{O-}\overset{4}{\text{N}}\text{H-}\overset{5}{\text{C}}\text{O-OH}$

1-hydrazido-2,4-diimidotricarbonic acid (PIN)

P-65.2.4.1.5 Substituent groups derived from polycarbonic acids

Names of substituent groups are formed by substitution or concatenation as required.

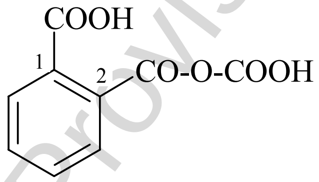
Examples:

HOOC-O-CO–

(carboxyoxy)carbonyl (PIN)
(carboxyoxy)formyl

HS-CS-S-CS–

[(dithiocarboxy)sulfanyl]carbonothioyl (PIN)
[(sulfanylcarbonothioyl)sulfanyl]carbonothioyl
[sulfanyl(thiocarbonyl)sulfanyl](thiocarbonyl)
[not (dithiocarboxy)sulfanyl]thioformyl]



2-[(carboxyoxy)carbonyl]benzoic acid (PIN)

P-65.3 Sulfur, selenium, and tellurium acids with chalcogen atoms directly linked to a parent hydride.

P-65.3.0 Introduction. The following acids are discussed in this section:

R-SO_3H	sulfonic acids	R-SO_2H	sulfinic acids
R-SeO_3H	selenonic acids	R-SO_2H	seleninic acids
R-TeO_3H	telluronic acids	R-TeO_2H	tellurinic acids

Table 6.1 Suffixes and prefixes used to denote sulfur, selenium, and tellurium acids with chalcogen atoms directly linked to a parent

Group	Suffix	Prefix
SO_2-OH	sulfonic acid	sulfo
SO-OH	sulfinic acid	sulfino
SeO_2-OH	selenonic acid	selenono
SeO-OH	seleninic acid	selenino
TeO_2-OH	telluronic acid	tellurono
TeO-OH	tellurinic acid	tellurino

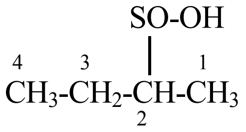
P-65.3.1 Substitutive nomenclature, suffix mode, for sulfonic, sulfinic, etc., acids

Sulfonic, sulfinic, etc., acids are named substitutively by adding an appropriate suffix listed in Table 6.1 to the name of a parent hydride name. Multiplying prefixes ‘di’, ‘tri’, ‘tetra’, etc. are used to denote multiplicity of suffixes.

Examples:

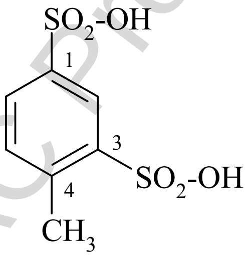
$C_6H_5\text{-}SO_2\text{-}OH$

benzenesulfonic acid (PIN)

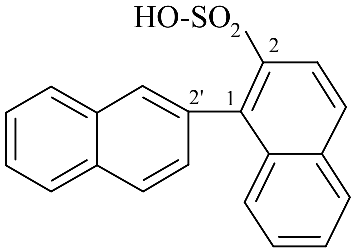


$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\underset{2}{\overset{SO\text{-}OH}{C}}H\text{-}\overset{1}{C}H_3$

butane-2-sulfinic acid (PIN)



4-methylbenzene-1,3-disulfonic acid (PIN)
(not toluene-2,4-disulfonic acid)



[1,2′-binaphthalene]-2-sulfonic acid (PIN)

P-65.3.1.1 Modification by functional replacement

Oxygen atoms of a suffix acid may be replaced by -OO- and/or other chalcogen analogues, –S– or =S, –Se– or =Se, –Te– or =Te, =NH and =N-NH_2 by functional replacement nomenclature. The general methodology is to modify the suffixes by infixes and use them in systematic substitutive nomenclature in the way prescribed for unmodified suffixes. If necessary, names are formed in accordance with the order of seniority, unmodified acids followed by –OO– > S > Se > Te . This seniority is fully exemplified in Section P-43 and in Appendix 1.

P-65.3.1.2 Peroxy acids

The suffixes given in Table 6.1 are modified by the infix ‘peroxo’ and used as such in substitutive nomenclature as illustrated by the following suffixes.

$-SO_2\text{-}OOH$
sulfonoperoxoic acid

$-SeO\text{-}OOH$
seleninoperoxoic acid

Examples:

$CH_3\text{-}SO_2\text{-}OOH$
methanesulfonoperoxoic acid (PIN)

$C_6H_5\text{-}TeO\text{-}OOH$
benzenetellurinoperoxoic acid (PIN)

P-65.3.1.3 Modification by other chalcogen atoms

Suffixes are modified by the infixes ‘thio’, for –S– or =S, ‘seleno’, for –Se – or =Se, and ‘telluro’, for –Te – or =Te, and used as such. Tautomers are denoted by symbols *S*, *Se* and *Te* placed in front of the term ‘acid’, to express positions of chalcogen atoms when known. The infixes ‘thioperoxo’, ‘selenoperoxo’, etc. are used to indicate functional replacement in peroxy acids.

$-SO_2\text{-}SH$
sulfonothioic *S*-acid

$-Se(=S)\text{-}OH$
seleninothioic *O*-acid

$-SO_2\text{-}OSH$
sulfono(thioperoxoic) *OS*-acid

$-TeO\text{-}SeSH$
tellurino(selenothioperoxoic) *SeS*-acid

Examples:

$CH_3\text{-}CH_2\text{-}CH_2\text{-}S\{O,Se\}H$
propane-1-sulfonoselenoic acid (PIN)

CH_3-CH_2-S(O)(S)-OH
ethanesulfonothioic *O*-acid (PIN)

CH_3-CH_2-Se(=S)-OH
ethaneseleninothioic *O*-acid (PIN)

P-65.3.1.4 Imidic and hydrazonic acids derived from sulfonic, sulfinic, etc., acids

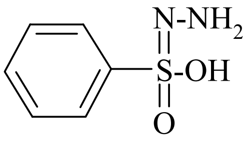
Imidic acids and hydrazonic acids derived from sulfonic, sulfinic, etc., acids are named by using suffixes such as ‘sulfinimidic acid’ for –S(O)(=NH)-OH, ‘sulfonohydrazonic acid’ for –S(O)(=NNH_2)-OH. The prefix ‘di’ is used to indicate the replacement of two oxygen atoms (=O) in sulfonic acids, for example, ‘sulfonodiimidic acid’ for –S$(=NH)_2$-OH,. Suffixes are listed in Table 4.3 and in Appendix 1.

Examples:

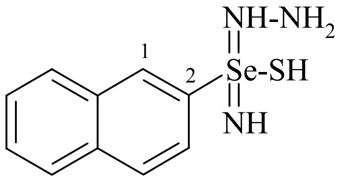
CH_3-S(=NH)-OH
methanesulfinimidic acid (PIN)

CH_3-CH_2-S$(=NH)_2$-OH
ethanesulfonodiimidic acid (PIN)

C_6H_5-Se$(=NH)_2$-OH
benzeneselenonodiimidic acid (PIN)



benzenesulfonohydrazonic acid (PIN)



naphthalene-2-selenonohydrazonimidothioic acid (PIN)

P-65.3.1.5 Hydroximic and hydroxamic acids derived from sulfonic, sulfinic, etc., acids

Hydroximic acids and hydroxamic acids derived from sulfonic, sulfinic, etc., acids are named as *N*-hydroxysulfonimidic acids and *N*-hydroxysulfonamides, etc. (see P-66.1.1.2), respectively.

Examples:

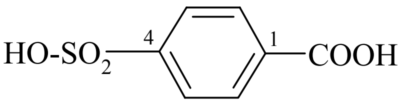
$CH_3\text{-S(O)(=}\overset{N}{\text{N}}\text{-OH)-OH}$
N-hydroxymethanesulfonimidic acid (PIN)

$CH_3\text{-}CH_2\text{-}CH_2\text{-SO-}\overset{N}{\text{N}}\text{H-OH}$
N-hydroxypropanesulfonamide (PIN)

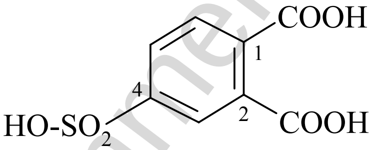
P-65.3.2 Substitutive nomenclature, prefix mode for sulfonic, sulfinic, etc., acids

P-65.3.2.1 When another group is also present that has seniority for citation as principal group (see P-41, P-42, P-43), or when all groups cannot be expressed as suffixes, organic oxoacids of sulfur, selenium or tellurium are named by adding to the name of the parent compound the appropriate prefix given in Table 6.1. These prefixes can be modified by prefixes designating chalcogen atoms in functional replacement nomenclature when the position of the chalcogen atom is not known or when it is not desirable to indicate such position.

Examples:



4-sulfobenzoic acid (PIN)



4-sulfobenzene-1,2-dicarboxylic acid (PIN)
4-sulfophthalic acid

$HO\text{-}SO_2\text{-}\overset{1}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_2\text{-}O\text{-}S\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}SO_2\text{-}OH$

4-({[(3-sulfopropoxy)methyl]sulfanyl}oxy)butane-1-sulfonic acid (PIN)

$HO\text{-}SO\text{-}CH_2\text{-}COOH$

sulfinoacetic acid (PIN)

$HOO\overset{1}{C}\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}SeO_2\text{-}OH$

3-selenonopropanoic acid (PIN)

$H\{O,S\}S\text{-}CH_2\text{-}CH_3\text{-}SO_2\text{-}OH$

2-(thiosulfino)ethane-1-sulfonic acid (PIN)

P-65.3.2.2 Acyl groups derived from sulfonic, sulfinic, etc., acids and their functional replacement analogues

P-65.3.2.2.1 Acyl sulfonic, sulfinic, selenonic, seleninic, telluronic, and tellurinic groups, R-EO_x–, –O_xE-R-EO_x–, or –O_xE-R-[R′-EO_x–]-R″-EO_x–, where E = S, Se, or Te, x = 1 or 2, and R, R′, and R″ are chains, rings, or ring systems, and their functional replacement analogues are groups derived by the removal of the hydroxy group from each sulfonic, sulfinic, or related selenium or tellurium acid group that is expressed as the principal characteristic group by an appropriate suffix.

P-65.3.2.2.2 Names for acyl groups derived from sulfonic and sulfinic acids, and their Se and Te counterparts, by removal of the –OH group from each sulfonic, sulfinic, etc. acid expressed as a suffix are formed by changing the ‘ic acid’ ending of the suffix to ‘yl’. When the suffix is modified by functional replacement nomenclature, the ending of the corresponding acyl group is ‘oyl’.

Examples:

C_6H_5-SO_2– benzenesulfonyl (PIN)	CH_3-SeO– methaneseleninyl (PIN)
CH_3-CH_2-S(O)(S)– ethanesulfonothioyl (PIN)	C_6H_5-S(Se)– benzenesulfinoselenoyl (PIN)
CH_3-CH_2-S(=NH)– ethanesulfinimidoyl (PIN)	

P-65.3.2.3 Substituent groups formed by concatenation

When the name of an acyl group cannot be derived directly from that of the acid expressed by a suffix, a concatenation procedure is used. For this procedure names of divalent mononuclear acyl groups are required. Acyl groups corresponding to sulfuric and sulfurous acids and the corresponding selenium and tellurium acids are formed from the acids by subtracting all -OH groups from the parent acid. The names used in the nomenclature of organic compounds are as follows:

–SO_2–	sulfonyl (PIN) sulfuryl	–SO–	sulfinyl (PIN) thionyl
–SeO_2–	selenonyl (PIN)	–SeO–	seleninyl (PIN)
–TeO_2–	telluronyl (PIN)	–TeO–	tellurinyl (PIN)

These acyl groups are modified by infixes in functional replacement nomenclature to indicate replacement by ‘=S’, ‘=Se’, ‘=Te’, ‘=NH’, and ‘=N-NH_2’.

Examples:

–S(=O)(=S)–	sulfonothioyl (PIN)
–S(=S)(=S)–	sulfonodithioyl (PIN)
–S(=NH)–	sulfinimidoyl (PIN)
–Se(=O)(=NNH_2)–	selenonohydrazonoyl (PIN)
–Se(=S)(=NH)–	selenonimidothioyl (PIN)

Prefixes denoting characteristic groups can then be attached to these divalent acyl group names. The prefix 'hydro-' for H can also be used. This traditional method generates preferred IUPAC names. Names of acyl groups derived directly from the names sulfuric acid and sulfurous acid, and their Se and Te congeners, are inappropriate because of ambiguity and incompleteness (see P-67.1.4.4.1). The name sulfamoyl for $H_2N-SO_2–$ is a retained name used as a preferred IUPAC name

Examples:

$CH_3O-SO_2–$
methoxysulfonyl (PIN)

$Cl-S(O)–$
chlorosulfinyl (PIN)

$H_2N-SO_2–$
sulfamoyl (PIN)
aminosulfonyl

$H-SO–$
hydrosulfinyl (PIN)

$CH_3-CO-O-SO_2–$
(acetyloxy)sulfonyl (PIN)

$CH_3-O-S(=NH)–$
S-methoxysulfinimidoyl (PIN)

$H-SeO_2–$
hydroselenonyl (PIN)

$HO-SO_2-O–$
sulfooxy

$–S-SO_2-S–$
sulfonylbis(sulfanediyl)

$–O-SO-O–$
sulfinobis(oxy)

P-65.3.4 Polyfunctional compounds

Polyfunctional compounds are named in accordance with the general order of seniority of suffixes described in Sections P-41 and P-43, and also in Appendix 1. When required, numbering is based on the following seniority order:

(a) fixed numbering of parent hydride (e.g. naphthalene, bicyclo[2.2.2]octane, etc.)

(b) heteroatoms in rings and chains

(c) indicated hydrogen [for unsubstituted compounds; a higher locant may be needed at another position to provide for a substituent suffix in accordance with the structural feature (d)].

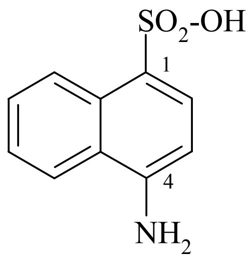
(d) principal group named as suffix

(e) added hydrogen (consistent with the structure of the compound and in accordance with further substitution)

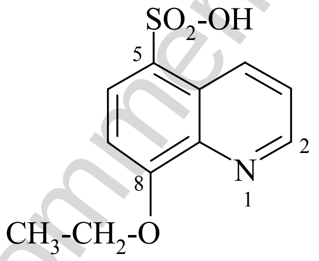
(f) unsaturation/saturation (ene/yne endings or hydro/dehydro prefixes)

(g) detachable (alphabetized) prefixes

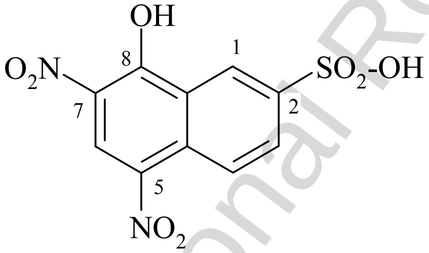
Examples:



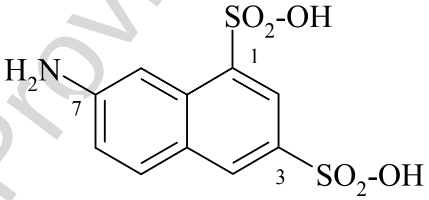
4-aminonaphthalene-1-sulfonic acid (PIN)



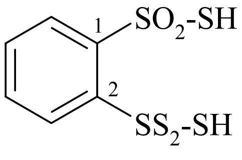
8-ethoxyquinoline-5-sulfonic acid (PIN)



8-hydroxy-5,7-dinitronaphthalene-2-sulfonic acid (PIN)



7-aminonaphthalene-1,3-disulfonic acid (PIN)



2-(trithiosulfo)benzene-1-sulfonothioic *S*-acid (PIN)

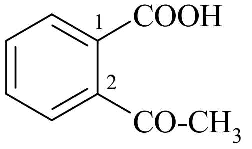
P-65.4. Acyl groups as substituent groups

P-65.4.1 General methodology

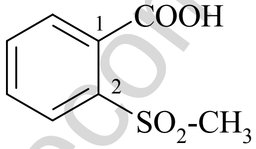
Acyl group nmaes that are described in preceding sections are used unchanged to denote substituent groups. Thus, the traditional way of using acyl groups derived from acyclic carboxylic acids to name ketones, pseudokeones and heterones is maintained (see P-64.4 for more examples).

This is a change in the case of acyl groups derived from carboxylic acids named by the suffix 'carboxylic acid' and for sulfonic, sulfinic, etc., acids; the traditional concatenation method denoting the parent hydride by a prefix is no longer recommended.

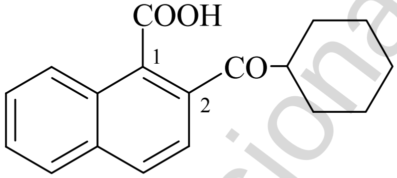
Examples:



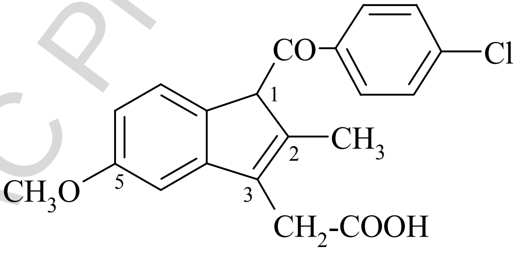
2-acetylbenzoic acid (PIN)



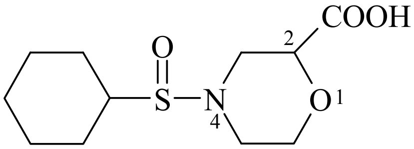
2-methanesulfonylbenzoic acid (PIN)
[not 2-(methylsulfonyl)benzoic acid]



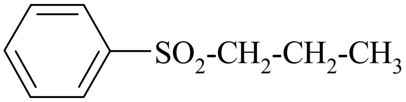
2-cyclohexanecarbonylnaphthalene-1-carboxylic acid (PIN)
[not 2-(cyclohexylcarbonyl)naphthalene-1-carboxylic acid]



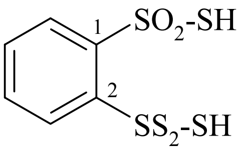
2-[1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1*H*-inden-3-yl]acetic acid (PIN)



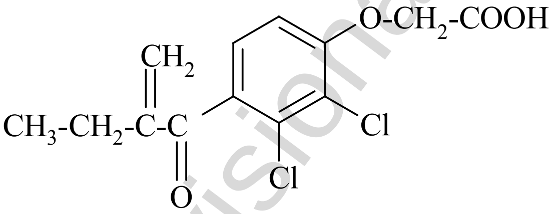
4-cyclohexanesulfinylmorpholine-2-carboxylic acid (PIN)
[not 4-(cyclohexylsulfinyl)morpholine-2-carboxylic acid]



propane-1-sulfonylbenzene (PIN)
[not (propylsulfonyl)benzene]



2-(trithiosulfo)benzene-1-sulfonothioic *S*-acid (PIN)



2-[2,3-dichloro-4-(2-methylidenebutanoyl)phenoxy]acetic acid (PIN)

P-65.5 Acyl halides and pseudohalides

P-65.5.1 Acyl halides from suffix acids

P-65.5.1.1 Acid halides in which hydroxy groups of all acid groups expressed as the suffix denoting the principal characteristic group (carboxylic, sulfonic, sulfinic, selenonic, etc. acids) have been replaced by halogen atoms (F, Cl, Br, and I) are named by citing the name of the acyl group (see P-65.1.7) followed by the name(s) of the specific class(es) as a separate word(s), in alphabetical order, each preceded by a multiplicative prefix, as needed.

The names formyl, acetyl, and benzoyl are retained.

Names of acid halides are functional class names (see Table 6.2)

Table 6.2. Halides and pseudohalides

Halide		Prefix	Pseudohalides		Prefix
–F	fluoride	fluoro	$–N_3$	azide	azido
–Cl	chloride	chloro	–CN	cyanide	cyano
–Br	bromide	bromo	–NC	isocyanide	isocyano
–I	iodide	iodo	–NCO	isocyanate	isocyanato
			–NCS	isothiocyanate	isothiocyanato
			–NCSe	isoselenocyanate	isoselenocyanato
			–NCTe	isotellurocyanate	isotellurocyanato

Examples:

$\overset{2}{C}H_3\text{-}\overset{1}{C}O\text{-}Cl$

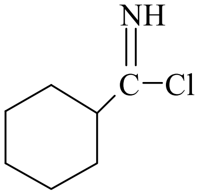
acetyl chloride (PIN)

HCO-Br

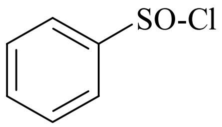
formyl bromide (PIN)

$\overset{6}{C}H_3\text{-}\overset{5}{C}H\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}F$

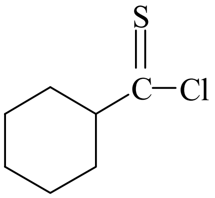
hexanoyl fluoride (PIN)



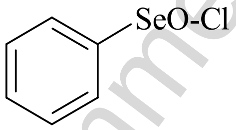
cyclohexanecarbonimidoyl chloride (PIN)



benzenesulfinyl chloride (PIN)



cyclohexanecarbothioyl chloride (PIN)



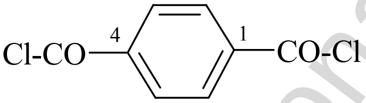
benzeneseleninyl chloride (PIN)

$Cl\text{-}CO\text{-}CH_2\text{-}CO\text{-}Cl$

propanedioyl dichloride (PIN)
malonyl dichloride

$Br\text{-}O_2S\text{-}CH_2\text{-}CH_2\text{-}SO_2\text{-}Br$

ethane-1,2-disulfonyl dibromide (PIN)



benzene-1,4-dicarbonyl dichloride (PIN)
terephthaloyl dichloride

P-65.5.2 Acyl pseudohalides from suffix acids

P-65.5.2.1 Acyl pseudohalides in which hydroxy groups of all acid groups expressed as the suffix denoting the principal characteristic group (carboxylic, sulfonic, sulfinic, selenonic, etc. acids) have been replaced by pseudohalogen groups (N_3, CN, NC, NCO, NCS, NCSe, NCTe) are named by citing the name of the acyl group (see P-65.1.7) followed by the name(s) of the class(es) as separate words, preceded by a multiplicative prefix, as needed. When a choice has to be made, the senior pseudohalide group is chosen in accordance with the decreasing order of seniority: N_3 > CN > NC > NCO > NCS > NCSe > NCTe. Halogen atoms are senior to pseudohalogen groups.

The names formyl, acetyl, and benzoyl are retained.

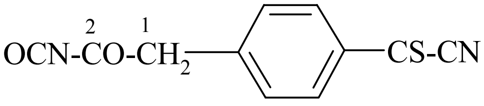
Examples:

$\overset{4}{H_3}\overset{3}{C}\text{-}CH_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}CN$

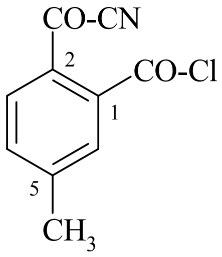
butanoyl cyanide (PIN)
butyryl cyanide

$CN\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}O\text{-}NCS$

butanedioyl isocyanate isocyanide (PIN)



4-(2-isocyanato-2-oxoethyl)benzenecarbothioyl cyanide (PIN)



2-(carbonocyanidoyl)-5-methylbenzoyl chloride (PIN)
2-(cyanocarbonyl)-5-methylbenzoyl chloride

P-65.5.3 Acyl halides and pseudohalides from carbonic, cyanic, oxalic, and the polycarbonic acids

P-65.5.3.1 Acyl groups derived from carbonic acid, carbamic acid, and related acids, such as ‘carbonyl’ from carbonic acid and ‘carbamoyl’ from carbamic acid, are used to form the names of the corresponding acyl halides.

Examples:

Cl-CO-Cl

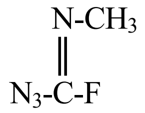
carbonyl dichloride (PIN)

$H_2N\text{-}CO\text{-}I$

carbamoyl iodide (PIN)

Br-CO-Cl

carbonyl bromide chloride (PIN)
(not carbonobromidic chloride)



$$\begin{array}{c} \text{N-CH}_3 \\ \| \\ \text{N}_3\text{-C-F} \end{array}$$

N-methylcarbonazidimidoyl fluoride (PIN)

NC-CO-Cl

carbonocyanidoyl chloride (PIN)

$H_2N\text{-}CO\text{-}NCO$

carbamoyl isocyanate (PIN)

P-65.5.3.2 The acyl group names oxalyl and oxalo from oxalic acid and oxamoyl from oxamic acid are **not** used to form preferred IUPAC names for acid halides and halogenoids; however, oxalyl and oxamoyl may be used in general nomenclature, but not oxalo. Names for acyl halides derived from oxalic acid, oxamic acid, and the polycarbonic acids are formed by using the name of the acid followed by the name(s) of the halides.

Examples:

HO-CO-CO-Cl

oxalic (mono)chloride (PIN)

$H_2N\text{-}CO\text{-}CO\text{-}Br$

oxamic bromide (PIN)
oxamoyl bromide

Cl-CO-CO-Cl

oxalic dichloride (PIN)
oxalyl chloride

ONC-CO-CO-Br

oxalic bromide isocyanate (PIN)
oxalyl bromide isocyanate

Cl-CO-O-CO-Cl

dicarbonic dichloride (PIN)

Cl-CO-O-CO-Br

dicarbonic bromide chloride (PIN)

1 2 3
Cl-CO-NH-CO-Cl

imidodicarbonic dichloride (PIN)

1 *N* 2 3 4 5
Cl-C(=NH)-NH-CO-S-C(S)-Br

1,2-diimido-4,5-dithiotricarbonic 1-chloride 5-bromide (PIN)

SCN-CO-CO-NCS

oxalic diisothiocyanate (PIN)
oxalyl diisothiocyanate

OCN-CO-O-CO-NCO

dicarbonic diisocyanate (PIN)
oxalyl diisocyanate

P-65.5.3.3 Acyl halides and pseudohalides from cyanic acid are formed in two ways:

(1) as acyl halides or pseudohalides of carbononitridic acid

(2) by citing the name of the halide or pseudohalide after the name of the acid:

Method (1) generates preferred IUPAC names.

Examples:

NC-Cl

carbononitridic chloride (PIN)
cyanic chloride

NC-N_3

carbononitridic azide (PIN)
cyanic azide

P-65.5.3 Acyl halides and pseudo halides as substituent groups

When another group is present that has priority for citation as principal group or when attached to another substituting group, an acyl halide or pseudohalide is expressed:

(1) by a prefix formed from the name of the acid;

(2) by a compound prefix composed of a halo or halogeno prefix and an appropriate bivalent acyl group, such as 'sulfonyl', for example, fluorosulfonyl;

(3) at the end of an acyclic carbon chain by a prefix denoting the halide or pseudohalide group and the prefix 'oxo', or a chalcogen analog of oxo, such as thioxo.

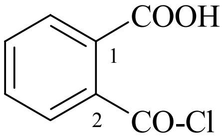
Method (1) leads to preferred IUPAC names when the suffix '-carboxylic acid' is used to name the corresponding acid; method (3) generates preferred IUPAC names for acyclic carbon chains.

Seniority for numbering follows that for acids, for which see P-65.1.2.3 or P-65.3.4.

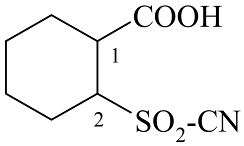
Examples:

$\text{Cl-}\overset{3}{\text{C}}\text{O-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{1}{\text{C}}\text{OOH}$

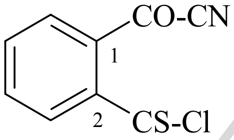
(3) 3-chloro-3-oxopropanoic acid (PIN)
(1) (carbonochloridoyl)acetic acid



(1) 2-(carbonochloridoyl)benzoic acid (PIN)
(2) 2-chlorocarbonylbenzoic acid



(1) 2-(cyanosulfonyl)cyclohexane-1-carboxylic acid (PIN)
(2) 2-sulfurocyanidoylcyclohexane-1-carboxylic acid



(1) 2-(carbonochloridothioyl)benzoyl cyanide (PIN)
(2) 2-(chlorocarbonothioyl)benzoyl cyanide

Br-CO-CO-CH_2-COOH

(3) 4-bromo-3,4-dioxobutanoic acid (PIN)
(2) 3-(bromooxalyl)acetic acid

Br-CO-O-CO-CH_2-COOH

(3) 3-[(carbonobromidoyl)oxy]-3-oxopropanoic acid (PIN)

P-65.6 Salts and esters

P-65.6.1 General methodology

Neutral salts and esters are both named using the name of the anion derived from the name of the acid. Anion names are formed by changing an '-ic acid' ending of an acid name to '-ate' and an '-ous acid' ending of an acid name to '-ite'. Then, salts are named using the names of cations, and esters the names of organyl groups, cited as separate words in front of the name of the anion.

P-65.6.2 Salts

P-65.6.2.1 Neutral salts of acids are named by citing the name of the cation(s) followed by the name of the anion (see P-7) as a separate word. Different cations are cited in alphabetical order. Formation of salts is a functionalization and not a substitution. Thus, all retained names, both those used as preferred IUPAC names and those used only for general nomenclature can be used without restriction. This rule applies equally to acids expressed by suffixes and carbonic, cyanic, oxalic, and the polycarbonic acids.

Examples:

$\mathrm{CH_3\text{-}CH_2\text{-}CH_2\text{-}COO^-\ \ K^+}$

potassium butanoate (PIN)
potassium butyrate

$\mathrm{CH_3\text{-}CH_2\text{-}CS\text{-}S^-\ \ Na^+}$

sodium propanedithioate (PIN)
sodium dithiopropionate

$\mathrm{(CH_3\text{-}COO^-)_2\ Ca^{2+}}$

calcium diacetate (PIN)

$\mathrm{C_6H_5\text{-}SO\text{-}O^-\ \ Na^+}$

sodium benzenesulfinate (PIN)

$\mathrm{K^+\ {}^-OOC\text{-}CH_2\text{-}CH_2\text{-}COO^-\ \ Na^+}$

potassium sodium butanedioate (PIN)
potassium sodium succinate

$\mathrm{NH_4^+\ {}^-OOC\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}COO^-\ \ K^+}$

ammonium potassium hexanedioate (PIN)
ammonium potassium adipate

$\mathrm{C(O)O_2^{2-}\ \ 2Na^+}$

disodium carbonate (PIN)

P-65.6.2.2 Acid salts

P-65.2.2.1 Acid salts of polybasic organic acids and organic derivatives of polybasic inorganic oxo acids are named in the same way as the neutral salts, the remaining acid hydrogen atom(s) being indicated by the word ‘hydrogen’ (preceded by a numerical prefix, ‘di’, ‘tri’, etc., as appropriate) inserted as a separate word between the name(s) of the cation(s) and the name of the anion. When required, cations are cited in names in alphabetical order. Anionic substitutents, such as $-COO^-$, $-SO_3^-$, $-SO_2^-$, are described by the prefix names ‘carboxylato’, ‘sulfonato’, and ‘sulfinato’, respectively, and similarly for the corresponding selenium and tellurium acids.

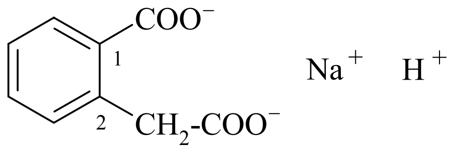
Examples:

$\mathrm{HOOC\text{-}[CH_2]_5\text{-}COO^-\ \ K^+}$

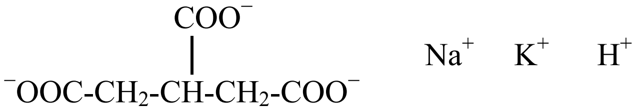
potassium hydrogen heptanedioate (PIN)

$\mathrm{HOOC\text{-}CH_2\text{-}CH_2\text{-}COO^-\ \ NH_4^+}$

ammonium hydrogen butanedioate (PIN)
ammonium hydrogen succinate



sodium hydrogen 2-(carboxylatomethyl)benzoate (PIN)



$$\overset{\displaystyle COO^{-}}{\overset{|}{}}\quad {}^{-}OOC\text{-}CH_2\text{-}CH\text{-}CH_2\text{-}COO^{-} \qquad Na^{+}\quad K^{+}\quad H^{+}$$

potassium sodium hydrogen propane-1,2,3-tricarboxylate (PIN)

$HO\text{-}CO\text{-}O^{-}\ Na^{+}$ $CH_3\text{-}P(O)(O^{-})_2\ K^{+}\ H^{+}$

sodium hydrogen carbonate (PIN) potassium hydrogen methylphosphonate (PIN)

P-66.6.2.2.2 In the nomenclature of inorganic chemistry (I-8.5.2, ref. 14), the term‘hydrogen’ is written directly in front of the name of the anion, without a space, to indicate that it is part of the anion.

Example:

$P(O)(O^{-})_3 \quad Na^{+} \quad 2\ H^{+}$ sodium dihydrogenphosphate

P-65.6.3 Esters, lactones and related compounds.

P-65.6.3.1 Definitions

Esters of oxoacids are organic compounds formally derived from an oxoacid$_z$ and an alcohol, phenol, heteroarenol, or enol by a formal loss of water from an acidic hydroxy group of the former and an hydroxy group of the latter. By extension, they are ‘acyl’ derivatives of alcohols, etc. Alcohols, phenols, enols, heteroarenols, ynols are hydroxy compounds in which one or more hydroxy groups are attached to (a) carbon atoms.

A new class, ‘pseudoesters’, is recommended. It includes compounds having the generic group formula $–E(=O)_x(OZ)$ and chalcogen analogues where $x = 1$ or 2 and Z is not a carbon atom but another element such as Si, Ge, B, Al, N, P, S, Se. Pseudoesters are ranked as esters in the seniority order of classes (see P-41).

P-65.6.3.2 Esters

P-65.6.3.2.1 Fully esterified acids are systematically named by placing the name(s) of the organyl group(s) (alkyl, aryl, etc.) in front of the name of the anion as separate word(s); they are cited in alphabetical order when more than one. When required, locants are cited at the front of the organyl groups. (For the endings ‘ate’ and ‘ite’, see P-65.6.1.). This rule applies equally to carboxylic, sulfonic, sulfinic, etc. acids, the other carbon acids, i. e., carbonic, oxalic, cyanic, and the polycarbonic acids and their replacement analogues.

Examples:

$CH_3\text{-}CO\text{-}O\text{-}CH_3$

ethyl acetate (PIN)

$H_3CO\text{-}OC\text{-}CH_2\text{-}CO\text{-}O\text{-}CH_2CH_3$

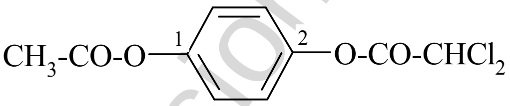
ethyl methyl propanedioate (PIN)
ethyl methyl malonate

$CH_3\text{-}CO\text{-}O\text{-}\overset{1}{C}H_2\overset{2}{C}H_2\text{-}O\text{-}CO\text{-}CH_3$

ethane-1,2-diyl diacetate (PIN)

$CH_3\text{-}O\text{-}CO\text{-}CO\text{-}O\text{-}CH_3$

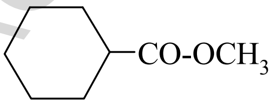
dimethyl oxalate (PIN)



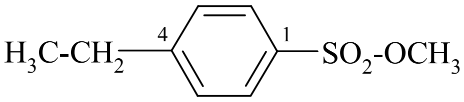
1,4-phenylene acetate dichloroacetate (PIN)
4-(acetyloxy)phenyl dichloroacetate

$HCO\text{-}O\text{-}CH_2\text{-}CO\text{-}CH_3$

methylene acetate formate (PIN)



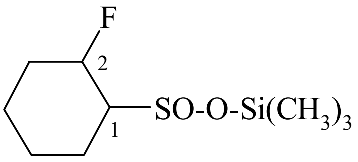
ethyl cyclohexanecarboxylate (PIN)



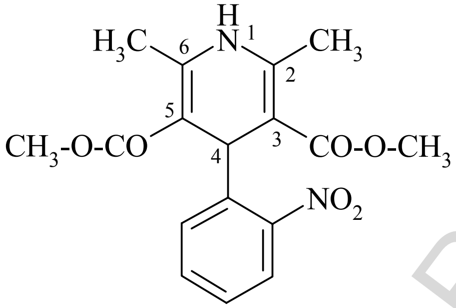
methyl 4-ethylbenzenesulfonate (PIN)

$\overset{4}{\mathrm{C}}\mathrm{H_3}\text{-}\overset{3}{\mathrm{C}}\mathrm{H(CO\text{-}O\text{-}CH_3)}\text{-}\overset{2}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{1}{\mathrm{C}}\mathrm{H(CO\text{-}O\text{-}CH_2CH_3)_2}$

1,1-diethyl 3-methyl butane-1,1,3-tricarboxylate (PIN)



trimethylsilyl 2-fluorocyclohexanesulfinate (PIN)



dimethyl 2,6-dimethyl-4-(2-nitrophenyl)-1,4-dihydropyridine-3,5-dicarboxylate (PIN)

P-65.6.3.2.2 When, in an ester another group is present that has priority for citation as a suffix or when all ester groups cannot be described by the above methods, an ester group is indicated by prefixes such as ‘acyloxy’ for the group R-CO-O–, or ‘alkyloxy-…oxo’ or ‘alkyloxycarbonyl’ for the group –CO-OR’.

The systematic name ‘acetyloxy’ is preferred to the contracted name ‘acetoxy’ that may be used in general nomenclature.

Seniority for numbering follows that for acids, for which see P-65.1.2.3 or P-65.3.4.

Examples:

$\mathrm{[CH_3CH_2\text{-}O\text{-}}\overset{3}{\mathrm{C}}\mathrm{O\text{-}}\overset{2}{\mathrm{C}}\mathrm{H_2}\overset{1}{\mathrm{C}}\mathrm{H_2\text{-}N^+(CH_3)_3]\ \ Br^-}$

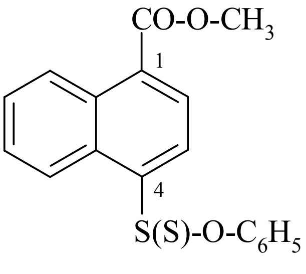
(3-ethoxy-3-oxopropyl)-*N,N,N*-trimethylazanium bromide (PIN)
[2-(ethoxycarbonyl)ethyl]-*N,N,N*-trimethylammonium bromide

$\mathrm{C_6H_5\text{-}CO\text{-}O\text{-}}\overset{3}{\mathrm{C}}\mathrm{H_2}\overset{2}{\mathrm{C}}\mathrm{H_2\text{-}}\overset{1}{\mathrm{C}}\mathrm{OOH}$

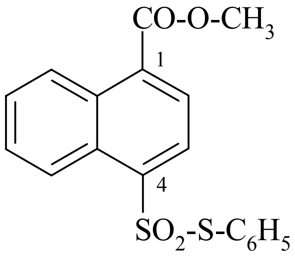
3-(benzoyloxy)propanoic acid (PIN)

$CH_3\text{-}\overset{2}{C}O\text{-}\overset{1}{O}\text{-}CH_2CH_2\text{-}S(O)_2\text{-}OH$

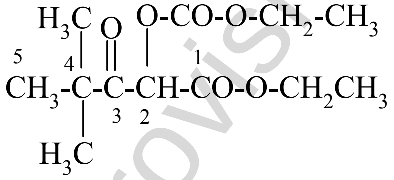
2-(acetyloxy)ethanesulfonic acid (PIN)
2-acetoxyethanesulfonic acid



methyl 4-(phenoxysulfinothioyl)naphthalene-1-carboxylate (PIN)

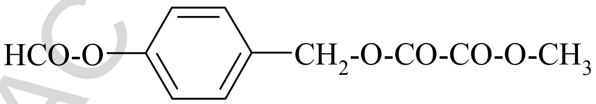


methyl 4-[(phenylsulfanyl)sulfonyl]naphthalene-1-carboxylate (PIN)

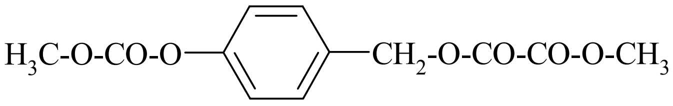


$$\overset{5}{C}H_3\text{-}\overset{4}{C}(CH_3)_2\text{-}\underset{3}{C}(=O)\text{-}\underset{2}{C}H(O\text{-}CO\text{-}O\text{-}CH_2\text{-}CH_3)\text{-}\overset{1}{C}O\text{-}O\text{-}CH_2CH_3$$

ethyl 2-[(ethoxycarbonyl)oxy]-4,4-dimethyl-3-oxopentanoate (PIN)



4-{[(methoxyoxalyl)oxy]methyl}phenyl formate (PIN)



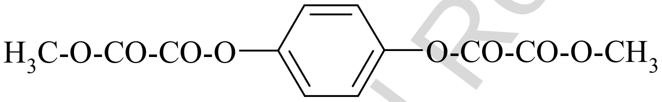
{4-[(methoxycarbonyl)oxy]phenyl}methyl methyl oxalate (PIN)
(not 4-{[(methoxyoxalyl)oxy]methyl}phenyl methyl carbonate;
oxalic acid preferred to carbonic acid)

P-65.6.3.2.3 Polyesters, i.e., esters between two or more acids, are named as described in P-65.6.3.1.1, then by using substitutive nomenclature, multiplicative nomenclature, skeletal (‘a’) replacement nomenclature, or phane nomenclature when the specific conditions are fulfilled.

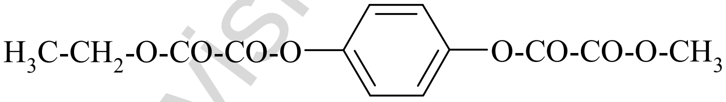
Examples:

$$\mathrm{CH_3\text{-}O\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_2\overset{3}{C}H_2\text{-}\overset{4}{C}O\text{-}O\text{-}CH_2CH_2\text{-}O\text{-}CO\text{-}CH_3}$$

2-(acetyloxy)ethyl methyl butanedioate (PIN)
2-acetoxyethyl methyl butanedioate



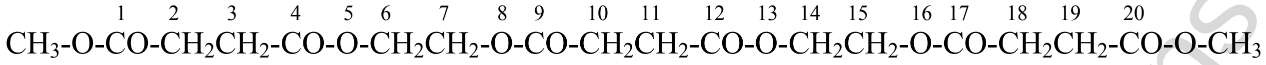
1,4-phenylenebis(methyl oxylate) (PIN)
4-[(methoxyoxalyl)oxy]phenyl methyl oxalate ;
(multiplicative name preferred to substitutive name)



4-[(ethoxyoxalyl)oxy]phenyl methyl oxalate (PIN)
(not ethyl 4-[(methoxyoxalyl)oxy]phenyl oxalate

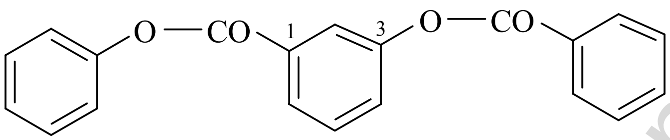
$$\mathrm{CH_3\text{-}O\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}O\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}\overset{4'}{C}O\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CO\text{-}CH_3}$$

2-(acetyloxy)ethyl methyl 4,4′-[ethane-1,2-diylbis(oxy)]bis(4-oxobutanoate) (PIN)
2-({4-[2-(acetyloxy)ethoxy]-4-oxobutanoyl}oxy)ethyl methyl butanedioate
2-(acetyloxy)ethyl 2-[(4-methoxy-4-oxobutanoyl)oxy]ethyl butanedioate]
(multiplicative name preferred to substitutive name, see P-51.2)

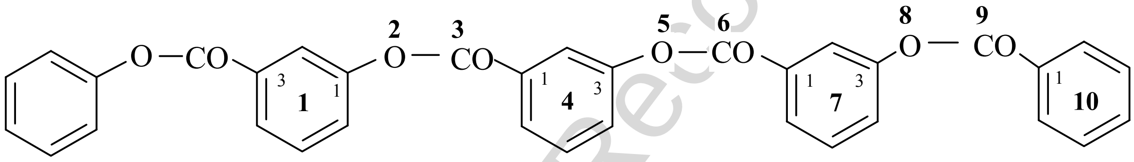


$$CH_3\text{-}O\text{-}\overset{1}{CO}\text{-}\overset{2}{CH_2}\overset{3}{CH_2}\text{-}\overset{4}{CO}\text{-}\overset{5}{O}\text{-}\overset{6}{CH_2}\overset{7}{CH_2}\text{-}\overset{8}{O}\text{-}\overset{9}{CO}\text{-}\overset{10}{CH_2}\overset{11}{CH_2}\text{-}\overset{12}{CO}\text{-}\overset{13}{O}\text{-}\overset{14}{CH_2}\overset{15}{CH_2}\text{-}\overset{16}{O}\text{-}\overset{17}{CO}\text{-}\overset{18}{CH_2}\overset{19}{CH_2}\text{-}\overset{20}{CO}\text{-}O\text{-}CH_3$$

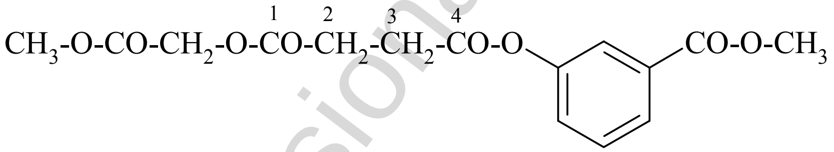
dimethyl 4,9,12,17-tetraoxo-5,8,13,16-tetraoxaicosanedioate (PIN)
[skeletal replacement (‘a’) name]
[ethane-1,2-diylbis(carbonyloxyethane-2,1-diyl)] dimethyl butanedioate
(multiplicative name)



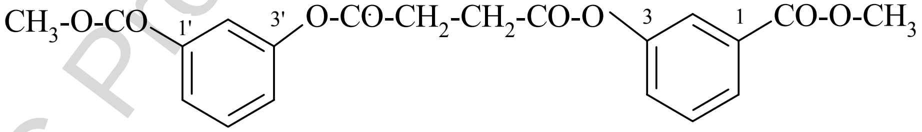
phenyl 3-(benzoyloxy)benzoate (PIN)



phenyl 3,6,9-trioxo-2,5,8-trioxa-1,10(1),4,7(1,3)-tetrabenzenadecaphane-1^3-carboxylate (PIN)



3-(methoxycarbonyl)phenyl 2-methoxy-2-oxoethyl butanedioate (PIN)



dimethyl 3,3′-[butanedioylbis(oxy)]dibenzoate (PIN)

P-65.6.3.2.4 Partial esters of polybasic acids and their salts are named by the procedure for neutral esters and acid salts; the components present are cited in the order, cation, organyl group, hydrogen, anion. Numerical locants and italic element symbols (see P-65.6.3.3.1) are added as necessary to provide specificity. The numbering of the polybasic acid is retained when the hydrogen method is applied to retained names.

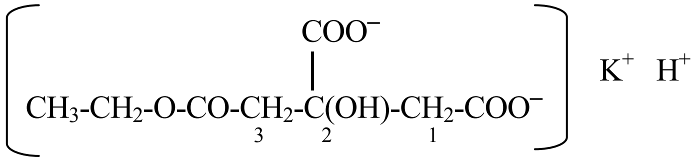
Examples:

$CH_3\text{-}CH_2\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}COO^-\ \ Na^+$

sodium ethyl succinate (PIN)

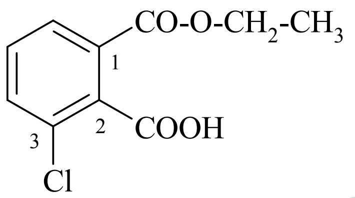
$CH_3\text{-}CH_2\text{-}S\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}\{O/S\}^-\ \ Li^+$

lithium 1-*S*-ethyl butanebis(thioate) (PIN)

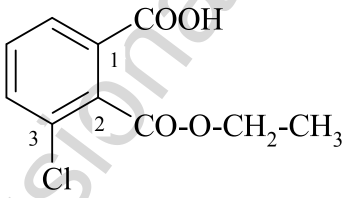


$$\left[CH_3\text{-}CH_2\text{-}O\text{-}CO\text{-}\underset{3}{C}H_2\text{-}\underset{2}{\overset{\displaystyle COO^-}{C}}(OH)\text{-}\underset{1}{C}H_2\text{-}COO^-\right]\ \ K^+\ \ H^+$$

potassium 3-ethyl hydrogen 2-hydroxypropane-1,2,3-tricarboxylate (PIN)
potassium 5-ethyl hydrogen citrate



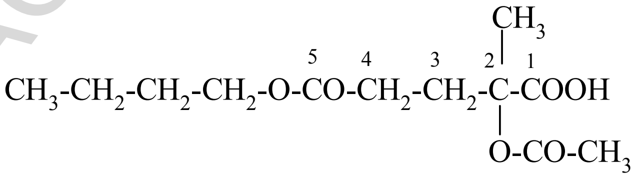
1-ethyl hydrogen 3-chlorobenzene-1,2-dicarboxylate (PIN)
1-ethyl hydrogen 3-chlorophthalate



2-ethyl hydrogen 3-chlorobenzene-1,2-dicarboxylate (PIN)
2-ethyl hydrogen 3-chlorophthalate

$CH_3\text{-}[CH_2]_3\text{-}O\text{-}\overset{5}{C}O\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H(CH_3)\text{-}\overset{1}{C}OOH$

5-butyl hydrogen 2-methylpentanedioate

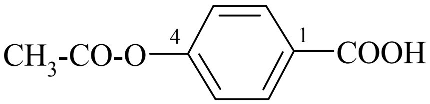


$$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}O\text{-}\overset{5}{C}O\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\underset{\displaystyle O\text{-}CO\text{-}CH_3}{\overset{\displaystyle CH_3}{\overset{2}{C}}}\text{-}\overset{1}{C}OOH$$

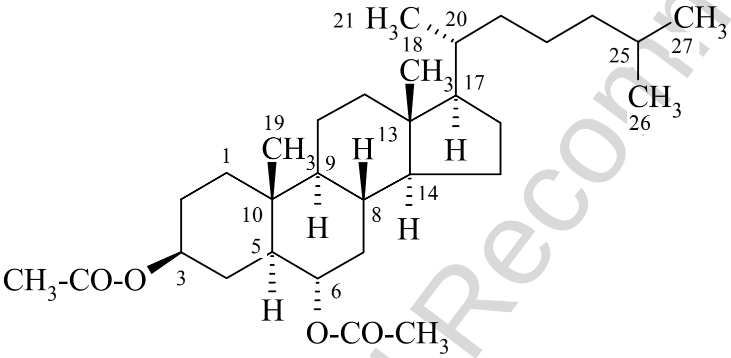
5-butyl hydrogen 2-(acetyloxy)-2-methylpentanedioate (PIN)

P-65.6.3.2.5 In the context of preferred IUPAC names, substitutive nomenclature is preferred over functional class nomenclature.

Examples:



4-(acetyloxy)benzoic acid (PIN)
4-hydroxybenzoic acid acetate



5α-cholestane-3β,6α-diyl diacetate (PIN)
5α-cholestane-3β,6α-diol diacetate

P-65.6.3.3 Esters of acids modified by functional replacement

P-65.6.3.3.1 With the exception of retained names, polycarbonic acids, oxalic acid, and cyanic acid that are described in P-65.6.3.3.3, names of esters are all derived from acids modified by functional replacement whose substitutive names are systematically formed, as indicated in sections P-65.1.3 to P-65.1.7.

Structural specification for esters of thio-, seleno- or tellurocarboxylic acids, thio-, seleno-, or tellurosulfonic acids and sulfinic acids and their peroxy analogues is provided by the appropriate italic element symbol, such as *S*, *O*, or *SO*, prefixed to the name of the organyl group.

Examples:

CH_3-$[CH_2]_4$-CO-S-CH_2-CH_3
S-ethyl hexanethioate (PIN)

CH_3-$[CH_2]_4$-CSe-O-CH_2-CH_3
O-ethyl hexaneselenoate (PIN)

CH_3-C(=NH)-O-CH_3
methyl ethanimidate (PIN)
methyl acetohydroximate

CH_3-CH_2-C(=N-NH_2)-O-C_2H_5
ethyl propanehydrazonate (PIN)
ethyl propionohydrazonate

C_6H_5-C(=NH)-S-CH_3

methyl benzenecarboximidothioate (PIN)

HC(=N-SH)-S-CH_2-CH_3

ethyl *N*-sulfanylbenzenecarboximidothioate (PIN)

C_6H_5-CO-S-O-CH_3

SO-methyl benzene(carbothioperoxoate) (PIN)

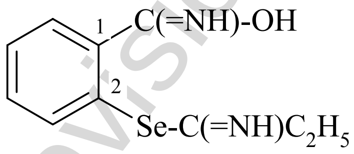
CH_3-CH_2-SO_2-O-S-C_2H_5

OS-ethyl ethanesulfono(thioperoxoate) (PIN)

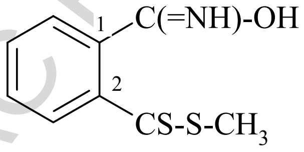
In the presence of a characteristic group having seniority for citation as suffix, an ester group is indicated by appropriate prefixes in accordance with the type of attachment of the substituent group, such as 'acylsulfanyl' for the group –S-CO-R, or 'alkylsulfanylcarbonothioyl', or alkylsulfanyl)…sulfanylidene' for the group –CS-SR.
Examples:

$CH_3\text{-S-}\overset{4}{C}\text{(=S)-}CH_2\text{-}CH_2\text{-}\overset{1}{C}\text{O-SH}$

4-(methylsulfanyl)-4-sulfanylidenebutanethioic *S*-acid



2-[(ethanimidoyl)selanyl]benzene-1-carboximidic acid (PIN)



2-[(methylsulfanyl)carbonothioyl]benzene-1-carboximidic acid

P-65.6.3.3.2 Esters of carbonic acid, oxalic acid, cyanic acid, and the polycarbonic acids modified by functional replacement.

P-65.6.3.3.2.1 Names of acids modified by functional replacement are used to generate preferred IUPAC names of corresponding esters. Element symbols *O*, *S*, etc. and locants are used to designate the location of organyl groups.

Examples:

$CH_3\text{-}S\text{-}\overset{1}{C}O\text{-}\overset{2}{O}\text{-}\overset{3}{C}O\text{-}\overset{4}{O}\text{-}\overset{5}{C}H_2\text{-}CH_3$

1-methyl 5-ethyl 1-thiodicarbonate (PIN)

$CH_3\text{-}S\text{-}CS\text{-}O\text{-}CH_3$

O,*S*-dimethyl carbonodithioate (PIN)

$CH_3\text{-}S\text{-}\overset{1}{C}O\text{-}\overset{2}{C}O\text{-}S\text{-}CH_3$

S,*S*-dimethyl 1,2-dithiooxlate (PIN)

$CH_3\text{-}O\text{-}\overset{2}{C}S\text{-}\overset{1}{C}(=NH)\text{-}S\text{-}CH_2\text{-}CH_3$

S-ethyl *O*-methyl 1-imido-1,2-dithiooxalate (PIN)

$CH_3\text{-}S\text{-}\overset{2}{C}O\text{-}\overset{1}{C}S\text{-}S\text{-}CH_2\text{-}CH_3$

1-ethyl 2-methyl 1,1,2-trithiooxalate

$(CH_3)_2CH\text{-}S\text{-}CN$

propan-2-yl thiocyanate

P-65.6.3.3.2.2 In the presence of a characteristic group having seniority for citation as suffix, an ester group is indicated by appropriate prefixes in accordance with the type of attachment of the substituent group.

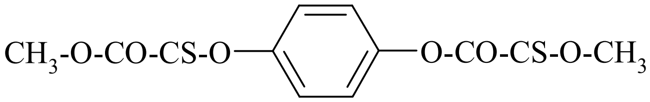
Examples:

$CH_3\text{-}S\text{-}CS\text{-}CO\text{-}O\text{-}CH_2\text{-}CS\text{-}SH$

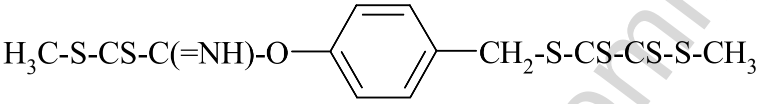
2-{[(methylsulfanyl)-2-thiooxalyl]oxy}ethanedithioic acid (PIN)

$\mathrm{NC{-}S{-}CH_2{-}CH_2{-}CO{-}S{-}CH_2{-}CH_3}$

S-ethyl 3-(cyanosulfanyl)propanethioate (PIN)



2-*O*-{4-[(methoxy-1-thiooxalyl)oxy]phenyl} *O*-methyl 1-thiooxalate (PIN)
(not 1-*O*-{4-[(methoxy-2-thiooxalyl)oxy]phenyl} methyl 1-thiooxalate;
1-thiooxalyl is senior to 2-thiooxalyl)



(4-{[(methylsulfanyl)-1-imido-2-thiooxalyl]oxy}phenyl)methyl methyl tetrathiooxalate (PIN)

P-65-6.3.4 Pseudoesters

Compounds having the generic formula R-CO-O-E, where E is not a carbon atom, belong to this class. Functional class names are constructed in the manner used for esters.

P-65.6.3.4.1 When E, in R-CO-O-E, is a nitrogen, phosphorus, arsenic, silicon, germanium, boron, or a chalcogen atom, pseudoesters are named as esters, unless other names must be selected in accordance with the seniority order of classes, in decreasing order: salts > acids > anhydrides > esters.

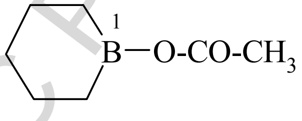
Examples:

$\mathrm{CH_3{-}CO{-}O{-}Si(CH_3)_3}$

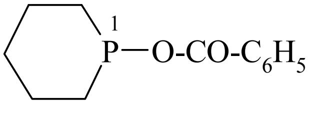
trimethylsilyl acetate (PIN)

$\mathrm{CH_3{-}CH_2{-}SO_2{-}S{-}Ge(CH_3)_3}$

S-(trimethylgermyl) ethanesulfonothioate (PIN)



borinan-1-yl acetate (PIN)



phosphinan-1-yl benzoate (PIN)

$\mathrm{(CH_3{-}CO{-}O)_3{-}B}$

triacetic boric trianhydride (PIN)

$\mathrm{H_2P{-}O{-}CO{-}CH_3}$

acetic phosphinous anhydride (PIN)

CH_3-CO-O-SSS-CH_3

methyltrisulfanyl acetate (PIN)

$(CH_3)_2$N-O-CO-CH_3

O-acetyl-*N*,*N*-dimethylhydroxylamine (PIN)
(hydroxylamine is a retained preferred
IUPAC name; see P-68.3.1.1.1)

CH_3-CO-O-P$(CH_3)_2$

acetic dimethylphosphinous anhydride (PIN; see P-67.1.3.2)

P.65.6.3.4.2 For compounds where E is an element belonging to Group 16, see also P-68.4.

P-65.6.3.5 Cyclic esters

Compounds that may be considered as derived from a hydroxy carboxylic acid or hydroxy sulfonic acid by loss of water intramolecularly are classified as 'lactones' and 'sultones', respectively. For these compounds heterocyclic names are preferred IUPAC names. Names derived from corresponding hydroxy acids are not recommended, but may be used in general nomenclature.

P-65.6.3.5.1 Lactones.

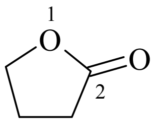
Intramolecular esters of hydroxy carboxylic acids are 'lactones' and are named in two ways.

(1) as heterocyclic pseudoketones by adding the suffix 'one', 'e', etc. to the name of the heterocyclic parent [Hantzsch-Widman names are used for monocycles with up to ten ring members; names for saturated heterocycles are used when the system is fully saturated; otherwise, names are based on mancude heterocycles; skeletal replacement ('a') nomenclature is used for monocyclic lactones having more than ten ring atoms].

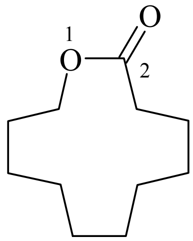
(2) by changing the 'ic acid' ending of a systematic 'oic acid' name for the non-hydroxylated parent acid to 'lactone', and inserting a locant designating the position of the hydroxy group between the 'o' and 'lactone'.

Method (1) gives preferred IUPAC names.

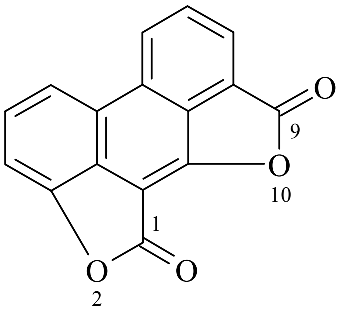
Examples:



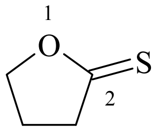
oxolan-2-one (PIN))
tetrahydrofuran-2-one
butano-4-lactone
(not γ-butyrolactone)



1-oxadodecan-2-one (PIN)
dodecano-12-lactone



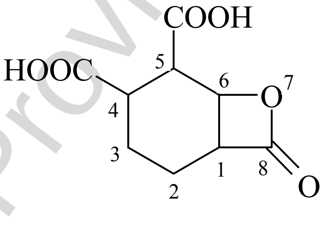
phenanthro[1,10-*bc*:9,8-*b'c'*]difuran-1,9-dione (PIN)
phenanthrene-1,10:9,8-dicarbolactone



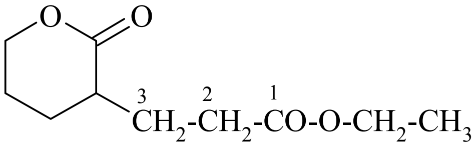
oxolane-2-thione (PIN)

A lactone, as a pseudoketone, ranks lower in the seniority of classes than an acid or an ester, but higher than an alcohol, amine, or imine.

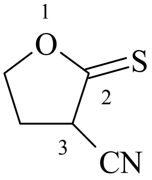
Examples:



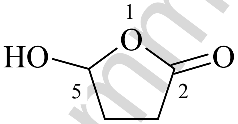
8-oxo-7-oxabicyclo[4.2.0]octane-4,5-dicarboxylic acid (PIN)
2-oxohexahydro-2*H*-benzooxete-5,6-dicarboxylic acid
(to be a preferred ring fusion name, there must be
a fusion site and two five membered rings, see P-52.5.2.1)



ethyl 3-(2-oxooxan-3-yl)propanoate (PIN)
ethyl 3-(2-oxotetrahydropyran-3-yl)propanoate
(saturated Hantzsch-Widman name preferred to hydrogenated retained name, see P-53.2.1 and P-53.2.2)



2-sulfanylideneoxolan-3-carbonitrile (PIN)



5-hydroxyoxolan-2-one (PIN)

P-65.6.3.5.2 Sultones and sultines are cyclic esters of hydroxy sulfonic acids and sulfinic acids, respectively.

P-65.6.3.5.2.1 Sultones and sultines may be named in three ways:

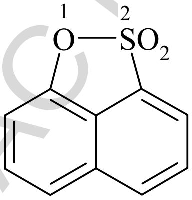
(1) as heterocyclic heterones;

(2) by citing the term ‘sultone’ or ‘sultine’ denoting the cyclic –O-SO$_2$– or –O-SO– group after the name of the appropriate parent hydride preceded by a pair of locants describing the points of attachment of the sulfonyl or sulfinyl group and the oxygen atom, respectively; the locant of the sulfonyl or sulfinyl group is cited first, and, if there is a choice, is the lower locant. Multiplying prefixes and pairs of locants separated by a colon are used to indicate two or more sultone or sultine rings.

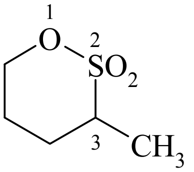
(3) as heterocycles according to functional class names using the class name ‘oxide’

Method (1) gives preferred IUPAC names.

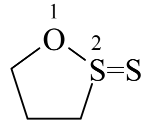
Examples:



2λ^6-naphtho[1,8-*cd*][1,2]oxathiole-2,2-dione (PIN)
naphthalene-1,8-sultone
naphtho[1,8-*cd*][1,2]oxathiole 2,2-dioxide



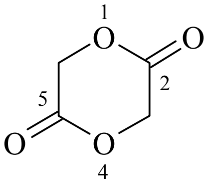
3-methyl-1,2λ^6-oxathiane-2,2-dione (PIN)
pentane-2,5-sultone
3-methyl-1,2-oxathiane 2,2-dioxide

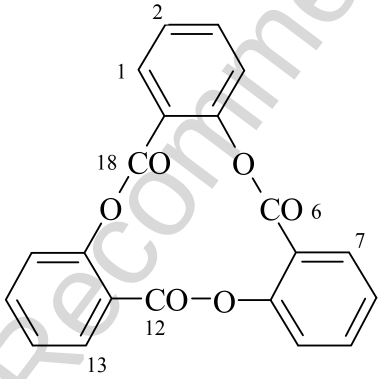


1,2λ^4-oxathiolan-2-thione (PIN)
1,2-oxathiolane 2-thiooxide

P-65.6.3.5.3 Lactides are cyclic esters derived by multiple esterification between two (or more) molecules of a hydroxy acid and are named as heterocyclic compounds.

Examples:



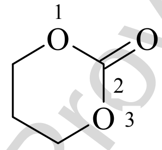


1,4-dioxane-2,5-dione (PIN)

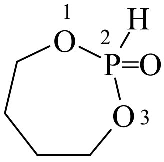
tribenzo[*b*,*f*,*j*][1,5,9]-trioxacyclododecin-6,12,18-trione (PIN)
(not trisalicylide)

P-65.6.3.5.4 Other cyclic esters derived from different hydroxy acids or from polybasic acids and polyhydroxy compounds are named as heterocycles.

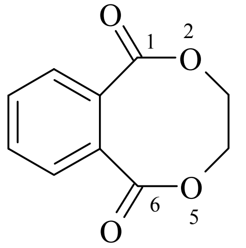
Examples:



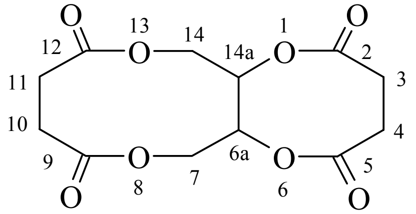
1,3-dioxan-2-one (PIN)



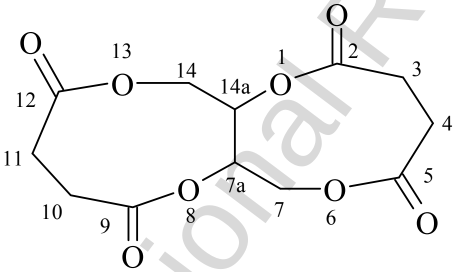
1,3,2λ^5-dioxaphosphepan-2-one (PIN)



3,4-dihydro-2,5-benzodioxepin-1,6-dione (PIN)
3,4-dihydrobenzo[*f*]dioxepin-1,6-dione



octahydro-1,6,8,13-tetraoxacycloocta[10]annulene-2,5,9,12-tetrone (PIN)



octahydro-1,6,8,13-tetraoxanonalene-2,5,9,12-tetrone (PIN)

P-65.6.3.6 Acylals

Acylals are a class of compounds with the general structures R-CH(O-CO-R′)$_2$, R′C(OCOR″)$_2$, etc. Specific compounds are named as esters.

Example:

2 1
CH_3-CH(O-CO-CH_2-CH_2-CH_3)$_2$

ethane-1,1-diyl dipropanoate (PIN)
(traditionally ethylidene dipropanoate)

P-65.7 Anhydrides and their analogues

P-65.7.0 Introduction

Anhydrides are compounds consisting of two acyl groups bonded to the same oxygen atom, i.e., acyl-O-acyl. Symmetric and mixed anhydrides have identical and different acyl groups, respectively. The central oxygen atom can be replaced by chalcogen atoms, a peroxy group and its chalcogen analogues, and by three consecutive oxygen atoms or any combination of three chalcogen atoms.

Polyanhydrides and polyfuctional anhydrides are also described in this Section.

P-65.7.1 Symmetric anhydrides

Symmetric anhydrides of monobasic acids, substituted or unsubstituted, are named by replacing the term ‘acid’ of an acid name by the class name ‘anhydride’.

Examples:

CH_3-CO-O-CO-CH_3

acetic anhydride (PIN)

C_6H_5-CS-O-CS-C_6H_5

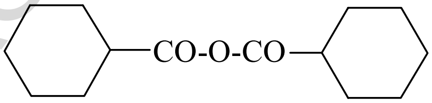
benzenecarbothioic anhydride (PIN)
(thiobenzoic) anhydride (PIN)

(CH_3-CH_2-CH_2-CH_2-CH_2-CO)$_2$O

hexanoic anhydride (PIN)

CH_3-CH_2-CS-O-CS-CH_2-CH_3

(propanethioic) anhydride (PIN)
(thiopropionic) anhydride



cyclohexanecarboxylic anhydride (PIN)

C_6H_5-SO_2-O-SO_2-C_6H_5

benzenesulfonic anhydride (PIN)

(Cl-CH_2-CO-O$)_2$O

chloroacetic anhydride (PIN)

(Cl-$\overset{2}{C}H_2$-$\overset{1}{C}H_2$-SO$)_2$O

2-chloroethanesulfinic anhydride (PIN)

P-65.7.2 Mixed anhydrides

Anhydrides derived from different monobasic acids are named by citing the names of the two acids, substituted or unsubstituted, without the class name ‘acid’ in alphabetical order, followed by the class name ‘anhydride’ as a separate word.

Examples:

CH_3-CO-O-CO-CH_2-CH_3

acetic propanoic anhydride (PIN)

C_6H_5-SO-O-SO_2-CH_2-CH_3

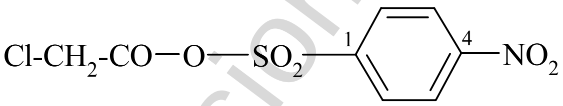
benzenesulfinic ethanesulfonic anhydride (PIN)

C_6H_5-CO-O-CS-CH_3

benzoic ethanethioic anhydride (PIN)
benzoic thioacetic anhydride

CH_3-CO-O-CO-CH_2-Cl

acetic chloroacetic anhydride (PIN)



chloroacetic 4-nitrobenzene-1-sulfonic anhydride (PIN)

Mixed anhydrides with carbonic acid, cyanic acid, and inorganic acids are named as anhydrides. Terms such as ‘monoanhydride’ are used with di-, tri- or tetrabasic acids to specify the appropriate number of anhydride linkages.

Examples:

CH_3-CO-O-CN

acetic cyanic anhydride (PIN)

C_6H_5-CO-O-PH_2

benzoic phosphinous anhydride (PIN)

HO−B(O-CO-$CH_3)_2$

acetic boric dianhydride (PIN)
(see also P-65.7.7)

P-65.7.3 Cyclic anhydrides

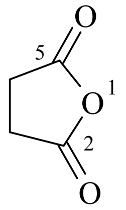
Cyclic anhydrides formed from two acid groups attached to the same parent hydride structure are named in two ways:

(1) as heterocyclic pseudoketones;

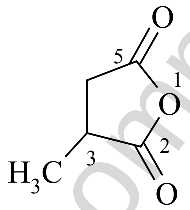
(2) by changing the class term 'acid' to 'anhydride' in the systematic or retained name of the dibasic acid.

Method (1) generates preferred IUPAC names

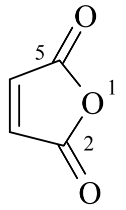
Examples:



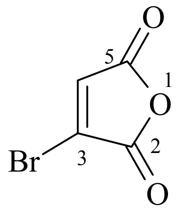
oxolane-2,5-dione (PIN)
3,4-dihydrofuran-2,5-dione
butanedioic anhydride
succinic anhydride



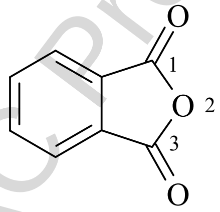
3-methyloxolane-2,5-dione (PIN)
3-methyl-3,4-dihydrofuran-2,5-dione
2-methylbutanedioic anhydride
methylsuccinic anhydride



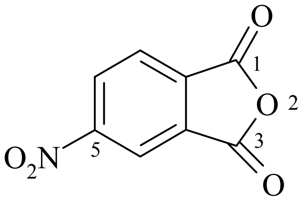
furan-2,5-dione (PIN)
maleic anhydride



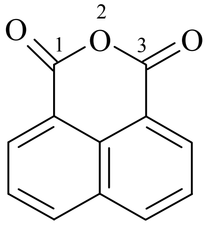
3-bromofuran-2,5-dione (PIN)
bromomaleic anhydride



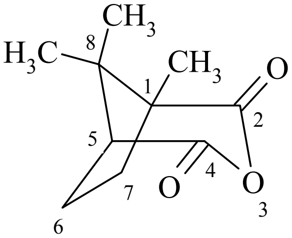
2-benzofuran-1,3-dione (PIN)
isobenzofuran-1,3-dione
benzo[*c*]furan-1,3-dione
phthalic anhydride



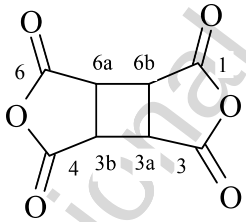
5-nitro-2-benzofuran-1,3-dione (PIN)
5-nitroisobenzofuran-1,3-dione
4-nitrophthalic anhydride
5-nitrobenzo[*c*]furan-1,3-dione



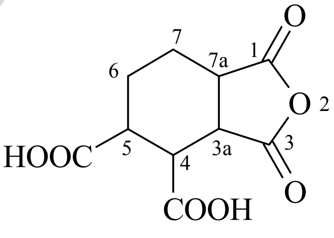
benzo[*d,e*]isochromene-1,3-dione (PIN)
naphthalene-1,8-dicarboxylic anhydride



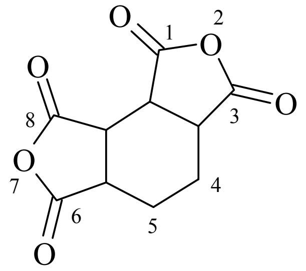
1,8,8-trimethyl-3-oxabicyclo[3.2.1]octane-2,4-dione (PIN)
(also known as camphoric anhydride)



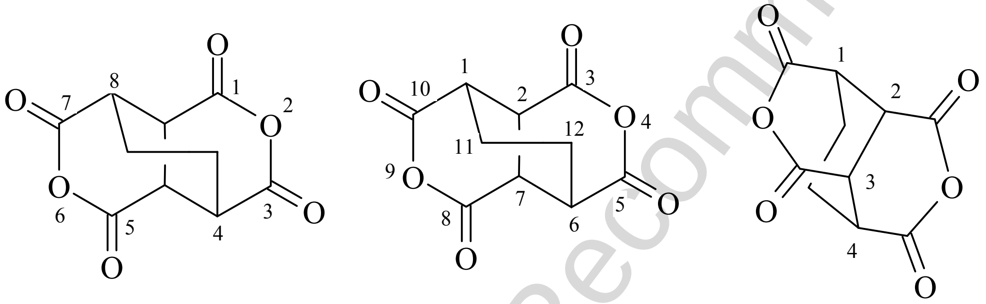
tetrahydrocyclobuta[1,2-*c*;3,4-c′]difuran-1,3,4,6-tetrone (PIN)
cyclobutane-1,2,3,4-tetracarboxylic 1,2:3,4-dianhydride



1,3-dioxooctahydro-2-benzofuran-4,5-dicarboxylic acid (PIN)
1,3-dioxooctahydroisobenzofuran-4,5-dicarboxylic acid
cyclohexane-1,2,3,4-tetracarboxylic acid 3,4-anhydride
1,3-dioxooctahydrobenzo[*c*]furan-4,5-dicarboxylic acid



hexahydrobenzo[1,2-*c*:3,4-*c*′]difuran-1,3,6,8-tetrone (PIN)
cyclohexane-1,2,3,4-tetracarboxylic 1,2:3,4-dianhydride



(I) (II) (III)

octahydro-4,8-ethanopyrano[4,3-*c*]pyran-1,3,5,8-tetrone (PIN)
[numbering shown in (I)]
4,9-dioxatricyclo[4.4.2.$0^{2,7}$]dodecane-3,5,8,10-tetrone
[numbering shown in (II)]
cyclohexane-1,2,3,4-tetracarboxylic 1,3:2,4-dianhydride
[numbering shown in (III)]

P-65.7.4 Thioanhydrides and analogues

Chalcogen analogues of anhydrides having the general structure −CO-X-CO−, −CO-X-CS−, or −CS-X-CS−, where X is −S −, −Se −, or −Te −, are named using the class names ‘thioanhydride’, ‘selenoanhydride’ or ‘telluroanhydride’, respectively.

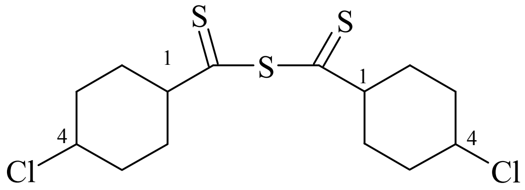
Examples:

C_6H_5-CO-S-CO-C_6H_5

benzoic thioanhydride (PIN)

CH_3-CH_2-SO_2-S-CS-C_6H_5

ethanesulfonic benzenecarbothioic thioanhydride (PIN)
ethanesulfonic thiobenzoic thioanhydride



4-chlorocyclohexane-1-carbothioic thioanhydride (PIN)

CH_3-CO-Se-CO-CH_3

acetic selenoanhydride (PIN)

The various unsymmetrical thioanhydrides derived from acetic propanoic anhydride are named as follows.

CH_3-CO-O-CO-CH_2-CH_3

acetic propanoic anhydride (PIN)
acetic propionic anhydride

CH_3-CO-O-CS-CH_2-CH_3

acetic propanethioic anhydride (PIN)
acetic thiopropionic anhydride

CH_3-CO-S-CO-CH_2-CH_3

acetic propanoic thioanhydride (PIN)
acetic propionic thioanhydride

CH_3-CS-O-CO-CH_2-CH_3

ethanethioic propanoic anhydride (PIN)
propionic thioacetic anhydride

CH_3-CS-O-CS-CH_2-CH_3

ethanethioic propanethioic anhydride (PIN)
thioacetic thiopropionic anhydride

CH_3-CS-S-CS-CH_2-CH_3

ethanethioic propanethioic thioanhydride (PIN)
thioacetic thiopropionic thioanhydride

CH_3-CH_2-CS-Se-CO-CH_3

acetic propanethioic selenoanhydride (PIN)
acetic thiopropionic selenoanhydride

CH_3-CS-S-CO-CH_2-CH_3

ethanethioic propanoic thioanhydride (PIN)
propionic thioacetic thioanhydride

P-65.7.5 Peroxyanhydrides and chalcogen analogues

Peroxyanhydrides, R-CO-OO-CO-R or R-CO-OO-COR', are named by replacing the term 'acid' of an acid or two different acids by the class name 'peroxyanhydride'.

Example:

CH_3-CO-OO-CO-CH_3

acetic peroxyanhydride (PIN)

Related anhydrides, in which the junction between two acyl groups is of the type −SS− −OS−, −SSe−, etc. are named as 'dithioperoxyanhydrides', 'thioperoxyanhydrides, 'selenothioperoxyanhydrides', etc.. When it is necessary to specify the position of the chalcogen atoms between two unsymmetrically substituted acyl groups or two different acyl group, the acyl group name is preceded by a the appropriate italicized capital element symbols indicating its attachment.

Examples:

CH_3-CO-S-O-CO-CH_3

acetic thioperoxyanhydride (PIN)

CH_3-CO-S-O-CO-CH_2-CH_3

S-acetic *O*-propanoic thioperoxyanhydride (PIN)

CH_3-CO-SS-CO-CH_3

acetic dithioperoxyanhydride (PIN)

P-65.7.6 Acyclic structures with three or more chalcogen atoms linking two acyl groups

P-65.7.6.1 Acyclic monoanhydrides named as pseudo ketones

Anhydrides derived from peroxy acids and their chalcogen analogues are named substitutively as pseudoketones (see P-64.3). Multiplicative names are preferred when the conditions for their use are fulfilled (see P-15.3).

Examples:

$\mathrm{CH_3\text{-}\overset{1''}{C}O\text{-}OOO\text{-}\overset{1}{C}O\text{-}CH_3}$

1,1′-trioxidanediylbis(ethan-1-one) (PIN)

$\mathrm{CH_3\text{-}CO\text{-}SSSS\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_3}$

1-(acetyltetrasulfanyl)propan-1-one (PIN)

CH_3-CO-S-O-S-CO-CH_3

1,1′-dithioxanediylbis(ethan-1-one) (PIN)

CH_3-CO-OO-S-CO-CH_3

1-[(acetylperoxy)sulfanyl]ethan-1-one (PIN)

P-65.7.6.2 Acyclic monoanhydrides are named by skeletal replacement (‘a’) nomenclature when the conditions for its use are fulfilled (see P-15.4).

Example:

1 2 3 4 5 6 7 8
CH_3-CO-O-Te-Se-S-CO-CH_3

3-oxa-6-thia-5-selena-4-telluraoctane-2,7-dione (PIN)

P-65.7.7 Polyanhydrides

Di- and trianhydrides have two and three –CO-O-CO– groups, respectively. They are named in different ways, depending on the general structure of the system.

P-65.7.7.1 Linear polyanhydrides

Linear polyanhydrides are formed by a continuous succession of anhydride linkages resulting from the elimination of water between two or more monobasic acids, called ‘exterior acids’ and one or more dibasic acids, called ‘interior acids’. They are named in the following way.

P-65.7.7.1.1 When interior acids are identical and symmetrical, exterior acids may be identical or different. Names are formed by citing the names of the characteristic part of acids, in alphanumerical order, as separate words followed by the term ‘anhydride’ preceded by a multiplying prefix denoting the number of anhydride linkages. Identical acids are named by using the appropriate multiplying prefixes.

Examples:

CH_3-CO-O-CO-CH_2-CH_2-CO-O-CO-CH_3

diacetic butanedioic dianhydride (PIN)

CH_3-CO-O-SO_2-CH_2-SO_2-O-CO-CH_2-CH_3

acetic methanedisulfonic propanoic dianhydride (PIN)

CH_3-CH_2-CO-O-CO-CH_2-CH_2-CO-O-CO- CH_2-CH_2-CH_3

butanedioic butanoic propanoic dianhydride (PIN)

CH_3-CO-O-CO-CH_2-CH_2-CO-O-CO-CH_2-CH_2-CO-O-CO-CH_2-CH_3

acetic dibutanedioic propanoic trianhydride (PIN)

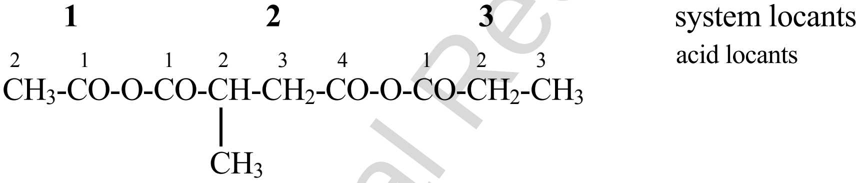
CH_3-CO-O-CO-CH_2-CO-O-CO-CH_2-CH_2-CO-O-CO-CH_3

diacetic butanedioic propanedioic trianhydride (PIN)

P-65.7.7.1.2 When the conditions required in P-65.7.7.1.1 are not fulfilled, the following methods are used.

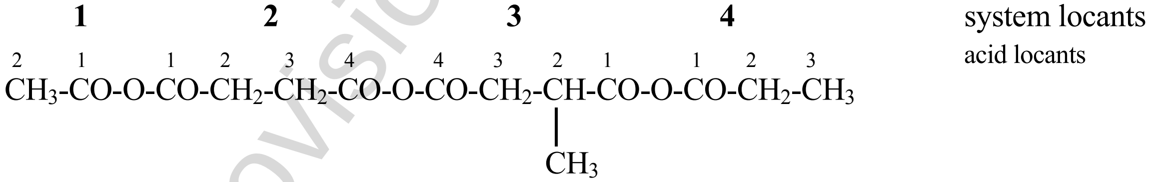
P-65.7.7.1.2.1 Acid residues constituting the polyanhydride are numbered consecutively alphanumerically and denoted by locants called ‘system locants’. Each acid residue is numbered systematically; these locants are called ‘acid locants’. Names are formed by citing the names of the acid residues in alphanumerical order of their ‘system locants’ followed by the term ‘anhydride’, which is preceded by the appropriate multiplying prefix denoting the number of anhydride linkages. This anhydride term is preceded by composite locants (formed by the system locant and the ‘acid locant’ cited as a superscript for each anhydride linkage) indicating the anhydride junctions, in a manner similar to that used in Phane Nomenclature (P-26.4.3) and ring assembly nomenclature (see P-29.3). If there is a choice of locants for interior acid residues, lowest locants are assigned in the order of the ‘system locants’.

Examples:



$CH_3\text{-CO-O-CO-}\underset{\displaystyle CH_3}{CH}\text{-}CH_2\text{-CO-O-CO-}CH_2\text{-}CH_3$

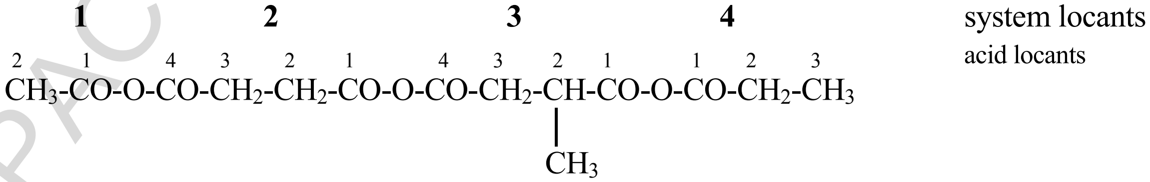
acetic 2-methylbutanedioic propanoic (1^{1},2^{1}:2^{4},3^{1})-dianhydride (PIN)



$CH_3\text{-CO-O-CO-}CH_2\text{-}CH_2\text{-CO-O-CO-}CH_2\text{-}\underset{\displaystyle CH_3}{CH}\text{-CO-O-CO-}CH_2\text{-}CH_3$

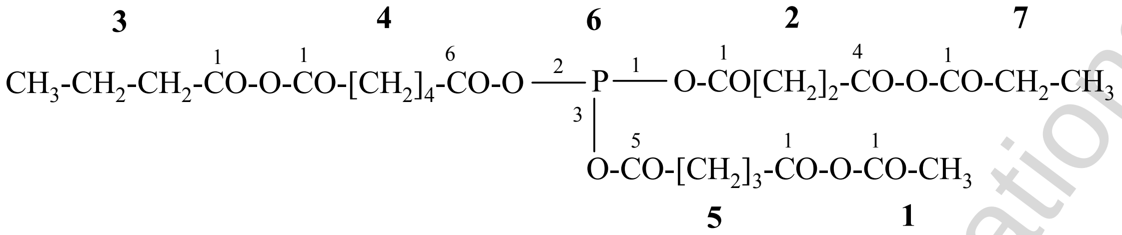
acetic butanedioic 2-methylbutanedioic propanoic (1^{1},2^{1}:2^{4},3^{4}:3^{1},4^{1})-trianhydride (PIN)

not



$CH_3\text{-CO-O-CO-}CH_2\text{-}CH_2\text{-CO-O-CO-}CH_2\text{-}\underset{\displaystyle CH_3}{CH}\text{-CO-O-CO-}CH_2\text{-}CH_3$

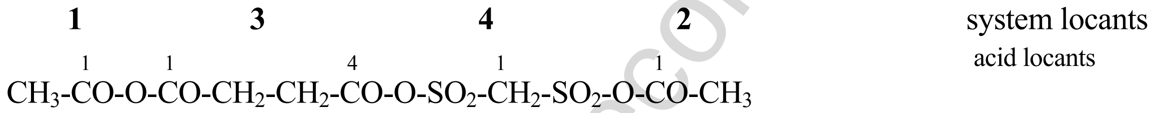
acetic butanedioic 2-methylbutanedioic propanoic (1^{1},2^{4}:2^{1},3^{4}:$3^{1}4^{1}$)-trianhydride



acetic butanedioic butanoic hexanedioic pentanedioic phosphoric propanoic
($1^1,5^1:2^1,6^1:2^4,7^1:3^1,4^1:4^6,6^2:5^5,6^3$)-hexaanhydride (PIN)

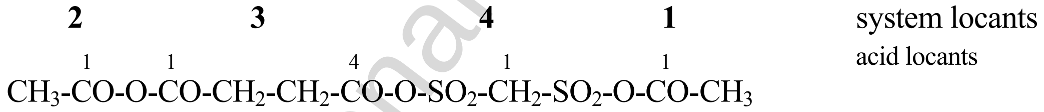
P-65.7.7.1.2.2 If there is choice in numbering involving system locants and acid locants, lowest locants are assigned to system locants so as to have the lowest locant set at the first point of difference.

Examples:

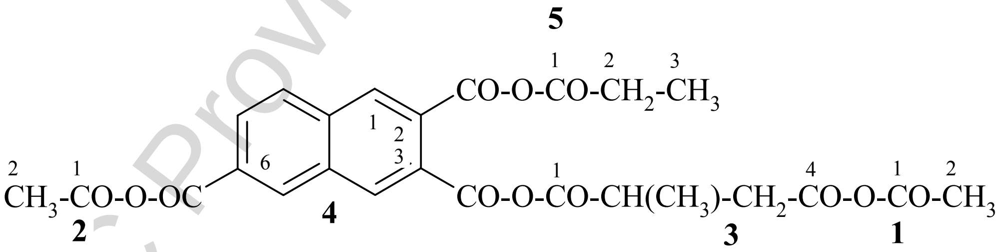

$CH_3\text{-}CO\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}O\text{-}SO_2\text{-}CH_2\text{-}SO_2\text{-}O\text{-}CO\text{-}CH_3$

diacetic butanedioic methanedisulfonic ($1^1,3^1:2^1,4^1:3^4,4^1$)-trianhydride (PIN)

not

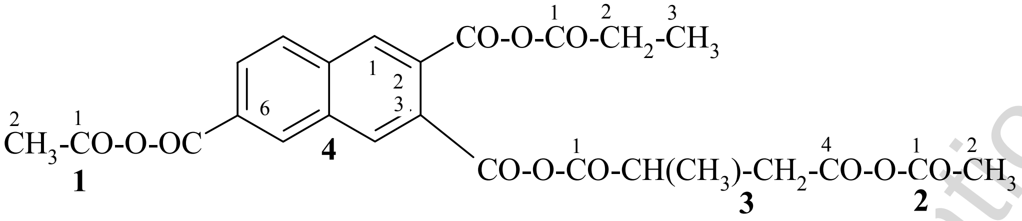

$CH_3\text{-}CO\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}O\text{-}SO_2\text{-}CH_2\text{-}SO_2\text{-}O\text{-}CO\text{-}CH_3$

diacetic butanedioic methanedisulfonic ($1^1,4^1:2^1,3^1:3^4,4^1$)-trianhydride
(the system locant set 1,3 in the correct name is lower than 1,4)



diacetic 2-methylbutanedioic naphthalene-2,3,6-tricarboxylic propanoic
($1^1,3^4:2^1,4^6:3^1,4^3:4^2,5^1$)-tetraanhydride (PIN)

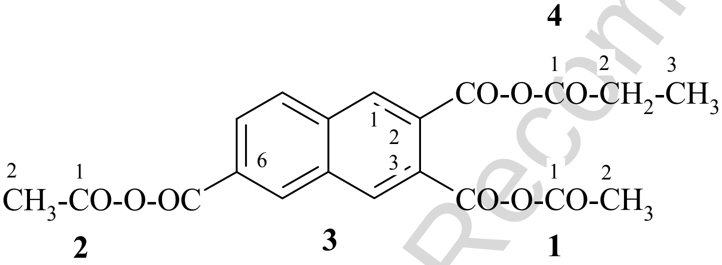
not



diacetic 2-methylbutanoic naphthalene-2,3,6-tricarboxylic propanoic $(1^1,4^6{:}2^1,3^4{:}3^1,4^3{:}4^2,5^1)$-tetraanhydride
(the system locant set 1,3 in the correct name is lower than 1,4)

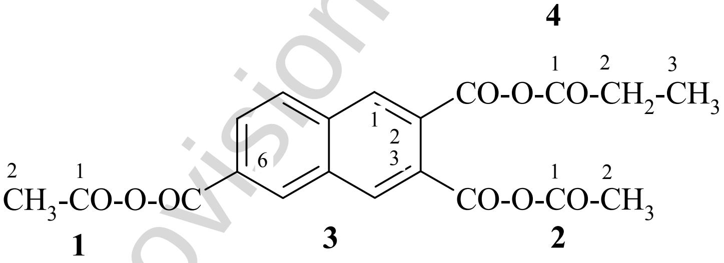
P-65.7.7.1.2.3 If a further choice is still possible because of a lack of difference between system locants, lowest locants are assigned so as to have the lowest set of locants in the order of citation.

Example:

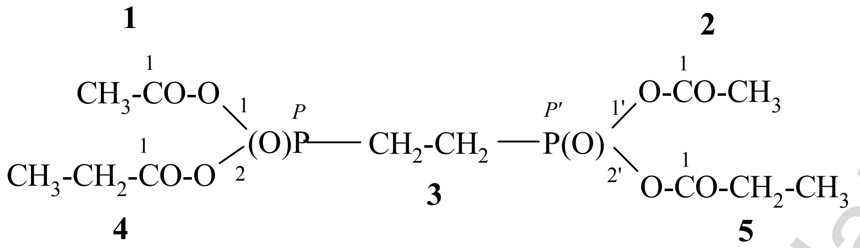


diacetic naphthalene-2,3,6-tricarboxylic propanoic $(1^1,3^3{:}2^1,3^6{:}3^2,4^1)$-trianhydride (PIN)

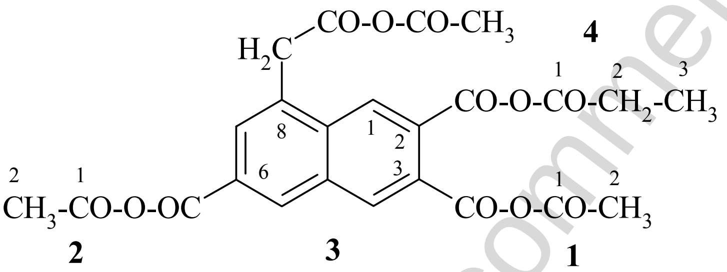
not



diacetic naphthalene-2,3,6-tricarboxylic propanoic $(1^1,3^6{:}2^1,3^3,3^2,4^1)$-trianhydride
(the set of locants $1^1,3^3{:}2^1,3^6{:}3^2,4^1$ is lower than $1^1,3^6{:}2^1,3^3,3^2,4^1$)



diacetic *P*,*P′*-ethane-1,2-diylbis(phosphonic) dipropanoic ($1^1,3^1{:}2^1,3^{1'}{:}3^2,4^1{:}3^{2'},5^1$)-tetraanhydride (PIN)



1,2-diacetic 3-{8-[2-(acetyloxy)-2-oxoethyl]naphthalene-2,3,6-tricarboxylic} propanoic ($1^1,3^3{:}2^1,3^6{:}3^2,4^1$)-trianhydride (PIN)

P-65.7.7.3 Chalcogen analogues of polyanhydrides

When chalcogen atoms are present in polyanhydrides, names are formed in different ways as follows.

P-65.7.7.3.1 When all anhydride linkages are identical, such as -CO-S-CO-, names are formed by using the class name, for example, ‘thioanhydride’, preceded by the multiplying prefixes ‘bis’, ‘tris’, etc.

Example:

$CH_3\text{-}CO\text{-}S\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}S\text{-}CO\text{-}CH_3$

diacetic butanedioic bis(thioanhydride) (PIN)

P-65.7.7.3.2 When mixed anhydride linkages are present, the usual seniority order established for chalcogen atoms, O > S > Se > Te, is used to determine the senior anhydride linkage. This senior anhydride is chosen as the basis of the name and other anhydride linkages are named substitutively.
Example:

$CH_3\text{-}CO\text{-}O\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_2\text{-}\overset{5}{C}O\text{-}S\text{-}CO\text{-}CH_3$

acetic 5-(acetylsulfanyl)-5-oxopentanoic anhydride (PIN)
acetic 4-[(acetylsulfanyl)carbonyl]butanoic acid

P-65.7.7.3.3 When the chalcogen atom replaces an oxygen atom in a carbonyl group, i.e. >C=S, thiocarboxylic acids and thioacyl groups are used in the manner described for anhydrides and polyanhydrides.

Examples:

$CH_3\text{-}CS\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}O\text{-}CO\text{-}CH_3$

acetic butanedioic ethanethioic dianhydride (PIN)

$CH_3\text{-}CO\text{-}O\text{-}CS\text{-}CH_2\text{-}CH_2\text{-}CS\text{-}O\text{-}CO\text{-}CH_3$

diacetic butanebis(thioic) dianhydride (PIN)

$CH_3\text{-}CO\text{-}O\text{-}CS\text{-}CH_2\text{-}CH_2\text{-}CS\text{-}S\text{-}CS\text{-}CH_3$

acetic 4-(ethanethioylsulfanyl)-4-thioxobutanethioic anhydride (PIN)

P-65.7.7.4 Skeletal replacement (‘a’) nomenclature and phane nomenclature.

P-65.7.7.4.1 Skeletal replacement (‘a’) nomenclature is used when four hetero units are present in acyclic anhydrides and other conditions are fulfilled (see P-15.4 and P-65.7.7.3.2)

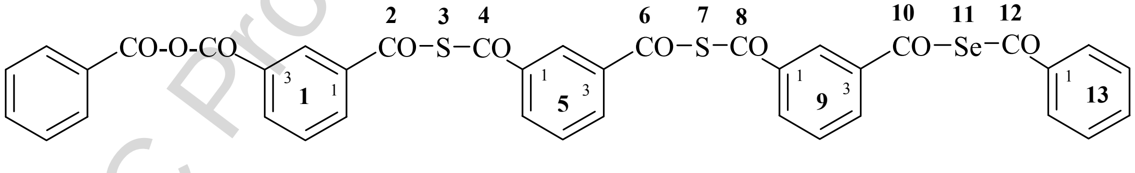
Example:

$$CH_3\text{-}CO\text{-}O\text{-}\overset{1}{CO}\text{-}\overset{2}{CH_2}\text{-}\overset{3}{O}\text{-}\overset{4}{CH_2}\text{-}\overset{5}{CO}\text{-}\overset{6}{S}\text{-}\overset{7}{CS}\text{-}\overset{8}{CH_2}\text{-}\overset{9}{O}\text{-}\overset{10}{CH_2}\text{-}\overset{11}{CS}\text{-}\overset{12}{S}\text{-}\overset{13}{CO}\text{-}\overset{14\text{-}15}{[CH_2]_2}\text{-}\overset{16}{CO}\text{-}O\text{-}CO\text{-}CH_3$$

5,13-dioxo-7,11-dithioxo-3,9-dioxa-6,12-dithiahexadecane1,16-dioic diacetic anhydride (PIN)

P-65.7.7.4.2 Phane nomenclature is used when the conditions for its use are fulfilled (see P-25.5 and P-65.7.7.3.2).

Example:



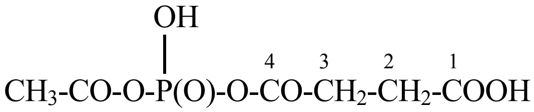
benzoic 2,4,6,8,10,12-hexaoxo-3,7-dithia-11-selena-1,13(1),5,9(1,3)-tetrabenzenatridecaphane-1^3-carboxylic anhydride (PIN)

P-65.7.8 Polyfunctional anhydrides

In the seniority of classes, acids are senior to anhydrides, and anhydrides are senior to esters and other classes (see P-41).

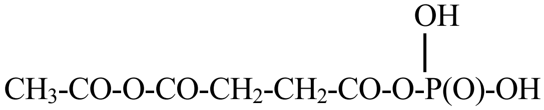
P-65.7.8.1 In presence of an acid, anhydrides are expressed by prefixes denoting the different components of the anhydride.

Examples:



$$CH_3\text{-}CO\text{-}O\text{-}\overset{\overset{OH}{|}}{P}(O)\text{-}O\text{-}\overset{4}{C}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$$

4-{[(acetyloxy)hydroxyphosphoryl]oxy}-4-oxobutanoic acid (PIN)



$$CH_3\text{-}CO\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}O\text{-}\overset{\overset{OH}{|}}{P}(O)\text{-}OH$$

{[4-(acetyloxy)-4-oxobutanoyl]oxy}phosphonic acid (PIN)

$CH_3\text{-}CO\text{-}O\text{-}CS\text{-}CH_2\text{-}CH_2\text{-}COOH$

4-(acetyloxy)-4-sulfanylidenebutanoic acid (PIN)
4-(acetyloxy)-4-thioxobutanoic acid

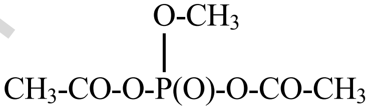
P-65.7.8.2 Nomenclature for assemblies of identical units is used when symmetry requirements for its use are fulfilled.

Example:

$$HOOC\text{-}CH_2\text{-}CH_2\text{-}\overset{4}{C}O\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}O\text{-}\overset{4'}{C}O\text{-}CH_2\text{-}CH_2\text{-}COOH$$

4,4′-[butanedioylbis(oxy)]bis(4-oxobutanoic acid) (PIN)

P-65.7.8.3 Anhydride nomenclature is applied when esters and other lower ranking characteristic groups are present.
Examples:



$$CH_3\text{-}CO\text{-}O\text{-}\overset{\overset{O\text{-}CH_3}{|}}{P}(O)\text{-}O\text{-}CO\text{-}CH_3$$

diacetic (methyl dihydrogen phosphate) dianhydride (PIN)

$$CH_3\text{-}CS\text{-}S\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}O\text{-}O\text{-}CH_3$$

ethanethioic (4-methoxy-4-oxobutanoic) thioanhydride (PIN)
(methyl hydrogen butanedioate) thioacetic thioanhydride

CH_3-CO-O-CO-CH_2-CN
acetic 2-cyanoacetic anhydride (PIN)

P-66 Amides, imides, hydrazides, nitriles, aldehydes, their chalcogen analogues and derivatives

P-66.0 Introduction

The classes dealt with in this Section have in common the fact that their retained names are derived from those of acids by changing the ‘ic acid’ ending to a class name, for example ‘amide’, ‘ohydrazide’, ‘nitrile’ or ‘aldehyde’. Their systematic names are formed substitutively by the suffix mode using one of two types of suffix, one that includes the carbon atom, for example, ‘carbonitrile’ for –CN, and one that does not, for example, ‘-nitrile’ for –(C)N,. Amidines are named as amides, hydrazidines as hydrazides, and amidrazones as amides or hydrazides.

P-66.1 Amides

P-66.1.0 Introduction

Amides are derivatives of oxoacids in which each hydroxy group has been replaced by an amino or substituted amino group. Chalcogen replacement analogues are called thio-, seleno- and telluroamides. Compounds having one, two or three acyl groups on a single nitrogen atom are generically included and may be designated as primary, secondary and tertiary amides, respectively.

P-66.1.1 Primary amides

P-66.1.1.1 Carboxamides

Names of carboxamides are formed in two ways:

P-66.1.1.1.1 Substitutive nomenclature
P-66.1.1.1.2 Modification of retained names for acids

P-66.1.1.1.1 Amide names formed by substitutive nomenclature

P-66-1.1.1.1.1 Aliphatic mono- and diamides are named substitutively by adding the suffix 'amide', to the appropriate parent hydride name, with elision of the final letter 'e' before 'a'. The multiplying prefix 'di' is used to name diamides.

Examples:

CH_3-$[CH_2]_4$-CO-NH_2
hexanamide (PIN)

H_2N-OC-CH_2-CH_2-CH_2-CO-NH_2
pentanediamide (PIN)

P-66-1.1.1.1.2 If an unbranched chain is directly linked to more than two –CO-NH_2 groups, these groups are named from the parent hydride by substitutive use of the suffix 'carboxamide'.

Example:

$$\mathrm{H_2N\text{-}CO\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H(CO\text{-}NH_2)\text{-}\overset{1}{C}H_2\text{-}CO\text{-}NH_2}$$

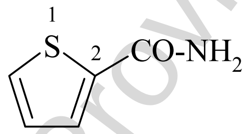
propane-1,2,3-tricarboxamide (PIN)

P-66-1.1.1.1.3 The suffix 'carboxamide' is always used to name amides having the –CO-NH_2 group attached to a ring or ring system or to a heteroatom.

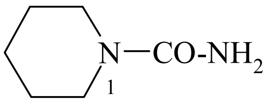
Examples:

H_2P-CO-NH_2
phosphanecarboxamide (PIN)

H_2N-NH-CO-NH_2
hydrazinecarboxamide (PIN)



thiophene-2-carboxamide (PIN)



piperidine-1-carboxamide (PIN)

P-66.1.1.1.2 Amide names formed by modifying retained names of acids

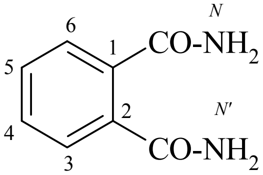
Names of amides derived from carboxylic acids listed in P-65.1.1 are formed by changing the 'ic acid' or '-oic acid' ending of the retained names of carboxylic acids into 'amide'. Names of amides formed by this method are either preferred IUPAC names or names only for use in general nomenclature according to the status of the corresponding acid; structures can be substituted in the same way as indicated for the corresponding acids (see P-65.1.1)

(a) Only the following two retained names are preferred IUPAC names and can be fully substituted. Systematic functional replacement names are used to generate acids modified by functional replacement.

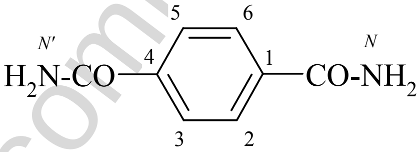
CH_3-CO-NH_2	C_6H_5-CO-NH_2
acetamide (PIN)	benzamide (PIN)

(b) For general nomenclature, only the names furamide, phthalamide, isophthalamide, and terephthalamide are retained with full substitution allowed (see P-34). Systematic names formed according to P-66.1.1.1.1 are the preferred IUPAC names.

Examples:



benzene-1,2-dicarboxamide (PIN)
phthalamide



benzene-1,4-dicarboxamide (PIN)
terephthalamide

(c) Amides derived from retained acid names given in P-65.1.1.2 are only used in general nomenclature; no substitution is allowed, even on amide nitrogen atoms. Preferred IUPAC names are given systematic names as given by P-66.1.1.1.1.

Examples:

$\overset{3}{CH_2}=\overset{2}{CH}-\overset{1}{CO}-NH_2$

prop-2-enamide (PIN)
acrylamide

$\overset{3}{CH_2}=\overset{2}{CH}-\overset{1}{CO}-NH-CH_3$

N-methylprop-2-enamide (PIN)
(not *N*-methylacrylamide; substitution not allowed on acrylamide)

$\overset{3}{CH_3}-\overset{2}{CH}(OH)-\overset{1}{CO}-NH_2$

2-hydroxypropanamide (PIN)
(not lactamide)

$\overset{3}{CH_3}-\overset{2}{CH}(OH)-\overset{1}{CO}-NH-CH_3$

2-hydroxy-*N*-methylpropanamide (PIN)
(not *N*-methyllactamide)

(d) The traditional name ‘formamide’ is retained for HCO-NH_2 and is the preferred IUPAC name. Substitution is permitted on the –NH_2 group. Substitution of the aldehydic hydrogen is subject to limitations (see P-65.2.2.1).

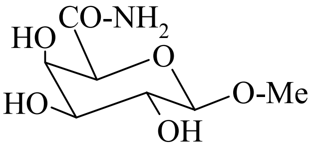
Examples:

$HCO\text{-}NH_2$ formamide (PIN)

$Cl\text{-}CO\text{-}NH_2$ carbonochloridic amide (PIN)
(not 1-chloroformamide)

(e) Names for amides derived from carbohydrate acids and α-amino acids are discussed in P-102.5.5.6.2.1 and P-103.2, respectively.

Examples:



R = –CO-NH$_2$

methyl β-D-galactopyranosiduronamide (PIN)

$H_2N\text{-}CH_2\text{-}CO\text{-}NH_2$
glycinamide (PIN)

P-66.1.1.2 Sulfonamides, sulfinamides, and related selenium and tellurium amides

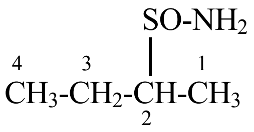
Sulfonamides, sulfinamides, and the analogous selenium and tellurium amides are named substitutively using the following suffixes:

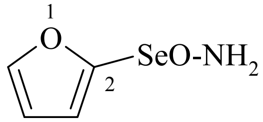
$-SO_2\text{-}NH_2$	sulfonamide	$-SO\text{-}NH_2$	sulfinamide
$-SeO_2\text{-}NH_2$	selenonamide	$-SeO\text{-}NH_2$	seleninamide
$-TeO_2\text{-}NH_2$	telluronamide	$-TeO\text{-}NH_2$	tellurinamide

These suffixes may be assigned to any position of a parent hydride.

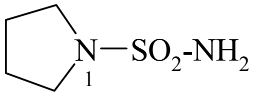
Examples:

$CH_3\text{-}SO_2\text{-}NH_2$
methanesulfonamide (PIN)


$$\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\underset{2}{C}H(SO\text{-}NH_2)\text{-}\overset{1}{C}H_3$$
butane-2-sulfinamide (PIN)



furan-2-seleninamide (PIN)



pyrrolidine-1-sulfonamide (PIN)

P-66.1.1.3 Substitution of primary amides

P-66.1.1.3.1 *N*-Substitution

P-66.1.1.3.1.1 Substituted primary amides, with general structures such as R-CO-NHR′ and R-CO-NR′R″, and the corresponding amides derived from chalcogen acids are named by citing the substituents R′ and R″ as prefixes preceded by the locant *N* when one amide group is present; the locants *N* and *N* ′ are used to distinguish between two equivalent amide groups, and *N* locants preceded by the locant denoting of the position of the amide group on the parent hydride to distinguish nonequivalent groups (see also P-62.2.1.2.2)

N-Substitution of primary amides is not allowed when amides having retained names designated as not substitutable.

Examples:

$\mathrm{HCO\text{-}\overset{\mathit{N}}{N}(CH_3)_2}$

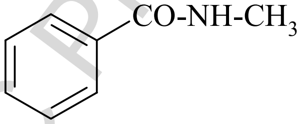
N,*N*-dimethylformamide (PIN)
dimethylformamide

$\mathrm{H_3C\text{-}CO\text{-}\overset{\mathit{N}}{N}H\text{-}CH(CH_3)_2}$

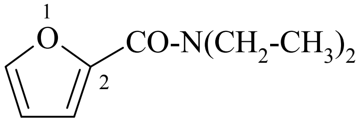
N-(propan-2-yl)acetamide (PIN)

$\mathrm{CH_3\text{-}CH_2\text{-}CO\text{-}\overset{\mathit{N}}{N}(CH_3)_2}$

N,N-dimethylpropanamide (PIN)
(not *N,N*-dimethylpropionamide;
substitution not allowed on
propionamide)



N-methylbenzamide (PIN)



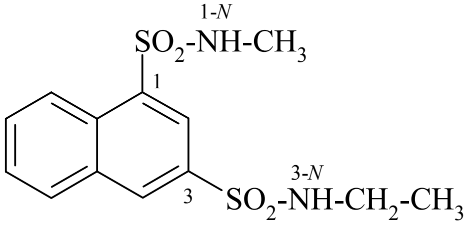
N,N-diethylfuran-2-carboxamide (PIN)
N,N-diethyl-2-furanamide

$\mathrm{CH_3\text{-}\overset{\mathit{N}}{NH}\text{-}\overset{1}{CO}\text{-}\overset{2}{CH_2}\text{-}\overset{3}{CH_2}\text{-}\overset{4}{CO}\text{-}NH_2}$

N-methylbutanediamide (PIN)

$\mathrm{CH_3\text{-}\overset{\mathit{N'}}{NH}\text{-}\overset{5}{CO}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CO}\text{-}\overset{\mathit{N}}{NH}\text{-}CH_3}$

N,*N*′ -dimethylpentanediamide (PIN)

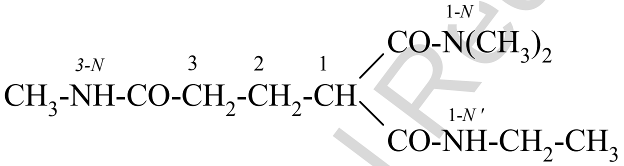


3-*N*-ethyl-1-*N*-methylnaphthalene-1,3-disulfonamide (PIN)

P-66.1.1.3.1.2 Locants for geminal carboxamide groups

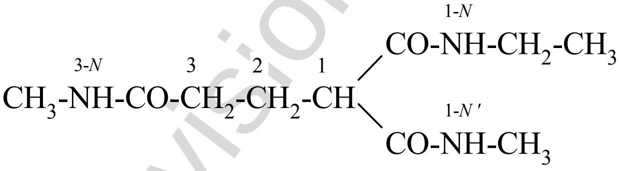
When geminal carboxamide groups are present, the locants *N*, *N*′, etc. are used in association with the numerical locant indicating the position of the groups on a chain or ring. Lowest locants are assigned to the most substituted group; when there is a choice, lowest locants are assigned to the first cited *N*-substituent. This system of *N*-locants in association with numerical locants is recommended for naming substituted amines (see P-62.2.1.2.2) and is extended to name geminal amidines (see P-66.4.1.3.3), amidrazones (see P-66.4.2.1), and hydrazidines (see P-66.4.3.1).

Examples:



$$\mathrm{CH_3\text{-}\overset{3\text{-}\mathit{N}}{N}H\text{-}CO\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H}\begin{matrix}\diagup\ \mathrm{CO\text{-}\overset{1\text{-}\mathit{N}}{N}(CH_3)_2} \\ \diagdown\ \mathrm{CO\text{-}\overset{1\text{-}\mathit{N}'}{N}H\text{-}CH_2\text{-}CH_3}\end{matrix}$$

1-*N*,1-*N*,3-*N*-trimethyl-1-*N*′-ethylpropane-1,1,3-tricarboxamide (PIN)



$$\mathrm{CH_3\text{-}\overset{3\text{-}\mathit{N}}{N}H\text{-}CO\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H}\begin{matrix}\diagup\ \mathrm{CO\text{-}\overset{1\text{-}\mathit{N}}{N}H\text{-}CH_2\text{-}CH_3} \\ \diagdown\ \mathrm{CO\text{-}\overset{1\text{-}\mathit{N}'}{N}H\text{-}CH_3}\end{matrix}$$

1-*N*-ethyl-1-*N*′,3-*N*-dimethylpropane-1,1,3-tricarboxamide (PIN)

P-66.1.1.3.2 Anilides

N-Phenyl derivatives of primary amides are called ‘anilides’ and may be named using the term ‘anilide’ in place of ‘amide’ in systematic or retained names of amides. The locants for substituents in the *N*-phenyl ring are primed numbers. However, names expressing *N*-substitution by a phenyl group on an amide are preferred IUPAC names.

Examples:

$\mathrm{HCO\text{-}NH\text{-}C_6H_5}$

N-phenylformamide (PIN)
formanilide

$CH_3\text{-}CO\text{-}NH\text{-}C_6H_5$

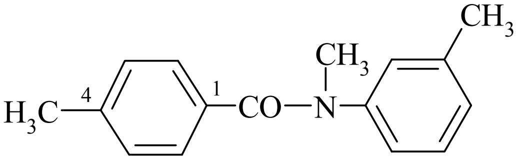
N-phenylacetamide (PIN)
acetanilide

$C_6H_5\text{-}CO\text{-}N(CH_3)\text{-}C_6H_5$

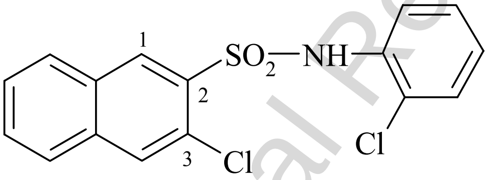
N-methyl-*N*-phenylbenzamide (PIN)
N-methylbenzanilide

$CH_3\text{-}[CH_2]_4\text{-}CO\text{-}NH\text{-}C_6H_5$

N-phenylhexanamide (PIN)
hexananilide



N,4-dimethyl-*N*-(3-methylphenyl)benzamide (PIN)
N,3′,4-trimethylbenzanilide



3-chloro-*N*-(2-chlorophenyl)naphthalene-2-sulfonamide (PIN)
2′,3-dichloronaphthalene-2-sulfonanilide

P-66.1.1.3.3 General substitution of amides

Substitution is expressed by prefixes; numerical and *N* and *N*′ locants are used as required.

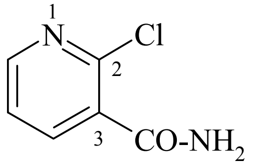
Examples:

$\mathrm{Cl\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}NH_2}$

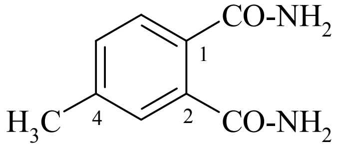
3-chloropropanamide (PIN)
(not 3-chloropropionamide;
no substitution on propionamide)

$\mathrm{Cl\text{-}\overset{4}{C}H_3\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}N(CH_3)_2}$

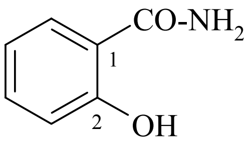
4-chloro-*N,N*-dimethylbutanamide (PIN)
(not 4-chloro-*N,N*-dimethylbutyramide;
no substitution on butyramide)



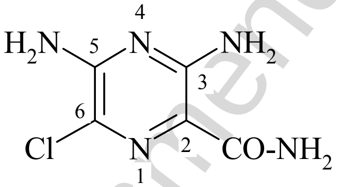
2-chloropyridine-3-carboxamide (PIN)
2-chloronicotinamide



4-methylbenzene-1,2-dicarboxamide (PIN)
4-methylphthalamide



2-hydroxybenzamide (PIN)
(not salicylamide)



3,5-diamino-6-chloropyrazine-2-carboxamide (PIN)

CH_3-CH_2-CO-NH-OH

N-hydroxypropanamide (PIN)
(not propanehydroxamic acid, see P-65.1.3.4)

P-66.1.1.4 Amides denoted as prefixes

Two different substituent groups can be derived from amides and expressed as prefixes in presence of a characteristic group having seniority for citation as suffix:

P-66.1.1.4.1 Substituents of the types −CO-NH$_2$ and −SO$_2$-NH$_2$;
P-66.1.1.4.2 Substituents of the types −NH-CO-R and −NH-SO$_2$-R

P-66.1.1.4.1 Substituent groups of the types −CO-NH$_2$ and −SO$_2$-NH$_2$ (and similar selenium and tellurium groups)

In presence of a characteristic group having priority for citation as suffix, the −CO-NH$_2$ group is named in three different ways:

(1) by using the two prefixes ‘amino’ and ‘oxo’ to denote such groups on terminal atoms of carbon chains having more than one carbon atom;

(2) by using the acyl group name ‘carbamoyl’;

(3) by using the prefix ‘aminocarbonyl’.

For generation of IUPAC preferred names, method (1) is preferred for chains and method (2) is preferred for rings and ring systems, heterogeneous chains, and on nonterminal atoms of carbon chains.

Deriatives of dicarboxylic acids having a retained name are called ‘amic acids’ when one carboxylic group has been changed to a carboxamide group. These acids may be named by replacing the ‘ic acid’ ending in the retained name by ‘amic acid’ (see P-65.1.6.1).

In presence of a characteristic group having priority for citation as suffix, the groups $-SO_2\text{-}NH_2$, $-SO\text{-}NH_2$ and related selenium and tellurium groups are named in two different ways corresponding to methods (2) and (3) for the $-CO\text{-}NH_2$ group above:

(2) by the acyl group ‘sulfamoyl’ (for sulfonamides only);

(3) by the the prefixes ‘amino-sulfonyl’, ‘-sulfinyl’, ‘-selenonyl’, -seleninyl’, -telluronyl’, or ‘tellurinyl’.

For generating preferred IUPAC names for $-SO_2\text{-}NH_2$, method (2) is preferred to method (3); method (3) is the sole method recommended for all other groups.

Substituted $-CO\text{-}NH_2$, $-SO_2\text{-}NH_2$, $-SO\text{-}NH_2$ and related selenium and tellurium groups are named by substituting the groups ‘carbamoyl’ and ‘sulfamoyl-’, and by using substituted amino groups along with the prefix ‘oxo’ or the prefixes ‘sulfonyl’, sulfinyl, selenonyl, etc.

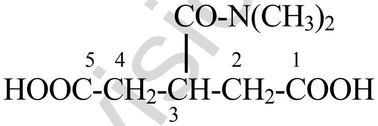
Examples:

$H_2N\text{-}\overset{10}{C}O\text{-}[CH_2\text{-}]_8\text{-}\overset{1}{C}OOH$

(1) 10-amino-10-oxodecanoic acid (PIN)
(2) 9-carbamoylnonanoic acid
(3) 9-(aminocarbonyl)nonanoic acid

$H_2N\text{-}\overset{3}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

(1) 3-amino-3-oxopropanoic acid (PIN)
(2) carbamoylacetic acid
(3) (aminocarbonyl)acetic acid
malonamic acid (see P-65.1.6.1)

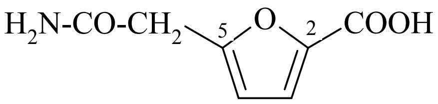


$$HOO\overset{5}{C}\text{-}\overset{4}{C}H_2\text{-}\underset{3}{\overset{\overset{\displaystyle CO\text{-}N(CH_3)_2}{|}}{C}}H\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$$

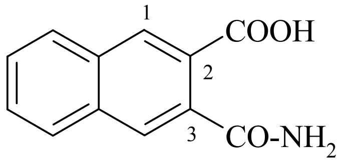
(2) 3-(dimethylcarbamoyl)pentanedioic acid (PIN)
(3) 3-[(dimethylamino)carbonyl]pentanedioic acid

$C_6H_5\text{-}NH\text{-}SO_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}O\text{-}CH_3$

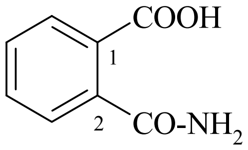
(2) methyl 3-(phenylsulfamoyl)propanoate (PIN)
(3) methyl 3-[(phenylamino)sulfonyl]propanoate



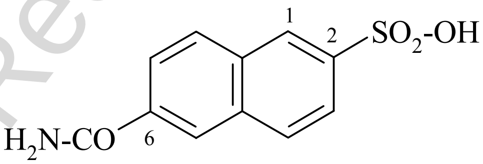
(1) 5-(2-amino-2-oxoethyl)furan-2-carboxylic acid (PIN)
(2) 5-(carbamoylmethyl)furan-2-carboxylic acid
(3) 5-[(aminocarbonyl)methyl]furan-2-carboxylic acid



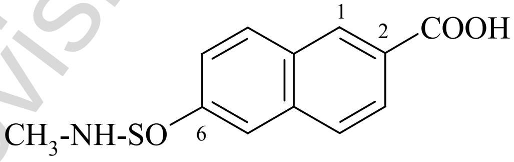
(2) 3-carbamoylnaphthalene-2-carboxylic acid (PIN)
3-carbamoyl-2-naphthoic acid
(3) 3-(aminocarbonyl)naphthalene-2-carboxylic acid
3-(aminocarbonyl)-2-naphthoic acid



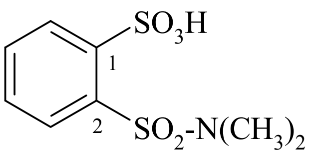
(2) 2-carbamoylbenzoic acid (PIN)
(3) 2-(aminocarbonyl)benzoic acid)
phthalamic acid (see P-65.1.6.1)



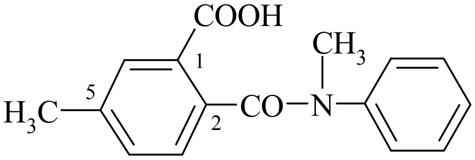
(2) 6-carbamoylnaphthalene-2-sulfonic acid (PIN)
(3) 6-(aminocarbonyl)naphthalene-2-sulfonic acid



(3) 6-[(methylamino)sulfinyl]naphthalene-2-carboxylic acid (PIN)
(3) 6-[(methylamino)sulfinyl]-2-naphthoic acid



(2) 2-(dimethylsulfamoyl)benzene-1-sulfonic acid (PIN)
(3) 2-[(dimethylamino)sulfonyl]benzene-1-sulfonic acid



(2) 5-methyl-2-[(methyl(phenyl)carbamoyl]benzoic acid (PIN)
(3) 5-methyl-2-[(*N*-methylanilino)carbonyl]benzoic acid

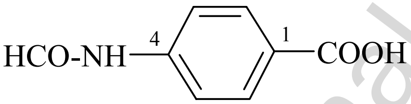
P-66.1.1.4.2 When a group having preference for citation as a principal characteristic group is present, the group R-CO-NH−, or R-SO_2-NH− (and selenium and tellurium analogues) of an *N*-substituted amide is named in two ways:

(1) substitutively, by using a prefix named formed by changing the final letter 'e' in the complete name of the amide to 'o', thus changing the suffixes 'amide' and 'carboxamide' into 'amido' and 'carboxamido', respectively, 'diamide' to 'diamido' or 'sulfonamide' to 'sulfonamido', etc.;

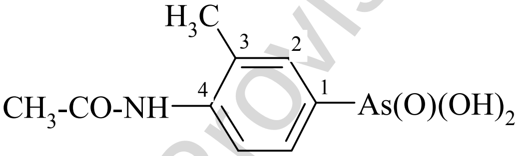
(2) substitutively, by using 'acylamino' prefixes formed by combining the name of the acyl group with that of the substituent group 'amino'

Method (1) generates preferred IUPAC names.

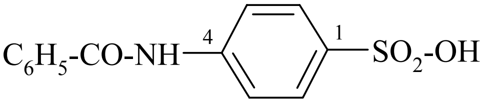
Examples:



4-formamidobenzoic acid (PIN)
4-(formylamino)benzoic acid



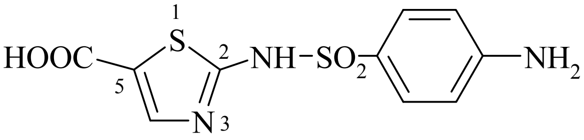
(4-acetamido-3-methylphenyl)arsonic acid (PIN)
[4-(acetylamino)-3-methylphenyl]arsonic acid



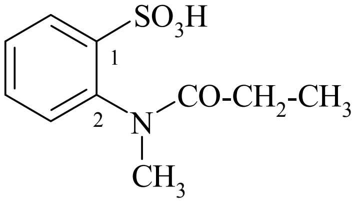
4-benzamidobenzesulfonic acid (PIN)
4-(benzoylamino)benzenesulfonic acid

$$CH_3\text{-}SO_2\text{-}NH\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$$

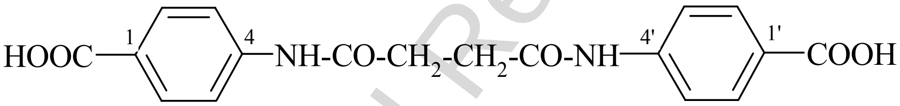
3-(methanesulfonamido)propanoic acid (PIN)
3-(methanesulfonylamino)propanoic acid



2-(4-aminobenzenesulfonamido)-1,3-thiazole-5-carboxylic acid (PIN)
(not 2-sulfanilamidothiazole-5-carboxylic acid;
sulfanilic acid is not a retained name)



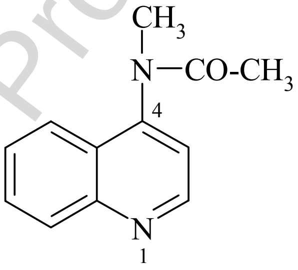
2-(*N*-methylpropanamido)benzene-1-sulfonic acid (PIN)
2-[methyl(propanoyl)amino]benzene-1-sulfonic acid



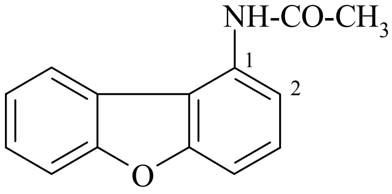
4,4′-butanediamidodibenzoic acid (PIN)
4,4′-succinamidodibenzoic acid

When an amide is the principal function, it must be named as such. The traditional method of considering amides as substituents on polycyclic ring systems, described in the 1993 Recommendations, should be avoided, even in general nomenclature.

Examples:



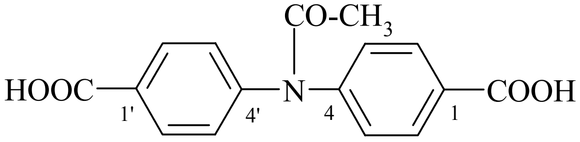
N-methyl-*N*-(quinolin-4-yl)acetamide (PIN)
(not 4-(*N*-methylacetamido)quinoline)
(not 4-[acetyl(methyl)amino]quinoline)



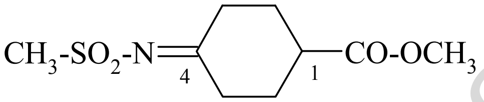
N-(dibenzofuran-1-yl)acetamide (PIN)
(not 1-acetamidodibenzofuran)
(not 1-(acetylamino)dibenzofuran)

P-66.1.1.4.3 When a group having preference for citation as a principal characteristic group is present, the groups R-CO-N< and R-CO-N=, or R-SO$_2$-N< and R-SO$_2$-N= (and selenium and tellurium analogues) of an *N*-substituted amide are named by combining acyl group names with those of the appropriate nitrogen substituent groups, azanediyl and imino, respectively.

Examples:



4,4′-(acetylazanediyl)dibenzoic acid (PIN)



methyl 4-(methanesulfonylimino)cyclohexane-1-carboxylate (PIN)

P-66.1.2 Secondary and tertiary amides

P-66.1.2.1 Amides having general formulas, (R-CO)$_2$NH, (R-SO$_2$)$_2$NH, etc., and (R-CO)$_3$N, (R-SO$_2$)$_3$N, etc., respectively, are named as *N*-acyl derivatives of the senior primary amide. Names based on the substitution of the parent hydride ‘azane’ or the pseudo parent hydride ‘amine’ by acyl groups, for example, diacetylazane or diacetylamine, as recommended in the 1993 Recommendations (ref 2) are not included in these recommendations, nor are trivial names such as diacetamide, triacetamide, dibenzamide and tribenzamide.

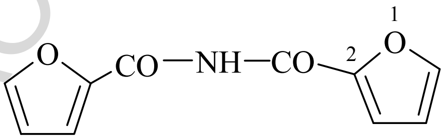
Examples:

HCO-NH-O-CH

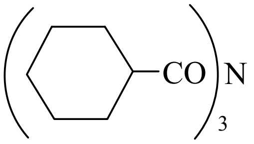
N-formylformamide (PIN)
(not diformylazane)
(not diformylamine)
(not diformamide)

CH_3-CO-NH-CO-CH_3

N-acetylacetamide (PIN)
(not diacetylazane)
(not diacetylamine)
(not diacetamide)



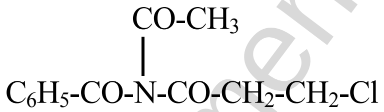
N-(furan-2-carbonyl)furan-2-carboxamide (PIN)
[not di(furan-2-carbonyl)azane]
[not di(furan-2-carbonyl)amine]



N,N-di(cyclohexanecarbonyl)cyclohexanecarboxamide (PIN)
[not tri(cyclohexanecarbonyl)azane]
[not tri(cyclohexanecarbonyl)amine]

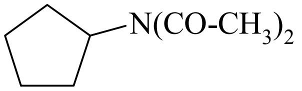
C_6H_5-CO-NH-CO-CH_3

N-acetylbenzamide (PIN)
[not acetyl(benzoyl)azane]
[not acetyl(benzoyl)amine]

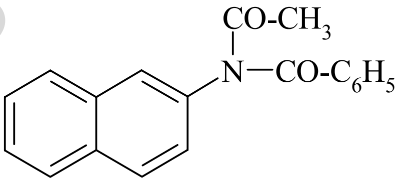


$\overset{\text{CO-CH}_3}{\overset{|}{\text{C}_6\text{H}_5\text{-CO-N-CO-CH}_2\text{-CH}_2\text{-Cl}}}$

N-acetyl-*N*-(3-chloropropanoyl)benzamide (PIN)
[not acetyl(benzoyl)(3-chloropropanoyl)azane]
[not acetyl(benzoyl)(3-chloropropanoyl)amine]



N-acetyl-*N*-cyclopentylacetamide (PIN)
[not diacetyl(cyclopentyl)azane]
[not diacetyl(cyclopentyl)amine]



N-acetyl-*N*-(naphthalen-2-yl)benzamide (PIN)
[not acetyl(benzoyl)(naphthalen-2-yl)azane]
[not acetyl(benzoyl)(naphthalen-2-yl)amine]

P-66.1.2.2 In the presence of a characteristic group higher than amide, a secondary amide group is expressed as an *N*-acylamido prefix or as a diacylamino prefix. The *N*-acylamido prefix method leads to preferred IUPAC names.

Example:

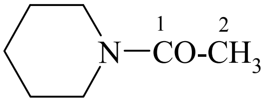
$(CH_3\text{-}CO)_2N\text{-}\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

3-(*N*-acetylacetamido)propanoic acid (PIN)
3-(diacetylamino)propanoic acid

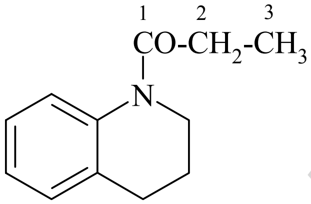
P-66.1.2.3 Hidden amides

An *N*-acyl group attached to a nitrogen atom of a heterocyclic system has been called a 'hidden amide', i.e., an amide that cannot be named as such. The traditional way to name such compounds by using acyl groups as substituents on the nitrogen atom of the heterocyclic system is discontinued. Such compounds are treated as pseudoketones (see P-64.3).

Examples:



1-(piperidin-1-yl)ethan-1-one (PIN)
(not 1-acetylpiperidine)



1-(1,2,3,4-tetrahydroquinolin-1-yl)propan-1-one (PIN)
(not 1-propanoyl-1,2,3,4-tetrahydroquinoline)
(not 1-propionyl-1,2,3,4-tetrahydroquinoline)

P-66.1.3 Chalcogen analogues of amides

Chalcogen analogues of amides are named systematically. Prefixes are no longer used with retained names.

P-66.1.3.1 Chalcogen amide suffixes

P-66.1.3.1.1 Names are formed by using suffixes modified by functional replacement nomenclature using prefixes and infixes.

Examples:

$-(C)S-NH_2$	thioamide
$-CS-NH_2$	carbothioamide
$-S(O)(S)-NH_2$	sulfonothioamide
$-S(S)(S)-NH_2$	sulfonodithioamide
$-S(S)-NH_2$	sulfinothioamide

For a more extended list, see Table 4.4.

Examples:

$HCS-NH_2$

methanethioamide (PIN)
thioformamide

$CH_3-CS-NH_2$

ethanethioamide (PIN)
thioacetamide

$C_6H_5-CS-NH_2$

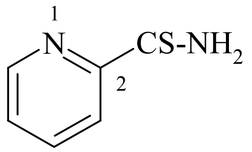
benzenecarbothioamide (PIN)
thiobenzamide

$CH_3\text{-}[CH_2]_4\text{-}CS\text{-}NH_2$

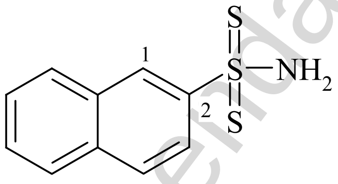
hexanethioamide (PIN)

$CH_3\text{-}CH_2\text{-}CS\text{-}NH_2$

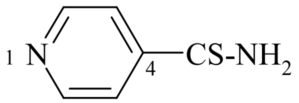
propanethioamide (PIN)
thiopropionamide



pyridine-2-carbothioamide (PIN)



naphthalene-2-sulfonodithioamide (PIN)



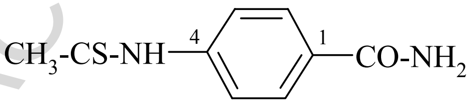
pyridine-4-carbothioamide (PIN)
thioisonicotinamide

P-66.1.3.1.2 In presence of a function having priority for citation as suffix, the amide function is expressed by the appropriate prefixes, such as amino in conjunction with sulfanylidene or thioxo, as well as carbonothioyl (not thiocarbonyl) for –CS– or carbamothioyl (not thiocarbamoyl) for –CS-NH$_2$.

Examples:

$H_2N\text{-}\overset{3}{C}S\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

3-amino-3-sulfanylidenepropanoic acid (PIN)
3-amino-3-thioxopropanoic acid
carbamothioylacetic acid
(aminocarbonothioyl)acetic acid



4-ethanethioamidobenzamide (PIN)
4-(ethanethioylamino)benzamide
[not 4-(thioacetamido)benzamide]

P-66.1.4 Lactams, lactims, sultams, sultims

P-66.1.4.1 Lactams and lactims

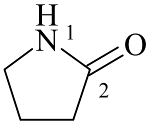
Intramolecular amides of amino carboxylic acids, –CO-NH–, are called 'lactams' and their tautomers, –C(OH)=N–, are 'lactims'. Lactams are named:

(1) as heterocyclic pseudoketones;

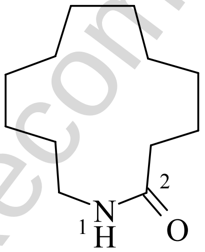
(2) by substituting 'lactam' for the 'ic acid' ending of a systematic 'oic acid' name for the parent acid without the amino substituent, and inserting a locant designating the position of the amino group between the 'o' and 'lactam'. Lactims are named in the same way, using 'lactim' in place of 'lactam'.

Method (1) generates preferred IUPAC names.

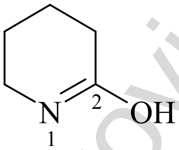
Examples:



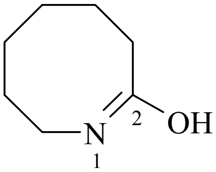
pyrrolidin-2-one (PIN)
butano-4-lactam
2-pyrrolidone
tetrahydropyrrol-2-one



1-azacyclotridecan-2-one (PIN)
dodecano-12-lactam



2,3,4,5-tetrahydropyridin-2-ol (PIN)
pentano-5-lactim



hexahydro-2,3,4,5,6,7-azocin-2-ol (PIN)
1,2-didehydroazocan-2-ol
heptano-7-lactim

P-66.1.4.2 Sultams, sultims, and intramolecular amides of sulfinic acids.

P-66.1.4.2.1 Intramolecular amides of amino sulfonic acids are called 'sultams' and may be named in three ways.

(1) as heterocyclic heterones;

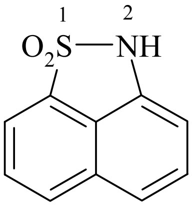
(2) by citing the term 'sultam' denoting the cyclic –NH-SO_2– group after the name of the appropriate parent hydride preceded by a pair of locants describing the points of

attachment of the sulfonyl group and the nitrogen atom, respectively; the locant of the sulfonyl group is cited first, and, if there is a choice, is the lower locant. Multiplying prefixes and pairs of locants separated by a colon are used to indicate two or more sultam rings.

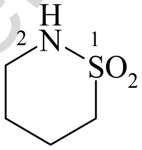
(3) as heterocycles according to functional class names using the class term ‘oxide’.

Method (1) leads to preferred IUPAC names.

Examples:



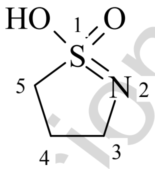
$1\lambda^{6}$-2*H*-naphtho[1,8-*cd*][1,2]thiazole-1,1-dione (PIN)
2*H*-naphtho[1,8-*cd*][1,2]thiazole 1,1-dioxide
naphthalene-1,8-sultam



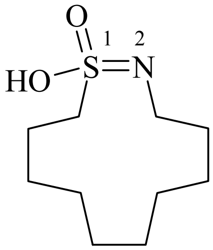
$1\lambda^{6}$,2-thiazinane-1,1-dione (PIN)
1,2-thiazinane 1,1-dioxide
butane-1,4-sultam

P-66.1.4.2.2 Sultims are tautomers of sultams and are named as described above for sultams, using the term ‘sultim’ in place of ‘sultam’.

Examples:



1-hydroxy-4,5-dihydro-3*H*-$1\lambda^{6}$,2-thiazol-1-one (PIN)
1-hydroxy-4,5-dihydro-3*H*-$1\lambda^{4}$,2-thiazole 1-oxide
propane-4-sultim

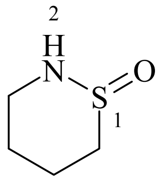


1-hydroxy-$1\lambda^{6}$-thia-2-azacyclododec-1-en-1-one (PIN)
1-hydroxy-$1\lambda^{4}$-thia-2-azacyclododec-1-ene 1-oxide
decane-11-sultim

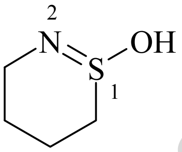
P-66.1.4.2.3 Intramolecular amides of amino sulfinic acids.

Cyclic amides of amino sulfinic acids and their tautomers are named as heterocyclic compounds.

Examples:



$1\lambda^4$,2-thiazinan-1-one (PIN)



3,4,5,6-tetrahydro-$1\lambda^4$,2-thiazin-1-ol (PIN)

P-66.1.5 Amides derived from carbonic, oxalic, cyanic, and the polycarbonic acids

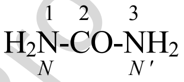
P-66.1.5.1 Amides derived from carbonic acid
P-66.1.5.2 Amides derived from cyanic acid
P-66.1.5.3 Amides derived from oxalic acid
P-66.1.5.4 Amides derived from polycarbonic acids

P-66.1.5.1 Amides derived from carbonic acid and related compounds

P-66.1.5.1.1 Urea, $H_2N\text{-}CO\text{-}NH_2$, and its derivatives
P-66.1.5.1.2 Isourea, $H_2N\text{-}C(=NH)\text{-}OH$, and its derivatives
P-66.1.5.1.3 Chalcogen analogues of urea and isourea
P-66.1.5.1.4 Condensed ureas

P-66.1.5.1.1 Urea and its substitutive derivatives

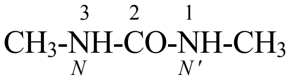
P-66.1.5.1.1.1 The compound $H_2N\text{-}CO\text{-}NH_2$ has the retained named 'urea', which is the preferred IUPAC name with locants 1,2, and 3 as shown below. The systematic name is 'carbonic diamide'with locants *N* and *N*′, as shown below.



$$H_2\underset{N}{\overset{1}{N}}\text{-}\overset{2}{C}O\text{-}\underset{N'}{\overset{3}{N}}H_2$$

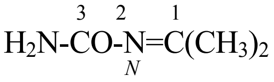
P-66.1.5.1.1.2 Derivatives of urea formed by substitution on the nitrogen atom(s) are named as substitution products in accordance with the seniority order of urea that is ranked as an amide of carbonic acid. Amides of the cyanic, oxalic, and the polycarboxylic acids follow the same seniority as the corresponding acid (see P-42.2)

Examples:



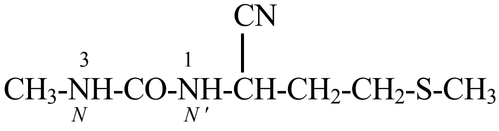
$$\mathrm{CH_3\text{-}}\underset{N}{\overset{3}{\mathrm{N}}}\mathrm{H\text{-}}\overset{2}{\mathrm{CO}}\mathrm{\text{-}}\underset{N'}{\overset{1}{\mathrm{N}}}\mathrm{H\text{-}CH_3}$$

1,3-dimethylurea (PIN)
N,*N′*-dimethylcarbonic diamide



$$\overset{3}{\mathrm{H_2N}}\mathrm{\text{-}}\overset{2}{\mathrm{CO}}\mathrm{\text{-}}\underset{N}{\overset{1}{\mathrm{N}}}\mathrm{=C(CH_3)_2}$$

propan-2-ylideneurea (PIN)
isopropylideneurea
N-(propan-2-ylidene)carbonic diamide



$$\mathrm{CH_3\text{-}}\underset{N}{\overset{3}{\mathrm{N}}}\mathrm{H\text{-}CO\text{-}}\underset{N'}{\overset{1}{\mathrm{N}}}\mathrm{H\text{-}}\overset{\overset{\mathrm{CN}}{|}}{\mathrm{C}}\mathrm{H\text{-}CH_2\text{-}CH_2\text{-}S\text{-}CH_3}$$

1-[1-cyano-3-(methylsulfanyl)propyl]-3-methylurea (PIN)
N-[1-cyano-3-(methylsulfanyl)propyl]-*N′*-methylcarbonic diamide

P-66.1.5.1.1.3 The prefixes for appropriate substituent groups derived from urea are systematically derived. The prefix names "ureido" and "ureylene" are not recommended.

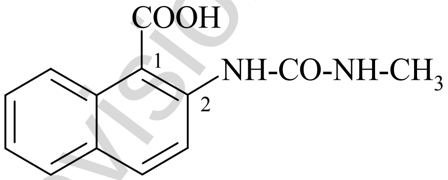
$\mathrm{H_2N\text{-}CO\text{-}NH}–$

carbamoylamino (PIN)
(not ureido)

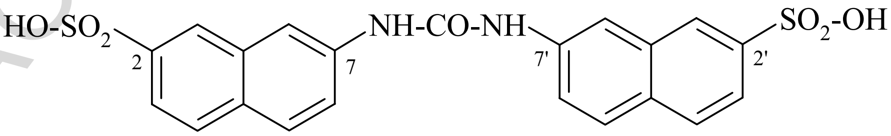
$–\mathrm{HN\text{-}CO\text{-}NH}–$

carbonylbis(azanediyl) (PIN)
(for use in multiplicative nomenclature)
(not ureylene)

Examples:



2-[(methylcarbamoyl)amino]naphthalene-1-carboxylic acid (PIN)
2-{[(methylamino)carbonyl]amino}-1-naphthoic acid
(not 2-ureidonaphthalene-1-carboxylic acid)



7,7′-[carbonylbis(azanediyl)]di(naphthalene-2-sulfonic acid) (PIN)
[not 7,7′-ureylenedi(naphthalene-1-carboxylic acid)]

$\mathrm{C_6H_5\text{-}CO\text{-}\overset{\mathit{N}}{N}H\text{-}CO\text{-}NH_2}$

N-carbamoylbenzamide (PIN)
N-(aminocarbonyl)benzamide

$\mathrm{C_6H_5\text{-}SO_2\text{-}\overset{\mathit{N}}{N}H\text{-}CO\text{-}NH_2}$

N-carbamoylbenzene-1-sulfonamide (PIN)
N-(aminocarbonyl)benzene-1-sulfonamide

$\mathrm{H_2N\text{-}CO\text{-}\overset{\mathit{N}}{N}H\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_2\text{-}C_6H_5}$

N-carbamoyl-2-phenylacetamide (PIN)
N-(aminocarbonyl)-2-phenylacetamide

P-66.1.5.1.1 4 Carboxylic acid derivatives of urea

Two carboxylic acids are related to urea; they have been known as ‘allophanic acid’ and ‘hydantoic acid’. These names are no longer recommended. Preferred IUPAC names for these two acids and their derivatives are formed systematically.

Examples:

$\mathrm{H_2\overset{3}{N}\text{-}\overset{2}{C}O\text{-}\overset{1}{N}H\text{-}COOH}$

carbamoylcarbamic acid (PIN)
(aminocarbonyl)carbamic acid

$\mathrm{H_2N\text{-}CO\text{-}NH\text{-}CO\text{–}}$

carbamoylcarbamoyl (PIN)
[(aminocarbonyl)amino]carbonyl

$\mathrm{H_2N\text{-}CO\text{-}NH\text{-}CH_2\text{-}COOH}$

N-carbamoylglycine (PIN)
(carbamoylamino)acetic acid

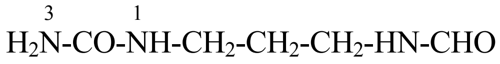
P-66.1.5.1.1.5 Seniority order of urea among amides

Amides are ranked in the same way than corresponding acids (see P-42). Thus, in substitutive nomenclature amides from carboxylic acids, which includes formamide, are senior to urea.

Examples:

$\mathrm{H_2N\text{-}CO\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}\overset{\mathit{N}}{N}H\text{-}CO\text{-}CH_3}$

N-[2-(carbamoylamino)ethyl]acetamide (PIN)
N-{2-[(aminocarbonyl)amino]ethyl}acetamide

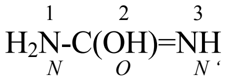


$$H_2\overset{3}{N}\text{-CO-}\overset{1}{N}\text{H-CH}_2\text{-CH}_2\text{-CH}_2\text{-HN-CHO}$$

[3-(carbamoylamino)propyl]formamide (PIN)
(not 1-(3-formamidopropyl)urea)
(not 1-[3-(formylamino)propyl]urea)
(formamide preferred to urea, see P-41)

P-66.1.5.1.2 Isourea

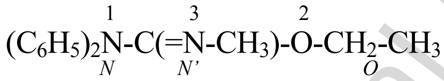
P-66.1.5.1.2.1 The imidic acid tautomer of urea, $H_2N\text{-}C(OH)\text{=}NH$, is named 'carbamimidic acid', a shortened form of the systematic functional replacement name 'carbonamidimidic acid'. The name 'isourea' is no longer recommended. Numerical locants are used in preferred IUPAC names when the positions of substituent groups are known; the locant *N* is used when the position of the double bond is unknown.



$$H_2\underset{N}{\overset{1}{N}}\text{-C(}\underset{O}{\overset{2}{O}}\text{H)=}\underset{N'}{\overset{3}{N}}\text{H}$$

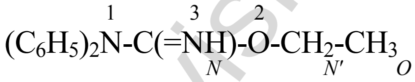
carbamimidic acid (PIN)

Examples:



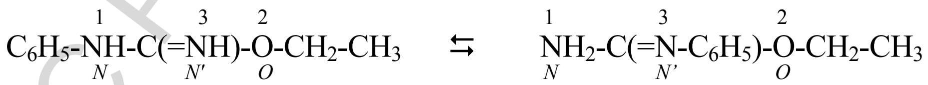
$$(C_6H_5)_2\underset{N}{\overset{1}{N}}\text{-C(=}\underset{N'}{\overset{3}{N}}\text{-CH}_3\text{)-}\overset{2}{O}\text{-C}\underset{O}{\text{H}_2}\text{-CH}_3$$

ethyl 3-methyl-1,1-diphenylcarbamimidate (PIN)
(not *O*-ethyl-*N′*-methyl-*N*,*N*-diphenylisourea)



$$(C_6H_5)_2\overset{1}{N}\text{-C(=}\overset{3}{N}\underset{N}{\text{H}}\text{)-}\overset{2}{O}\text{-C}\underset{N'}{\text{H}_2}\text{-CH}_3{}_{O}$$

ethyl 1,1-diphenylcarbamimidate (PIN)
(not *O*-ethyl-*N*,*N*-diphenylisourea)



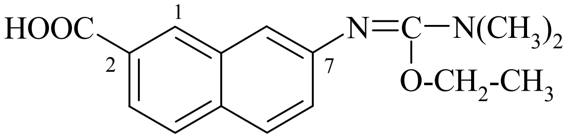
$$C_6H_5\text{-}\underset{N}{\overset{1}{N}}\text{H-C(=}\underset{N'}{\overset{3}{N}}\text{H)-}\underset{O}{\overset{2}{O}}\text{-CH}_2\text{-CH}_3 \quad \leftrightarrows \quad \underset{N}{\overset{1}{N}}\text{H}_2\text{-C(=}\underset{N'}{\overset{3}{N}}\text{-C}_6\text{H}_5\text{)-}\underset{O}{\overset{2}{O}}\text{-CH}_2\text{-CH}_3$$

ethyl *N*-phenylcarbamimidate (PIN)
(not *O*-ethyl-*N*-phenylisourea)

P-66.1.5.1.2.2 The groups $HN\text{=}C(OH)\text{-}NH-$ and $-N\text{=}C(OH)\text{-}NH_2$ are named '(*C*-hydroxycarbonimidoyl)amino' and '[amino(hydroxy)methylidene]amino', respectively. The letter locant '*C*' is used in the former to prevent possible ambiguity with *N*-substitution and parentheses are used around 'hydroxy' to emphasize that 'amino' is not substituted by 'hydroxy'.

The prefixes 1-isoureido and 3-isoureido are no longer recommended.

Example:



7-{[(dimethylamino)(ethoxy)methylidene]amino}naphthalene-2-carboxylic acid (PIN)
(not 7-(2-ethyl-1,1-dimethyl-3-isoureido)naphthalene-2-carboxylic acid)

P-66.1.5.1.3 Chalcogen analogues of urea and isourea

P-66.1.5.1.3.1 Chalcogen analogues of urea are named by functional replacement nomenclature using the prefixes ‘thio’, ‘seleno’ and ‘telluro’. Preferred IUPAC names use numerical locants.

Examples:

$H_2\underset{N}{\overset{3}{N}}\text{-}\overset{2}{C}S\text{-}\underset{N'}{\overset{1}{N}}H_2$

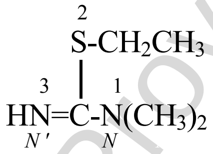
thiourea (PIN)
carbonothioic diamide

$H_2\underset{N'}{\overset{3}{N}}\text{-}\overset{2}{C}Se\text{-}\underset{N}{\overset{1}{N}}H\text{-}C(CH_3)\text{-}CH_2\text{-}CH_3$

1-(butan-2-yl)selenourea (PIN)
N-(butan-2-yl)carbonoselenoic diamide

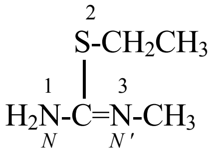
P-66.1.5.1.3.2 Chalcogen analogues of isourea are named by functional replacement nomenclature using the appropriate chalcogen infixes. Preferred IUPAC names use the locants *N* and *N'*. When the position of the double bond is not known, locants *S, Se, Te* and *N* are used to assign substituents to the appropriate atoms.

Examples:



$$\underset{N'}{\overset{3}{HN}}=C(\overset{2}{S}\text{-}CH_2CH_3)\text{-}\underset{N}{\overset{1}{N}}(CH_3)_2$$

ethyl *N*,*N*-dimethylcarbamimidothioate (PIN)
(not 2-ethyl-1,1-dimethylisothiourea)



$$H_2\underset{N}{\overset{1}{N}}\text{-}C(\overset{2}{S}\text{-}CH_2CH_3)=\underset{N'}{\overset{3}{N}}\text{-}CH_3$$

ethyl *N′*-methylcarbamimidothioate (PIN)
(not 2-ethyl-3-methylisothiourea)

For the second example, when the position of the double bond is not known the names are ethyl *N*-methylcarbamimidothioate (PIN) and *S*-ethyl *N*-methylisothiourea.

P-66.1.5.1.3.3 Prefix names for the groups $H_2N\text{-}CS\text{-}NH–$, $HN=C(SH)\text{-}NH–$, and $–N=C(SH)\text{-}NH_2$, are ‘carbamothioylamino’, ‘(*C*-sulfanylcarbonimidoyl)amino’, and ‘[amino(sulfanyl)methylidene]amino’, respectively.

Example:

$$\mathrm{H_2N\text{-}CS\text{-}NH\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH}$$

3-(carbamothioylamino)propanoic acid

P-66.1.5.1.4 Condensed ureas

Condensed ureas, $H_2N\text{-}[CO\text{-}NH]_n\text{-}H$, where $n = 2, 3$, or 4 are named systematically as diamides of triimidodicarbonic acid, pentaimidotricarbonic acid, and heptatriimidotetracarbonic acid. The names biuret, triuret, etc., are no longer recommended as preferred IUPAC names. Chalcogen analogues are described by functional replacement prefixes. Locants, as shown, are used to indicate the positions of substituents and functional replacement prefixes, where needed. Preferred IUPAC names use the locants prescribed for the amides of imidopolycarbonic acids (see P-66.1.5.4).

$$\mathrm{H_2\underset{1}{\overset{\mathit{N}}{N}}\text{-}\underset{2}{\overset{1}{C}}O\text{-}\underset{3}{\overset{2}{N}}H\text{-}\underset{4}{\overset{3}{C}}O\text{-}\underset{5}{\overset{\mathit{N}'}{N}}H_2}$$

2-imidodicarbonic diamide (PIN)
(numbering above structure)
biuret (numbering below structure)

$$\mathrm{H_2\underset{1}{\overset{\mathit{N}}{N}}\text{-}\underset{2}{\overset{1}{C}}O\text{-}\underset{3}{\overset{2}{N}}H\text{-}\underset{4}{\overset{3}{C}}O\text{-}\underset{5}{\overset{4}{N}}H\text{-}\underset{6}{\overset{5}{C}}O\text{-}\underset{7}{\overset{\mathit{N}'}{N}}H_2}$$

2,4-diimidotricarbonic diamide (PIN)
(numbering above structure)
triuret (numbering below structure)

Examples:

$$\mathrm{CH_3\text{-}\overset{\mathit{N}}{N}H\text{-}CO\text{-}NH\text{-}CO\text{-}NH_2}$$

N-methyl-2-imidodicarbonic diamide (PIN)

$$\mathrm{CH_3\text{-}\overset{\mathit{N}}{N}H\text{-}\overset{1}{C}S\text{-}\overset{2}{N}H\text{-}\overset{3}{C}O\text{-}\overset{\mathit{N}'}{N}H_2}$$

N-methyl-2-imido-1-thiodicarbonic diamide (PIN)

$$\mathrm{CH_3\text{-}\overset{\mathit{N}}{N}H\text{-}\overset{1}{C}O\text{-}\overset{2}{N}H\text{-}\overset{3}{C}S\text{-}\overset{4}{N}H\text{-}\overset{5}{C}O\text{-}\overset{\mathit{N}'}{N}H_2}$$

N-methyl-2,4-diimido-3-thiotricarbonic diamide (PIN)

For polyurets, where $n = 5$ and higher, skeletal replacement (‘a’) nomenclature leads to preferred IUPAC names.

Example:

1 2 3 4 5 6 7 8 9
H_2N-CO-NH-CO-NH-CO-NH-CO-NH-CO-NH_2

3,5,7-trioxo-2,4,6,8-tetraazanonanediamide (PIN)
pentauret

P-66.1.5.2 Amides derived from cyanic acid.

The traditional name ‘cyanamide’ is retained for NC-NH_2 and is the preferred IUPAC name. Substitution is allowed on the –NH_2 group.

Examples:

NC-NH-CH$(CH_3)_2$	NC-N$(CH_2$-$CH_3)_2$
(propan-2-yl)cyanamide (PIN) (not propan-2-ylcarbononitridic amide)	diethylcyanamide (PIN) (not diethylcarbononitridic amide)

P-66.1.5.3 Amides of oxalic acid

The name ‘oxamide’ is retained for H_2N-CO-CO-NH_2 and is the preferred IUPAC name. Substitution is allowed. The structure is numbered as shown below.

N 1 2 *N′*
H_2N-CO-CO-NH_2

Example:

N *N′*
CH_3-CH_2-NH-CO-CO-NH-CH_3

N-ethyl-*N′*-methyloxamide (PIN)
N-ethyl-*N′*-methyloxalic diamide

Chalcogen analogues are described by functional replacement prefixes.

Example:

N 1 2
$(CH_3)_3$C-NH-CS-CO-NH_2

N-*tert*-butyl-1-thiooxamide (PIN)
N-*tert*-butyl-1-thiooxalic diamide

The prefixes used to indicate appropriate substituent groups derived from oxamide are:

H_2N-CO-CO-NH–	oxamoylamino (PIN) carbamoylformamido aminooxoacetamido

$\mathrm{H_2N\text{-}CO\text{-}CO\text{-}N{=}}$	oxamoylimino (PIN)
$\mathrm{H_2N\text{-}CO\text{-}CO\text{-}N{<}}$	oxamoylazanediyl (PIN)
$\mathrm{–HN\text{-}CO\text{-}CO\text{-}NH–}$	oxalylbis(azanediyl) (PIN) (used in multiplicative nomenclature)
$\mathrm{{>}N\text{-}CO\text{-}CO\text{-}N{<}}$	oxalyldinitrilo (PIN) (used in multiplicative nomenclature)
$\mathrm{{=}N\text{-}CO\text{-}CO\text{-}N{=}}$	oxalylbis(azanylylidene) (PIN) (used in multiplicative nomenclature)

P-66.1 5.4 Amides of the polycarbonic acids.

Systematic names are formed by adding the functional class name ‘amide’ to that of the corresponding acid, preceded by the numerical prefix ‘di’ to indicate the presence of two $–NH_2$ groups. Chalcogen analogues are described by functional replacement prefixes. Numerical and letter locants are used to number the structures.

$\overset{N}{\mathrm{H_2N}}\text{-}\overset{1}{\mathrm{CO}}\text{-}\overset{2}{\mathrm{O}}\text{-}\overset{3}{\mathrm{CO}}\text{-}\overset{N'}{\mathrm{NH_2}}$

dicarbonic diamide (PIN)

$\overset{N}{\mathrm{H_2N}}\text{-}\overset{1}{\mathrm{CO}}\text{-}\overset{2}{\mathrm{O}}\text{-}\overset{3}{\mathrm{CO}}\text{-}\overset{4}{\mathrm{O}}\text{-}\overset{5}{\mathrm{CO}}\text{-}\overset{N'}{\mathrm{NH_2}}$

tricarbonic diamide (PIN)

Examples:

$\mathrm{(CH_3)_2CH}\text{-}\overset{N}{\mathrm{NH}}\text{-}\mathrm{CO\text{-}O\text{-}CO\text{-}NH_2}$

N-(propan-2-yl)dicarbonic diamide (PIN)
N-isopropyldicarbonic diamide

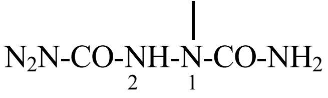
$\mathrm{CH_3}\text{-}\overset{N}{\mathrm{NH}}\text{-}\overset{1}{\mathrm{CO}}\text{-}\overset{2}{\mathrm{S}}\text{-}\mathrm{CO\text{-}O\text{-}CO\text{-}NH_2}$

N-methyl-2-thiotricarbonic diamide (PIN)

P-66.1.6 Polyfunctional amides

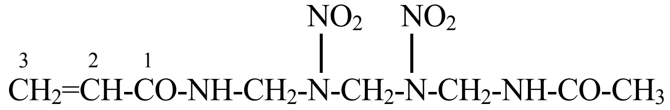
Amides follow acids, anhydrides, esters, and acid halides in the seniority order of compound classes expressed by suffixes (see P-41) and within the amide class, amides rank in the same order as the corresponding acid. Seniority for numbering polyfunctional amides follows that described for acids for which see P-65.1.2.3 and P-65.3.4.

Examples:



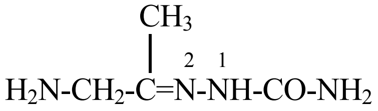
$\mathrm{N_2N\text{-}CO}\text{-}\underset{2}{\mathrm{NH}}\text{-}\overset{\mathrm{CH(NO_2)_2}}{\underset{1}{\mathrm{N}}}\text{-}\mathrm{CO\text{-}NH_2}$

1-(dinitromethyl)hydrazine-1,2-dicarboxamide (PIN)



$$\overset{3}{\mathrm{C}}\mathrm{H_2}=\overset{2}{\mathrm{C}}\mathrm{H}-\overset{1}{\mathrm{C}}\mathrm{O}-\mathrm{NH}-\mathrm{CH_2}-\overset{\mathrm{NO_2}}{\overset{|}{\mathrm{N}}}-\mathrm{CH_2}-\overset{\mathrm{NO_2}}{\overset{|}{\mathrm{N}}}-\mathrm{CH_2}-\mathrm{NH}-\mathrm{CO}-\mathrm{CH_3}$$

N-[({[(acetamidomethyl)nitroamino]methyl}nitroamino)methyl]prop-2-enamide (PIN)
N- {[({[(acetylamino)methyl]nitroamino}methyl)nitroamino]methyl}prop-2-enamide



$$\mathrm{H_2N}-\mathrm{CH_2}-\overset{\mathrm{CH_3}}{\overset{|}{\mathrm{C}}}=\overset{2}{\mathrm{N}}-\overset{1}{\mathrm{N}}\mathrm{H}-\mathrm{CO}-\mathrm{NH_2}$$

2-(1-aminopropan-2-ylidene)hydrazine-1-carboxamide (PIN)

$$\mathrm{HO}-\mathrm{CH_2}-\mathrm{CH_2}-\mathrm{NH}-\overset{4}{\mathrm{C}}\mathrm{H_2}-\overset{3}{\mathrm{C}}\mathrm{H_2}-\overset{2}{\mathrm{C}}\mathrm{H_2}-\overset{1}{\mathrm{C}}\mathrm{O}-\mathrm{NH}-\mathrm{CH_2}-\mathrm{CH_2}-\mathrm{NH}-\mathrm{CH_2}-\mathrm{CH_2}-\mathrm{OH}$$

4-[(2-hydroxyethyl)amino]-*N*-{2-[(2-hydroxyethyl)amino]ethyl}butanamide (PIN)

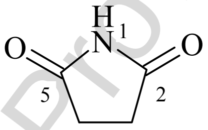
$$\mathrm{H_2N}-\overset{2}{\mathrm{C}}\mathrm{H_2}-\overset{1}{\mathrm{C}}\mathrm{O}-\mathrm{N(CH_3)}-\mathrm{CH_2}-\mathrm{CHOH}-\mathrm{CH_2OH}$$

2-amino-*N*-(2,3-dihydroxypropyl)-*N*-methylacetamide (PIN)

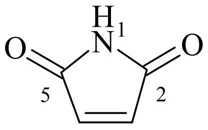
P-66.2 Imides

Imides are compounds containing the structural grouping –CO-NH-CO–. Acyclic imides are named according to P-66.1.2. Cyclic imides are preferably named as heterocyclic pseudoketones. They may also be named by replacing the suffixes 'dioic acid', or 'dicarboxylic acid' of the corresponding dibasic acid, or 'ic acid' in retained names of diacids, by 'imide' or 'dicarboximide'.

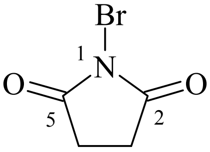
Examples:



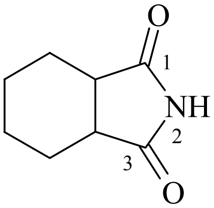
pyrrolidine-2,5-dione (PIN)
succinimide



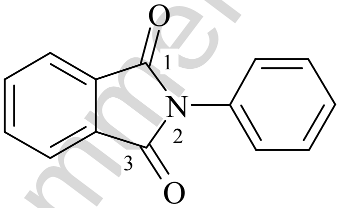
1*H*-pyrrole-2,5-dione (PIN)
pyrrole-2,5-dione



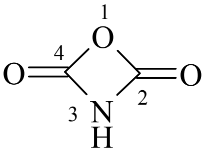
1-bromopyrrolidine-2,5-dione (PIN)
(not *N*-bromosuccinimide; substitution not allowed on succinimide)



hexahydroisoindole-1,3-dione (PIN)
cyclohexane-1,2-dicarboximide



2-phenylisoindole-1,3-dione (PIN)
N-phenylphthalimide



2*H*-1,3-oxazete-2,4(3*H*)-dione (PIN)

P-66.3 Hydrazides

P-66.3.0 Definition

Hydrazides are compounds derived from oxoacids by replacing –OH groups by –NR-NR′R″ groups (R groups are commonly H).

P-66.3.1 Systematic names

Hydrazides of the type R-CO-NH-NH_2 are named in two ways:

P-66.3.1.1 substitutive nomenclature;
P-66.3.1.2 modification of retained names of carboxylic acids.

P-66.3.1.1 Substitutive names

Hydrazides may be named substitutively in two ways:

(1) by the following suffixes:

–(C)O-NH-NH_2	hydrazide
–CO-NH-NH_2	carbohydrazide
–SO_2-NH-NH_2	sulfonohydrazide (and corresponding Se and Te suffixes)
–SO-NH-NH_2	sulfinohydrazide (and corresponding Se and Te suffixes)

> The suffix ‘hydrazide’ is recommended in place of ‘ohydrazide’ in accordance with the general use of suffixes that are added to names of parent hydrides, for example pentanehydrazide for CH_3-CH_3-CH_2-CH_2-CO-NH-NH_2, not pentanohydrazide.

The suffix ‘hydrazide’ is used to name acyclic compounds. The suffix ‘carbohydrazide’ is used to denote the –CO-NH-NH_2 characteristic group attached to cyclic compounds and in chains having more than two –CO-NH-NH_2 characteristic groups, or when the group is attached to a heteroatom of a heterocycle. Multiplicative nomenclature may be used when the symmetry conditions for its use are met.

(2) as acyl derivatives of hydrazine; multiplicative nomenclature is used when conditions allow this type of nomenclature.

Method (1) leads to preferred IUPAC names.

The nitrogen atoms in hydrazides are identified by *N* and *N′* locants as $-\text{CO-}\overset{N}{\text{NH}}\text{-}\overset{N'}{\text{NH}_2}$, even though hydrazine, itself, is numbered using the numerical locants 1 and 2, as $\overset{1}{\text{NH}_2}\text{-}\overset{2}{\text{NH}_2}$.

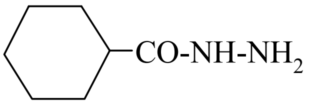
Examples:

$\overset{5}{\text{CH}_3}\text{-}\overset{4}{\text{CH}_2}\text{-}\overset{3}{\text{CH}_2}\text{-}\overset{2}{\text{CH}_2}\text{-}\overset{1}{\text{CO}}\text{-NH-NH}_2$

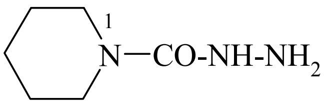
(1) pentanehydrazide (PIN)
(2) pentanoylhydrazine

$\text{H}_2\text{N-NH-}\overset{4}{\text{CO}}\text{-}\overset{3}{\text{CH}_2}\text{-}\overset{2}{\text{CH}_2}\text{-}\overset{1}{\text{CO}}\text{-NH-NH}_2$

(1) butanedihydrazide (PIN)
succinohydrazide (see P-66.2.1.3)
(2) (ethane-1,2-diyldicarbonyl)dihydrazine
succinyldihydrazine



cyclohexanecarbohydrazide (PIN)
(cyclohexanecarbonyl)hydrazine



piperidine-1-carbohydrazide (PIN)
[(piperidin-1-yl)carbonyl]hydrazine

CH_3-SO_2-NH-NH_2

methanesulfonohydrazide (PIN)

P-66.3.1.2 Names formed by modifying retained names of carboxylic acids

Names of hydrazides are formed by changing the 'ic acid' or '-oic acid' ending of the retained names of carboxylic acids into 'ohydrazide', as described in P-34.4.3.

(a) Only the following two retained names are preferred IUPAC names and can be fully substituted. Systematic substitutive names are used to generate acids modified by functional replacement.

HCO-NH-NH_2

formohydrazide (PIN)
hydrazinecarbaldehyde (see P-66.6.1.4)

CH_3-CO-NH-NH_2

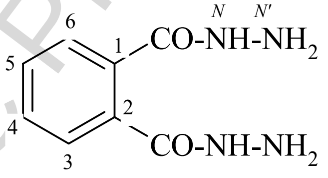
acetohydrazide (PIN)

C_6H_5-CO-NH-NH_2

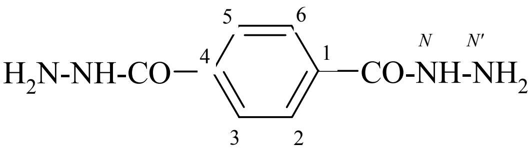
benzohydrazide (PIN)

(b) For general nomenclature, only the names furohydrazide, phthalohydrazide, isophthalohydrazide, and terephthalohydrazide are retained with full substitution allowed (see P-34). Systematic names are preferred IUPAC names (see P-66-3.1.1).

Examples:



benzene-1,2-dicarboxamide (PIN)
phthalohydrazide



benzene-1,4-dicarboxamide (PIN)
terephthalohydrazide

(c) Retained names for carboxylic acids (see P-65.1.1.2) are used only in general nomenclature and hydrazide formation is governed by the above rule; but substitution is not allowed, including substitution on the nitrogen atom(s) of the hydrazides.

Example:

$\mathrm{CH_3\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}NH\text{-}NH_2}$

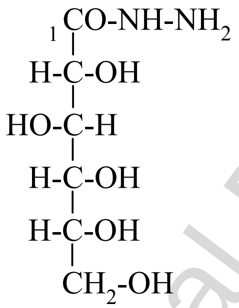
butanehydrazide (PIN)
butyrohydrazide
(substitution not allowed)

(d) Hydrazides derived from carbohydrate acids and α-amino acids are discussed in P-102.5.5.6.2.1 and P-103.2, respectively.

Examples:

$\mathrm{NH_2\text{-}CH_2\text{-}CO\text{-}NH\text{-}NH_2}$

glycinohydrazide (PIN)



gluconohydrazide (PIN)

P-66.3.2. Substituent groups derived from hydrazides

Substituent groups corresponding to hydrazides are of two types;

P-66.3.2.2.1 Substituent groups of the type $-\mathrm{CO\text{-}NH\text{-}NH_2}$, $-\mathrm{SO_2\text{-}NH\text{-}NH_2}$, etc.;
P-66.3.2.2.2 Substituent groups of the type $-\mathrm{NH\text{-}NH\text{-}CO\text{-}R}$, $-\mathrm{NH\text{-}NH\text{-}SO_2\text{-}R}$, etc.

P-66.3.2.1 Substituent groups of the type $-\mathrm{CO\text{-}NH\text{-}NH_2}$, $-\mathrm{SO_2\text{-}NH\text{-}NH_2}$, etc., may be named in two ways:

(1) as acyl groups derived from the corresponding acids or the appropriate carbonohydrazidoyl acyl prefix; the former are preferred IUPAC names:

$\mathrm{H_2N\text{-}NH\text{-}COOH}$	$\mathrm{H_2N\text{-}NH\text{-}CO-}$
hydrazinecarboxylic acid (PIN) carbonohydrazidic acid	hydrazinecarbonyl (PIN; (see P-68.3.1.2.1.2) carbonohydrazidoyl

$H_2N\text{-}NH\text{-}SO_2OH$ — hydrazinesulfonic acid (PIN)

$H_2N\text{-}NH\text{-}SO_2\text{–}$ — hydrazinesulfonyl (PIN; see P-68.3.1.2.1.2)

(2) by the prefixes ‘hydrazinyl’ and ‘oxo’ when the –CO-NHNH$_2$ group is located at the end of a chain.

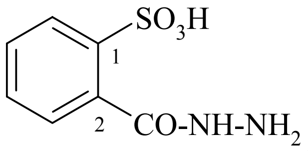
Examples:

$H_2N\text{-}NH\text{-}\overset{3}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

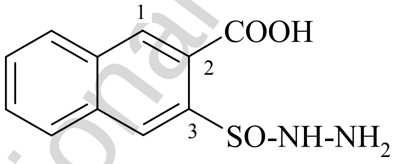
(1) 3-hydrazinyl-3-oxopropanoic acid (PIN)
(2) 2-hydrazinecarbonylacetic acid
2-carbonohydrazidoylacetic acid

$H_2N\text{-}NH\text{-}SO_2\text{-}CH_2\text{-}COOH$

(1) hydrazinesulfonylacetic acid (PIN)



(1) 2-hydrazinecarbonylbenzene-1-sulfonic acid (PIN)
2-carbonohydrazonoylbenzene-1-sulfonic acid



(1) 3-(hydrazinesulfinyl)naphthalene-2-carboxylic acid (PIN)

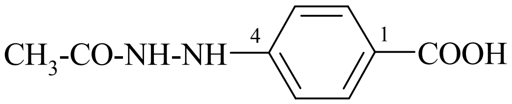
P-66.3.2.2 When a group having priority for citation as a principal characteristic group is present, a hydrazide group of the type R-CO-NH-NH–, or R-SO$_2$-NH-NH– (or related selenium and tellurium group) is named:

(1) as an acylhydrazinyl compound; the hydrazinyl group is numbered by using numerical locants 1 and 2; the locant ‘1’ is the nitrogen atom adjacent to the free valence;

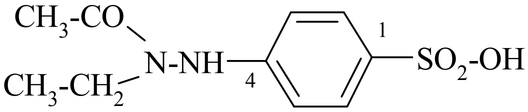
(2) by expressing the corresponding hydrazide as a prefix by replacing the final letter ‘e’ in the name of the hydrazide by the letter ‘o’, for example, ‘acetohydrazido’, ‘propanehydrazido’, and ‘benzenecarbohydrazido’. The locant *N* designates the nitrogen atom adjacent to the –CO– group.

Method (1) generates preferred IUPAC names.

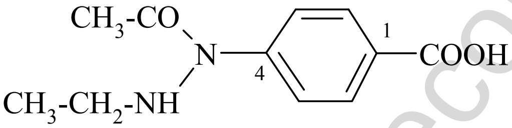
Example:



4-(2-acetylhydrazin-1-yl)benzoic acid (PIN)
4-(acetohydrazido)benzoic acid



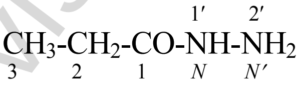
4-(2-acetyl-2-ethylhydrazin-1-yl)benzene-1-sulfonic acid (PIN)
4-(*N*-ethylacetohydrazido)benzene-1-sulfonic acid



4-(1-acetyl-2-ethylhydrazin-1-yl)benzoic acid (PIN)
4-(*N′*-ethylacetohydrazido)benzoic acid

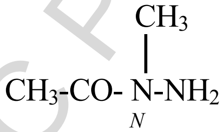
P-66.3.3 Substituted hydrazides

P-66.3.3.1 Alkyl, aryl, cycloalkyl, etc substituents on the nitrogen atoms of hydrazides are described by the appropriate prefix names and the locants *N* or 1′ for the imido nitrogen atom and *N′* or 2′ for the amino nitrogen atom as illustrated below. Preferred IUPAC names use the locants *N* and *N′* rather than the locants 1′ and 2′.



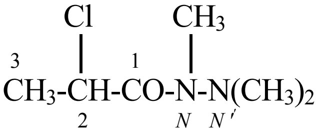
$$\underset{3}{CH_3}\text{-}\underset{2}{CH_2}\text{-}\underset{1}{CO}\text{-}\underset{N}{\overset{1'}{NH}}\text{-}\underset{N'}{\overset{2'}{NH_2}}$$

Examples:



$$CH_3\text{-}CO\text{-}\underset{N}{\overset{\overset{CH_3}{|}}{N}}\text{-}NH_2$$

N-methylacetohydrazide (PIN)
1-acetyl-1-methylhydrazine

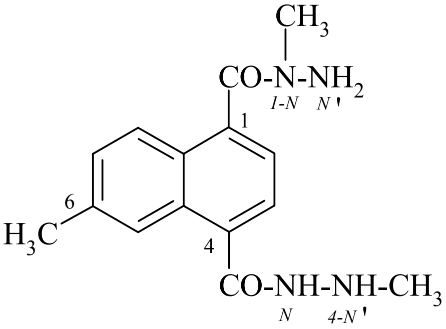


$$\overset{3}{CH_3}\text{-}\underset{2}{\overset{\overset{Cl}{|}}{CH}}\text{-}\overset{1}{CO}\text{-}\underset{N}{\overset{\overset{CH_3}{|}}{N}}\text{-}\underset{N'}{N}(CH_3)_2$$

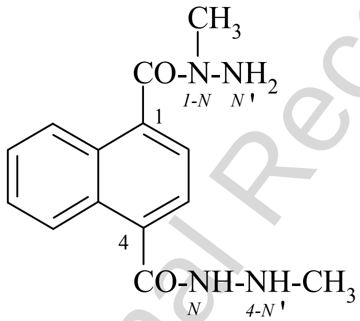
2-chloro-*N,N′,N′*-trimethylpropanehydrazide (PIN)
1-(2-chloropropanoyl)-1,2,2-trimethylhydrazine

When two hydrazide groups are present, each is identified by the locants *N* and *N′*. To distinguish the four nitrogen atoms, the symbols are preceded by the locant of the skeletal atom of the parent structure to which the hydrazide group is attached, followed by a hyphen.

Examples:



1-*N*,4-*N*′,6-trimethylnaphthalene-1,4-dicarbohydrazide (PIN)
(the numbering for this compound is based on the lowest set of locants for the three substituent groups)



1-*N*,4-*N*′-dimethylnaphthalene-1,4-dicarbohydrazide (PIN)
(numbering is based on the lower set of locants: since *N* is lower than *N*′, the set 1-*N*, 4-*N*′ is lower than 1-*N*′,4-*N*)

P-66.3.3.2 Acyl, diacyl, and triacyl derivatives of hydrazides are named:

(1) by substituting the senior hydrazide by the appropriate acyl groups (the senior hydrazide is the one derived from the senior acid), or

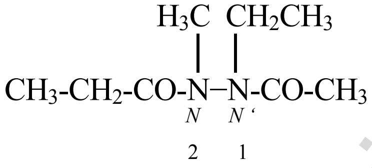
(2) by substituting the parent hydride, hydrazine (hydrazine, a retained name, is preferred to diazane for preferred IUPAC names).

Method (1) leads to preferred IUPAC names.

Examples:

$$C_6H_5\text{-}\overset{1}{C}O\text{-}\overset{2}{\underset{N}{N}}H\text{-}\underset{N'}{N}H\text{-}CO\text{-}C_6H_5$$

N′-benzoylbenzohydrazide (PIN)
1,2-dibenzoylhydrazine



$$CH_3\text{-}CH_2\text{-}CO\text{-}\underset{\substack{N\\2}}{\overset{\substack{H_3C\\|}}{N}}-\underset{\substack{N'\\1}}{\overset{\substack{CH_2CH_3\\|}}{N}}\text{-}CO\text{-}CH_3$$

N′-acetyl-*N*′-ethyl-*N*-methylpropanehydrazide (PIN)
1-acetyl-1-ethyl-2-methyl-2-propanoylhydrazine

P-66.3.4 Functional replacement by chalcogen atoms

Thiohydrazides may be named in three ways; seleno and tellurohydrazides may be named in a similar manner.

(1) substitutively using suffixes formed by functional replacement, i.e., ‘thiohydrazide’, ‘-carbothiohydrazide’, ‘sulfonothiohydrazide’, etc.;

(2) by substituting hydrazine with appropriately modified acyl groups;

(3) retained names modified by the prefixes ‘thio’, ‘seleno’, telluro’.

Examples:

CH_3-CH_2-CS-NH-NH_2

(1) propanethiohydrazide (PIN)
(2) (propanethioyl)hydrazine
(thiopropionyl)hydrazine

C_6H_5-CS-NH-NH_2

(1) benzenecarbothiohydrazide (PIN)
(2) benzenecarbothioylhydrazine
(thiobenzoyl)hydrazine

P-66.3.5 Hydrazides from carbonic, cyanic, oxalic, and the polycarbonic acids

P-66.3.5.1 Preferred IUPAC names of hydrazides derived from carbonic and cyanic acids are as follows:

H_2N-NH-CN	cyanohydrazide (PIN) hydrazinecarbonitrile carbononitridic hydrazide
H_2N-NH-CO-OH	hydrazinecarboxylic acid (PIN) carbonohydrazidic acid
H_2N-NH-CO-NH-NH_2	hydrazinecarbohydrazide (PIN) carbonic dihydrazide

P-66.3.5.2 Names of hydrazides derived from oxalic and the polycarbonic acids are formed by adding the functional class name ‘hydrazide’ to that of the corresponding acid, preceded by the numerical locant ‘di’ to express multiplicity of hydrazide groups, when necessary. Chalcogen and other replacement analogues are described by the appropriate functional replacement prefix.

Examples:

$\overset{N'}{H_2N}\text{-}\overset{N}{NH}\text{-CO-CO-}\overset{N''}{NH}\text{-}\overset{N'''}{NH_2}$ oxalic dihydrazide (PIN)

$\overset{N'}{H_2N}\text{-}\overset{N}{NH}\text{-CO-O-CO-}\overset{N''}{NH}\text{-}\overset{N''''}{NH_2}$ dicarbonic dihydrazide (PIN)

$\overset{N'}{H_2N}\text{-}\overset{N}{NH}\text{-}\overset{2}{CO}\text{-}\overset{1}{CS}\text{-}\overset{N''}{NH}\text{-}\overset{N'''}{NH_2}$ 1-thiooxalic dihydrazide (PIN)

$\overset{N''}{H_2N}\text{-}\overset{N'}{NH}\text{-}\overset{1}{CO}\text{-}\overset{2}{CO}\text{-}\overset{N}{NH_2}$ 2-amidooxalic hydrazide
2-hydrazidooxamide (PIN)

P-66.3.5.3 Corresponding substituent groups

When a group having priority for citation as a principal characteristic group is present, the hydrazide group is named:

(1) as an acylhydrazinyl compound; the hydrazinyl group is numbered by using numerical locants 1 and 2;

(2) by expressing the corresponding hydrazide as a prefix by replacing the final letter 'e' in the name of the hydrazide by the letter 'o', for example, 'formohydrazido'. The locant *N* designates the nitrogen atom adjacent to the –CO– group

Method (1) generates preferred IUPAC names.

Examples:

$OHC\text{-NH-NH-}CH_2\text{-}CH_2\text{-COOH}$

3-(2-formylhydrazin-1-yl)propanoic acid (PIN)
3-formohydrazidopropanoic acid

$H_2N\text{-NH-CO-NH-NH-}CH_2\text{-COOH}$

2-(2-hydrazinecarbonylhydrazin-1-yl)acetic acid (PIN)
2-hydrazinecarbohydrazidoacetic acid

$H_2N\text{-NH-CO-O-CO-NH-NH-}\overset{4}{CH_2}\text{-}CH_2\text{-}CH_2\text{-}\overset{1}{COOH}$

4-{2-[(hydrazinecarbonyloxy)carbonyl]hydrazin-1-yl}butanoic acid (PIN)

P-66.3.6 Semioxamazones

Semioxamazones have the general structure R=N-NH-COCO-NH$_2$ and are named as substituted hydrazido oxamides.

Example:

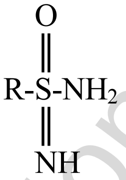
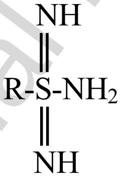
$$C_6H_5\text{-}CH{=}\overset{N}{N}\text{-}NH\text{-}COCO\text{-}NH_2$$

N′-benzylidene-2-hydrazidooxamide (PIN)
2-(2-benzylidenehydrazin-1-yl)-2-oxoacetamide

P-66.4 Amidines, amidrazones, and hydrazidines, and amide oximes (amidoximes)

P-66.4.1 Amidines

Compounds having the general structure R-C(=NH)-NH$_2$ are generically known as ‘(carbox)amidines’; those having the general structure R-S(=NH)-NH$_2$ are ‘sulfinamidines’.

Compounds with the structure $\mathrm{R{-}\overset{O}{\overset{\|}{\underset{\underset{NH}{\|}}{S}}}{-}NH_2}$ or $\mathrm{R{-}\overset{NH}{\overset{\|}{\underset{\underset{NH}{\|}}{S}}}{-}NH_2}$ are generically called ‘sulfonimidamides’ and not amidines.

P-66.4.1.1 Suffixes for amidines

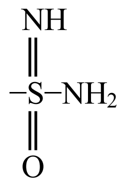
Amidines are named as amides in which the =O atom has been replaced by the =NH group by functional replacement nomenclature. As a principal characteristic group they are designated by the following suffixes, formed by functional replacement by using the prefix or the infix ‘imido’.

$-(C)(=NH)-NH_2$ imidamide

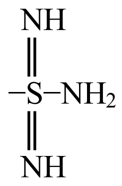
$-C(=NH)-NH_2$ carboximidamide

The suffixes ‘amidine’ and ‘carboxamidine’ are no longer recommended.

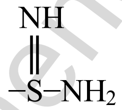
Suffixes for sulfonic acid, sulfinic acid and selenium and tellurium analogues are named similarly.


$-\overset{\overset{NH}{\|}}{\underset{\underset{O}{\|}}{S}}-NH_2$

sulfonimidamide

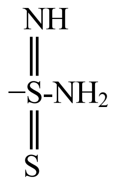

$-\overset{\overset{NH}{\|}}{\underset{\underset{NH}{\|}}{S}}-NH_2$

sulfonodiimidamide


$-\overset{\overset{NH}{\|}}{S}-NH_2$

sulfinimidamide

The suffixes for groups containing S, Se and Te in place of O in a sulfonimidamide suffix are named by functional replacement, for example:


$-\overset{\overset{NH}{\|}}{\underset{\underset{S}{\|}}{S}}-NH_2$

-sulfonimidothioamide

The suffix ‘imidamide’ is used to denote an acyclic amidine with one terminal amidine characteristic group; two terminal amidine characteristic groups on an acyclic parent hydride are denoted by the suffix ‘bis(imidamide)’ (the multiplicative prefix ‘bis’ is used to avoid the possibility of ambiguity). All the other suffixes are used to name acyclic polyamidines and all amidines having the suffix attached to a cyclic parent hydride or a heteroatom of a heteroacyclic parent hydride.

Retained names of amidines are formed by replacing the ‘amide’ ending in names of amides by ‘imidamide’, but are not preferred IUPAC names; preferred IUPAC names are derived systematically. Other than that, the nomenclatural properties of amides are transferred to amidines; thus, names of amidines correspond to preferred names of amides; and amides that are not substitutable generate nonsubstitutable amidines.

Examples:

$\overset{6}{C}H_3-[CH_2]_4-\overset{1}{C}(=NH)-NH_2$

hexanimidamide (PIN)
(no longer hexanamidine)

$C_6H_{11}-C(=NH)-NH_2$

cyclohexanecarboximidamide (PIN)
(no longer cyclohexanecarboxamidine)

$\mathrm{CH_3{-}C({=}NH){-}NH_2}$

ethanimidamide (PIN)
acetimidamide
(no longer acetamidine)

$\mathrm{CH_3{-}S({=}NH){-}NH_2}$

methanesulfinimidamide (PIN)
(no longer methanesulfinamidine)

$\mathrm{HC({=}NH){-}NH_2}$

methanimidamide (PIN)
formimidamide
(no longer formamidine)

$\mathrm{H_2N{-}C({=}NH){-}CH_2{-}CH_2{-}CH_2{-}C({=}NH){-}NH_2}$

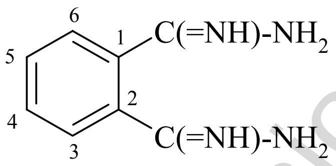
pentanebis(imidamide) (PIN)
(no longer pentanediamidine)

$\mathrm{H_2N{-}C({=}NH){-}SiH_2{-}SiH_2{-}C({=}NH){-}NH_2}$

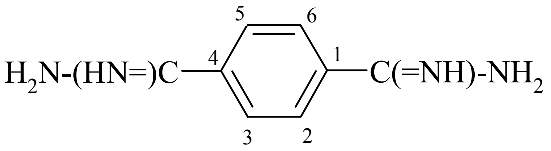
disilanedicarboximidamide (PIN)
(no longer disilanedicarboxamidine)

$\mathrm{H_2N{-}C({=}NH){-}CH_2{-}CH_2{-}C({=}NH){-}NH_2}$

butanebis(imidamide) (PIN)
succinimidamide



benzene-1,2-dicarboximidamide (PIN)
phthalimidamide
(no longer benzene-1,2-dicarboxamidine)

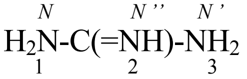


benzene-1,4-dicarboximidamide (PIN)
terephthalimidamide
(no longer benzene-1,4-dicarboxamidine)

P-66.4.1.2 Amidines of carbonic, oxalic, and the polycarbonic acids

P-66.4.1.2.1 Guanidine, $\mathrm{H_2N{-}C({=}NH){-}NH_2}$, and its derivatives

P-66.4.1.2.1.1 The preferred IUPAC name for the ‘amidine’ related to carbonic acid, $\mathrm{H_2N{-}C({=}NH){-}NH_2}$, is the retained name ‘guanidine’; the locants 1, 2, and 3 are used, not N, N' and N''.



$$\overset{N}{\underset{1}{\mathrm{H_2N}}}\mathrm{{-}C({=}}\overset{N''}{\underset{2}{\mathrm{NH}}}\mathrm{){-}}\overset{N'}{\underset{3}{\mathrm{NH_2}}}$$

The systematic functional replacement name ‘carbonimidic diamide’ may be used in general nomenclature and uses the locants N, N' and N''.

P-66.4.1.2.1.2 Hydrocarbyl derivatives are named as substituted guanidines. The locants *N* and *N′* are used when the position of the double bond is unknown; when there is a choice, a minimum number of primes is used.

Examples:

$(CH_3)_2\underset{1}{\overset{N}{N}}\text{-C(=}\underset{2}{\overset{N''}{N}}\text{-}C_6H_5\text{)-}\underset{3}{\overset{N'}{N}}(CH_3)_2$

1,1,3,3-tetramethyl-2-phenylguanidine (PIN)
N,*N*,*N′*,*N′*-tetramethyl-*N″*-phenylguanidine
N,*N*,*N′*,*N′*-tetramethyl-*N″*-phenylcarbonimidic diamide

$CH_3\text{-}\underset{3}{\overset{N''}{N}}H\text{-C(=}\underset{2}{\overset{N''}{N}}H\text{)-}\underset{1}{\overset{N}{N}}(CH_3)_2$

1,1,3-trimethylguanidine (PIN)
N,*N*,*N′*-trimethylguanidine
N,*N*,*N′*-trimethylcarbonimidic diamide

P-66.4.1.2.1.3 In presence of a characteristic group having seniority over guanidine (see P-42.2), the following prefixes are used. The prefix guanidino is no longer recommended.

$\overset{N'}{H_2N}\text{-C(=}\overset{N''}{NH}\text{)-}\overset{N}{NH}\text{–}$

carbamimidamido (PIN)
carbamimidoylamino
(not guanidino)

$(H_2N)_2C\text{=N–}$

(diaminomethylidene)amino (PIN)

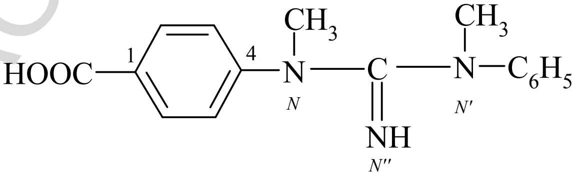
Examples:

$(H_2N)_2C\text{=N-}CH_2\text{-COOH}$

N-(diaminomethylidene)glycine (PIN)
[(diaminomethylidene)amino]acetic acid

$(H_2N)_2C\text{=N-}\overset{4}{C}H_2\text{-}CH_2\text{-}CH_2\text{-}\overset{1}{C}OOH$

4-[(diaminomethylidene)amino]butanoic acid (PIN)



4-(*N*,*N′*-dimethyl-*N′*-phenylcarbamimidamido)benzoic acid (PIN)
4-[methyl(*N*-methyl-*N*-phenylcarbamimidoyl)amino]benzoic acid

$H_2N-C(=NH)-NH-CHO$

N-carbamimidoylformamide (PIN)
(not *N*-formylguanidine)

$H_2N-C(=NH)-NH-CO-NH_2$

carbamimidoylurea (PIN)
(not *N*-carbamoylguanidine)

N 1 2
$H_2N-C(=NH)-NH-CO-CH_3$

N-(*C*-aminocarbonimidoyl)acetamide (PIN)
(not *N*-acetylguanidine)

P-66.4.1.2.2 Condensed guanidines.

The names biguanide, triguanide, etc., are no longer recommended. Condensed guanidines, $H_2N-[C(=NH)-NH]_n-H$, where n = 2, 3, or 4 are named systematically as the diamides of triimidodicarbonic acid, pentaimidotricarbonic acid, and heptatriimidotetracarbonic acid. Locants, as shown, are used to indicate the positions of substituents.

N 1 *N''* 2 3 *N'''* *N'*
$H_2N-C(=NH)-NH-C(=NH)-NH_2$

1,2,3-triimidodicarbonic diamide (PIN)

N 1 *N''* 2 3 *N'''* 4 5 *N''''* *N'*
$H_2N-C(=NH)-NH-C(=NH)-NH-C(=NH)-NH_2$

1,2,3,4,5-pentadiimidotricarbonic diamide (PIN)

Example:

N' 3 *N'''* 2 1 *N''* *N*
$H_2N-C(=NH)-NH-C(=N-CH_2-CH_3)-N(C_6H_5)_2$
3 2 1

N,N-diphenyl-*N″*-ethylimidodicarbonodiimidic diamide (PIN)

For polyguanides, where n = 5 and higher skeletal replacement (‘a’) nomenclature leads to preferred IUPAC names

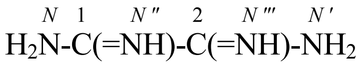
Example:

1 2 3 4 5 6 7 8 9
$H_2N-C(=NH)-NH-C(=NH)-NH-C(=NH)-NH-C(=NH)-NH-C(=NH)-NH_2$

3,5,7-triimino-2,4,6,8-tetraazanonanebis(imidamide) (PIN)

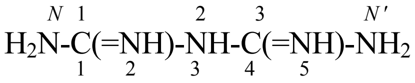
P-66.4.1.2.3 Preferred names for amidines related to oxalic acid and the polycarbonic acids are diamides of imido acids in which the imido groups are indicated by the functional replacement prefix imido (see also P-66-1.5.6.1.2).

Examples:



$$\overset{N}{\mathrm{H_2N}}\text{-}\overset{1}{\mathrm{C}}(=\overset{N''}{\mathrm{N}}\mathrm{H})\text{-}\overset{2}{\mathrm{C}}(=\overset{N'''}{\mathrm{N}}\mathrm{H})\text{-}\overset{N'}{\mathrm{N}}\mathrm{H_2}$$

1,2-diimidooxalic diamide (PIN)
(not oxalimidamide; see P-65.2.5)



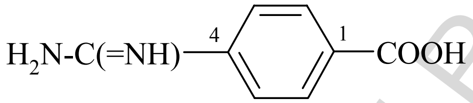
$$\overset{N}{\mathrm{H_2N}}\text{-}\overset{1}{\underset{1}{\mathrm{C}}}(=\underset{2}{\mathrm{N}}\mathrm{H})\text{-}\overset{2}{\underset{3}{\mathrm{N}}}\mathrm{H}\text{-}\overset{3}{\underset{4}{\mathrm{C}}}(=\underset{5}{\mathrm{N}}\mathrm{H})\text{-}\overset{N'}{\mathrm{N}}\mathrm{H_2}$$

1,2,3-triimidodicarbonic diamide (PIN)

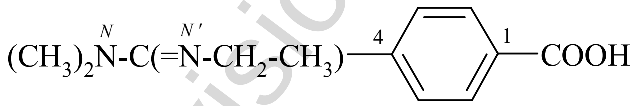
P-66.4.1.3 Prefixes for the amidine characteristic group

P-66.4.1.3.1 The systematic name for the group $-C(=NH)-NH_2$ is ‘carbamimidoyl’; it is the name of the acyl group derived from the name carbamimidic acid, $HO-C(=NH)-NH_2$. The prefix ‘amidino’ is no longer recommended. In the acyl group, the $-NH_2$ group is denoted by the locant *N* and the =NH group by *N*′.

Examples:



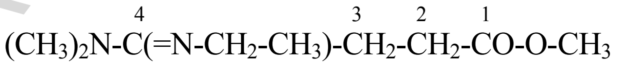
4-carbamimidoylbenzoic acid (PIN)
(no longer 4-amidinobenzoic acid)



4-(*N*′-ethyl-*N*,*N*-dimethylcarbamimidoyl)benzoic acid (PIN)
[no longer 4-(*N*′-ethyl-*N*,*N*-dimethylamidino)benzoic acid]

P-66.4.1.3.2 When the carbon atom of the $H_2N-C(=NH)-$ group terminates a chain, the groups $-NH_2$ and =NH are designated by the prefixes ‘amino’ and ‘imino’, respectively.

Example:

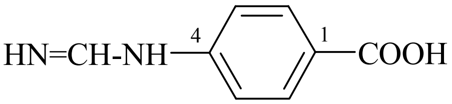


$$\mathrm{(CH_3)_2N}\text{-}\overset{4}{\mathrm{C}}(=\mathrm{N}\text{-}\mathrm{CH_2}\text{-}\mathrm{CH_3})\text{-}\overset{3}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{2}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{1}{\mathrm{C}}\mathrm{O}\text{-}\mathrm{O}\text{-}\mathrm{CH_3}$$

methyl 4-(dimethylamino)-4-(ethylimino)butanoate (PIN)
(not methyl 3-[*C*-(dimethylamino)-*N*-ethylcarbonimidoyl]propanoate)
(not methyl 3-(N^2-ethyl-N^1,N^1-dimethylamidino)propionate)

P-66.4.1.3.3 The substituent group HN=CH-NH− is named 'methaneimidamido'; it can also be named as a compound substituent 'formimidoylamino' or '(iminomethyl)amino'. The name 'methanimidamido' leads to preferred IUPAC names. The substituent group H_2N-CH=N− can only be named as a compound substituent group, '(aminomethylidene)amino'.

Example:



4-methanimidamidobenzoic acid (PIN)
4-[(iminomethyl)amino]benzoic acid
4-(formimidoylamino)benzoic acid

P-66.4.1.3.4 Substituent prefixes corresponding to the suffixes sulfonimidamide, sulfinimidamide, and related selenium and tellurium suffixes are formed systematically by concatenation using the prefix 'amino-' and the the name of the appropriate acyl group:

$-S(O)(=NH)-NH_2$	$-S(=NH)_2-NH_2$	$-S(=NH)-NH_2$
S-aminosulfonimidoyl	*S*-aminosulfonodiimidoyl	*S*-aminosulfinimidoyl

The italic letter locant '*S* ' is used to avoid potential ambiguity regarding substitution on the imido nitrogen atom

Example:

$$H_2N\text{-}S(=NH)\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$$

3-(*S*-aminosulfinimidoyl)propanoic acid (PIN)

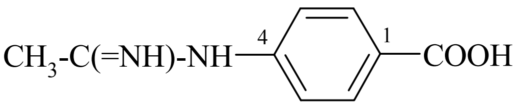
P-66.4.1.3.5 In the presence of a characteristic group cited as a suffix, the group R-C(=NH)NH−, or R-S(O)(=NH)NH− (and selenium and tellurium analogues) is named in two ways.

(1) substitutively, by using a prefix named formed by changing the final letter 'e' in the complete name of the amide to 'o', thus changing the suffixes 'imidamide' and 'carboximidamide' into 'imidamido' and 'carboximidamido', respectively, or 'sulfonimidamide' to 'sulfonimidamido', etc..

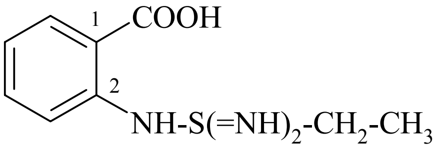
(2) substitutively, by using 'acylamino' prefixes formed by substituting the name of the acyl group to the substituent 'amino'

Method (1) generates preferred IUPAC names.

Examples:



4-ethanimidamidobenzoic acid (PIN)
4-(acetimidoylamino)benzoic acid
4-acetimidamidobenzoic acid

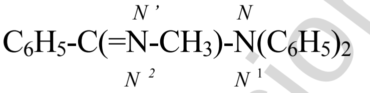


2-ethanesulfonodiimidamidobenzoic acid (PIN)
2-(ethanesulfonodiimidoylamino)benzoic acid

P-66.4.1.4 Substituted amidines

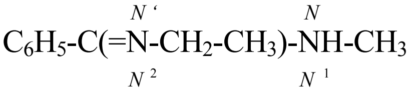
P-66.4.1.4.1 *N*-Substituted amidines are named by prefixing the name of the appropriate substituent to the name of the unsubstituted amidine, with *N* or N^1 and N'or N^2 locants; *N* or N^1 refers to the amino group and N' or N^2 refers to the imino group. Because of tautomerism, the plain locant *N* is used when only one substituent is present. The locants *N* and N' are used in preferred IUPAC names.

Examples:



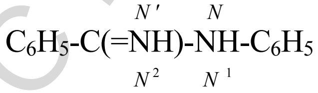
$C_6H_5\text{-}C(=\underset{N^{2}}{\overset{N'}{N}}\text{-}CH_3)\text{-}\underset{N^{1}}{\overset{N}{N}}(C_6H_5)_2$

N'-methyl-*N*,*N*-diphenylbenzenecarboximidamide
(PIN)
N^2-methyl-N^1,N^1-diphenylbenzamidine
(no longer *N*′-methyl-*N*,*N*-diphenyl-benzamidine)



$C_6H_5\text{-}C(=\underset{N^{2}}{\overset{N'}{N}}\text{-}CH_2\text{-}CH_3)\text{-}\underset{N^{1}}{\overset{N}{N}}H\text{-}CH_3$

N'-ethyl-*N*-methylbenzenecarboximidamide
(PIN)
N^2-ethyl-N^1-methylbenzamidine
(no longer *N*′-ethyl- *N*–methyl-benzamidine)

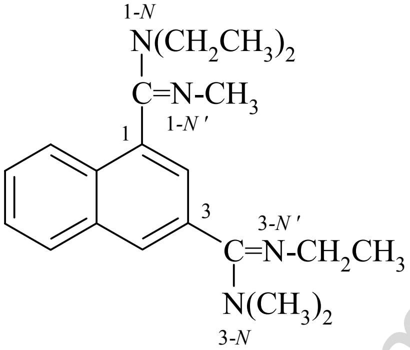


$C_6H_5\text{-}C(=\underset{N^{2}}{\overset{N'}{N}}H)\text{-}\underset{N^{1}}{\overset{N}{N}}H\text{-}C_6H_5$

N-phenylbenzenecarboximidamide (PIN)
(no longer *N*-phenylbenzamidine)
(not benzimidanilide)

P-66.4.1.4.2 When it is necessary to identify the position of substituents in a polyamidine system, the *N* locants described above are preceded by the locant of the position occupied by each amidine characteristic group.

Example:

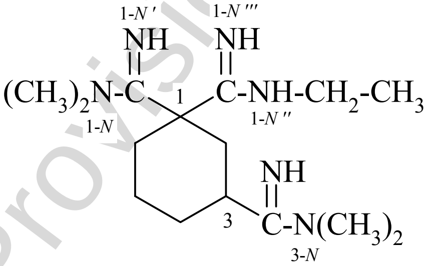


1-*N*,1-*N*,3-*N* ′-triethyl-1-*N* ′,3-*N*,3-*N*-trimethylnapthalene-1,3-dicarboximidamide (PIN)

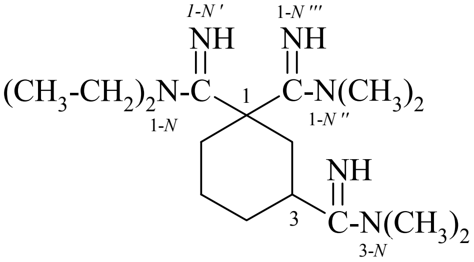
P-66.4.1.4.3 Geminal carboxamidine groups

When geminal carboximidamide groups are present, the locants *N*, *N*’, etc. are used in association with the numerical locant indicating the position of the groups on a chain or cycle. Lowest locants are assigned to the most substituted group; when there is a choice, lowest locants are assigned to the first cited *N*-substituent. This system of *N*-locants in association with numerical locants is recommended for naming substituted amines (see P-62.2.1.2.2) and substituted amides (see P-66.1.1.3.1.2).

Examples:



1-*N*,1-*N*,3-*N*,3-*N*-tetramethyl-1-*N*″-ethylcyclohexane-1,1,3-tricarboximidamide (PIN)



1-*N*,1-*N*-diethyl-1-*N*″,1-*N*″,3-*N*-,3-*N*-tetramethylcyclohexane-1,1,3-tricarboximidamide (PIN)

P-66.4.1.5 Formamidine disulfides.

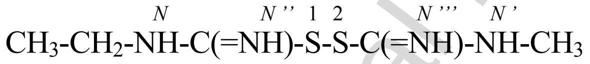
The compound $\overset{N}{\mathrm{H_2N}}\text{-}\overset{1}{\mathrm{C}}(=\overset{N''}{\mathrm{NH}})\text{-}\overset{2}{\mathrm{S}}\text{-}\overset{3}{\mathrm{S}}\text{-}\overset{4}{\mathrm{C}}(=\overset{N'''}{\mathrm{NH}})\text{-}\overset{N'}{\mathrm{NH_2}}$ and its derivatives have been named previously on the basis of the parent structure ‘formamidine disulfides’. They are now named on the basis of:

(1) the parent hydride ‘disulfane’; or

(2) the parent compound ‘dicarbonic acid’.

Method (1) generates preferred IUPAC names.

Example:



$$\mathrm{CH_3\text{-}CH_2\text{-}\overset{\mathit{N}}{NH}\text{-}C(=\overset{\mathit{N''}}{NH})\text{-}\overset{1}{S}\text{-}\overset{2}{S}\text{-}C(=\overset{\mathit{N'''}}{NH})\text{-}\overset{\mathit{N'}}{NH}\text{-}CH_3}$$

N-ethyl-*N*′-methyldisulfanedicarboximidamide (PIN)
N-ethyl-*N*′ -methyl(dithioperoxy)dicarbonimidic diamide
(traditionally N^1-ethyl-N^2-methyl-α,α′-dithiobisformamidine)

P-66.4.1.6 Diamidides

Diamidides are analogues of acyclic carboxylic anhydrides in which the =O atoms have been replaced by =NR groups and the anhydride oxygen atom by −NR− giving the general formula RC(=NR′)-NR″-(=NR‴)CR‴′. They are named systematically as *N*-imidoylimidamides.

Example:

$$\mathrm{CH_3\text{-}C(=NH)\text{-}\overset{\mathit{N}}{NH}\text{-}C(=\overset{\mathit{N'}}{NH})\text{-}CH_3}$$

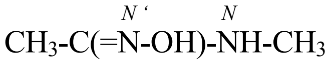
N-ethanimidoylethanimidamide (PIN)
N-acetimidoylacetimidamide (PIN)

P-66.4.1.7 Amide oximes

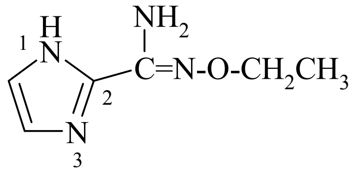
Amide oximes are formally oximes of carboxamides, i.e., compounds having the general structure R-C(=N-OH)-NH_2 and derivatives formed by substitution. Preferred IUPAC names are

N′-hydroxy- or *N′*-alkyloxy- derivatives of carboximidamides (amidines). Suffixes such as ‘amide oxime’ or ‘carboxamide oxime’ are no longer recommended.

Example:


$CH_3\text{-}C(=\overset{N'}{N}\text{-}OH)\text{-}\overset{N}{N}H\text{-}CH_3$

N′-hydroxy-*N*-methylacetimidamide (PIN)
(no longer *N*-methylacetamide oxime)

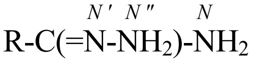


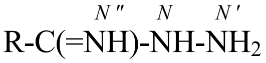
N′ -ethoxyimidazole-2-carboximidamide (PIN)
(no longer imidazole-2-carboxamide *O*-ethyloxime)

P-66.4.2 Amidrazones

P-66.4.2.1 Amidrazone suffixes

Compounds having the general structure R-C(-NH_2)=N-NH_2 or the tautomeric R-C(=NH)-NH-NH_2 have the class name ‘amidrazones’ and are named substitutively using the suffixes ‘hydrazonamide’ or ‘imidohydrazide’, respectively, or ‘carbohydrazonamide’ or ‘carboximidohydrazide’, respectively. *N*-Substitution, when the position of the double bond is known, is designated according to the following numbering:

for carbohydrazonamides  $R\text{-}C(=\overset{N'}{N}\text{-}\overset{N''}{N}H_2)\text{-}\overset{N}{N}H_2$

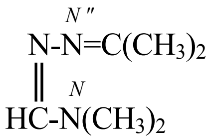
for carboximidohydrazides  $R\text{-}C(=\overset{N''}{N}H)\text{-}\overset{N}{N}H\text{-}\overset{N'}{N}H_2$

Locants *N*, *N′* and *N″* as shown are recommended. The previous methods of naming amidrazones as ‘amide hydrazones’ or ‘hydrazide imides’, or amidrazones when the structure is not known are no longer recommended.

When the position of the double bond is unknown, the senior characteristic group, carbohydrazonamide, is chosen to denote the tautomers, with appropriate locants *N* and *N″* to denote substitution. When the position of the substituted suffixes must be indicated in a name, locants designating the positions of the suffixes are added in front of the appropriate *N* locants, separated by a hyphen.

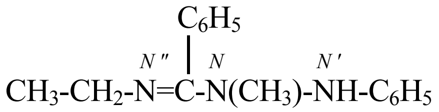
Retained names of amidrazones are formed by replacing the ‘amide’ ending in names of amides by ‘ohydrazonamide’ and are only used in general nomenclature. Preferred IUPAC names of amidrazones are formed systematically. Otherwise, the nomenclatural properties of amides are transferred to amidrazones; thus, preferred names of amidrazones correspond to preferred names of amides and amides that are not substitutable generate nonsubstitutable amidrazones.

Examples:



$$\begin{array}{l} N\text{-}\overset{N''}{N}{=}C(CH_3)_2 \\ \| \\ HC\text{-}\overset{N}{N}(CH_3)_2 \end{array}$$

N,*N*-dimethyl-*N*″-propan-2-ylidenemethanehydrazonic amide (PIN)
N,*N*-dimethyl-*N*″-isopropylideneformohydrazonic amide
(not *N*,*N*-dimethylformamide isopropylidenehydrazone)

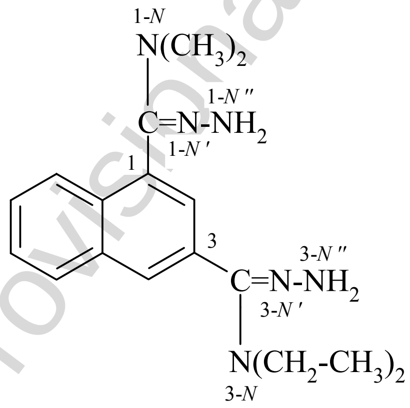


$$CH_3\text{-}CH_2\text{-}\overset{N''}{N}{=}\overset{C_6H_5}{C}\text{-}\overset{N}{N}(CH_3)\text{-}\overset{N'}{N}H\text{-}C_6H_5$$

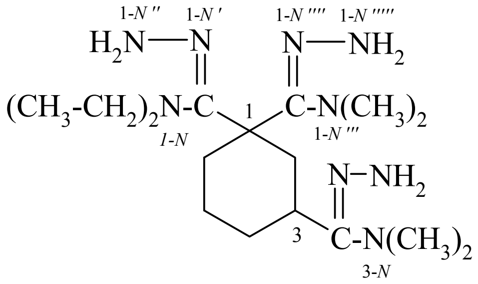
N″-ethyl-*N* -methyl-*N*′-phenylbenzenecarboximidohydrazide (PIN)
(not N^1-methyl-N^2-phenylbenzohydrazide ethylimide)

$$H_2N\text{-}C({=}NH)\text{-}\overset{1}{N}H\text{-}\overset{2}{N}H\text{-}\overset{3}{N}{=}\overset{4}{N}\text{-}C({=}NH)\text{-}\overset{1}{N}H\text{-}\overset{2}{N}H\text{-}NO$$

4-[*C*-(2-nitrosohydrazinecarbonimidoyl)tetraaz-3-ene-1-carboximidamide (PIN)
[an imidamide is senior to an imidohydrazide (an amidrazone)]



3-*N*,3-*N*-diethyl-1-*N*,1-*N*-dimethylnaphthalene-1,3-dicarbohydrazonamide (PIN)



1-*N*,1-*N*-diethyl-1-*N*‴,1-*N*‴,3-*N*,3-*N*-tetramethylcyclohexane-1,1,3-tricarbohydrazonamide (PIN)
(for locants *N,N*′, etc. in association with numerical locants, see P-62.2.1.2.2 and P-66.4.1.3.3)

Amidrazones derived from sulfonic acid, and similar acids, are named in accordance with the same principles.

Example:

$C_6H_5\text{-}S(=NNH_2)\text{-}NH_2$

benzenesulfinohydrazonamide (PIN)

P-66.4.2.2 Amidrazones of carbonic, oxalic, and the polycarbonic acids

The general methodology discussed in P-65.2 is applied to generate the names for amidrazones derived from carbonic, oxalic, and the polycarbonic acids.

Examples:

2 1 *N*'' *N* *N*'
$H_2N\text{-}NH\text{-}C(=NH)\text{-}NH\text{-}NH_2$

hydrazinecarboximidohydrazide (PIN)
carbonimidic dihydrazide

$H_2N\text{-}C(=N\text{-}NH_2)\text{-}NH_2$

carbonohydrazonic diamide (PIN)

1 2 3
$H_2N\text{-}NH\text{-}C(=NH)\text{-}O\text{-}C(=NH)\text{-}NH\text{-}NH_2$

1,3-diimidodicarbonic dihydrazide (PIN)

1 2 3
$H_2N\text{-}C(=N\text{-}NH_2)\text{-}O\text{-}C(=N\text{-}NH_2)\text{-}NH_2$

1,3-dihydrazonodicarbonic diamide (PIN)

$\mathrm{H_2N\text{-}NH\text{-}C(=NH)\text{-}O\text{-}C(=NNH_2)\text{-}NH_2}$

(hydrazinecarboximidoyloxy)formohydrazonic amide (PIN)
(carbamohydrazonoyloxy)methanimidohydrazide

$\mathrm{H_2N\text{-}NH\text{-}\overset{1}{C}(=NH)\text{-}\overset{2}{C}(=NH)\text{-}NH\text{-}NH_2}$

1,2-diimidooxalic dihydrazide (PIN)

$\mathrm{H_2N\text{-}\overset{1}{C}(=N\text{-}NH_2)\text{-}\overset{2}{C}(=N\text{-}NH_2)\text{-}NH_2}$

1,2-dihydrazonooxalic diamide (PIN)

$\mathrm{H_2N\text{-}NH\text{-}C(=NH)\text{-}C(=N\text{-}NH_2)\text{-}NH_2}$

hydrazinecarboximidoylmethanehydrazonic amide (PIN)
carbamohydrazonoylmethanimidohydrazide

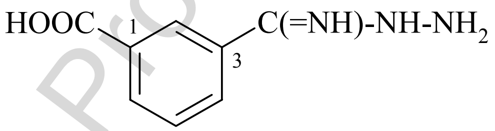
P-66.4.2.3 Amidrazone prefixes

P-66.4.2.3.1 The prefix name for the group $\mathrm{-C(=NH)\text{-}NHNH_2}$ is ‘hydrazinecarboximidoyl’. When this group is located at the end of a carbon chain, the prefixes ‘imino’ and ‘hydrazinyl’ are preferred in order to avoid fragmenting the chain.

Examples:

$\mathrm{H_2N\text{-}NH\text{-}(HN=)\overset{3}{C}\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH}$

3-imino-3-hydrazinylpropanoic acid (PIN)
hydrazinecarboximidoylacetic acid



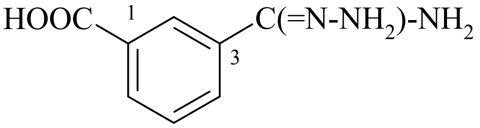
3-hydrazinecarboximidoylbenzoic acid (PIN)

P-66.4.2.3.2 The prefix name for the group $\mathrm{-C(=N\text{-}NH_2)\text{-}NH_2}$ is ‘carbamohydrazonoyl’. When this group is located at the end of a carbon chain, the prefixes ‘amino’ and ‘hydrazinylidene’ are preferred in order to avoid fragmenting the chain.

Examples:

$H_2N\text{-}\overset{3}{C}(=N\text{-}NH_2)\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

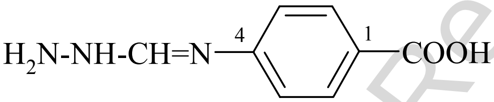
3-amino-3-hydrazinylidenepropanoic acid (PIN)
carbamohydrazonoylacetic acid



3-carbamohydrazonoylbenzoic acid (PIN)

P-66.4.2.3.3 The prefix names for the groups $-NH\text{-}CH{=}N\text{-}NH_2$ and $-N{=}CH\text{-}NH\text{-}NH_2$ are compound prefixes and are ‘(hydrazinylidenemethyl)amino’ and ‘(hydrazinylmethylidene)amino’, respectively.

Example:



4-[(hydrazinylmethylidene)amino]benzoic acid (PIN)

P-66.4.2.3.4 Prefix names for the $H_2N\text{-}CH{=}N\text{-}NH-$, $HN{=}CH\text{-}NH\text{-}NH-$, and $HC(=NNH_2)\text{-}NH-$ groups are compound prefixes, which are: 2-(aminomethylidene)hydrazinyl (PIN)’, ‘2-methanimidoylhydrazinyl (PIN)’ or ‘methanimidohydrazido’ or ‘2-(iminomethyl)hydrazinyl’, and ‘methanehydrazonoylamino (PIN)’ or methanehydrazonamido, respectively.

Example:

$H_2N\text{-}CH{=}NH\text{-}NH\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

3-[2-(aminomethylidene)hydrazin-1-yl]propanoic acid (PIN)

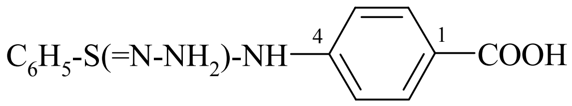
P-66.4.2.3.5 When a group having preference for citation as a principal characteristic group is present, the group $R\text{-}C(=N\text{-}NH_2)\text{-}NH-$, or $R\text{-}S(O)(=N\text{-}NH_2)\text{-}NH-$ (and selenium and tellurium analogues) of an *N*-substituted amide is named in two ways.

(1) substitutively, by using a prefix named formed by changing the final letter ‘e’ in the complete name of the amide to ‘o’;

(2) substitutively, by using ‘acylamino’ prefixes formed by substituting the name of the acyl group to the substituent ‘amino’

Method (1) generates preferred IUPAC names.

Example:



4-benzenesulfinohydrazonamidobenzoic acid (PIN))
4-(benzenesulfinohydrazonoylamino)benzoic acid

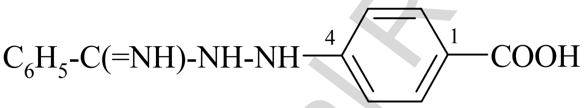
P-66.4.2.3.6 When a group having priority for citation as a principal characteristic group is present, a hydrazide group of the type R-C(=NH)-NHNH–, or R-S(=NH)$_2$-NHNH– (or analogous selenium and tellurium group) is named:

(1) as an acylhydrazinyl prefix; the hydrazinyl group is numbered by using the numerical locants 1 and 2;

(2) by expressing the corresponding hydrazide as a prefix by replacing the final letter ‘e’ in the name of the hydrazide by the letter ‘o’.

Method (1) generates preferred IUPAC names.

Example:



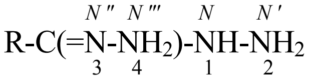
4-(2-benzenecarboximidoylhydrazin-1-yl)benzoic acid (PIN)
4-(2-benzenecarboximidohydrazido)benzoic acid

P-66.4.3 Hydrazidines

P-66.4.3.1 Hydrazidine suffixes

Compounds with the general structure R-C(NH-NH$_2$)=N-NH$_2$ have the class name ‘hydrazidines’ and are named substitutively by using the suffixes ‘hydrazonohydrazide’ and ‘carbohydrazonohydrazide’ as prescribed for hydrazides. The former method of naming hydrazidines as hydrazones of the corresponding hydrazides is no longer recommended.

Locants are assigned to nitrogen atoms as follows:



$$\text{R-C(=}\underset{3}{\overset{N''}{\text{N}}}\text{-}\underset{4}{\overset{N'''}{\text{NH}_2}}\text{)-}\underset{1}{\overset{N}{\text{NH}}}\text{-}\underset{2}{\overset{N'}{\text{NH}_2}}$$

When necessary, the appropriate *N* locants are preceded by the locant indicating the position of the hydrazidine characteristic group on the parent structure.

Names of hydrazidines formally derived from carboxylic acids having retained names, formed by replacing the ‘ohydrazide’ ending in names of hydrazides by ‘hydrazonohydrazide’ may be used in general nomenclature. Preferred IUPAC names are formed systematically. Otherwise, the nomenclatural properties of hydrazides are transferred to hydrazidines; thus, preferred names of hydrazidines correspond to preferred names of hydrazides, and hydrazides that are not substitutable generate nonsubstitutable hydrazidines.

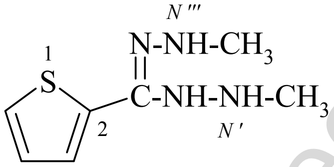
Examples:

$\mathrm{HC(=NNH_2)\text{-}NH\text{-}NH_2}$

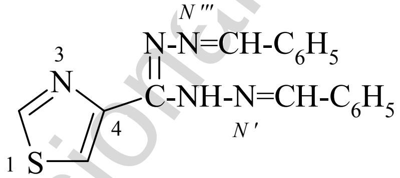
methanehydrazonohydrazide (PIN)
(not methanehydrazide hydrazone)

$\mathrm{CH_3\text{-}CH_2\text{-}CH_2\text{-}C(=NNH_2)\text{-}NHNH_2}$

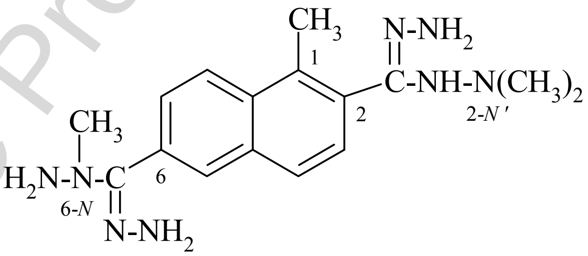
butanehydrazonohydrazide (PIN)
(not butanehydrazide hydrazone)



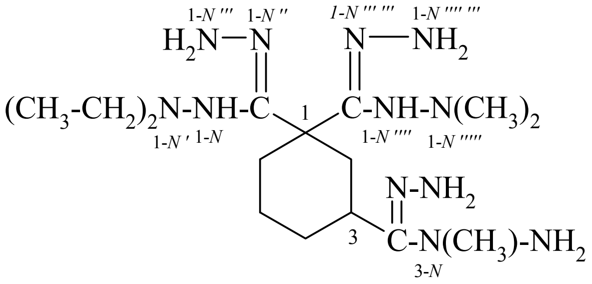
N′,*N*‴-dimethylthiophene-2-carbohydrazonohydrazide (PIN)
(not N^2,N^4-dimethyl-2-thenohydrazide hydrazone)



N′,*N*‴-dibenzylidene-1,3-thiazole-4-carbohydrazonohydrazide (PIN)
(not N^2,N^4-dibenzylidenethiazole-4-carbohydrazide hydrazone)



1,2-*N*′,2-*N*′,6-*N*-tetramethylnaphthalene-2,6-dicarbohydrazonohydrazide (PIN)



1-*N*′,1-*N*′-diethyl-1-*N*‴ ″,1-*N*‴ ″,3-*N*-trimethylcyclohexane-1-1-3-tricarbohydrazonohydrazide (PIN)
(for locants *N*,*N*′, etc. in association with numerical locants, see P-62.2.1.2.2, P-66.4.1.3.3 and P-66.4.2.1).

P-66.4.3.2 Hydrazidines derived from sulfonic acid, and similar selenium and tellurium acids, are named in accordance with the same principles.

Example:

$C_6H_5\text{-}S(=NNH_2)\text{-}NH\text{-}NH_2$

benzenesulfinohydrazonohydrazide (PIN)

P-66.4.3.3 Hydrazidines derived from carbonic acid, oxalic acid, and the polycarbonic acid follow the procedure for the corresponding hydrazides given above (see P-66.3.5).

Example:

$H_2N\text{-}NH\text{-}C(=N\text{-}NH_2)\text{-}NH\text{-}NH_2$

hydrazinecarbohydrazonohydrazide (PIN)
carbonohydrazonic dihydrazide

$H_2N\text{-}NH\text{-}\overset{1}{C}(=N\text{-}NH_2)\text{-}\overset{2}{O}\text{-}\overset{3}{C}(=N\text{-}NH_2)\text{-}NH\text{-}NH_2$

dihydrazonodicarbonic dihydrazide (PIN)

$H_2N\text{-}NH\text{-}\overset{1}{C}(=N\text{-}NH_2)\text{-}\overset{2}{C}(=N\text{-}NH_2)\text{-}NH\text{-}NH_2$

dihydrazonooxalic dihydrazide (PIN)

$\overset{N'}{H_2N}\text{-}\overset{N}{NH}\text{-}(H_2\overset{N''''}{NN}=)\overset{1}{C}\text{-}\overset{2}{C}(=\overset{N'''''}{NNH_2})\text{-}\overset{N''}{NH}\text{-}\overset{N'''}{NH_2}$

dihydrazonooxalic dihydrazide (PIN)

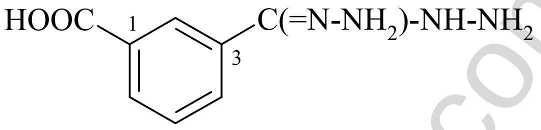
P-66.4.3.4 Hydrazidine prefixes

P-66.4.3.4.1 Prefix names for the group $-C(=NNH_2)\text{-}NH\text{-}NH_2$ are ‘hydrazinecarbohydrazonoyl’ or ‘*C*-hydrazinylcarbonohydrazonoyl’; preferred IUPAC names use the former prefix. When this group is located at the end of a carbon chain, the prefixes ‘hydrazinyl’ and ‘hydrazinylidene’ are preferred in order to avoid fragmenting the chain.

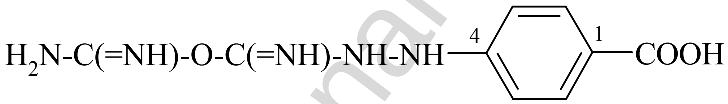
Examples:

$$\mathrm{H_2N\text{-}NH\text{-}(H_2N\text{-}N{=})\overset{3}{C}\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH}$$

3-hydrazinyl-3-hydrazinylidenepropanoic acid (PIN)
2-hydrazinecarbohydrazonoyl)acetic acid
2-(*C*-hydrazinylcarbonohydrazonoyl)acetic acid



3-(hydrazinecarbohydrazonoylbenzoic acid (PIN)
3-(*C*-hydrazinylcarbonohydrazonoyl)benzoic acid



4-{2-[(carbamimidoyloxy)methanimidoyl]hydrazin-1-yl}benzoic acid (PIN)

P-66.4.3.4.2 The prefix names for the groups $-NH\text{-}NH\text{-}CH{=}N\text{-}NH_2$ and $-NH\text{-}N{=}CH\text{-}NH\text{-}NH_2$ are compound prefixes and are: ‘2-(hydrazinylidenemethyl)hydrazinyl’ or ‘(2-methanehydrazonoyl-hydrazin-1-yl) (PIN)’ and ‘2-(hydrazinylmethylidene)hydrazinyl (PIN)’, respectively.

Example:

$$\mathrm{H_2N\text{-}NH\text{-}CH{=}N\text{-}NH\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH}$$

2-(2-methanehydrazonoylhydrazin-1-yl)acetic acid (PIN)
[2-(hydrazinylmethylidene)hydrazin-1-yl]acetic acid

P-66.5 Nitriles

P-66.5.0 Introduction

Compounds with the general structure R-C≡N are called ‘nitriles’ or ‘cyanides’. Nitriles and cyanides are derived from hydrocyanic acid, HC≡N. When the point of attachment of the −C≡N group to R is a carbon atom or a heteroatom, these compounds form the class of nitriles and are named substitutively as nitriles. They may also be named as cyanides according to the principles of functional class nomenclature. These two types of nomenclature are fully discussed in this Section.

P-66.5.1 Nomenclature for generating preferred names of nitriles

Compounds of the general structure R-C≡N have the class names ‘nitriles’ and are named in three ways:

(a) substitutively, using the suffixes ‘nitrile’ for –(C)N and carbonitrile’ for –CN

(b) by changing the ‘ic acid’ or ‘oic acid’ endings in retained names of carboxylic acids into ‘onitrile’; the nomenclatural properties of acids are transferred to nitriles; thus, preferred names of nitriles correspond to preferred names of carboxylic acids (see P-55) and carboxylic acids that are not substitutable generate nonsubstitutable nitriles (see P-65.1.1.1.2)

(c) by functional class nomenclature, using the class name ‘cyanide’

P-66.5.1.1 Substitutive and functional class names for nitriles

P-66.5.1.1.1 Acyclic mono- and dinitriles are named in the following two ways:

(1) substitutively by using the suffix ‘nitrile’, and

(2) by functional class nomenclature using the class name ‘cyanide’.

Method (1) leads to preferred IUPAC names.

Examples:

$\overset{6}{C}H_3\text{-}[CH_2]_4\text{-}\overset{1}{C}N$

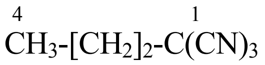
hexanenitrile (PIN))
pentyl cyanide

$N\overset{5}{C}\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}N$

pentanedinitrile (PIN))
propane-1,3-diyl dicyanide

P-66.5.1.1.2 If an unbranched alkane is linked to more than two terminal cyano groups, all cyano groups are named from the parent hydride by the substitutive suffix ‘carbonitrile’, preceded by appropriate multiplying prefix and locants.

Example:



$\overset{4}{C}H_3\text{-}[CH_2]_2\text{-}\overset{1}{C}(CN)_3$

butane-1,1,1-tricarbonitrile (PIN)

P-66.5.1.1.3 The suffix ‘carbonitrile’ is always used to name nitriles having the −CN group attached to a ring or ring system or to an acyclic heteroatom.

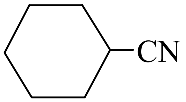
Examples:

$H_3Si\text{-}CN$

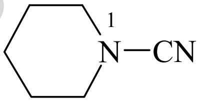
silanecarbonitrile (PIN)
silyl cyanide

$H_2N\text{-}NH\text{-}CN$

hydrazinecarbonitrile (PIN)
hydrazinyl cyanide



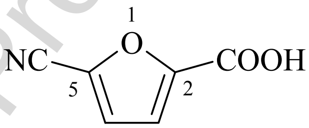
cyclohexanecarbonitrile (PIN)
cyclohexyl cyanide



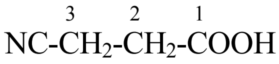
piperidine-1-carbonitrile (PIN)

P-66.5.1.1.4 When a group is present that has priority for citation as the principal characteristic group or when all −CN groups cannot be expressed as the principal characteristic group, the −CN group is designated by the prefix ‘cyano’. The prefix ‘cyano’ **must** also be used when the −CN group is located at the end of a chain.

Examples:

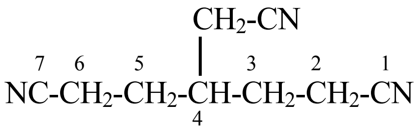


5-cyanofuran-2-carboxylic acid (PIN)
5-cyano-2-furoic acid



$N\overset{3}{C}\text{-}\overset{2}{C}H_2\text{-}CH_2\text{-}\overset{1}{C}OOH$

3-cyanopropanoic acid (PIN)



$$\overset{7}{N}C\text{-}\overset{6}{C}H_2\text{-}\overset{5}{C}H_2\text{-}\underset{4}{\overset{CH_2\text{-}CN}{C}}H\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}N$$

4-(cyanomethyl)heptanedinitrile (PIN)

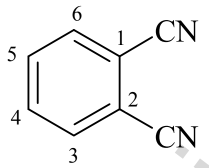
P-66.5.1.2 Names of nitriles derived from retained names of carboxylic acids

(a) The following names are retained as preferred names, with unlimited substitution, except for formonitrile whose substitution rules are the same as formic acid (see P-65.1.8)

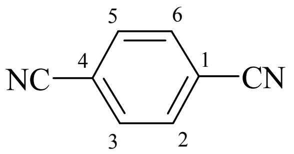
HCN	$CH_3\text{-}CN$	$C_6H_5\text{-}CN$
formonitrile (PIN) methanenitrile hydrogen cyanide	acetonitrile (PIN) ethanenitrile	benzonitrile (PIN) benzenecarbonitrile

(a) For general nomenclature, only the names furocarbonitrile, phthalonitrile, isophthalonitrile, and terephthalonitrile are retained with full substitution allowed (see P-34). Systematic names (P-66.1.1.1.1) are the preferred IUPAC names.

Examples:



benzene-1,2-dicarbonitrile (PIN)
phthalonitrile



benzene-1,4-dicarbonitrile (PIN)
terephthalonitrile

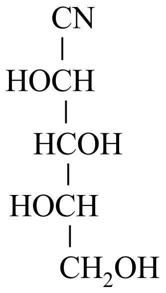
(c) Nitriles derived from retained acid names given in P-65.1.1.2 are only used in general nomenclature; no substitution is allowed. Preferred IUPAC names are given systematic names (P-66.5.1.1).

Examples:

$CH_3\text{-}CH_2\text{-}CN$	$NC\text{-}CH_2\text{-}CH_2\text{-}CN$
propiononitrile propanenitrile (PIN)	succinonitrile butanedinitrile (PIN)

(d) Names of nitriles derived from carbohydrate acids and amino acids are discussed in P-102.5.5.6.2.1 and P-103.2, respectively.

Examples:



$$\begin{array}{c} \mathrm{CN} \\ | \\ \mathrm{HOCH} \\ | \\ \mathrm{HCOH} \\ | \\ \mathrm{HOCH} \\ | \\ \mathrm{CH_2OH} \end{array}$$

L-xylononitrile (PIN)

H_2N-CH_2-CN

glycinonitrile (PIN)

P-66.5.1.3 Functional class nomenclature for generating preferred IUPAC names of cyanides

Functional class nomenclature is used, when needed, to name compounds in accordance with the seniority of classes and to name compounds that cannot be named substitutively, for example, cyanides corresponding to sulfonic and sulfinic acids, selenium and tellurium analogues, carbonic acid, and inorganic acids.

P-66.5.1.3.1 Nitriles with an α-oxo group.

Compounds of the type R-CO-CN can be named as acyl cyanides in a way similar to that of acid halides. Since acyl cyanides are senior to nitriles, in the seniority of classes, functional class nomenclature must be used to correctly express the seniority order.

Examples:

HCO-CN	CH_3-CO-CN	CH_3-$[CH_2]_5$-CO-CN
formyl cyanide (not oxoacetonitrile)	acetyl cyanide (PIN) (not pyruvonitrile)	heptanoyl cyanide (PIN) (not 2-oxooctanenitrile) (not 2-oxopropanenitrile)

P-66.5.1.3.2 Cyanides corresponding to the sulfur, selenium, and tellurium acid suffixes

Cyanides formally formed by replacing the –OH group in sulfonic acids, sulfinic acids, and similar Se and Te acids, are named by functional class nomenclature.

Examples:

CH_3-SO_2-CN	C_6H_5-SeO-CN
methanesulfonyl cyanide (PIN)	benzeneseleninyl cyanide (PIN)

P-66.5.2 Substituted nitriles

Substituents on the parent hydrides are denoted as prefixes. Nitriles, in the seniority order of classes, are senior to ketones, pseudoketones, heterones, hydroxy compounds, amines and imines; these classes must be cited as prefixes in the presence of a nitrile group. Seniority for numbering polyfunctional amides follows that described for acids, for which see P-65.1.2.3 and P-65.3.4.

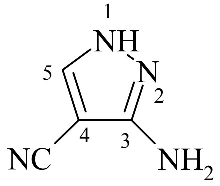
Examples:

$\overset{6}{C}H_2\text{-}\overset{5}{C}O\text{-}[CH_2]_3\text{-}\overset{1}{C}N$

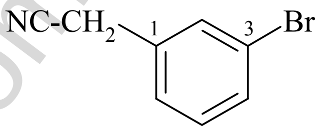
5-oxohexanenitrile (PIN)

$HO\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}N$

4-hydroxybutanenitrile (PIN)
4-hydroxybutyronitrile



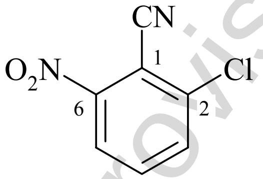
3-amino-1*H*-pyrazole-4-carbonitrile (PIN)



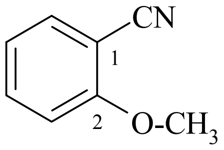
(3-bromophenyl)acetonitrile (PIN)
3-bromobenzyl cyanide

$NC\text{-}CH_2\text{-}CH_2\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}CN$

3,3′-iminodipropanenitrile (PIN)
3,3′-iminodipropionitrile



2-chloro-6-nitrobenzonitrile (PIN)



2-methoxybenzonitrile (PIN)

$Cl\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}CN$

3-chloropropanoyl cyanide (PIN)
(not 3-chloropropionyl cyanide)
(not 4-chloro-2-oxopropanenitrile)

P-66.5.3 Nitriles/cyanides corresponding to carbonic, oxalic, and the polycarbonic acids

P-66.5.3.1 Nitriles corresponding to carbonic acid and related compounds, oxalic acid and the polycarbonic acids are named by functional class nomenclature

Eamples:

NC-CO-CN

carbonyl dicyanide (PIN)
(not 2-oxopropanedinitrile)
(not oxomalononitrile; no substitution
allowed on malononitrile)

NC-C(=NH)-CN

carbonimidoyl dicyanide (PIN)
(not 2-iminopropanedinitrile)

NC-C(=NNH_2)-CN

carbonohydrazonoyl dicyanide (PIN)
(not 2-hydrazonopropanedinitrile)

H_2N-CO-CN

carbamoyl cyanide (PIN)

NC-CO-CO-CN

oxalic dicyanide (PIN)

NC-CO-O-CO-CN

dicarbonic dicyanide (PIN)

P-66.5.4 Nitrile oxides

P-66.5.4.1 Compounds with the general structure R-C≡NO have the generic name ‘nitrile oxides’. As zwitterions, they are classed with the zwitterion class in the order of compound classes. They are named by three methods.

(1) by the term ‘oxide’ added to the name of the nitrile;

(2) by applying the λ-convention and oxo substitution to the nitrogen atom (see P-14.1)

(3) as zwitterions (see P-74.2.2.2)

Methods (1) and (2) lead to preferred IUPAC names.

Example:

C_6H_5-C≡N^+-O^-

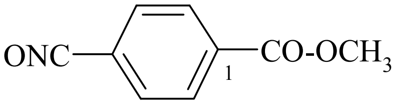
(1) benzonitrile oxide (PIN)
(2) benzylidyne(oxo)-λ^5-azane
(3)_(benzylidyneammoniumyl)oxidanide

$HC{\equiv}N^{+}\text{-}O^{-}$

(1) formonitrile oxide (PIN)
(2) methylidyne(oxo)-λ^5-azane
(3) (methylidyneammoniumyl)oxidanide

P-66.5.4.2 When necessary to cite the group –C≡NO group as a substituent prefix, method (2) is applied.

Example:



methyl 4-[(oxo-λ^5-azanylidene)methyl]benzoate (PIN)
(no longer methyl 4-fulminatobenzoate)

P-66.6 Aldehydes

P-66.6.0 Introduction.

The class name ‘aldehyde’ traditionally refers to compounds containing a −CH=O group attached to a carbon atom. However, when the attachment is to a heteroatom it is convenient to call the compound a pseudoaldehyde.

P-66.6.1 Systematic names of aldehydes

Aldehydes are systematically named in two ways:

(1) substitutively, using the suffixes ‘al’ for −(C)HO and ‘carbaldehyde’ for −CHO;

(2) by changing the ‘ic acid’ or ‘oic acid’ endings of retained names of carboxylic acids into ‘aldehyde’; the nomenclatural properties of acids are transferred to aldehydes; thus, preferred names of aldehydes correspond to preferred names of acids and carboxylic acids that are not substitutable generate nonsubstitutable aldehydes.

P-66.6.1.1 Systematic substitutive names for aldehydes

Aldehydes are named substitutively using the suffixes ‘al’ or ‘carbaldehyde’, or the prefix ‘oxo’, denoting =O, or ‘formyl-’, denoting the substituent group −CHO.

P-66.6.1.2 Mono- and dialdehydes derived from alkanes are named substitutively using the suffix ‘al’ added to the name of the parent hydride with elision of the final letter ‘e’ of the parent hydride before ‘a’.

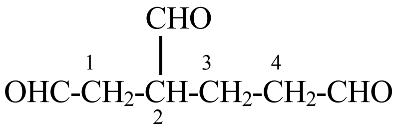
Examples:

$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CHO$
pentanal (PIN)

$OHC\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CHO$
pentanedial (PIN)

P-66.6.1.3 The suffix ‘carbaldehyde’ is used when more than two −CHO groups are attached to an alkane.

Example:

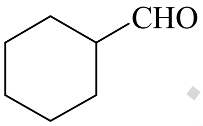


$$OHC\text{-}\overset{1}{C}H_2\text{-}\underset{2}{\overset{\overset{CHO}{|}}{C}}H\text{-}\overset{3}{C}H_2\text{-}\overset{4}{C}H_2\text{-}CHO$$

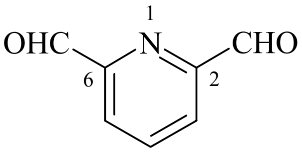
butane-1,2,4-tricarbaldehyde (PIN)

P-66.6.1.4 The suffix ‘carbaldehyde’ is used when the −CHO group is attached to a carbon atom of a ring or ring system, or to a heteroatom.

Examples:



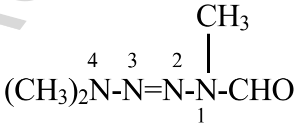
cyclohexanecarbaldehyde(PIN)



pyridine-2,6-dicarbaldehyde (PIN)

$H_2P\text{-}CHO$
phosphanecarbaldehyde (PIN)

$H_2NNH\text{-}CHO$
hydrazinecarbaldehyde
formohydrazide (PIN)
(a hydrazide is senior to an aldehyde)



$$(CH_3)_2\overset{4}{N}\text{-}\overset{3}{N}\text{=}\overset{2}{N}\text{-}\underset{1}{\overset{\overset{CH_3}{|}}{N}}\text{-}CHO$$

1,4,4-trimethyltetraaz-2-ene-1-carbaldehyde (PIN)

P-66.5.1.2 Names of aldehydes derived from retained names of carboxylic acids

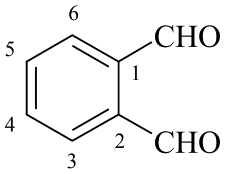
Names of aldehydes are formed by changing the ‘ic acid’ or ‘oic acid’ ending of the retained names of carboxylic acids to ‘aldehyde’. Substitution of aldehydes parallels that of corresponding carboxylic acids.

(a) The following names are retained as preferred IUPAC names, with, except for formaldehyde, unlimited substitution. Substitution rules for formaldehyde are the same as for formic acid (see P-65.1.8)

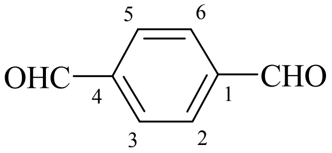
HCHO	CH_3-CHO	C_6H_5-CHO
formaldehyde (PIN) methanal	acetaldehyde (PIN) ethanal	benzaldehyde (PIN) benzenecarboxaldehyde

(b) For general nomenclature, only the names furaldehyde, phthalaldehyde, isophthalaldehyde, and terephthalaldehyde are retained with full substitution allowed (see P-34). Systematic names (P-66.6.1.1) are the preferred IUPAC names.

Examples:



benzene-1,2-dicarbaldehyde (PIN)
phthalalaldehyde



benzene-1,4-dicarbaldehyde (PIN)
terephthalaldehyde

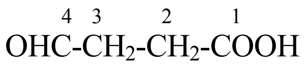
(c) Aldehydes derived from retained acid names given in P-65.1.1.2 are only used in general nomenclature; no substitution is allowed. Preferred IUPAC names are given systematic names (P-66.6.1.1).

Examples:

CH_3-CH_2-CHO	OHC-CH_2-CH_2-CHO
propionaldehyde propanal (PIN))	succinaldehyde butanedial (PIN)

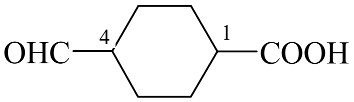
P-66.6.1.3 In the presence of a characteristic group having priority to be cited as a suffix or when present on a side chain, a –CHO group is expressed by the prefix, ‘oxo’, if located at an end of a carbon chain, or, in other cases, by the prefix ‘formyl’.

Examples:

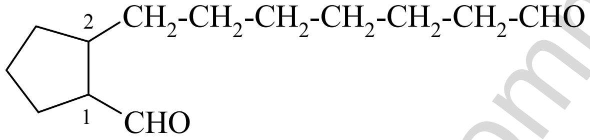


$\overset{4}{\text{OHC}}\text{-}\overset{3}{\text{C}}\text{H}_2\text{-}\overset{2}{\text{C}}\text{H}_2\text{-}\overset{1}{\text{C}}\text{OOH}$

4-oxobutanoic acid (PIN)
3-formylpropanoic acid



2-formylcyclohexane-1-carboxylic acid (PIN)



2-(7-oxoheptyl)cyclopentane-1-carbaldehyde (PIN)
7-(2-formylcyclopentyl)heptanaldehyde
(ring preferred to chain: see P-44.1.2.2)

P-66.6.2 Aldehydes from oxalic acid and the polycarbonic acids

P-66.6.2.1 The retained name oxaldehyde is the preferred IUPAC name for the dialdehyde from oxalic acid. Substitution follows the rules for substituting formaldehyde or formic acid.

Example:

$O=CH-CH=O$

oxaldehyde (PIN)
(a shortened form of oxalaldehyde)
(not ethanedial)

P-66.6.2.2 Aldehydes from di- and polycarbonic acids are named on the basis of the higher compound class. Multiplicative names based on formaldehyde can be used (see P-65.2.2.2)

Example

$O=CH-O-CH=O$

formic anhydride (PIN)
(anhydride preferred to aldehyde)
oxydiformaldehyde

$O=CH-O-CO-O-CH=O$

carbonic diformic dianhydride (PIN)
(anhydride preferred to ester)
bis(oxomethyl) carbonate
[carbonylbis(oxy)]diformaldehyde

P-66.6.3 Chalcogen analogues of aldehydes

Chalcogen analogues of aldehydes are named by using the following suffixes and prefixes modified by functional replacement. In the seniority order of classes, aldehydes are senior to ketones, hydroxy compounds, amines and imines. Names of chalcogen analogues corresponding to aldehydes with retained names are all systematically formed.

Group	Suffix	Prefix
–(C)HO	al	oxo
–(C)HS	thial	sulfanylidene (preferred to thioxo)
–(C)HSe	selenal	selanylidene (preferred to selenoxo)
–(C)HTe	tellural	tellanylidene (preferred to telluroxo)
–CHO	carbaldehyde	formyl
–CHS	carbothialdehyde	methanethioyl (preferred to thioformyl)
–CHSe	carboselenaldehyde	methaneselenoyl (preferred to selenoformyl)
–CHTe	carbotelluraldehyde	methanetelluroyl (preferred to telluroformyl)

Examples:

$\overset{2}{C}H_3\text{-}\overset{1}{C}HS$

ethanethial (PIN)
thioacetaldehyde

$C_6H_5\text{-}CHS$

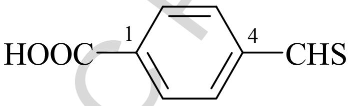
benzenecarbothialdehyde (PIN)
thiobenzaldehyde

$\overset{6}{C}H_3\text{-}[CH_2]_4\text{-}\overset{1}{C}HSe$

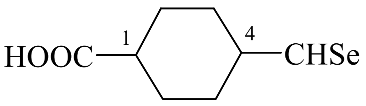
hexaneselenal (PIN)

$S\overset{5}{H}\overset{4}{C}\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}CHS$

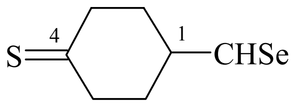
pentanedithial (PIN)



4-(methanethioyl)benzoic acid (PIN)
4-(thioformyl)benzoic acid



4-(methaneselenoyl)cyclohexane-1-carboxylic acid (PIN)
4-(selenoformyl)cyclohexane-1-carboxylic acid



4-sulfanylidenecyclohexane-1-carboselenaldehyde (PIN)
4-thioxocyclohexane-1-carboselenaldehyde

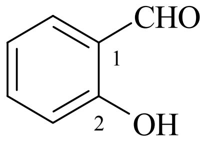
P-66.6.4 Polyfunctional aldehydes

In presence of an aldehyde group, ketones, pseudoketones, heterones, hydroxy compounds, amines and imines are expressed by prefixes. Seniority for numbering polyfunctional aldehydes follows that described for acids, for which see P-65.1.2.3 and P-65.3.4.

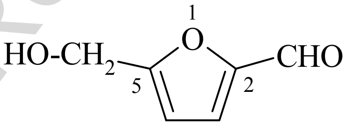
Examples:

$\overset{4}{\mathrm{CH_3}}\text{-}\overset{3}{\mathrm{CO}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{CHO}}$

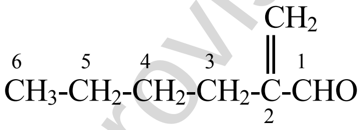
3-oxobutanal (PIN)
3-oxobutyraldehyde



2-hydroxybenzaldehyde (PIN)
(not salicylaldehyde)

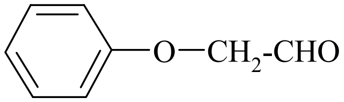


5-(hydroxymethyl)furan-2-carbaldehyde (PIN)
5-(hydroxymethyl)-2-furaldehyde
(not 5-(hydroxymethyl)furfural)

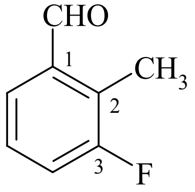


$\overset{6}{\mathrm{CH_3}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{CH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\underset{2}{\overset{\overset{\mathrm{CH_2}}{\|}}{\mathrm{C}}}\text{-}\overset{1}{\mathrm{CHO}}$

2-methylidenehexanal (PIN)
[not 2-butylprop-2-enal, the longest chain is the principal chain (see P-44.3)]



phenoxyacetaldehyde (PIN)



3-fluoro-2-methylbenzaldehyde (PIN)

P-66.6.5 Acetals and ketals, hemiacetals and hemiketals, and chalcogen analogues

P-66.6.5.1 Acetals and ketals

P-66.6.5.1.1 Compounds with the general structure RR′C(O-R″)(O-R‴), where only R and R′ may be, but need not be, hydrogen, have the class name 'acetals'. 'Ketals' constitute a subclass of acetals wherein neither R nor R′ may be hydrogen. Acetals (ketals) are named in two ways:

(1) substitutively as 'alkoxy', 'aryloxy', etc. derivatives of an appropriate parent hydride or functional parent compound;

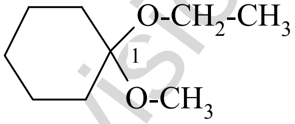
(2) by functional class nomenclature by citing the name of the aldehyde or ketone, the names of the *O*-substituents, in alphanumerical order if required, and finally the class terms 'acetal' or 'ketal'

Method (1), the substitutive method, leads to preferred IUPAC names.

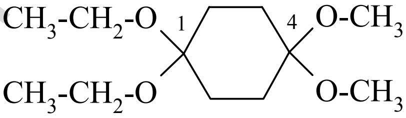
Examples:

$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H(OCH_2\text{-}CH_3)_2$

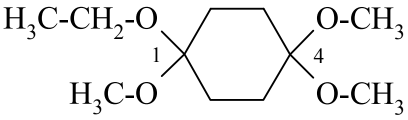
(1) 1,1-diethoxypropane (PIN)
(2) propanal diethyl acetal



(1) 1-ethoxy-1-methoxycyclohexane (PIN)
(2) cyclohexanone ethyl methyl ketal



(1) 1,1-diethoxy-4,4-dimethoxycyclohexane
(2) cyclohexane-1,4-dione 1-(diethyl ketal) 4-(dimethyl ketal)



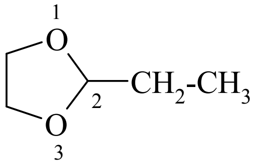
(1) 1-ethoxy-1,4,4-trimethoxycyclohexane (PIN)
(2) cyclohexanedione 1-ethyl 1,4,4-trimethyl diketal

P-66.6.5.1.2 Cyclic acetals and ketals

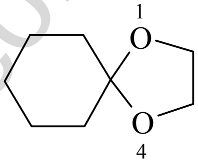
Cyclic acetals as the principal function are named as heterocyclic compounds and these names are preferred IUPAC names; cyclic ketals are spiro compounds that are named in accordance with the rules described in Section P-24 giving preferred IUPAC names.

Functional class nomenclature using the name of the appropriate divalent substituent groups may also be used.

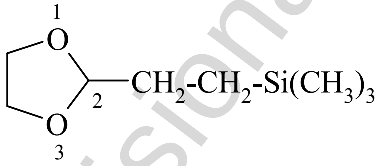
Examples:



2-ethyl-1,3-dioxolane (PIN)
propanal ethylene acetal



1,4-dioxaspiro[4.5]decane (PIN)
cyclohexanone ethylene ketal

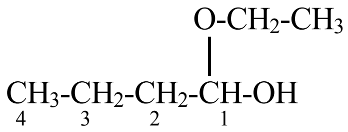


[2-(1,3-dioxolan-2-yl)ethyl]trimethylsilane (PIN)
3-(trimethylsilyl)propanal ethylene ketal

P-66.6.5.2 Hemiacetals and hemiketals.

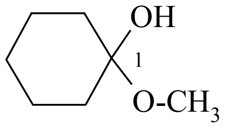
Compounds with the general structure RR′C(OH)(O-R″) have the class name ‘hemiacetals’. They are named substitutively as ‘alkoxy’, ‘aryloxy’, etc., derivatives of an appropriate hydroxy parent compound, such as an alcohol; these names are the preferred IUPAC names. Other names are formed by functional class nomenclature with the class name ‘hemiacetal’; similarly derivatives of ketones are denoted by the class name ‘hemiketal’.

Examples:



$$\underset{4}{\mathrm{CH_3}}\text{-}\underset{3}{\mathrm{CH_2}}\text{-}\underset{2}{\mathrm{CH_2}}\text{-}\underset{1}{\overset{\overset{\displaystyle\mathrm{O\text{-}CH_2\text{-}CH_3}}{|}}{\mathrm{CH}}}\text{-}\mathrm{OH}$$

1-ethoxybutanol (PIN)
butanal ethyl hemiacetal

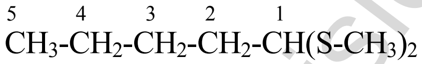


1-methoxycyclohexan-1-ol (PIN)
cyclohexanone methyl hemiketal

P-66.6.5.3 Chalcogen analogues of acetals and ketals

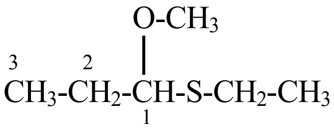
Sulfur analogues of acetals and ketals with the general structures RR′C(S-R″)(S-R‴) or RR′C(S-R″)(O-R‴), have the class names ‘dithioacetals’ or ‘monothioacetals’, respectively. They are named substitutively as ‘alkylsulfanyl’, ‘arylsulfanyl’, ‘alkoxy’, or ‘aryloxy’ derivatives, as appropriate, of a parent hydride; these names are preferred IUPAC names. Other names can be generated by functional class nomenclature, using class names such as ‘monothioacetal’ and ‘dithioketal’. Capital italic letter locants are used to provide structural specificity. Selenium, tellurium and mixed analogues are treated in the same way as their sulfur analogues.

Examples:



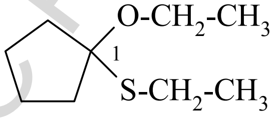
$$\overset{5}{\mathrm{CH_3}}\text{-}\overset{4}{\mathrm{CH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{CH}}\mathrm{(S\text{-}CH_3)_2}$$

1,1-bis(methylsulfanyl)pentane (PIN)
pentanal diethyl dithioacetal

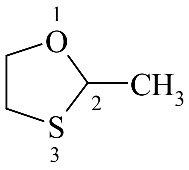


$$\overset{3}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\underset{1}{\overset{\overset{\displaystyle\mathrm{O\text{-}CH_3}}{|}}{\mathrm{CH}}}\text{-}\mathrm{S\text{-}CH_2\text{-}CH_3}$$

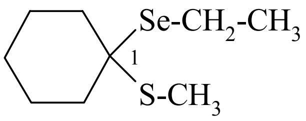
1-(ethylsulfanyl)-1-methoxypropane (PIN)
propanal *S*-ethyl *O*-methyl monothioacetal



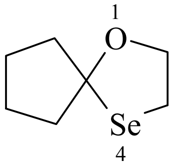
1-ethoxy-1-(ethylsulfanyl)cyclopentane (PIN)
cyclopentanone diethyl monothioketal



2-methyl-1,3-oxathiolane (PIN)
ethan-1-one ethylene monothioketal



1-(ethylselanyl)-1-(methylsulfanyl)cyclohexane (PIN)
cyclohexanone *Se*-ethyl *S*-methyl selenothioketal

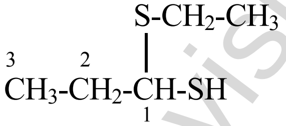


1-oxa-4-selenaspiro[4.4]nonane (PIN)
cyclopentanone ethylene monoselenoketal

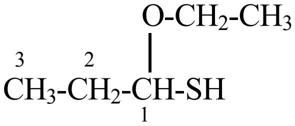
P-66.6.5.4 Chalcogen analogues of hemiacetals and hemiketals

Sulfur analogues of hemiacetals and hemiketals with the general structures RR′C(SH)(S-R″), RR′C(OH)(S-R″) or RR′C(SH)(O-R″), have the class names 'dithiohemiacetals' or 'monothiohemiacetals', respectively. They are named substitutively as 'alkylsulfanyl', 'arylsulfanyl', 'alkoxy', or 'aryloxy' derivatives, as appropriate, of a hydroxy parent compound; these are preferred IUPAC names. Other names can be generated by functional class nomenclature. Capital italic letter locants are used to provide structural specificity. Selenium, tellurium, and mixed analogues are treated in the same way as their sulfur analogues; generically, they are 'monoselenohemiacetals', 'ditellurohemiacetals, 'selenothiohemiacetals', etc.

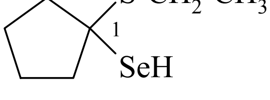
Examples:


$$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\underset{1}{C}H(\text{S-CH}_2\text{-CH}_3)\text{-SH}$$

1-(ethylsulfanyl)propane-1-thiol (PIN)
propanal ethyl dithiohemiacetal


$$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\underset{1}{C}H(\text{O-CH}_2\text{-CH}_3)\text{-SH}$$

1-ethoxypropane-1-thiol (PIN)
propanal *O*-ethyl monothiohemiacetal



1-(ethylsulfanyl)cyclopentane-1-selenol (PIN)
cyclopentanone *S*-ethyl selenothiohemiketal

P-67 Mononuclear and polynuclear noncarbon acids and their functional replacement analogues as parents for naming organic compounds

P-67.0 Introduction

Mono-, di-, and polynuclear noncarbon oxoacids and their chalcogen analogues having retained names are used as parent structures to generate names of carbon containing compounds. In these recommendations, the names for these compounds are preselected names (see P-12)

Names of chalcogen analogues of oxoacids are formed by functional replacement nomenclature. This type of nomenclature is also used to create derived classes, for example, acid halides and pseudohalides, amides, hydrazides, and amidines. With regard to functional replacement, mono- di- and polynuclear acids do not constitute a homogeneous group. Names of mononuclear oxoacids are modified by infixes, with the exception of silicic acid, nitrous acid, nitric acid and halogen acids. Names of di- and polynuclear oxoacids are modified by prefixes. Functional class nomenclature is used to generate names for esters, organic anhydrides, carbon containing pseudohalides such as cyanides and isocyanates, and organic derivatives of amides, imides, and hydrazides.

Mononuclear oxoacids are discussed first, then di- and polynuclear oxoacids such as diphosphoric acid, $(HO)_2P(O)$-O-P(O)(OH), that are named as acids, not as anhydrides, and hypodiphosphoric acid, $(HO)_2P(O)-P(O)(OH)_2$. Systematization has been achieved, taking into consideration the nomenclature of inorganic compounds (ref. 14), that has restricted the use of retained names and of prefixes such as ‘hypo’, ‘ortho’, ‘iso’ added to the names of mononuclear oxoacids to generate retained names. However, the traditional nomenclature of organic compounds derived from mono- di-, and polynuclear oxoacids has been maintained.

For carbonic, cyanic, oxalic, and the polynuclear carbonic acids, see P-65.

P-67.1 Mononuclear noncarbon acids

Retained names for mononuclear noncarbon oxoacids have the following elements as central atoms: N, P, As, Sb, Si, B, S, Se, Te, F, Cl, Br, and I. They are used as parent structures and also for derivation of prefixes to be used in the presence of classes that have seniority for being named as parent compounds. These parent structures have retained names that are traditional names used as preselected names (see P-12). They may also have systematic additive or substitutive names, but these names are not recommended for generating preselected names (see P-17).

Functional replacement nomenclature is discussed first; next the formation of esters and anhydrides using functional class nomenclature; and finally, substitutive nomenclature using prefixes is described. Application of the seniority order of oxoacids and their derivatives, described in Section P-42, is discussed. The Section ends with the nomenclature of *aci*-nitro compounds that are named as derivatives of azinic acid.

P-67.1.1 Names for mononuclear acids and their derivatives
P-67.1.2 Functional replacement nomenclature applied to acids
P-67.1.3 Esters and anhydrides of acids
P-67.1.4 Derived substituent groups expressed as prefixes
P-67.1.5 Seniority order among acids and derivatives
P-67.1.6 *aci*-Nitro compounds

P-67.1.1 Names for mononuclear acids and their derivatives

Preselected names (see P-12.2) of the mononuclear noncarbon oxoacids used for deriving preferred IUPAC names for organic compounds and names for general organic nomenclature are noted in the following list, given in alphabetical order.

$H_2As(O)(OH)$	arsinic acid
$H_2As(OH)$	arsinous acid
$HAs(O)(OH)_2$	arsonic acid
$HAs(OH)_2$	arsonous acid
$As(O)(OH)_3$	arsoric acid (formerly arsenic acid)
$As(OH)_3$	arsorous acid (formerly arsen(i)ous acid)
$H_2N(O)(OH)$	azinic acid
$H_2N(OH)$	azinous acid
$HN(O)(OH)_2$	azonic acid
$HN(OH)_2$	azonous acid
$N(O)(OH)_3$	azoric acid (hypothetical)
$N(OH)_3$	azorous acid (hypothetical)
$B(OH_3)$	boric acid
H_2B-OH)	borinic acid
$HB(OH)_2$	boronic acid
$Br(O)_2(OH)$	bromic acid
$Br(O)(OH)$	bromous acid
$Cl(O)_2(OH)$	chloric acid
$Cl(O)(OH)$	chlorous acid
$Br(OH)$	hypobromous acid
$Cl(OH)$	hypochlorous acid
$F(OH)$	hypoflurous acid
$I(OH)$	hypoiodous acid
$I(O)_2(OH)$	iodic acid
$I(O)(OH)$	iodous acid
$HO-NO_2$	nitric acid

HO-NO	nitrous acid
$Br(O)_3(OH)$	perbromic acid
$Cl(O)_3(OH)$	perchloric acid
$F(O)_3(OH)$	perfluoric acid
$I(O)_3(OH)$	periodic acid
$H_2P(O)(OH)$	phosphinic acid
$H_2P(OH)$	phosphinous acid
$HP(O)(OH)_2$	phosphonic acid
$HP(OH)_2$	phosphonous acid
$P(O)(OH)_3$	phosphoric acid
$P(OH)_3$	phosphorous acid
$Se(O)_2(OH)_2$	selenic acid
$Se(O)(OH)_2$	selenous acid
$Si(OH)_4$	silicic acid (formerly orthosilicic acid)
$H_2Sb(O)(OH)$	stibinic acid
$H_2Sb(OH)$	stibinous acid
$HSb(O)(OH)_2$	stibonic acid
$HSb(OH)_2$	stibonous acid
$Sb(O)(OH)_3$	stiboric acid (formerly antimonic acid)
$Sb(OH)_3$	stiborous acid (formerly antimonous acid)
$S(O)_2(OH)_2$	sulfuric acid
$S(O)(OH)_2$	sulfurous acid
$Te(O)_2(OH)_2$	telluric acid
$Te(O)(OH)_2$	tellurous acid

P-67.1.2 Functional replacement nomenclature applied to mononuclear oxo acids

Mononuclear oxo acids are modified by either infixes or prefixes in functional replacement nomenclature.

P-67.1.2.1 Mononuclear acids modified by infixes, The following acids are modified by infixes; they are listed in group order B, N, P, As, Sb, S, Se, Te:

$B(OH_3)$	boric acid
$HB(OH)_2$	boronic acid
$H_2B-OH)$	borinic acid
$N(O)(OH)_3$	azoric acid (hypothetical)
$N(OH)_3$	azorous acid (hypothetical)
$HN(O)(OH)_2$	azonic acid
$H_2N(O)(OH)$	azinic acid
$H_2N(OH)$	azinous acid
$HN(OH)_2$	azonous acid
$P(O)(OH)_3$	phosphoric acid
$P(OH)_3$	phosphorous acid
$P(O)(OH)_2$	phosphonic acid
$HP(OH)_2$	phosphonous acid
$H_2P(O)(OH)$	phosphinic acid
$H_2P(OH)$	phosphinous acid
$As(O)(OH)_3$	arsoric acid (formerly arsenic acid)
$As(OH)_3$	arsorous acid (formerly arsen(i)ous acid)
$HAs(O)(OH)_2$	arsonic acid
$HAs(OH)_2$	arsonous acid
$H_2As(O)(OH)$	arsinic acid
$H_2As(OH)$	arsinous acid
$Sb(O)(OH)_3$	stiboric acid (formerly antimonic acid)
$Sb(OH)_3$	stiborous acid (formerly antimonous acid)
$HSb(O)(OH)_2$	stibonic acid
$HSb(OH)_2$	stibonous acid
$H_2Sb(O)(OH)$	stibinic acid
$H_2Sb(OH)$	stibinous acid
$S(O)_2(OH)_2$	sulfuric acid
$S(O)(OH)_2$	sulfurous acid
$Se(O)_2(OH)_2$	selenic acid
$Se(O)(OH)_2$	selenous acid

$Te(O)_2(OH)_2$	telluric acid
$Te(O)(OH)_2$	tellurous acid

P-67.1.2.2 Mononuclear acids modified by prefixes. The following acids are modified by prefixes; they are listed in the order Si, N, F, Cl, Br, I.

$Si(OH)_4$	silicic acid (formerly orthosilicic acid)
$HO\text{-}NO_2$	nitric acid
HO-NO	nitrous acid
$F(O)_3(OH)$	perfluoric acid
$F(O)_2(OH)$	fluoric acid
F(O)(OH)	fluorous acid
F(OH)	hypoflurous acid
$Cl(O)_3(OH)$	perchloric acid
$Cl(O)_2(OH)$	chloric acid
Cl(O)(OH)	chlorous acid
Cl(OH)	hypochlorous acid
$Br(O)_3(OH)$	perbromic acid
$Br(O)_2(OH)$	bromic acid
Br(O)(OH)	bromous acid
Br(OH)	hypobromous acid
$I(O)_3(OH)$	periodic acid
$I(O)_2(OH)$	iodic acid
I(O)(OH)	iodous acid
I(OH)	hypoiodous acid

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P-67.1.2.3 General methodology for functional replacement nomenclature using infixes

Functional replacement nomenclature (see P-15.5) using infixes generates functional class names for the following classes: acid halides and pseudo halides (azides, cyanides, isocyanides, and isocyanates), amides, hydrazides, and also imidic, hydrazonic and nitridic acids. Chalcogen analogues are also described by infixes.

Preferred IUPAC names are retained names modified by functional nomenclature. The the use of infixes is restricted to acids listed in P-67.1.2.1 and leads to preferred IUPAC names. Prefixes are used as recommended for acids listed in P-67.1.2.2, and in general nomenclature for all mononuclear acids. Substitutive names and names modified by prefixes are used only in special occasions (see P-67.1.4.1.1 (f) and P-67.3.1).

$(C_6H_5)P\text{-}SH$	diphenylphosphinothious acid (PIN) (not diphenylphosphanethiol) (not diphenyl(sulfanyl)phosphane)

P-67.1.2.3.1 The following infixes are used to describe the replacement of =O and −OH by chalcogen analogues (in decreasing order of seniority):

(1)	–OO–	peroxo
(2)	–OS– or –SO–	thioperoxo (similarly, selenoperoxo, telluroperoxo)
(3)	–SS–	dithioperoxo (similarly, diselenoperoxo, telluroperoxo)
(4)	–SSe– or –SeS–	selenothioperoxo (similarly for other mixed chalcogens)
(5)	–S– or =S	thio
(6)	–Se– or =Se	seleno
(7)	–Te– or =Te	telluro

P-67.1.2.3.2 Infixes denoting classes (in decreasing order of seniority except for halides that have the same rank but are cited in alphabetical order and pseudohalides that have the same rank but are cited in alphabetical order)

(1)	–Br	bromido
	–Cl	chlorido
	–F	fluorido
	–I	iodido
(2)	$–N_3$	azido
	–CN	cyanido
	–NC	isocyanido
	–NCO	isocyanatido
	–NCS	isothiocyanatido
	–NCSe	isoselenocyanatido
	–NCTe	isotellurocyanatid
(3)	$–NH_2$	amido
(4)	$–NH\text{-}NH_2$	hydrazido
(5)	≡N	nitrido
(6)	=NH	imido
(7)	$=NNH_2$	hydrazono

P-67.1.2.3.3 Prefixes denoting chalcogen analogues of acids by replacing oxygen atoms (in decreasing order of seniority):

(1)	−OO−	peroxy
(2)	−OS− or −SO−	thioperoxy (similarly, selenoperoxy, telluroperoxy)
(3)	−SS−	dithioperoxoy(similarly, diselenoperoxy, telluroperoxy)
(4)	−SSe− or −SeS−	selenothioperoxy (similarly for other mixed chalcogens)
(5)	−S− or =S	thio
(6)	−Se− or =Se	seleno
(7)	−Te− or =Te	telluro

P-67.1.2.3.4 Prefixes denoting classes (in decreasing order of seniority except for halides that have the same rank but are cited in alphabetical order and pseudohalides that have the same rank but are cited in alphabetical order)

(1)	−Br	bromo		−NCS	isothiocyanato
	−Cl	chloro		−NCSe	isoselenocyanato
	−F	fluoro		−NCTe	isotellurocyanato
	−I	iodo	(3)	$-NH_2$	amido
(2)	$-N_3$	azido	(4)	$-NH\text{-}NH_2$	hydrazido
	−CN	cyano	(5)	≡N	nitrido
	−NC	isocyano	(6)	=NH	imido
	−NCO	isocyanato	(7)	$=NNH_2$	hydrazono

P-67.1.2.3.5 The appropriate infix is indicated (in alphabetical order if more than one) before the ‘ic acid’ or ‘ous acid’ ending in the parent name, with elision of the letter ‘o’ before a vowel, with the exception of the infixes ‘thio’, ‘seleno’, telluro’ and ‘peroxo’ which are cited as such, with no elision of the letter ‘o’, before the ‘ic ending’. A euphonic letter ‘o’ also may be added when necessary. Multiplying an infix by multiplying prefixes ‘di’ or tri’ does not change its place in the alphabetical order.

The appropriate prefix is indicated (in alphabetical order if there is more than one) before the name of the acid; no elision is recommended. Multiplying a prefix by multiplying prefixes ‘di’ or tri’ does not change its place in the alphabetical order.

P-67.1.2.4 Mononuclear acids modified by functional replacement

Mononuclear noncarbon acids have preselected names used for deriving preferred IUPAC names for organic compounds.

As long as there is at least one −OH group left in an acid having a retained name, the acid modified by functional replacement is classified as an acid and denoted by class name ‘acid’.

P-67.1.2.4.1 Acids with substitutable hydrogen atoms

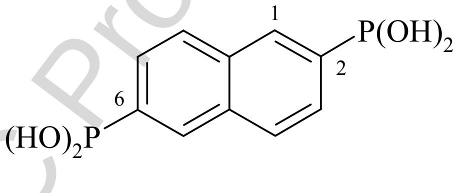
P-67.1.2.2.1 Acids with hydrogen atoms attached to the central atom (substitutable hydrogen)

Acids of the type $HE(O)(OH)_2$, $HE(OH)_2$, $H_2E(O)(OH)$, or $H_2E(O)(OH)$ where E is B, N, P, As, or Sb having hydrogen atoms attached directly to the central atom are named substitutively by organyl groups, leading to names such as ethylphosphonic acid Another method has been suggested which would treat the acid as a suffix (like sulfonic acid leading to names such as benzenephosphonic acid. This suggestion has been rejected because in cases where the acid has two substitutable hydrogen atoms, the use of additional letter locants would be required leading to unnecessarily more cumbersome names.

Acids with hydrogen atoms attached to the central atom may be substituted by organyl groups and prefered IUPAC names are formed substitutively. Use of acid names as suffixes is not recommended.

Examples:

C_2H_5-$P(O)(OH)_2$	ethylphosphonic acid (PIN) (not ethanephosphonic acid)
$(C_2H_5)_2P(O)(OH)$	diethylphosphinic acid (PIN) (not *P*-ethyldiethanephosphinic acid
$(C_6H_5)_2As(OH)$	diphenylarsinous acid (PIN)
$C_6H_5Sb(OH)_2$	phenylstibonous acid (PIN)



naphthalene-2,6-bis(phosphonous acid) (PIN)

P-67.1.2.4.2 Functional replacement of the oxoacids specifically listed in P-67.1.2 is expressed by infixes or prefixes. Substitution of nonacidic hydrogen atoms is indicated by prefixes, with a letter locant *B*, *N*, *P, As* or *Sb* as needed. Tautomers may be distinguished by prefixing italic elements symbols, such as *S* and *O*, to the term ‘acid’. Parentheses are needed to enclose infixes modified by prefixes, for example, ‘thioperoxoic’. In addition to infixes and prefixes listed in P-67.1.2.3, the prefix ‘cyanato’ and the infix ‘cyanatido’, for −OCN, are used to modify acids as indicated in P-67.1.2.4.2.3.

P-67.1.2.4.2.1 Examples of acids modified by infixes:

CH_3-B(OH)(SH)	methylboronothioic acid (PIN)
CH_3-B(NH-CH_3)(OH)	*B*,*N*-dimethylboronamidic acid (PIN)
CH_3-N(OH)(SH)	methylazonothious acid
$(C_2H_5)_2$P(S)(SH)	diethylphosphinodithioic acid (PIN)
$(CH_3)_2$N-P(O)$(OH)_2$	*N*,*N*-dimethylphosphoramidic acid (PIN)
$(C_6H_5)_2$P(=N-CH_3)(OH)	*N*-methyl-*P*,*P*-diphenylphosphinimidic acid (PIN)
C_6H_5-P(=N-C_6H_5)(Cl)(SH)	*N*,*P*-diphenylphosphonochloridimidodothioic acid (PIN)
C_6H_5-P(S)(NH-CH_3)(OH)	*N*-methyl-*P*-phenylphosphonamidothioic *O*-acid (PIN)
$CH_3)_2$N-P(O)(NCS)(SH)	*N*,*N*-dimethylphosphoramido(isothiocyanatido)thioic *S*-acid (PIN)
$(CH_3)_2$N-P(=N-C_6H_5)(SCN)(OH)	*N*,*N*-dimethyl-*N*′-phenylphosphoramidimido(thiocyanatidic) *O*-acid (PIN)
(C_6H_5)P(OH)(SH)	phenylphosphonothious *S*-acid (PIN)
C_6H_5-P(≡N)(OH)	phenylphosphononitridic acid (PIN)
C_6H_5-P(O)(Cl)(OH)	phenylphosphorochloridic acid (PIN)
CH_3-CH_2-P(Se)$(OH)_2$	ethylphosphonoselenoic *O*,*O*-acid (PIN)
CH_3-CH_2-P(O)(OH)(SeH)	ethylphosphonoselenoic *Se*-acid (PIN)
P(=NH)(NH-NH_2)$(OH)_2$	phosphorohydrazidimidic acid (preselected name)

$P(O)(OH)(SH)(SSH)$	phosphoro(dithioperoxo)thioic *S*-acid (preselected name)
$P(O)(OH)_2(OSH)$	phosphoro(thioperoxoic) *OS*-acid (preselected name)
$As(O)(OH)(SH)_2$ or $As(S)(OH)_2(SH)$	arsorodithioic acid (preselected name)
$As(S)(OH)_3$	arsorothioic *O*,*O*,*O*-acid (preselected name)
$(C_6H_5)_2As(SH)$	diphenylarsorothious acid (PIN)
$HO-SO_2-SH$	sulfurothioic *S*-acid (preselected name)
H_2N-SO_2-OH	sulfamic acid (preselected name) (a contraction of sulfuramidic acid)
$H_2S_2O_3$	sulfurothioic acid (preselected name; the position of the sulfur atom is undetermined)
$HO-SO_2-NC$	sulfurisocyanidic acid (preselected name)
$HO-SO-NCS$	sulfuro(thiocyanatidic) acid (preselected name)
$HO-SO_2-CN$	sulfurocyanidic acid (preselected name)
$HS-SO_2-NH_2$	sulfamothioic *S*-acid (preselected name) sulfuramidothioic *S*-acid
$HS-TeO_2-NH_2$	telluramidothioic acid (preselected name)

P-67.1.2.4.2.2 Examples of acids modified by prefixes**:**

$Si(OH)_3(SH)$	thiosilicic acid (preselected name)
$S=N-OH$	thionitrous *O*-acid (preselected name)
$Cl(S)_2-OH$	dithiochloric *O*-acid (preselected name)

P-67.1.2.4.2.3 Specific use of the prefix 'cyanato' and the infix 'cyanatido'

When attached to the central atom of an oxo acid, the group −OCN creates an anhydride linkage (see P-67.1.3.3). In order to respect the seniority order of classes, this group is used, therefore, in functional replacement nomenclature to name acids; acids are senior to anhydrides. For the prefixes 'cyanato', 'thiocyanato', 'selenocyanato' and 'tellurocyanato', see P-65.2.2.

Examples:

CH_3-P(OCN)OH	methylphophonocyanatidic acid (PIN)
P(O)$(OCN)_2$OH	phosphorodicyanatidic acid (PIN)
Si(OCN)$(OH)_3$	cyanatosilicic acid

P-67.1.2.4.3 Comment on name construction. The names phosphonous, phosphinous, phosponic and phosphinic acid (and similarly for arsenic and antimony acids) can only be used when P, As or Sb is attached to atoms of hydrogen, carbon or another atom of a parent hydride such as N, As, Si. Thus, C_6H_5-P(O)Cl(OH) is phenylphosphonochloridic acid and not chlorophenylphosphinic acid; $(C_5H_{10}N)$-P(O)Cl(OH) is piperidin-1-ylphosphonochloridic acid and not chloropiperidin-1-yl-phosphinic acid; and ClP(O)$(OH)_2$ is phosphorochloridic acid and not chlorophosphonic acid.

P-67.1.2.5 Acid halides and pseudohalides

Except for the boron acids and silicic acid, preferred IUPAC names of acid halides and pseudohalides are formed by adding the class name(s) of a halide or pseudohalide to that of the acid. Exceptionally, in accordance with tradition and the recommended nomenclature of inorganic compounds (ref. 14), halides and pseudohalides formed of identical atoms or groups derived from phosphoric acid, sulfuric acid, selenic acid and telluric acid are named by adding the class name(s) to the acyl group name 'phosphoryl', 'sulfuryl', 'sulfamoyl', 'selenonyl' and 'telluronyl', and not to the name of the acid itself. In accordance with the seniority order of halides and pseudohalides, names are formed on the basis of the senior class, as described in P-67.1.2.1.

Preferred IUPAC names of acid halides and pseudohalides derived from the boron acids and silicic acid are formed on the basis of the parent hydride names borane and silane, respectively..

Examples:

CH_3-N(O)-Cl_2	methylazonic dichloride
P(O)$(NCO)_3$	phosphoryl triisocyanate (PIN)
$(C_6H_5)_2$P-Cl	diphenylphosphinous chloride (PIN)
$(C_6H_5)_2$Sb-NCO	diphenylstibinous isocyanate (PIN)
C_6H_5-PCl_2	phenylphosphonous dichloride (PIN)

C_6H_5-PBrCl	phenylphosphonous bromide chloride (PIN) phenylphosphonobromidous chloride
$(C_6H_5)_2P(=N-C_6H_5)Cl$	*N*,*P*,*P*-triphenylphosphinimidic chloride (PIN)
$(CH_3-CH_2)_2P(S)Cl$	diethylphosphinothioic chloride (PIN)
$C_6H_5-P(O)Cl_2$	phenylphosphonic dichloride (PIN)
$CH_3-CH_2-P(O)[N(CH_3)_2]Cl$	*P*-ethyl-*N*,*N*-dimethylphosphonamidic chloride (PIN)
$(CH_3)_2N-P(O)(NCO)Cl$	*N*,*N*-dimethylphosphoramidisocyanatidic chloride (PIN)
$HP(O)(NCO)_2$	phosphonic diisocyanate (PIN)
$P(=NH)(NCS)_3$	phosphorimidic tris(isothiocyanate) (PIN)
$(CH_3)_2PN_3$	dimethylphosphinous azide (PIN)
$SO_2(NCO)_2$	sulfuryl diisocyanate (PIN)
$S(=NH-CH_3)-Cl_2$	*N*-methylsulfurimidous dichloride (PIN)
$F-SO_2-NCO$	sulfurisocyanatidic fluoride (PIN)
F-S(=NH)(NCO)	sulfurimidisocyanatidous fluoride (PIN)
$CH_3-NH-SO_2Cl$	*N*-methylsulfamoyl chloride (PIN)
C_6H_5-B(Cl)(Br)	chloro(bromo)phenylborane (PIN) phenylboronic bromide chloride phenylboronobromidic chloride

$SiCl_4$	tetrachlorosilane (preselected name) (not silicic tetrachloride) silicon tetrachloride

P-67.1.2.6 Amides and hydrazides

Amides and hydrazides are named by functional class nomenclature by replacing the term ‘acid’ in the name of the corresponding acid by ‘amide’ or ‘hydrazide’. Amides and hydrazides of nitric acid and nitrous acid have been discussed in P-61.5.3; azorous acid, azinous acid and azonous acid.are exceptions discussed below. Preferred IUPAC names of amides and hydrazides are denoted by the class name ‘amide’ or ‘hydrazide’:

(a) when all –OH groups in the corresponding acid have been replaced by $-NH_2$ or $-NH-NH_2$ groups, and

(b) when the amide or hydrazide is the principal functional group in accordance with the following order of seniority:

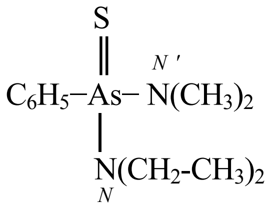
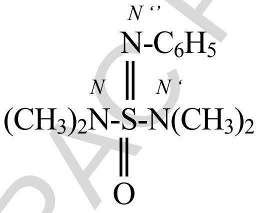
Br, Cl, F, I, N_3, CN, NC, NCO, ONC, $\boxed{NH_2 \text{ (amide)}, \overset{1}{N}H\overset{2}{N}H_2 \text{ (hydrazide)}}$

> Note that this order is not quite the same as that used by CAS (where amide follow the halogens and precedes the pseudohalogens) but it is consistent with the order of compound classes in P-41.

Substituents on the nitrogen atoms are denoted by letter locants such as, *N* (primed and double primed as required), in addition to *P, As,* and *Sb*. Locants to denote hydrazides are 1 and 2, primed and double primed as required.

Examples:

$[(CH_3)_2N]_3PO$	hexamethylphosphoric triamide (PIN) hexamethylphosphoramide (not phosphoric tris(dimethylamide)
$(CH_3)_2P(O)[N(CH_3)_2]$	*N*,*N*,*P*,*P*-tetramethylphosphinic amide (PIN) (not dimethylphosphinic dimethylamide)
$C_6H_5-P(O)(NHCH_3)_2$	*N*,*N*′-dimethyl-*P*-phenylphosphonic diamide (PIN) (not phenylphosphonic bis(methylamide)
$C_6H_5-P(S)[N(CH_3)_2]_2$	*N*,*N*,*N*′,*N*′-tetramethyl-*P*-phenylphosphonothioic diamide (PIN)

$C_6H_5\text{-}Sb(S)[N(CH_3)_2][N(CH_2\text{-}CH_3)_2]$	*N*,*N*-diethyl-*N*′,*N*′-dimethyl-*Sb*-phenylstibonothioic diamide (PIN)
$(CH_3)_2N\text{-}P(O)Cl_2$	*N*,*N*-dimethylphosphoramidic dichloride (PIN)
 $C_6H_5\text{-}\underset{\underset{\underset{N}{N(CH_2\text{-}CH_3)_2}}{\vert}}{\overset{\overset{S}{\Vert}}{As}}\text{-}\overset{N'}{N}(CH_3)_2$	*N*,*N*-diethyl-*N*′,*N*′-dimethyl-*As*-phenylarsonothioic diamide (PIN)
$P(O)[\overset{1,1',1''}{N}(CH_3)\text{-}\overset{2,2',2''}{NH_2}]_3$	1,1′,1″-trimethylphosphoric trihydrazide (PIN)
$P(S)[\overset{1,1',1''}{NH}\text{-}\overset{2,2',2''}{N}(CH_3)_2]_3$	2,2,2′,2′,2″,2″-hexamethylphosphorothioic trihydrazide (PIN) (not phosphorothioic tris(2,2-dimethylhydrazide)
$CH_3\text{-}\overset{N}{NH}\text{-}SO\text{-}\overset{N'}{NH_2}$	*N*-methylsulfurous diamide (PIN)
$(CH_3)_2\overset{N}{N}\text{-}SO_2\text{-}\overset{N'}{NH_2}$	*N*,*N*-dimethylsulfuric diamide (PIN) (not *N*,*N*-dimethylsulfamide)
$(CH_3)_2\overset{N}{N}\text{-}S(=\overset{N''}{N}CH_3)\text{-}\overset{N'}{N}(CH_3)_2$	pentamethylsulfurimidous diamide (PIN)
$CH_3\text{-}NH\text{-}S(O)(=N\text{-}CH_3)\text{-}Br$	*N*,*N*′-dimethylsulfurimidic bromide (PIN)
 $(CH_3)_2\overset{N}{N}\text{-}\underset{\underset{O}{\Vert}}{\overset{\overset{\overset{N''}{N\text{-}C_6H_5}}{\Vert}}{S}}\text{-}\overset{N'}{N}(CH_3)_2$	*N*,*N*,*N*′,*N*′-tetramethyl-*N*″-phenylsulfurimidic diamide (PIN)
$B(NH_2)_3$	boric triamide (preselected name) (not boranetriamine)

$B(\overset{1,1',1''}{N}H\text{-}\overset{2,2',2''}{N}H_2)_3$	boric trihydrazide (preselected name) (not 1,1′,1″-boranetriyltris(hydrazine)
$Si(NH_2)_4$	silicic tetramide (preselected name) (not silanetetramine)
$Si(\overset{1}{N}H\text{-}\overset{2}{N}H_2)_4$	silicic tetrahydrazide (preselected name) (not 1,1′,1″,1‴-silanetetrayltetrakis(hydrazine)

Exceptions: names of amides and hydrazides of azorous acid, azinous acid and azonous acid are exceptions to the general rule. They are named as di- and polyazanes.

Examples:

$H_2N\text{-}N(NH_2)\text{-}NH_2$	2-aminotriazane (preselected name) (not azorous trimide)
$H_2N\text{-}NH_2$	hydrazine (retained name) (not azinous amide)
$H_2N\text{-}NH\text{-}NH_2$	triazane (not azinous hydrazide)

P-67.1.3 Salts, esters and anhydrides

The methodology discussed in this section is applicable to all mononuclear oxo acids whether or not they have retained names or names using infixes or prefixes.

P-67.1.3.1 Salts
P-67.1.3.2 Esters
P-67.1.3.3 Anhydrides

P-67.1.3.1 Salts

Neutral salts of oxo acids are named by citing the cation(s) followed by the name of the anion as a separate word. Names of anions are formed by changing the ‘ic acid’ ending to ‘ate’ and the ‘ous acid’ ending to ‘ite’. Different cations are cited in alphabetical order.

Examples:

$Na_2(CH_3\text{-}PO_2)$	disodium methylphosphonite (PIN)
$K[(CH_3)_2As(O)O]$	potassium dimethylarsinate (PIN)

Acid salts of polybasic acids are named in the same way as neutral salts, the remaining acid hydrogen atom(s) being indicated by the word "hydrogen' (or 'dihydrogen', etc., as appropriate) ionserted between the name of the cation(s) and the name of the anion from which it is separated by spaces.

Example:

$Na^+ [B(OH)(OCN)(O^-)]$	sodium hydrogen borocyanatidate

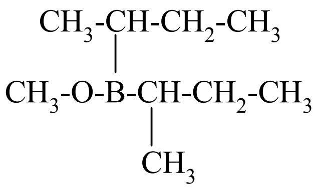
P-67.1.3.2 Esters

Esters of noncarbon acids are named in the same way as esters of organic acids (see P-65.6.3). Alkyl groups, aryl groups, etc. are cited as separate words, in alphanumerical order when more than one, and followed by the name of the appropriate anion. Partial (acid) esters of polybasic acids are named by citing alkyl groups, aryl groups, etc. as separate word, in alphanumeric order if more than one, followed by the word 'hydrogen' (with the appropriate multiplying prefix denoting multiplicity) also cited as a separate word, and the name of the appropriate anion. Salts of partial (acid esters) are named by citing the name of the cation before the name of the organic group; remaining acids groups are denoted by the word 'hydrogen' as described above. Structural specificity for esters of chalcogen acids is provided by the appropriate italic element symbols *O*, *S*, *Se*, and *Te*, prefixed to the name of the group, as needed.

Examples:

$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}O\text{-}NO$	pentyl nitrite (PIN)
$CH_3\text{-}S\text{-}NO_2$	*S*-methyl thionitrate
$(C_6H_5)_2P\text{-}O\text{-}CH_3$	methyl diphenylphosphinite (PIN)
$CH_3\text{-}P(Cl)(S\text{-}CH_2\text{-}CH_3)$	ethyl methylphosphonochloridothioite (PIN)
$CH_3\text{-}P(NH\text{-}CH_3)(OCH_3)$	methyl *N*,*P*-dimethylphosphonamidite (PIN)
$P(OCH_3)_3$	trimethyl phosphite (PIN)
$P(Cl)[N(CH_3)_2](O\text{-}CH_3)$	methyl *N*,*N*-dimethylphosphoramidochloridite (PIN)
$P(O)(CH_3)_3$	trimethyl phosphate (PIN)
$P(O)(O\text{-}C_2H_5)(O\text{-}CH_3)(O\text{-}C_6H_5)$	ethyl methyl phenyl phosphate (PIN)

$\mathrm{P(O)(O{-}CH_3)(OH)_2}$	methyl dihydrogen phosphate (PIN)
$\mathrm{C_6H_5{-}HAs(S)(O{-}CH_3)}$	*O*-methyl phenylarsinothioate
$\mathrm{CH_3{-}O{-}P(O)(OH){-}O^{-}\ Na^{+}}$	sodium methyl hydrogen phosphate (PIN)
$\mathrm{HP(O)(O{-}CH_3)_2}$	dimethyl phosphonate (PIN)
$\mathrm{(CH_3{-}CH_2)_2P(S)(S{-}CH_2{-}CH_3)}$	ethyl diethylphosphinodithioate (PIN)
$\mathrm{(CH_3)_2As(O)(S{-}CH_3)}$	*S*-methyl dimethylarsinothioate (PIN)
$\mathrm{CH_3{-}P(O)(O{-}CH_2{-}CH_3)_2}$	diethyl methylphosphonate (PIN)
$\mathrm{C_6H_5{-}P(O)(O{-}CH_3)(S{-}CH_2{-}CH_3)}$	*S*-ethyl *O*-methyl phenylphosphonothioate (PIN)
$\mathrm{C_6H_5{-}P(O)(Cl)(O{-}CH_3)}$	methyl phenylphosphonochloridate (PIN)
$\mathrm{(CH_3)_2N{-}P(O)(O{-}CH_3)_2}$	dimethyl *N*,*N*-dimethylphosphoramidate (PIN)
$\mathrm{(CH_3{-}CH_2)_2N{-}P(O)(NCS)(O{-}CH_2{-}CH_3)}$	ethyl *N*,*N*-diethylphosphoramido(isothiocyanatidate) (PIN)
$\mathrm{As(O)(F)(O{-}CH_3)_2}$	dimethyl arsorofluoridate (PIN)
$\mathrm{Sb(O)(F_2)(S{-}CH_3)}$	*S*-methyl stiborodifluoridothioate (PIN)
$\mathrm{(CH_3)_2B{-}O{-}C_6H_5}$	phenyl dimethylborinate (PIN)
$\mathrm{CH_3{-}O{-}SO_2{-}OH}$	methyl hydrogen sulfate (PIN)
$\mathrm{C_6H_5{-}O{-}F}$	phenyl hypofluorite (PIN)
$\mathrm{CH_3{-}S{-}Cl}$	methyl thiohypochlorite (PIN)
$\mathrm{CH_3{-}CO{-}CH_2{-}CH_2{-}O{-}BrO_2}$	3-oxobutyl bromate (PIN)



$$\begin{array}{l} \mathrm{CH_3\text{-}CH\text{-}CH_2\text{-}CH_3} \\ \qquad | \\ \mathrm{CH_3\text{-}O\text{-}B\text{-}CH\text{-}CH_2\text{-}CH_3} \\ \qquad\quad | \\ \qquad\quad \mathrm{CH_3} \end{array}$$

methyl bis(1-hydroxypropan-2-yl)borinate (PIN)

$Si(S-CH_3)_3(O-CH_2-CH_3)$	O-ethyl *S,S,S*-trimethyl silicate (PIN)

P-67.1.3.2 Anhydrides

Neutral anhydrides formed between acids named by suffixes and mononuclear oxoacids described in P-67.1.1 are named in the way described for anhydrides derived from carboxylic acids and sulfur acids named by suffixes (see P-65.7). The names of the acids are cited in alphabetical order followed by the name of the class ‘anhydride’ prefixed by a numerical term indicating the number of anhydride linkages (the numerical prefix mono is not used); such names lead to preferred IUPAC names rather than names formed acyl groups substituting the name of the phosphorus, arsenic or antimony oxoacid modified by the ending ‘ate’. Halogen oxoacids form anhydrides with acids expressed by suffixes.

Acidic anhydrides are named as described in P-67.3.1 by using the senior acid as parent, or by using systematic substitutive nomenclature.

Examples:

$(CH_3)_2B-O-CO-CH_3$	acetic dimethylborinic anhydride (PIN)
$CH_3-CO-O-As(O)(CH_3)_2$	acetic dimethylarsinic anhydride (PIN) acetyl dimethylarsinate
$[(CH_3)_2CH]_2Sb-S-C(S)-N(CH_2-CH_3)_2$	diethylcarbamothioic di(propan-2-yl)stibinous thioanhydride (PIN)
$B(O-CO-CH_3)_3$	triacetic boric trianhydride (PIN)
$C_6H_5-CO-O-I$	benzoic hypoiodous anhydride (PIN)
$(CH_3)_2B-O-O-B(CH_3)_2$	dimethylborinic peroxyanhydride (PIN)
$B(OCN)_3$	tricyanic boric trianhydride (PIN)
$CH_3-HP(O)(OCN)$	cyanic methylphosphinic anhydride (PIN)

P-67.1.4 Substitutent prefix groups

P-67.1.4.1 Substituent groups derived from nitrogen, phosphorus, arsenic, and antimony acids

P-67.1.4.1.1 Substituent prefix groups have retained names and systematic names corresponding to simple or compound acyl groups. The preselected names are formed by applying the following seniority order, in the order given, until a decision is reached.

(a) Retained names

A few names denoting monovalent acidic groups are retained These names are preselected names when unsubstituted or for chalcogen analogues when the position of chalcogen atoms introduced by functional replacement is not known or it is not necessary to specify their position(s): the chalcogen atoms are expressed by prefixes.

$-N(O)(OH)_2$	azono (preselected name)
$-P(O)(OH)_2$	phosphono (preselected name)
$-As(O)(OH)_2$	arsono (preselected name)
$-Sb(O)(OH)_2$	stibono (preselected name)
$-P(O)(OH)(SH)$ or $-P(S)(OH)_2$	thiophosphono (preselected name)
$-P(S)(SH)_2$	trithiophosphono (preselected name)

(b) Basic acyl groups

Acyl prefix groups are formed by removing all -OH groups from an oxo acid having the general structures $E(=O)(OH)_3$, $R\text{-}E(=O)(OH)_2$ or $R,R'E(=O)OH$, where R and R′ = H or an organyl group. Names of acyl groups derived from the names of acids, modified or not by functional replacement, by elimination of all hydroxy groups or their chalcogen analogues, are formed by changing the 'ic acid' ending in the name of the acid to 'oyl', with the exception of 'azoryl' (preferred to 'nitroryl' -N(O)<); 'phosphoryl', -P(O)<: 'arsoryl', -As(O)<; and 'stiboryl', -Sb(O)<. Names formed in this manner are preferred IUPAC names. For example, the group ‘phosphoryl’ −P(O)<, is derived from phosphoric acid, $P(O)(OH)_3$ or phosphorothioic *S*-acid, $P(O)(OH)_2(SH)$.

The name ‘azoryl’, for the acyl group >N(O)–, derived from the hypothetical acid $N(O)(OH)_3$, named azoric acid, has been recommended in 1993 (see R-3.3, ref. 2). The name ‘azoryl’ is the preferred IUPAC name; it is preferred to ‘nitroryl’.

Examples:

$N(O)(OH)_3$	azoric acid (preselected name) nitroric acid	>N(O)–	azoryl (preselected name) nitroryl
$P(O)(OH)_3$	phosphoric acid (preselected name)	>P(O)–	phosphoryl (preselected name)
$As(O)(OH)_3$	arsoric acid (preselected name) (not arsenic acid)	>As(O)–	arsoryl (preselected name) (not arsenyl)
$Sb(O)(OH)_3$	stiboric acid (preselected name) (not antimonic acid)	>Sb(O)–	stiboryl (preselected name) (not antimonyl)
$NH(O)(OH)_2$	azonic acid (preselected name)	>NH(O)	azonoyl (preselected name)
$NH_2(O)(OH)$	azinic acid (preselected name)	$-NH_2(O)$	azinoyl (preselected name)
$PH(O)(OH)_2$	phosphonic acid (preselected name)	>PH(O)	phosphonoyl (preselected name)
$PH_2(O)(OH)$	phosphinic acid (preselected name)	$-PH_2(O)$	phosphinoyl (preselected name)
$AsH(O)(OH)_2$	arsonic acid (preselected name)	>AsH(O)	arsonoyl (preselected name)

$AsH_2(O)OH$	arsinic acid (preselected name)	$-AsH_2(O)$	arsinoyl (preselected name)
$SbH(O)(OH)_2$	stibonic acid (preselected name)	$>SbH(O)$	stibonoyl (preselected name)
$SbH_2(O)OH$	stibinic acid (preselected name)	$-SbH_2(O)$	stibinoyl (preselected name)

(c) Names of substituted basic acyl groups

Names of substituted basic acyl groups are formed directly from those of the acids generated by the method described in P-67.1.2.2.1. Preferred IUPAC names of acyl groups are those derived from the preferred names of acids. The addition of hydrogen atoms to acyl groups by the method of concatenation, described in P-67.1.4.1.2, is not allowed.

Examples:

CH_3-$P(O)(OH)_2$	CH_3-$P(O)<$
methylphosphonoic acid (PIN)	methylphosphonoyl (PIN)
CH_3-CH_2-$SbH(O)OH$	CH_3-CH_2-$SbH(O)-$
ethylstibinic acid (PIN)	ethylstibinoyl (PIN)
C_6H_5-$As(CH_3)(O)OH$	C_6H_5-$As(CH_3)(O)-$
methyl(phenyl)arsenic acid (PIN)	methyl(phenyl)arsinoyl (PIN)

(d) Names of acyl groups modified by functional replacement nomenclature

Preferred IUPAC names are formed by the methodology indicated in Section P-65.2.1.5 for acyl groups derived from carbonic acids modified by the infixes and prefixes in functional replacement nomenclature. All infixes and prefixes listed in Table 1.6 and cited in P-65.2.1.5 are allowed. Applied to the B, N, P, As and Sb oxo acids, the method consists of achieving functional replacement in acids, then removing all remaining –OH groups. Preselected names use infixes to denote functional replacement.

Examples:

$P(S)(OH)_3$	$>P(S)-$
phosphorothioic *O*,*O*,*O*-acid (preselected name) thiophosphoric *O*,*O*,*O*-acid	phosphorothioyl (preselected name) thiophosphoryl

$As(=NH)(OH)_3$	$>As(=NH)-$
arsorimidic acid (preselected name)	arsorimidoyl (preselected name)
imidoarsoric acid	imidoarsoryl
$Sb(=NNH_2)(OH)_3$	$>Sb(=NNH_2)-$
stiborohydrazonic acid (preselected name)	stiborohydrazonoyl (preselected name)
hydrazonostiboric acid	hydrazonostiboroyl
$NH(S)(OH)_2$	$>NH(S)$
azonothioic acid (preselected name)	azonothioyl (preselected name)
thioazonic acid	thioazonoyl
$PH_2(=NH)(OH)$	$-PH_2(=NH)$
phosphinimidic acid (preselected name)	phosphinimidoyl (preselected name)
imidophosphinic acid	imidophosphinoyl
$(CH_3)_2P(Se)(OH)$	$(CH_3)_2P(Se)-$
dimethylphosphinoselenoic acid (PIN)	dimethylphosphinoselenoyl (PIN)
dimethyl(selenophosphinic acid)	dimethyl(selenophosphinoyl)
$C_6H_5\text{-}P(O)Cl(OH)$	$C_6H_5\text{-}P(O)(Cl)-$
phenylphosphonochloridic acid (PIN)	phenylphosphonochloridoyl (PIN)
phenyl(chlorophosphonic acid)	phenyl(chlorophosphonoyl)
$P(\equiv N)(OH)_2$	$>P(\equiv N)$
phosphoronitridic acid (preselected name)	phosphoronitridoyl (preselected name)
nitridophosphoric acid	nitridophosphoryl
$P(=NH)(NHNH_2)(OH)_2$	$>P(=NH)(NHNH_2)$
phosphorohydrazidimidic acid (preselected name)	phosphorohydrazidimidoyl (preselected name)
hydrazidimidophosphoric acid	hydrazidimidophosphoryl
$P(O)Cl_2(OH)$	$P(O)(Cl)_2-$
phosphorodichloridic acid (preselected name)	phosphorodichloridoyl (preselected name)
dichlorophosphoric acid	dichlorophosphoryl

$(CH_3)_2N\text{-}P(O)(OH)_2$

dimethylphosphoramidic acid (PIN)
(dimethylamido)phosphoric acid

$(CH_3)_2N\text{-}P(O)<$

dimethylphosphoramidoyl (PIN)
(dimethylamido)phosphoryl

$P(O)(OH)_2(OOH)$

phosphoroperoxoic acid (preselected name)
peroxyphosphoric acid

$>P(O)(OOH)$

phosphoroperoxoyl (preselected name)
peroxyphosphoryl

$P(O)(OH)_2(OSH)$ or $P(O)(OH)_2(SOH)$

phosphoro(thioperoxoic) acid (preselected name)
(thioperoxy)phosphoric acid

$>P(O)(OSH)$ or $>P(O)(SOH)$

phosphoro(thioperoxoyl) (preselected name)
(thioperoxy)phosphoryl

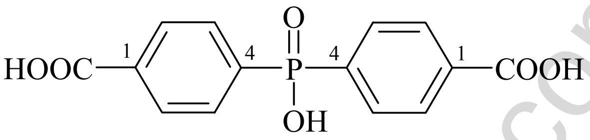
(e) Names of acyl groups and substituted acyl groups formed by concatenation

Concatenation is used to generate preferred IUPAC names or prselected names of acyl groups substituted by hydroxy groups or their chalcogen and peroxy analogues; this is the recommended method to reintroduce in substituent groups the hydroxyl groups and their chalcogen analogues or to introduce groups that are not treated as infixes in functional replacement nomenclature, such as '−OR', '−SR', etc. It is important to respect the concatenation procedure that is an additive operation using acyl groups only. The following acyl groups are allowed: basic acyl groups described in (b) above, substituted basic acyl groups described in (c) above, and acyl groups modified by functional replacement described in (d) above. Substitution of hydrogen atoms attached to the central atom (substitutable hydrogen) in the basic acyl groups described in (b) above is not allowed.

Examples:

$-NH(O)(OH)$	hydroxyazonoyl (preselected name)
$-P(Se)(OCH_3)_2$	dimethoxyphosphoroselenoyl (PIN) dimethoxy(selenophosphoryl)
$-P(O)(OH)(SH)$	hydroxy(sulfanyl)phosphoryl (preselected name)
$-P(O)(SH)_2$	bis(sulfanyl)phosphoryl (preselected name)
$-PH(O)(SeH)$	selanylphosphinoyl (preselected name)

–PH(S)(SH)	sulfanylphosphinothioyl (preselected name) sulfanyl(thiophosphinoyl)
>P(O)(OSH)	(sulfanyloxy)phosphoryl (preselected name) (*OS*-thiohydroperoxy)phosphoryl
–P(S)(SOH)	(hydroxysulfanyl)phosphorothioyl (preselected name) (*SO*-thiohydroperoxy)thiophosphoryl
CH_3-P(O)(OH)–	hydroxy(methylphosphonoyl) (PIN)



4,4′-(hydroxyphosphoryl)dibenzoic acid (PIN)

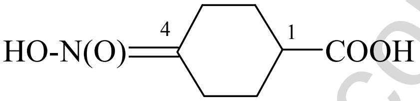
(f) Names formed by substitutive nomenclature

Substitutive nomenclature based on parent hydrides BH_3, PH_3, AsH_3, SbH_3, PH_5, AsH_5, and SbH_5 is used to generate names of substituent groups for which acyl group names cannot be generated by the methods in P-67.1.4.1.1.1 through P-67.1.4.1.1.5, for example ‘phosphonous acid’, ‘phosphinous acid’, and the corresponding As and Sb acids. It is also used to indicate a different type of free valencies, for example an ‘ylidene’ type instead of the ‘diyl’ observed in a substituent group derived from the acid in criteria (b) and (d).

Examples:

$-P(OH)_2$	dihydroxyphosphanyl (preselected name)
–AsH(OH)	hydroxyarsanyl (preselected name)
–AsHCl	chloroarsanyl (preselected name)
$-P(NH_2)$	diaminophosphanyl
>Sb(OH)	hydroxystibanediyl (preselected name)
=P(OH)	hydroxyphosphanylidene (preselected name)

=B(O-CH_3)	methoxyboranylidene (preselected name)
–P(O-CH_3)$_2$	dimethoxyphosphanyl (PIN)
=P(O)(OH)	hydroxy(oxo)-λ^5-phosphanylidene (preselected name)
=As(O)(OCH_3)	methoxy(oxo)-λ^5-arsanylidene (PIN)
=N(O)OH	4-[hydroxy(oxo)-λ^5-azanylidene] (preselected name) (no longer *aci*-nitro; see P-67.1.6)



4-[hydroxy(oxo)-λ^5-azanylidene]cyclohexane-1-carboxylic acid (PIN)
(see *aci*-nitro compounds, P-67.1.6)

P-67.1.4.1.2 The prefix hydro may be added by concatenation for use in general nomenclature only.

Examples:

>PH(O)	hydrophosphoryl phosphonoyl (preselected name)
>PH(S)	hydro(thiophosphoryl) phosphonothioyl (preselected name)

P-67.1.4.1.3 Compound and complex substituent groups

If a B, N, P, As, or Sb containing group is attached by an oxygen or other chalcogen atom or a nitrogen atom to a compound that also contains another substituent having priority over the B, N, P, As, or Sb containing group for citation as principal group, then the B, N, P, As, or Sb containing group is named by a compound or complex prefix built from prefixes described above and arranged in the order in which the components occur in the compound.

Examples:

$(HO)_2P(O)\text{-}O\text{-}CH_2\text{-}COOH$

2-(phosphonooxy)acetic acid (PIN)

$(CH_3O)_2P(O)\text{-}S\text{-}CH_2\text{-}CH_2\text{-}COOH$

3-[(dimethoxyphosphoryl)sulfanyl]propanoic acid (PIN)

$(HO)(HS)P(S)\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}COOH$

3-{[hydroxy(sulfanyl)phosphorothioyl]amino}propanoic acid (PIN)

P-67.1.4.2 Substituent groups derived from the boron acids and silicic acid

All substituent groups from boron and silicon mononuclear compounds are all formed by substituting the parent hydride names ‘borane’ and ‘silane’. The name borono, for $–B(OH)_2$, is retained and in the preferred IUPAC name.

The name boryl has been used for the substituent group $H_2B–$, now named boranyl as the preferred IUPAC name, and consequently is not be used for the prefix group derived from boric acid by removal of all three –OH groups.

Examples:

$–B(OH)_2$

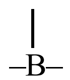
borono (preselected name)

$–BH_2$

boranyl (preselected name)
(not borinoyl)

$>BH$

boranediyl (preselected name)
(not boronoyl)



$–\overset{|}{B}–$

boranetriyl (preselected name)
(not boryl)

$=BH$

boranylidene (preselected name)
(not boronoyl)

$\equiv B$

boranylidyne (preselected name)
(not boryl)

$–B(NH_2)_2$

diaminoboranyl (preselected name)
(not borodiamidoyl)_

$–BH(O\text{-}CH_3)$

methoxyboranyl (PIN)
(not hydromethoxyboryl)

$-Si(OH)_3$
trihydroxysilyl (preselected name)

$-Si(OH)_2(SH)$
dihydroxy(sulfanyl)silyl (preselected name)

$-SiCl_2(NH_2)$
aminodichlorosilyl (preselected name)

$-Si(O\text{-}CH_3)_3$
trimethoxysilyl (PIN)

P-67.1.4.3 Substituent groups derived from nitric acid, nitrous acid, and the analogous phosphorus and arsenic acids.

The names ‘nitro’, ‘nitroso’, phospho, phosphoroso, arso, and arsoroso are used to denote the groups $-NO_2$, $-NO$, $-PO_2$, $-PO$, $-AsO_2$, and AsO, respectively. These names can be modified by functional replacement nomenclature using prefixes. These prefixes are treated as compulsory prefixes (see P-61.5). Traditionally, the groups ‘nitro’ and ‘nitroso’ are added to a nitrogen atom, thus constituting an exception to the principle of using the longest possible chain as parent hydride.

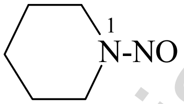
Examples:

$-N{=}S$
thionitroso (PIN)

$-O\text{-}NO_2$
nitrooxy (PIN)

$-S\text{-}N{=}S$
(thionitroso)sulfanyl (PIN)

$-NH\text{-}NO_2$
nitramido (PIN)



1-nitrosopiperidine (PIN)

$CH_3\text{-}O\text{-}P(O)_2$
(phosphooxy)methane (PIN)
methoxy-λ^5-phosphanedione
(formerly methyl metaphosphate)

P-67.1.4.4 Substituent groups derived from chalcogen acids

P-67.1.4.4.1 Acyl groups

There are two methods to generate names of acyl groups derived from the chalcogen acids for use as substituent groups.

(1) The methodology described in P-65.3.2.3 in which infixes denote functional replacement by –S-, -Se-, -Te-, =NH, and $=NNH_2$, and concatenation is used for other atoms or groups.

(2) The general method described in P-65.2.1.5 for deriving acyl groups from derivatives of carbonic acid, and applied in P-67.1.4.1.2.2 for acyl groups derived from phosphoric, phosphonic and phosphinic acids and their arsenic and antimony congeners is applied to sulfuric acid and its functional replacement analogues.

Method (1) produces preselected names.

Examples:

$–SO_2–$	sulfonyl (preselected name) sulfuryl
–S(O)(S)–	sulfonothioyl (preselected name) sulfurothioyl
$–S(S)_2–$	sulfonodithioyl (preselected name) sulfurodithioyl
–S(O)(=NH)–	sulfonimidoyl (preselected name) sulfurimidoyl
$–S(=NH)_2–$	sulfonodiimidoyl (preselected name) sulfurodiimidoyl
$–S(O)(=NNH_2)–$	sulfonohydrazonoyl (preselected name) sulfurohydrazonoyl
$–S(=NNH_2)_2–$	sulfonodihydrazonoyl (preselected name) sulfurodihydrazonoyl
$–SO_2$-Cl	chlorosulfonyl (preselected name) sulfurochloridoyl
$–SO_2$-CN	cyanosulfonyl (PIN) sulfurocyanidoyl
$–SO_2$-NCS	isothiocyanatosulfonyl (PIN) sulfuroisothiocyanatidoyl
–S(O)(S)-NCS	isothiocyanatosulfonothioyl (PIN) sulfuro(isothiocyanatido)thioyl
$–SO_2$-O-CH_3	methoxysulfonyl (PIN) methoxysulfuryl

–S(=O)-Cl chlorosulfinyl (preselected name)

Method (2) cannot be applied to sulfurous acid, selenic acid and selenous acid, and telluric acid and tellurous acid, because of ambiguous results.

P-67.1.4.4.2 If a sulfur containing group is attached by oxygen (chalcogen) or nitrogen to a compound that contains also another substituent having priority over the sulfur-containing group for citation as principal group, then the sulfur-containing group is named by an appropriate prefix as described in P-65.3 and P-67.1.4.4.1.
Examples:

$HO\text{-}SO_2\text{-}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

3-(sulfooxy)propanoic acid (PIN)

$CH_3O\text{-}SO\text{-}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

3-[(methoxysulfinyl)oxy]propanoic acid (PIN)

$Cl\text{-}\overset{3}{S}O_2\text{-}\overset{2}{O}\text{-}\overset{1}{C}H_2\text{-}CH_2\text{-}COOH$

3-[(chlorosulfonyl)oxy]propanoic acid (PIN)
3-(sulfurochloridoyloxy)propanoic acid

$H_2N\text{-}SO_2\text{-}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

3-(sulfamoyloxy)propanoic acid (PIN)
3-(sulfuramidoyloxy)propanoic acid
[not (sulfonamidoyloxy)propanoic acid; the name sulfonamidic acid is not an approved name]

$H_2N\text{-}SO\text{-}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$

3-[(aminosulfinyl)oxy]propanoic acid (PIN)
[not 3-(sulfinamidoyloxy)propanoic acid; the name sulfinamidic acid is not an approved name]

$CH_3O\text{-}SO_2\text{-}NH\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$ (PIN)

3-[(methoxysulfonyl)amino]propanoic acid

P-67.1.4.5 Substituent groups derived from halogen acids

Names of prefixes derived from halogen acids and their chalcogen analogues are used as compulsory prefixes in substitutive nomenclature. They are listed in Table 5.1 and discussed in P-61.3.2.

OCl–	chlorosyl (preselected name)
SCl–	thiochlorosyl (preselected name)
O_2Cl–	chloryl (preselected name)
O_3Cl–	perchloryl (preselected name)

The corresponding Br, F and I groups are named in a similar manner..

Example:

C_6H_5-BrO	bromosylbenzene (PIN)

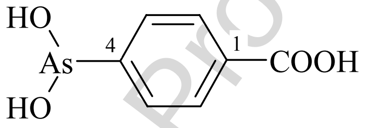
P-67.1.5 Seniority order for inorganic acids and their derivatives

P-67.1.5.1 When a characteristic group having priority to be cited as principal group is present (see seniority order of classes, P-42, and of acids, P-44), prefixes having retained names or names systematically formed (see Tables 6.3 and 6.4) are used to denote inorganic acids.

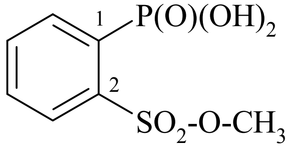
Examples:

$(HO)_2P(O)$-CH_2-COOH

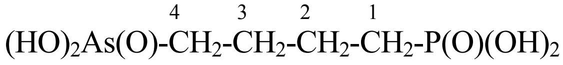
phosphonoacetic acid (PIN)



(dihydroxyarsanyl)benzoic acid (PIN)
[-COOH is senior to -$As(OH)_2$]



2-[(methoxysulfonyl)phenyl]phosphonic acid (PIN)
(an acid is senior to an ester)



$$(HO)_2As(O)\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}P(O)(OH)_2$$

(4-arsonobutyl)phosphonic acid (PIN)
(a phosphorus acid is senior to an arsenic acid)

C_6H_5-SO_2-N=P(NH-C_6H_5)$_3$

N-[tris(phenylamino)-λ^5-phosphanylidene]benzenesulfonamide (PIN)
(not *N*,*N′*,*N″*-triphenyl-*N‴*-benzenesulfonylphosphorimidic triamide;
nor *N‴*-benzenesulfonylphosphorimidic tris(phenylamide)

P-67.1.5.2 When derivatives of mononuclear acids are named by functional class nomenclature, the seniority order is established in accordance with the greater number of atoms linked to the central atom and appearing as early as possible in the list: O, OO, S, Se, Te for the acids, then F, Cl, Br, I, then the pseudohaliodes in the order N_3, CN, NC, NCO, NCS, NCSe, NCTe, then amides and hydrazides.

Examples:

Br_2P(O)-CH_2-CH_2-P(O)Cl_2

(2-phosphorodibromidoylethyl)phosphonic dichloride (PIN)
(Cl is senior to Br in the seniority order of classes)

Br_2P(O)-CH_2-CH_2-P(S)Cl_2

(2-phosphorodichloridothioylethyl)phosphonic dibromide (PIN)
(phosphonic dibromide is preferred to phosphonothioic dichloride;
O > S is considered before Cl > Br)

Cl_2P(O)-O-CH_2-CH_2-O-P(O)Cl(NH_2)

2-(phosphoramidochloridoyloxy)ethyl phosphorodichloridate (PIN)
(phosphorodichloridic acid preferred to phosphoramidochloridic acid)

P-67.1.6 *aci*-Nitro compounds

aci-Nitro compounds deserve a special mention. They are tautomers of nitro compounds and have the general structure R=N(O)OH or R_2N(O)OH and are named as derivatives of azinic acid, H_2N(O)OH. The substitutive prefix '*aci*-nitro' is no longer recommended to denote the principal characteristic group.

Example:

CH_2=N(O)-OH

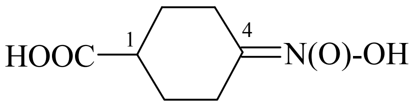
methylideneazinic acid (PIN)
(no longer *aci*-nitromethane)

When needed, the R_2N(O)− group is designated by a prefix derived from 'azinoyl', that is preferred to 'nitroryl' (see P-67.1.4.1.5). The group =N(O)OH is named 'hydroxy(oxo)-λ^5-azanylidene'.

Examples:

$(CH_3)_2N(O)\text{-}CH_2\text{-}CN$

(dimethylazinoyl)acetonitrile (PIN)
[not (dimethylnitroryl)acetonitrile]



4-[hydroxy(oxo)-λ^5-azanylidene]cyclohexane-1-carboxylic acid (PIN)
(formerly *aci*-nitro)

P-67.2 Polynuclear noncarbon acids

Like mononuclear acids, polynuclear acids have retained names that are used as preselected names. Substitutive or additive names are not recommended. Retained names are used as parents and are modifiable by functional replacement in the same manner that mononuclear acids are, except that only prefixes are used for functional replacement.

Di- and polynuclear acids, whose central atoms are B, P, As, Sb, S, Se, are described here. They are divided into three types. Di- and trinuclear are exemplified for each central atom. In some cases higher polynuclear acids are known. Their names are formed by using the appropriate multiplying prefixes to indicate the number of central atoms. Di- and polynuclear noncarboxylic carbon acids are discussed in Sections P-65.2 and P-66.1.5.

Insofar as their structures are known and conform to those of the phosphorus acids, arsenic and antimony acids are named in the same way as those of phosphorus, with 'ars' and 'stib', respectively, in place of 'phosp'. Similarly, tellurium acids are named in the same way as those of selenium, by changing 'selen' to 'tellur' in the names of acids.

P-67.2.1 Preselected names

The following traditional names are retained as preselected names (for consistency in the names of polynuclear oxoacids, the numerical infix 'di' has been uniformly used in naming dinuclear 'hypo' acids). Although the 'meta' acids are for general nomenclature only, they are preferred IUPAC names if the structure is unknown.

$(HO)_2B\text{-}O\text{-}B(OH)_2$	diboric acid (preselected name)

$(HO)BH\text{-}O\text{-}BH(OH)$	diboronic acid (preselected name)
$(HO)HP(O)\text{-}O\text{-}HP(O)(OH)$	diphosphonic acid (preselected name)
$HO\text{-}PH\text{-}O\text{-}PH\text{-}OH$	diphosphonous acid (preselected name)
$(HO)_2P(O)\text{-}O\text{-}P(O)(OH)_2$	diphosphoric acid (preselected name)
$(HO)_2P\text{-}O\text{-}P(OH)_2$	diphosphorous acid (preselected name)
$HO\text{-}SeO_2\text{-}O\text{-}SeO_2\text{-}OH$	diselenic acid (preselected name)
$HO\text{-}SO_2\text{-}O\text{-}SO_2\text{-}OH$	disulfuric acid (preselected name
$HO\text{-}SO\text{-}SO\text{-}OH$	disulfurous acid (preselected name)
$(HO)_2(O)P\text{-}P(O)(OH)_2$	hypodiphosphoric acid (preselected name)
$(HO)_2P\text{-}P(OH)$	hypodiphosphorous acid (preselected name)
$HO\text{-}SO_2\text{-}SO_2\text{-}OH$	hypodisulfuric acid (preselected name) dithionic acid (see below for polythionic acids)
$[HAsO_3]_n = (\text{-}As(O)(OH)O\text{-})_n$	metaarsoric acid (preselected name; for general nomenclature only)
$[HAsO_2]_n = (\text{-}As(OH)O\text{-})_n$	metaarsorous acid (preselected name; for general nomenclature only)
$[HBO_{2n} = (\text{-}B(OH)O\text{-})_n$	metaboric acid (preselected name; for general nomenclature only)
$[HPO_3]_n = (\text{-}P(O)(OH)O\text{-})_n$	metaphosphoric acid (preselected name; for general nomenclature only)
$[HPO_2]_n = (\text{-}P(OH)O\text{-})_n$	metaphosphorous acid (preselected name; for general nomenclature only)
$[H_2SiO_3]_n = (\text{-}Si(OH)_2O\text{-})_n$	metasilicic acid (preselected name; for general nomenclature only)
$[HSbO_3]_n = (\text{-}Sb(O)(OH)O\text{-})_n$	metastiboric acid (preselected name; for general nomenclature only)

$[HSbO_2]_n$ = $(\text{-Sb(OH)O-})_n$	metastiborous acid (preselected name; for general nomenclature only)
(HO)HP(O)-O-HP(O)(OH)-O-HP(O)(OH)	triphosphonic acid (preselected name)
$(HO)_2P(O)\text{-}O\text{-}P(O)(OH)\text{-}O\text{-}P(O)(OH)_2$	triphosphoric acid (preselected name)
$HO\text{-}SeO_2\text{-}O\text{-}SeO_2\text{-}O\text{-}SeO_2\text{-}OH$	triselenic acid (preselected name)
$HO\text{-}SO_2\text{-}O\text{-}SO_2\text{-}O\text{-}SO_2\text{-}OH$	trisulfuric acid (preselected name)

P-67.2.2 Derivatives formed by functional replacement

P-67.2.2.1 General methodology

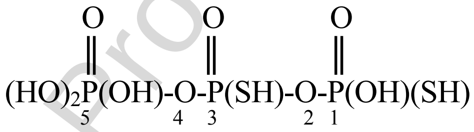
Prefixes are used to indicate functional replacement. They are listed in Table 4.2.. Each acid is numbered from one end to the other, starting from and finishing at a central atom. Prefixes are cited in alphabetical order in front of the retained name of the polyacid, with appropriate locants as required.

P-67.2.2.2 Replacement by –OO–, –S–, =S, –Se–, =Se, –Te–, =Te, –NH–, and =NH

Functional replacement of oxygen atom(s) is denoted by prefixes, i.e., peroxy, for –OO–; thio, for –S– or =S; seleno, for –Se– or =Se; telluro, for –Te– or =Te; and imido, for –NH– or =NH. The position of each replaced oxygen atom is denoted by the appropriate a numerical locant.

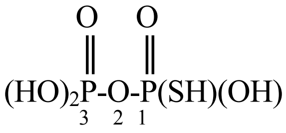
Italic letter locants *N*, *N'*, etc. are used to designate substitution on nitrogen atoms that are not linkages between central atoms (aza anhydrides).

Examples:



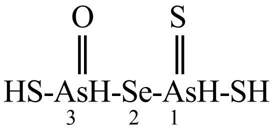
$(HO)_2\underset{5}{\overset{\overset{O}{\|}}{P}}(OH)\text{-}\underset{4}{O}\text{-}\underset{3}{\overset{\overset{O}{\|}}{P}}(SH)\text{-}\underset{2}{O}\text{-}\underset{1}{\overset{\overset{O}{\|}}{P}}(OH)(SH)$

1,3-dithiotriphosphoric 1-*S*,3-*S*-acid (preselected name)



$(HO)_2\underset{3}{\overset{\overset{O}{\|}}{P}}\text{-}\underset{2}{O}\text{-}\underset{1}{\overset{\overset{O}{\|}}{P}}(SH)(OH)$

1-thiodiphosphoric 1-*S*-acid
(preselected name)

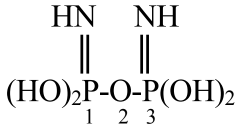


$HS\text{-}\underset{3}{\overset{\overset{O}{\|}}{As}}H\text{-}\underset{2}{Se}\text{-}\underset{1}{\overset{\overset{S}{\|}}{As}}H\text{-}SH$

2-seleno-1,1,3-trithiodiarsonic 3-*S*-acid
(preselected name)

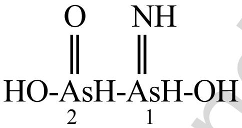
$\text{HS-}\underset{3}{\text{P}}\text{H(O)-}\underset{2}{\text{O}}\text{-}\underset{1}{\text{P}}\text{H(S)-OH}$

1,3-dithiodiphosphonic 1-*O*,3-*S*-acid (preselected name)



$(\text{HO})_2\overset{\text{HN}}{\overset{\|}{\underset{1}{\text{P}}}}\text{-}\underset{2}{\text{O}}\text{-}\overset{\text{NH}}{\overset{\|}{\underset{3}{\text{P}}}}(\text{OH})_2$

1,3-diimidodiphosphoric acid
(preselected name)



$\text{HO-}\overset{\text{O}}{\overset{\|}{\underset{2}{\text{As}}}}\text{H-}\overset{\text{NH}}{\overset{\|}{\underset{1}{\text{As}}}}\text{H-OH}$

1-imidohypodiarsonic acid
(preselected name)

$\text{HO-}\overset{3}{\text{S}}\text{O}_2\text{-}\overset{2}{\text{O}}\text{-}\overset{1}{\text{S}}\text{O}_2\text{-SH}$

1-thiodisulfuric 1-*S*-acid
(preselected name)

$\text{H}_2\text{N-}\overset{3}{\text{S}}\text{O}_2\text{-}\overset{2}{\text{O}}\text{-}\overset{1}{\text{S}}\text{O}_2\text{-SeH}$

3-amido-1-selenodisulfuric 1-*Se*-acid
(preselected name)

$\text{HO-}\overset{1}{\text{S}}\text{O}_2\text{-}\overset{2}{\text{S}}\text{-}\overset{3}{\text{S}}\text{O}_2\text{-OH}$

2-thiodisulfuric acid (PIN)
sulfanedisulfonic acid
trithionic acid (traditional name)

$\text{HO-}\overset{1}{\text{S}}\text{O}_2\text{-}\overset{2}{\text{S-S}}\text{-}\overset{3}{\text{S}}\text{O}_2\text{-OH}$

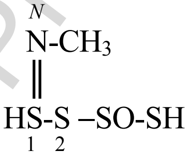
2-(dithioperoxy)disulfuric acid (PIN)
disulfanedisulfonic acid
tetrathionic acid (traditional name)

$\text{HO-}\underset{1}{\text{S}}\text{O}_2\text{-}\underset{2}{\text{N}}\text{H-}\underset{3}{\text{S}}\text{O}_2\text{-}\underset{4}{\text{N}}\text{H-}\underset{5}{\text{S}}\text{O}_2\text{-OH}$

2,4-diimidotrisulfuric acid
(preselected name)

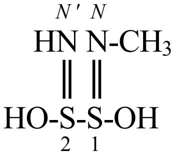
$\text{H}_2\overset{N}{\text{N}}\text{-}\underset{1}{\text{S}}\text{O}_2\text{-}\underset{2}{\text{N}}\text{H-}\underset{3}{\text{S}}\text{O}_2\text{-}\underset{4}{\text{N}}\text{H-}\underset{5}{\text{S}}\text{O}_2\text{-}\overset{N'}{\text{N}}\text{H}_2$

2,4-diimidotrisulfuric diamide
(preselected name)



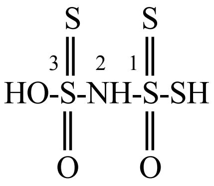
$\text{HS-}\overset{\overset{N}{\text{N-CH}_3}}{\overset{\|}{\underset{1}{\text{S}}}}\text{ –}\underset{2}{\text{S}}\text{O-SH}$

N-methyl-1-imido-1,2-dithiodithionous 2-*S*-acid
(preselected name)
(not 1-(methylimido)-1,2-dithionous 2-*S*-acid)



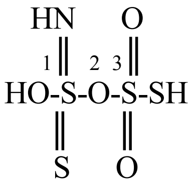
$\text{HO-}\overset{\overset{N'}{\text{HN}}}{\overset{\|}{\underset{2}{\text{S}}}}\text{-}\overset{\overset{N}{\text{N-CH}_3}}{\overset{\|}{\underset{1}{\text{S}}}}\text{-OH}$

N-methyl-1,2-diimidodithionous acid
(preselected name)



$$\text{HO-}\overset{\overset{\text{S}}{\|}}{\underset{\underset{\text{O}}{\|}}{\overset{3}{\text{S}}}}\text{-}\overset{2}{\text{NH}}\text{-}\overset{\overset{\text{S}}{\|}}{\underset{\underset{\text{O}}{\|}}{\overset{1}{\text{S}}}}\text{-SH}$$

2-imido-1,1,3-trithiodisulfuric 1-*S*,3-*O*-acid
(preselected name)



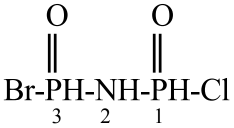
$$\text{HO-}\overset{\overset{\text{HN}}{\|}}{\underset{\underset{\text{S}}{\|}}{\overset{1}{\text{S}}}}\text{-}\overset{2}{\text{O}}\text{-}\overset{\overset{\text{O}}{\|}}{\underset{\underset{\text{O}}{\|}}{\overset{3}{\text{S}}}}\text{-SH}$$

1-imido-1,3-dithiodisulfuric 1-*O*,3-*S*-acid
(preselected name)

P-67.2.3 Acid halides and pseudohalides

Acid halides and pseudohalides, in which all OH groups have been replaced by halides or pseudohalide atoms or groups, are named by functional class nomenclature by replacing the name ‘acid’ by the name of the appropriate halide or pseudohalide. Halides are cited in alphabetical order. When halides and pseudohalides are present, the seniority order for selecting the principal class is as follows: halides (in alphabetical order), N_3, CN, NC, NCO, NCS, NCSe, NCTe.

Examples:



$$\text{Br-}\overset{\overset{\text{O}}{\|}}{\underset{3}{\text{PH}}}\text{-}\underset{2}{\text{NH}}\text{-}\overset{\overset{\text{O}}{\|}}{\underset{1}{\text{PH}}}\text{-Cl}$$

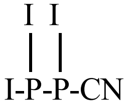
2-imidodiphosphonic bromide chloride
(preselected name)

$$\overset{1}{Cl_2P(O)}\text{-}\overset{2}{S}\text{-}\overset{3}{P(O)Cl_2}$$

2-thiodiphosphoric tetrachloride
(preselected name)

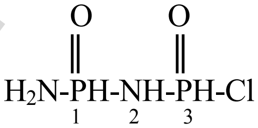
$$(OCN)_2\underset{1}{P}(O)\text{-}\underset{2}{O}\text{-}\underset{3}{P}(O)(NCO)_2$$

diphosphoric tetraisocyanate
(preselected name)



$$\text{I-}\overset{\overset{\text{I}}{|}}{\text{P}}\text{-}\overset{\overset{\text{I}}{|}}{\text{P}}\text{-CN}$$

cyanohypodiphosphorous triiodide
(preselected name)



$$H_2N\text{-}\overset{\overset{\text{O}}{\|}}{\underset{1}{\text{PH}}}\text{-}\underset{2}{\text{NH}}\text{-}\overset{\overset{\text{O}}{\|}}{\underset{3}{\text{PH}}}\text{-Cl}$$

1-amido-2-imidodiphosphonic chloride (preselected name)

$F\text{-}SO_2\text{-}NCO$

isocyanatosulfuric fluoride
(preselected name)

F-S-(=NH)-NCO

sulfurimidoisocyanatous fluoride
(preselected name)

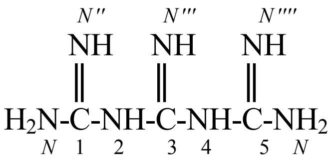
$CH_3–NH–SO_2–Cl$

methylsulfamoyl chloride (preselected name)

P-67.2.4 Amides and hydrazides

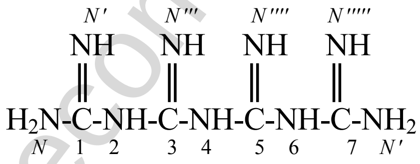
Polynuclear carbonic compounds in which all −OH groups have been replaced by $−NH_2$ or $−NHNH_2$ groups are named as amides or hydrazides, respectively by functional class nomenclature. The amide groups are expressed by the class name ‘amide’, preceded by an appropriate multiplying prefix, ‘di’, ‘tri’, etc. Amides of imidodicarbonimidic acid, diimidotricarboniimidic amide, etc., are biuret, triuret, etc., for which see P-66.1.5.6.1.2. Substituents are described by prefixes cited before the whole name, not in front of the class name.

Examples:



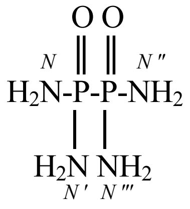
$H_2N\text{-}\overset{\overset{NH}{\|}}{C}\text{-}NH\text{-}\overset{\overset{NH}{\|}}{C}\text{-}NH\text{-}\overset{\overset{NH}{\|}}{C}\text{-}NH_2$

pentaimidotricarbonic diamide
(preselected name)



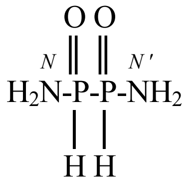
$H_2N\text{-}\overset{\overset{NH}{\|}}{C}\text{-}NH\text{-}\overset{\overset{NH}{\|}}{C}\text{-}NH\text{-}\overset{\overset{NH}{\|}}{C}\text{-}NH\text{-}\overset{\overset{NH}{\|}}{C}\text{-}NH_2$

heptaimidotetracarbonic diamide
(preselected name)



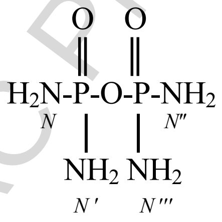
$H_2N\text{-}\underset{\underset{H_2N}{|}}{\overset{\overset{O}{\|}}{P}}\text{-}\underset{\underset{NH_2}{|}}{\overset{\overset{O}{\|}}{P}}\text{-}NH_2$

hypodiphosphoric tetraamide
(preselected name)



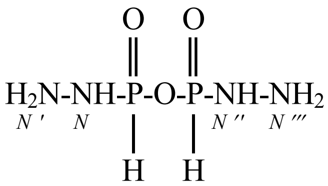
$H_2N\text{-}\underset{\underset{H}{|}}{\overset{\overset{O}{\|}}{P}}\text{-}\underset{\underset{H}{|}}{\overset{\overset{O}{\|}}{P}}\text{-}NH_2$

hypodiphosphonic diamide
(preselected name)



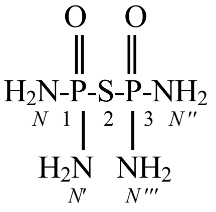
$H_2N\text{-}\underset{\underset{NH_2}{|}}{\overset{\overset{O}{\|}}{P}}\text{-}O\text{-}\underset{\underset{NH_2}{|}}{\overset{\overset{O}{\|}}{P}}\text{-}NH_2$

diphosphoric tetraamide
(preselected name)

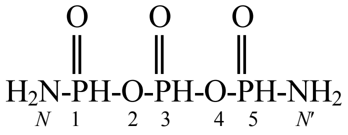


$H_2N\text{-}NH\text{-}\underset{\underset{H}{|}}{\overset{\overset{O}{\|}}{P}}\text{-}O\text{-}\underset{\underset{H}{|}}{\overset{\overset{O}{\|}}{P}}\text{-}NH\text{-}NH_2$

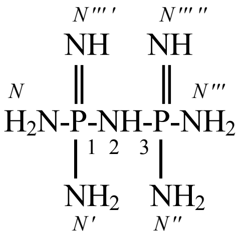
diphosphonic dihydrazide
(preselected name)


$H_2N\text{-}P\text{-}S\text{-}P\text{-}NH_2$

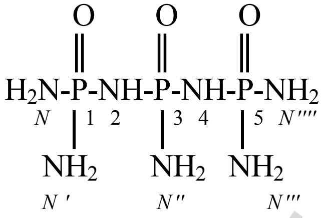
2-thiodiphosphoric tetraamide
(preselected name)


$H_2N\text{-}PH\text{-}O\text{-}PH\text{-}O\text{-}PH\text{-}NH_2$

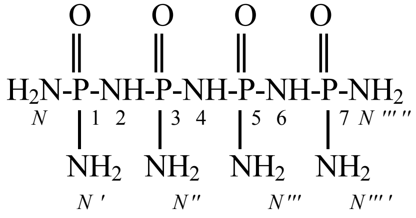
triphosphonic diamide
(preselected name)


$H_2N\text{-}P\text{-}NH\text{-}P\text{-}NH_2$

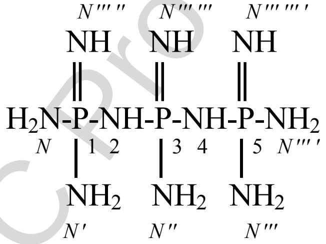
1,2,3-triimidodiphosphoric tetraamide (preselected name)


$H_2N\text{-}P\text{-}NH\text{-}P\text{-}NH\text{-}P\text{-}NH_2$

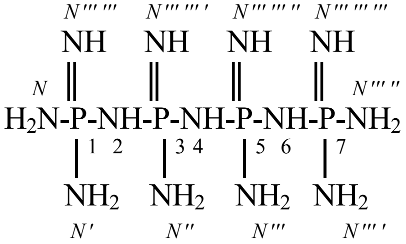
2,4-diimidotriphosphoric pentaamide
(preselected name)


$H_2N\text{-}P\text{-}NH\text{-}P\text{-}NH\text{-}P\text{-}NH\text{-}P\text{-}NH_2$

2,4,6-triimidotetraphosphoric hexaamide
(preselected name)


$H_2N\text{-}P\text{-}NH\text{-}P\text{-}NH\text{-}P\text{-}NH_2$

pentaimidotriphosphoric pentaamide
(preselected name)


$H_2N\text{-}P\text{-}NH\text{-}P\text{-}NH\text{-}P\text{-}NH\text{-}P\text{-}NH_2$

heptaimidoimidotetraphosphoric hexaamide
(preselected name)

$H_2N\text{-}SO_2\text{-}O\text{-}SO_2\text{-}NH_2$

disulfuric diamide (preselected name)

$H_2N\text{-}SeO_2\text{-}O\text{-}SeO_2\text{-}NH_2$

diselenic diamide (preselected name)

P-67.2.2.5 Esters and anhydrides

P-67.2.2.5.1 Esters
P-67.2.2.5.2 Anhydrides

P-67.2.2.5.1 Esters

Fully esterified acids are named as neutral salts, except that names of allowed groups (alkyl groups, aryl groups, etc.), cited in alphanumerical order when more than one, replace the name of the cations. Partial (acid) esters of polybasic acids and their salts are named by the procedures for neutral esters and acid salts, except that the name ‘hydrogen’ denoting acid hydrogen atoms is indicated by the separate word ‘hydrogen’ (with the appropriate multiplying prefix denoting multiplicity) inserted between the name of the cation or of the organic group and the name of the anion.

Examples:

$CH_3\text{-}S\text{-}\overset{1}{P}H\text{-}\overset{2}{P}H\text{-}O\text{-}CH_3$

dimethyl thiohypodiphosphonite (PIN)

$HS\text{-}\overset{1}{P}H\text{-}\overset{2}{P}H\text{-}S\text{-}CH_3$

methyl hydrogen dithiohypodiphosphonite (PIN)

$CH_3\text{-}O\text{-}SO_2\text{-}O\text{-}SO_2\text{-}S\text{-}CH_2\text{-}CH_3$

S-ethyl *O*-methyl thiodisulfate (PIN)

$(CH_3)_2CH\text{-}O\text{-}SO\text{-}O\text{-}SO\text{-}O\text{-}CH_3)_2$

di(propan-2-yl) disulfite (PIN)

P-67.2.2.5.2 Anhydrides

Neutral anhydrides formed between organic acids and polynuclear noncarbon acids having preselected names are named by citing, in alphabetical order, the names of the acids followed by the name of the class ‘anhydride’; multiplying prefixes ‘di’, ‘tri’, etc. are used to indicate the multiplicity of the anhydride linkages.

Acidic anhydrides are named using the senior acid as parent or by using systematic substitutive nomenclature as described in P-67.3.1.

Examples:

$(CH_3\text{-}CO\text{-}O)_2P(O)\text{-}P(O)(O\text{-}CO\text{-}CH_3)_2$

tetraacetic hypodiphosphoric tetraanhydride (PIN)

$CH_3\text{-}CO\text{-}O\text{-}SO\text{-}SO\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_3$

acetic hypodisulfurous propanoic dianhydride (PIN)
acetic dithionous propanoic dianhydride

P-67.2.2.6 Substituent groups derived from polyacids

In presence of a characteristic group having precedence for citation as principal group, oxoacids are cited as prefixes. The names of these prefixes are formed by:

(1) combinations of acyl groups;

(2) on the basis of the names of the group which includes the greatest number of P, As, Sb, S, Se, and Te central atoms.

(3) skeletal replacement nomenclature, when conditions for its use are satisfied.

When there is a choice for parent substituent, seniority is given to parent substituents having the largest size, then, if needed, to alphanumerical order.

Examples:

$$(HO)_2P(O)\text{-}O\text{-}P(O)(OH)\text{-}O\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$$

3-(1,3,3-trihydroxy-1,3-dioxo-$1\lambda^5$,$3\lambda^5$-diphosphoxan-1-yl)propanoic acid (PIN)
3-{[(phosphonooxy)phosphoryl]oxy}propanoic acid

$$\overset{1}{C}H_3\text{-}\overset{2}{O}\text{-}S(O)\text{-}O\text{-}S(O)\text{-}O\text{-}S(O)\text{-}O\text{-}CH_2\text{-}\overset{10}{C}OOH$$

3,5,7-trioxo-2,4,6,8-tetraoxa-$3\lambda^4$,$5\lambda^4$,$7\lambda^4$-trithiadecan-10-oic acid (PIN)
{[({[(methoxysulfinyl)oxy]sulfinyl}oxy)sulfinyl]oxy}acetic acid
(5-methoxy-1,3,5-trioxo-$1\lambda^4$,$3\lambda^4$,$5\lambda^4$-trisulfoxan-1-yl)acetic acid

$$CH_3\text{-}S\text{-}S(S)\text{-}S\text{-}S(S)\text{-}S\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH$$

3,5-disulfanylidene-2,$3\lambda^4$,4,$5\lambda^4$,6-pentathianonan-9-oic acid (PIN)
3-(5-methyl-2,4-sulfanylidene-$2\lambda^4$,$4\lambda^4$-pentasulfanyl)propanoic acid
3-[({[(methylsulfanyl)sulfinothioyl]sulfanyl}sulfinothioyl)sulfanyl]propanoic acid

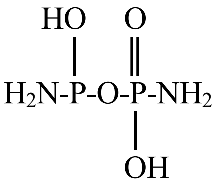
P-67.3 Substitutive names and functional class names of polyacids

P-67.3.1 Names of polyacids that cannot be formed from basic acids are either class names such as anhydrides or they are formed substitutively. Anhydride names are preferred to substitutive names.

Some names are also included in this Section because their structure does not correspond to the name implied by a diacid or a hypodiacid, for example the name 'disulfurous acid', exemplified below.

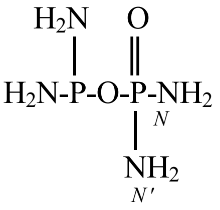
Names of derivatives of acids that cannot be formed directly by functional replacement are generated by substitution of acids with preferred names such as phosphonic acid and phosphinic acid; or they are class names such as 'anhydride'. The parent is chosen in accordance with the seniority order of classes: acids, acid halides, azides, amides, hydrazides, cyanides, isocyanides, isocyanates (and chalcogen analogues in the order O > S > Se > Te), imides, and nitrides and the maximum number of groups representing senior classes.

Examples:



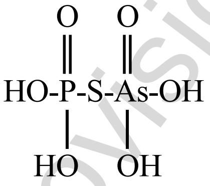
$H_2N\text{-}\underset{}{\overset{HO}{P}}\text{-}O\text{-}\underset{OH}{\overset{O}{P}}\text{-}NH_2$

{[amino(hydroxy)phosphanyl]oxy}phosphonamidic acid (preselected name)
(phosphonamidic acid is senior to phosphonamidous acid)
phosphoramidic phosphoramidous monoanhydride
(an acid is preferred to an anhydride in the seniority order of classes)



$H_2N\text{-}\overset{H_2N}{P}\text{-}O\text{-}\underset{\underset{N'}{NH_2}}{\overset{O}{P}}\text{-}\underset{N}{NH_2}$

phosphorodiamidic phosphorodiamidous anhydride (preselected name)
[(diaminophosphanyl)oxy]phosphonic diamide
(an anhydride is senior to an amide)



$HO\text{-}\underset{HO}{\overset{O}{P}}\text{-}S\text{-}\underset{OH}{\overset{O}{As}}\text{-}OH$

(arsonosulfanyl)phosphonic acid (preselected name)
arsoric phosphoric thiomonoanhydride
(an acid is senior to an anhydride; the phosphorus acid is senior to the arsenic acid)

$(HO)HP(O)\text{-}\overset{N}{N}H\text{-}P(O)(OH)_2$

N-(hydroxyphosphonoyl)phosphoramidic acid
(a substitutive name only is possible in this case)

$(HO)_2P\text{-}HP(O)\text{-}OH$

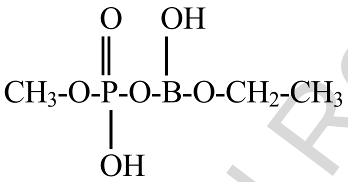
(dihydroxyphosphanyl)phosphinic acid (preselected name)

$(CH_3\text{-}O)_2P(O)\text{-}O\text{-}HP(O)\text{-}O\text{-}CH_3$

methyl [(dimethoxyphosphoryl)oxy]phosphinate (PIN)
(phosphonic acid is preferred to phosphoric acid; see P-41)
(formerly trimethyl isohypophosphate)

$HO\text{-}\overset{1}{S}I_2\text{-}\overset{2}{S}\text{-}CN$

1-hydroxy-1,1-diodo-1λ^4-disulfane-2-carbonitrile (preselected name)
(formerly diiodo(thiocyanatido)orthosulfurous acid)
(not orthosulfurodiiodidothiocyanatous acid)



$$CH_3\text{-}O\text{-}\underset{\displaystyle OH}{\overset{\displaystyle O}{\overset{\|}{P}}}\text{-}O\text{-}\overset{\displaystyle OH}{\overset{|}{B}}\text{-}O\text{-}CH_2\text{-}CH_3$$

methyl hydrogen ([ethoxy(hydroxy)boranyl]oxy}phosphonate (PIN)
(ethyl dihydrogen borate) (methyl dihydrogen phosphate) anhydride

$CH_3\text{-}CO\text{-}O\text{-}P(OH)_2$	(acetyloxy)phosphonic acid (PIN) acetic phosphoric monoanhydride monoacetyl phosphate
$HO\text{-}SeO_2\text{-}O\text{-}SO_2\text{-}OH$	(selenonooxy)hydroxy-λ^6-sulfanedione (preselected name) selenic sulfuric anhydride
$CH_3\text{-}CH_2\text{-}CO\text{-}O\text{-}B(OH)_2$	(propanoyloxy)boronic acid (PIN) boric propanoic monoanhydride
$CH_3\text{-}CO\text{-}O\text{-}CO\text{-}O\text{-}CO\text{-}OH$	{[(acetyloxy)carbonyl]oxy}formic acid (PIN) acetic dicarbonic monoanhydride

P-67.3.2 The disulfurous acid name dilemna

The name disulfurous acid must correspond to the structure HO-SO-O-SO-OH implied for all homogeneous diacids in accordance with the definition given in P-67.2. As the reported structure is HO-SO-SO_2-OH, a different name must be assigned to this structure. A substitutive name is appropriate in this situation.

HO-S(=O)-O-S(=O)-OH	HO-S(=O)-S$(=O)_2$-OH
disulfurous acid (preselected name)	1,2-dihydroxydisulfane-1,1,2-trione (preselected name)

P-68 Nomenclature of organic compounds of the Groups 13, 14, 15, 16, and 17 elements not included in Sections 62-67.

P-68.0 Introduction

The nomenclature of organic compounds is based on two approaches. General principles, rules and conventions are applicable, with some rare exceptions, to all compounds belonging to Groups 13 through 17. They have been described and illustrated in previous Chapters. Another approach is based on the identical treatment of compounds within one Group. Up until now the nomenclature of compounds of Group 13 was essentially that of boron compounds. The nomenclature of aluminium, gallium, indium and thallium compounds in these recommendations has been modeled on that of boron compounds. It is thus advantageous to describe all compounds of a Group, to clearly identify their similarities and underline exceptions, if any. This way should facilitate the naming of new compounds by comparison with established models.

Another aspect of nomenclature described Group by Group is to easily grasp the general patterns of the different Groups. The nomenclature of Group 15 is diversified. Suffixes are associated with nitrogen; mononuclear and polynuclear acids are the base of many derivatives of phosphorus, arsenic and antimony compounds; bismuth compounds are all named substitutively. In comparison, compounds of Group 14 are essentially named by substitutive nomenclature. Thus, the compound C_6H_5-PH-OCH_3 is named as an ester, methyl phenylphosphinate, but the compound, C_6H_5-$SnH(OCH_3)_2$ is named substitutively as dimethoxy(phenyl)stannane or phenylstannanebis(ylium) dimethanolate, inspite of their apparent similarity of structures.

A third purpose is assigned to this Section. Substitutive nomenclature treats equally metal, semi-metals, and non-metals when the central atom is directly linked to carbon. The Group treatment is illustrating many aspects of the nomenclature of organometallic compounds, again facilitating the naming of new compounds by applying the general rules recommended for the nomenclature of organic compounds. This is particularly evident for the nomenclature of compounds of Groups 13 and 14, for which the extensive and well known nomenclature of boron and carbon compounds serves as models to name the other compounds of the Group.

P-68.1 Nomenclature of compounds of Group 13

Except for the polynuclear boron hydrides, boron compounds have traditionally been included in the recommendations for naming inorganic compounds; substitutive nomenclature has been applied on the basis of parent hydrides, substituent groups and appropriate operations to complement the nomenclature of polynuclear compounds, for example names formed by skeletal replacement (‘a’) nomenclature, multiplicative names, and names derived from functional parent acids. The nomenclature of Al, Ga, In, and Tl compounds, including formal organometallic compounds, is patterned on boron nomenclature, with the exception of boronic acid, $B(OH)_3$, boronic acid, $HB(OH)_2$, and borinic acid, $H_2B(OH)$ which are retained names of functional parent compounds.

P-68.1.1 Parent hydrides
P-68.1.2 Substituent groups derived from parent hydrides
P-68.1.3 Modification of the degree of hydrogenation
P-68.1.4 Parent structures
P-68.1.5 Substitutive nomenclature
P-68.1.6 Adducts

P-68.1.1 Parent hydrides

P-68.1.1.1 Mononuclear hydrides
P-68.1.1.2 Acyclic polynuclear hydrides
P-68.1 1.3 Cyclic hydrides

P-68.1.1.1 Mononuclear hydrides

The names of the mononuclear hydrides are listed in Table 1.2. The standard bonding number is 3; the λ-convention (see P-14.1) is used to indicate nonstandard bonding numbers. The names of these parent hydrides are preselected names (see P-12.2).

Examples:

BH_3	BH	AlH_3	InH_3	TlH_3
borane	λ^1-borane	alumane	indigane	thallane

P-68.1.1.2 Acyclic polynuclear hydrides

P-68.1.1.2.1 Acyclic di- and polynuclear parent hydrides are named by citing the number of skeletal atoms in the molecule as a multiplying prefix, ‘di’, ‘tri’, etc. in front of the name of the mononuclear parent hydride. The number of hydrogen atoms in the molecule is designated by an arabic numeral enclosed in parentheses immediately following the name derived as above. These numbers are omitted when there is no ambiguity or by convention in the names of acyclic polynuclear hydrides. A specific nomenclature is used to name polycyclic polyboranes; these names are described in Chapter I-11 of ref. 14. Parent hydrides are preselected preferred IUPAC names.

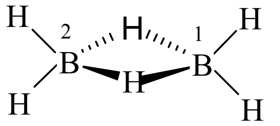
Examples:

$H_2\overset{2}{B}\text{-}\overset{1}{B}H_2$

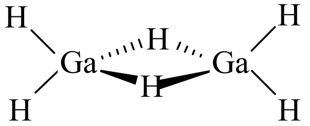
diborane(4) (preselected name)

$H_2\overset{3}{B}\text{-}\overset{2}{B}H\text{-}\overset{1}{B}H_2$

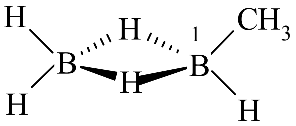
triborane(5) (preselected name)



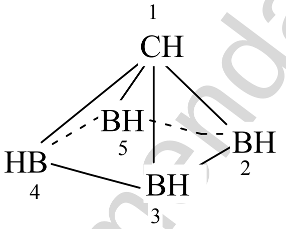
diborane(6) (preselected name)



digallane(6) (preselected name)



1-methyldiborane(6) (PIN)



1-carbapentaborane(5) (PIN)

P-68.1.1.2.2 Compounds formed of alternating heteroatoms are considered as nonfunctional parent structures having preselected names.

Examples:

3 2 1
$(CH_3)_2B\text{-}O\text{-}B(CH_3)_2$

tetramethyldiboroxane (PIN)

5 4 3 2 1
$H_2Al\text{-}O\text{-}AlH\text{-}O\text{-}AlH_2$

trialuminoxane (preselected name)

P-68.1.1.2.3 Compounds named by skeletal replacement (‘a’) nomenclature

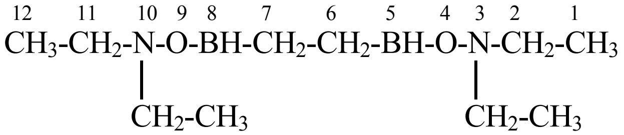
Examples:

10 9 8 7 6 5 4 3 2 1
$CH_3\text{-}B(CH_3)\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}B(CH_3)\text{-}CH_3$

2,9-dimethyl-4,7-dioxa-2,9-diboradecane (PIN)
[ethane-1,2-diylbis(oxymethylene)]bis(dimethylborane)
B,B,B′,B′-tetramethyl[ethane-1,2-diylbis(oxymethylene)]bis(borane)

9 8 7 6 5 4 3 2 1
$H_2B\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SHi_2\text{-}CH_2\text{-}BH_2$

3,5,7-trisila-1,9-diboranonane (PIN)
[silanediylbis(methylene)]bis[(boranylmethyl)silane]
Si,Si′-bis(boranylmethyl)[silanediylbis(methylene)]bis(silane)



$$\overset{12}{CH_3}\text{-}\overset{11}{CH_2}\text{-}\overset{10}{\underset{CH_2\text{-}CH_3}{N}}\text{-}\overset{9}{O}\text{-}\overset{8}{BH}\text{-}\overset{7}{CH_2}\text{-}\overset{6}{CH_2}\text{-}\overset{5}{BH}\text{-}\overset{4}{O}\text{-}\overset{3}{\underset{CH_2\text{-}CH_3}{N}}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CH_3}$$

3,10-diethyl-4,9-dioxa-3,10-diaza-5,8-diboradodecane (PIN)
O,O′-[(ethane-1,2-diylbis(boranediyl))bis(*N*,*N* ′-diethylhydroxylamine)

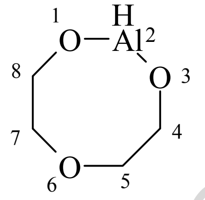
P-68.1.1.3 Cyclic parent hydrides

Nomenclature of polyhedral polyboranes constitute a rich and diversified system characterized by specific prefixes. It has been described and illustrated in the Section I-11.2 (ref. 14)(Red Book); it is not reproduced in these recommendations.

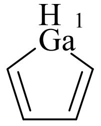
Cyclic parent hydrides containing Group 13 atom(s) belong to all the different classes of rings and ring systems described in Chapter 2. Preferred names are selected according to the general rules given for each class.

P-68.1.1.3.1 Hantzsch-Widman names (see P-22.2.2) are preferred for monocyclic rings with three through ten ring members. Names formed by skeletal replacement (‘a’) nomenclature are not recommended.

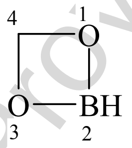
Examples:



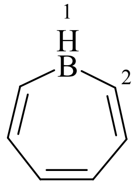
1,3,6,2-trioxaaluminocane (PIN)



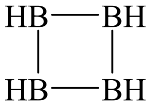
1*H*-gallole (PIN)



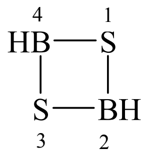
1,3,2-dioxaboretane (PIN)



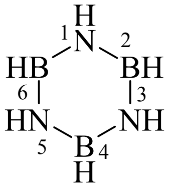
1*H*-borepine (PIN)



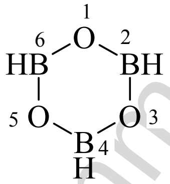
tetraboretane (preselected name; see P-12; P-22.2.4)
cyclotetraborane(4)



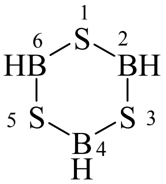
1,3,2,4-dithiadiboretane (preselected name; see P-12, P-22.2.5)
cyclodiborathiane



1,3,5,2,4,6-triazatriborinane
(preselected name)
borazine
cyclotriborazane



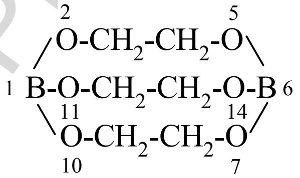
1,3,5,2,4,6-trioxatriborinane
(preselected name)
boroxin
cyclotriboroxane



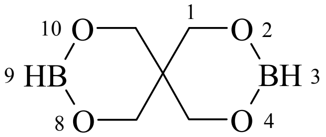
1,3,5,2,4,6-trithiatriborinane (preselected name)
borthiin
cyclotriborathiane

P-68.1.1.3.2 von Baeyer and spiro compounds

Examples:



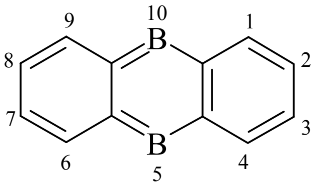
2,5,7,10,11,14-hexaoxa-1,6-diborabicyclo[4.4.4]tetradecane (PIN)



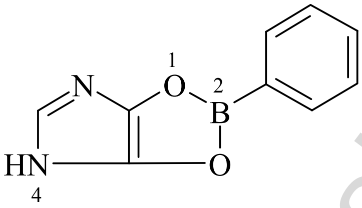
2,4,8,10-tetraoxa-3,9-diboraspiro[5.5]undecane (PIN)

P-68.1.1.3.3 Fused ring systems

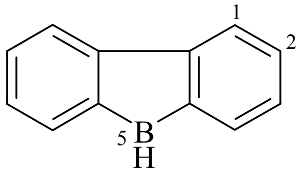
Examples:



boranthrene (PIN)



2-phenyl-4*H*-[1,3,2]dioxaborolo[4,5-*d*]imidazole (PIN)



5*H*-dibenzoborole (PIN)

P-68.1.2 Names of substituent groups derived from parent hydrides

Names of substituent groups $-BH_2$ and $=BH$ derived from borane are formed by the method described in P-29.2.2; these are preselected preferred IUPAC names.

Examples:

$-BH_2$

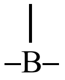
boranyl (preselected name)
(not boryl)

$=BH$

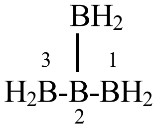
boranylidene (preselected name)
(not borylidene)

$>BH$

boranediyl (preselected name)
(not borylidene)
(not borylene)


$-\overset{|}{B}-$

boranetriyl (preselected name)
(not borylidyne)



$$\overset{BH_2}{H_2B\text{-}B\text{-}BH_2}$$

2-boranyltriborane(5) (preselected name)

1 2 3
$–BH\text{-}BH\text{-}BH_2$

triboran(5)-1-yl (preselected name)

$–BH\text{-}O\text{-}BH_2$

diboroxanyl (preselected name)

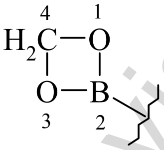
1 2 3
$–BH\text{-}NH\text{-}BH_2$

diborazan-1-yl (preselected name)

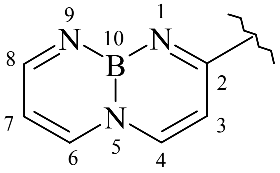
$H_2Al–$	alumanyl (preselected name)
$H_2In–$	indiganyl (preselected name)
$H_2Ga–$	gallanyl (preselected name)
$H_2Tl–$	thallanyl (preselected name)

1 2 4 6 8 9
$CH_3\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}SiH_2\text{-}CH_2\text{-}BH\text{-}CH_2–$

2,4,6-trisila-8-boranonan-9-yl (PIN)



1,3,2-dioxaboretan-2-yl
(preselected name)



[1,3,2]-diazaborino[1,2-*a*][1,3,2]-diazaborin-2-yl (PIN)

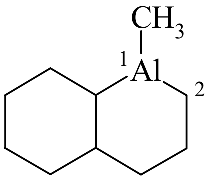
P-68.1.3 Modification of the degree of hydrogenation

Double bonds are denoted by the ‘ene’ ending, as described in Section P-31.1, and ‘hydro’ prefixes as indicated in P-33.2.

Example:

1 2 3
$HB{=}B\text{-}BH_2$

triborene(5) (preselected name)



1-methyldecahydro-1-benzoaluminine (PIN)

P-68.1.4 Functional parents

P-68.1.4.1 The names boric acid, boronic acid, and borinic acid are preselected retained names denoting the compounds $B(OH)_3$, $HB(OH)_2$, and $H_2B(OH)$, respectively (see P-67.1.1). They are used as preferred IUPAC names to form the names of the corresponding salts, esters, or anhydrides; or when substituted, for example methylboronic acid for $CH_3\text{-}B(OH)_2$. Chalcogen analogues are named using infixes to denote functional replacement of oxygen by S, Se, and Te.

Acid names such as these are not used for other elements of Group 13, which are named using substitutive nomenclature based on the appropriate parent hydride. For names such as methaneboronic acid vs. methylboronic acid for $CH_3\text{-}B(OH)_2$, see P-67.1.2.4.1.

Examples:

$CH_3\text{-}B(O^-)_2\ \ 2Na^+$

disodium methylboronate (PIN)

$CH_3\text{-}B(O^-)(OH)\ \ Na^+$

sodium hydrogen methylboronate (PIN)

$CH_3\text{-}B(OH)_2$

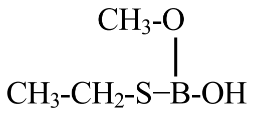
methylboronic acid (PIN)
methylboranediol

$(CH_3)_2B(SH)$

dimethylborinothioic acid (PIN)
dimethyl(thioborinic) acid
dimethylboranethiol

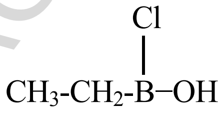
$B(SCH_3)_3$

trimethyl borotrithioate (PIN)
trimethyl trithioborate



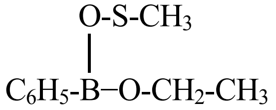
$CH_3\text{-}CH_2\text{-}S{-}\overset{CH_3\text{-}O}{\overset{|}{B}}\text{-}OH$

S-ethyl *O*-methyl hydrogen borothioate (PIN)
S-ethyl *O*-methyl hydrogen thioborate



$CH_3\text{-}CH_2\text{-}\overset{Cl}{\overset{|}{B}}{-}OH$

ethylboronochloridic acid (PIN)
(not chloro(ethyl)boronic acid)



$$C_6H_5\text{-}\underset{}{\overset{\displaystyle O\text{-}S\text{-}CH_3}{\overset{|}{B}}}\text{-}O\text{-}CH_2\text{-}CH_3$$

O-ethyl *OS*-methyl phenylborono(thioperoxoate) (PIN)
O-ethyl *OS*-methyl phenyl(thioperoxy)boronate

$(CH_3)_2Al\text{-}O^- \ Na^+$

sodium dimethylalumanolate (PIN)

$$(C_6H_5)_2\overset{6}{B}\text{-}\overset{5}{N}H\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{N}H\text{-}\overset{1}{B}(C_6H_5)_2$$

N,*N*-ethane-1,2-diylbis(diphenylborinic amide) (PIN)
(not *N*,*N′*-bis(diphenylboryl)ethane-1,2-diamine)
(not *N*,*N’*-ethane-1,2-diylbis(diphenylborananine)
(not 1,1,6,6-tetraphenyl-2,5-diaza-1,6-diborahexane)

P-68.1.4.2 Substituent groups for the boron acids

The general methodology for forming substituent groups derived from boron acids has been described in P-67.1.4.2.1. Their names are formed substitutively on the basis of the parent hydride ‘borane’, BH_3. The name ‘borono’, for $(HO)_2B$–, is retained.

Examples:

$(HO)_2B$–

borono (preselected name)
dihydroxyboranyl

$(HS)BH$–

sulfanylboranyl (preselected name)

$(HO)(HS)B$–

thioborono (preselected name)
hydroxyl(sulfanyl)boranyl

$(HSe)_2B$–

diselenoborono (preselected name)
bis(selanyl)boranyl

$Cl\text{-}BH$–

chloroboranyl (preselected name)

$(H_2N)_2B$–

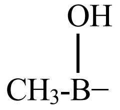
diaminoboranyl (preseleted name)

$(CH_3)_2B\text{-}O$–

(dimethylboranyl)oxy (PIN)

$CH_3\text{-}BH\text{-}NH$–

(methylboranyl)amino (PIN)



$\mathrm{CH_3{-}B(OH){-}}$

methyl(hydroxy)boranyl (PIN)

P-68.1.5 Substitutive nomenclature

Derivatives of borane, BH_3, are named as substitution products, the substituents being denoted by suffixes and prefixes in accordance with the principles, rules and conventions of substitutive nomenclature. The three acids described in P-68.1.4 have retained names that are preferred IUPAC names.

Derivatives are named in accordance with the seniority of classes described by the general rule in Section P-41. Thus, acids having retained names have seniority over other suffixes. Suffixes are used when recommended in substitutive nomenclature, in accordance with the general rule described in Section P-43. In the absence of a suffix that has priority for naming organic compounds, when a choice is possible for selecting the parent hydride, the seniority order is as follows: N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl > O > S > Se > Te > C (substituent groups).

P-68.1.5.1 Suffix nomenclature

Suffixes, when available, are used to denote characteristic groups; prefixes are not recommended. Suffixes containing a carbon atom generate preferred IUPAC names.

Examples:

$H_2B\text{-}CN$

boranecarbonitrile (PIN)

$(HO)_2B\text{-}B(OH)_2$

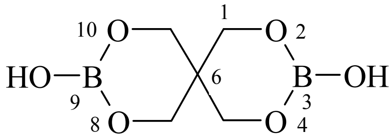
hypodiboric acid (preselected PIN; see P-67)
diborane(4)tetrol

$(CH_3)_2Tl\text{-}OH$

dimethylthallanol (PIN)

$(CH_3)_2Tl\text{-}O^-\ Na^+$

sodium dimethylthallanolate (PIN)



2,4,8,10-tetraoxa-3,9-diboraspiro[5.5]undecane-3,9-diol (PIN)

P-68.1.5.2 Prefix nomenclature

P-68.1.5.2.1 Substituted parent hydrides;
P-68.1.5.2.2 Compounds with bridging prefixes
P-68.1.5.2.3 Compounds with groups of higher seniority.

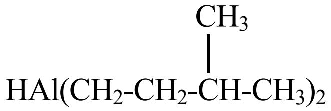
P-68.1.5.2.1 Substituted parent hydrides

Normal prefix names are used to describe substituents of the B, Al, In, Tl parent hydrides.

Examples:

$B(CH_3)_3$
trimethylborane (PIN)

$Al(C_2H_5)_3$
triethylalumane (PIN)


$HAl(CH_2\text{-}CH_2\text{-}\overset{\overset{\displaystyle CH_3}{|}}{C}H\text{-}CH_3)_2$
bis(3-methylbutyl)alumane (PIN)

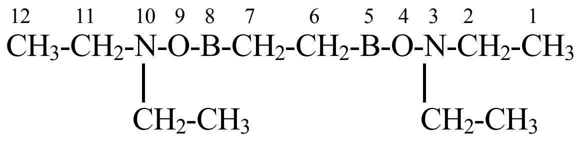
$Al(O\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3)_3$
tributoxyalumane (PIN)

$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}\overset{5}{B}H\text{-}\overset{4}{N}H\text{-}\overset{3}{B}H\text{-}\overset{2}{N}H\text{-}\overset{1}{B}H\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3$

1,5-dibutyltriborazane (PIN)
[not *N*,*N*′-bis(butylboranyl)boranediamine;
triborazane is a nonfunctional parent hydride]

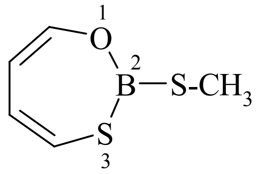
$\overset{10}{C}H_3\text{-}\overset{9}{B}(CH_3)\text{-}\overset{8}{C}H_2\text{-}\overset{7}{O}\text{-}\overset{6}{C}H_2\text{-}\overset{5}{C}H_2\text{-}\overset{4}{O}\text{-}\overset{3}{C}H_2\text{-}\overset{2}{B}(CH_3)\text{-}\overset{1}{C}H_3$

2,9-dimethyl-4,7-dioxa-2,9-diboradecane (PIN)
[(ethane-1,2-diylbis(oxymethylene))bis(dimethylborane)

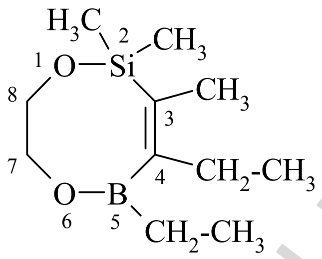


$$\overset{12}{CH_3}\text{-}\overset{11}{CH_2}\text{-}\underset{CH_2\text{-}CH_3}{\overset{10}{N}}\text{-}\overset{9}{O}\text{-}\overset{8}{B}\text{-}\overset{7}{CH_2}\text{-}\overset{6}{CH_2}\text{-}\overset{5}{B}\text{-}\overset{4}{O}\text{-}\underset{CH_2\text{-}CH_3}{\overset{3}{N}}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{CH_3}$$

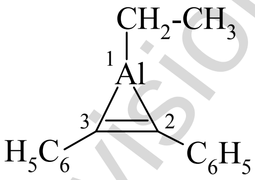
3,10-diethyl-4,9-dioxa-3,10-diaza-5,8-diboradodecane (PIN)
O,*O*′-[(ethane-1,2-diyldiboranediyl)bis(*N*,*N*-diethylhydroxylamine)



2-(methylsulfanyl)-1,3,2-oxathiaborepine (PIN)



4,5-diethyl-2,2,3-trimethyl-2,5,7,8-tetrahydro-1,6,2,5-dioxasilaborocine (PIN)



1-ethyl-2,3-diphenylaluminirene (PIN)

P-68.1.5.2.2 Compounds with bridging atoms or groups

Derivatives of di- and polyheteranes of the Group 13 elements, such as diborane, the polyboranes, and related Al, In, and Tl congeners, are named using substitutive nomenclature. When a nonbridging hydrogen is substituted, locants are used in the customary way. Bridging atoms or groups are indicated as follows:

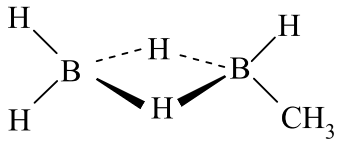
(a) a bridging substituent is indicated by adding the Greek letter μ (mu) immediately before the name of the substituent and separating its prefix name from that of the rest of the name by hyphens;

(b) two or more bridging substituents of the same kind are indicated by 'di-μ' or 'bis-μ', and so on;

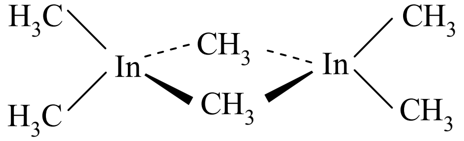
(c) bridging substituents are listed with the other substituents in alphanumerical order;

(d) where the same substituent is present as a bridging group and a nonbridging substituent it is cited first as a bridging substituent.

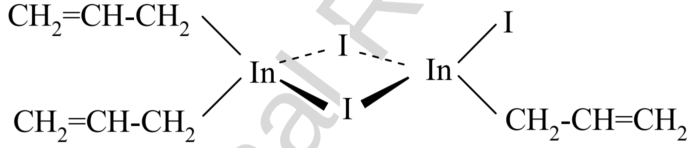
Examples:



methyldiborane(6) (PIN)



di-μ-methyl-tetramethyldiindigane(6) (PIN)



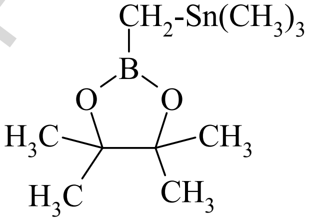
di-μ-iodo-iodotri(prop-2-en-1-yl)diindigane(6) (PIN)

For more examples of the application of the symbol μ, see Rule I-11.4.3.2, ref. 14.

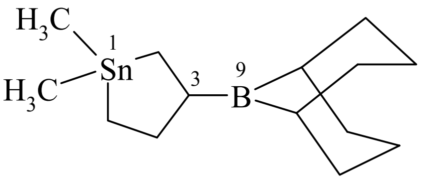
P-68.1.5.2.3 Compounds with groups of higher seniority.

When required, parent structures and prefixes are chosen in accordance with the seniority of classes.

Examples:



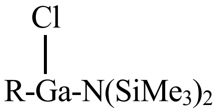
trimethyl[(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)methyl]stannane (PIN)
(Sn is senior to B)



3-(9-borabicyclo[3.3.1]nonan-9-yl)-1,1-dimethylstannolane (PIN)

$[Si(CH_3)_3]_2N\text{-}BH\text{-}N[Si(CH_3)_3]_2$

2,2′-boranediylbis(1,1,1,3,3,3-hexamethyldisilazane (PIN)
(not *N*,*N*,*N*′,*N*′-tetrakis(dimethylsilyl)boranediamine;
disilazane is a nonfunctional parent hydride; N is senior to B)



$R\text{-}\overset{Cl}{Ga}\text{-}N(SiMe_3)_2$ [R– = 2,4,6-tri-*tert*-butylphenyl-]

2-[chloro(2,4,6-tri-*tert*-butylphenyl)gallanyl]-1,1,1,3,3,3-hexamethyldisilazane (PIN)
(disilazane is a nonfunctional parent hydride; N is senior to Ga;)

$R\text{-}In[N(SiCH_3)_2]_2$ [R– = 2,4,6-tri-*tert*-butylphenyl-]

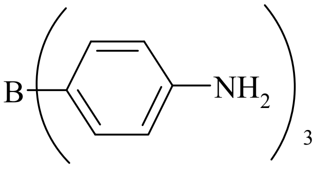
2,2′-[(2,4,6-tri-*tert*-butylphenyl)indiganediyl]bis(1,1,1,3,3,3-trimethyldisilazane) (PIN)
(disilazane is a nonfunctional parent hydride; N is senior to In)

$R\text{-}Ga[PH\text{-}Ar]_2$ [R– = 2,4,6-tri-*tert*-butylphenyl-]

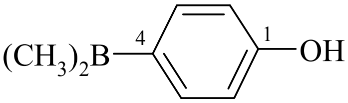
[(2,4,6-tri-*tert*-butylphenyl)gallanediyl]bis[(2,4,6-tri-*tert*-butylphenyl)phosphane] (PIN)
(P is senior to In)

$R\text{-}In[P(H)Ar]_2$ [R– = 2,4,6-tri-*tert*-butylphenyl-]

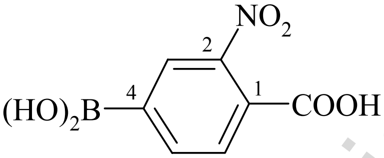
[(2,4,6-tri-*tert*-butylphenyl)indiganediyl]bis[(2,4,6-tri-*tert*-butylphenyl)phosphane] (PIN)
(P is senior to In)



4,4′,4′′-boranetriyltrianiline (PIN; a multiplicative name)



4-(dimethylboranyl)phenol (PIN)



4-borono-2-nitrobenzoic acid (PIN)

$(CH_3)_3Si\text{-}BF_2$

(difluoroboranyl)trimethylsilane (PIN)
(Si is senior to B)
(not (dimethylsilyl)boronic difluoride)

$Ga(S\text{-}S\text{-}CH_2\text{-}CH_3)_3$

tris(ethyldisulfanyl)gallane (PIN)
tris[ethyl(dithioperoxy)]gallane

$Al(O\text{-}CO\text{-}[CH_2]_{16}\text{-}CH_3)_3$

alumanetriyl trioctadecanoate (PIN)

P-68.1.6 Adducts

Adducts are chemical species A/B, each molecular entity of which is formed by direct combination (addition) of two molecular entities A and B in such a way that there is change in connectivity, but no loss of atoms within the moieties A and B. Stoichiometries other than 1:1 are also possible, e.g. (2:1), a bis-adduct. An intramolecular adduct is formed when A and B are groups contained within the same molecular entity.

'Adduct' is a general term which, whenever appropriate, should be used in preference to the less explicit term 'complex'. It is also used specifically for products of an addition reaction. Lewis adducts and π-adducts are discussed in this Subsection. Meisenheimer adducts are discussed in Section P-76.2)

P-68.1.6.1 Formulas of Lewis adducts

In the formulas of addition compounds the component molecules are cited in order of increasing number; if they occur in equal numbers, they are cited in alphabetical of the first symbols. Addition compounds containing boron compounds or water are exceptional, in that the water or boron component is cited last. If both are present, the boron compounds precede water. Components are separated by a centered dot.

P-68.1.6.1.1 General method

Adducts (addition compounds) between neutral Lewis bases and Lewis acids are named by citing the name of each component in the order given for the structure and connecting the name of each component by a dash (see P-16.2.5). The number of molecules of each component is denoted by two methods:

(1) appropriate multiplying prefixes, except for mono; or,

(2) by indicating the proportions of the species after the name by arabic numbers separated by a solidus (/)and placed in parentheses. A boron component, if present, is cited last in the name; water, if present, is cited last, after any boron component.

Method (1) leads to preferred IUPAC names.

Examples:

$BF_3 \bullet 2\ H_2O$

trifluoroborane–water (1/2) (preselected name)
boron trifluoride–bis(water)

$CH_3)_3N \bullet BCl_3$

N,*N*-dimethylmethamine–trichloroborane (1/1) (PIN)
N,*N*-dimethylmethamine–trichloroborane

$(C_2H_5)_2S \bullet BH_2(CH_3)$

(ethylsulfanyl)ethane–methylborane(1/1) (PIN)
(ethylsulfanyl)ethane–methylborane

$H_2N\text{-}CH_2\text{-}CH_2\text{-}NH_2 \bullet 2\ BH_3$

ethane-1,2-diamine–borane (1/2) (PIN)
ethane-1,2-diamine–bis(borane)

$2\ C_2H_5\text{-}NH_2 \bullet B_5H_9$

ethanamine–pentaborane(9) (2/1) (PIN)
bis(ethanamine)–pentaborane(9)

$(CH_3)_2S \bullet (CH_3)_3N \bullet B_{12}H_{10}$

N,*N*-dimethylmethanamine–(methylsulfanyl)methane–dodecaborane(10) (1/1/1) (PIN)
N,*N*-dimethylmethanamine–(methylsulfanyl)methane–dodecaborane(10)

When there is more than one possible donor molecule, the points of attachment to the boron component are indicated by italicized atomic symbols joined by a dash (see P-16.2.5), enclosed in parentheses, and cited between the names of each component of the adduct. Each atomic symbol refers to the component nearest to it. The names of components and the atomic symbols are cited in the sequence donor-acceptor. The locant of a component is added before the appropriate atomic symbols, as required.

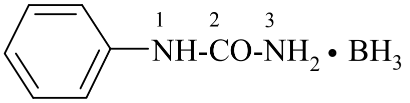
Examples:

$CH_3\text{-}O\text{-}NH_2 \bullet BH_3$

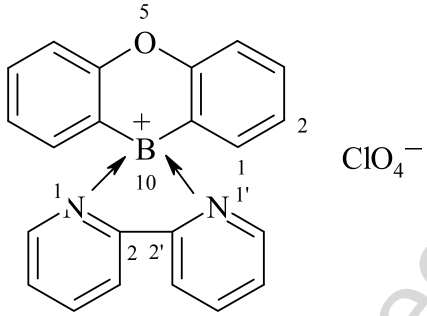
O-methylhydroxylamine(*N*–*B*)borane (PIN)

$(CH_3)_2NPF_2 \bullet B_4H_8$

N,*N*-dimethylphosphoramidous difluoride(*P*–*B*)tetraborane(8) (PIN)



1-phenylurea(3-*N*–*B*)borane (PIN)

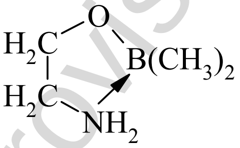


2,2′-bipyridine(*N*,*N*′–*B*)-10*H*-phenoxaborin-10-ylium perchlorate(1-) (PIN)

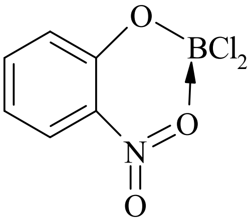
P-68.1.6.1.2 Intramolecular adducts

An intramolecular adduct between a group acting as a Lewis base and another group acting as a Lewis acid in the same molecule is denoted by atomic symbol pairs in the order donor-acceptor as described in Rule P-69.1.1, but cited in front of the complete name of the compound.

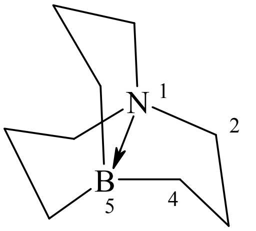
Examples:



(*N*–*B*)-2-aminoethyl dimethylborinate (PIN)

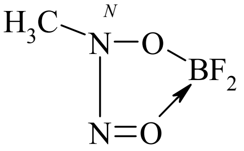


(*O*–*B*)-2-nitrophenyl borodichloridate (PIN)
(*O*–*B*)-dichloro(2-nitrophenoxy)borane

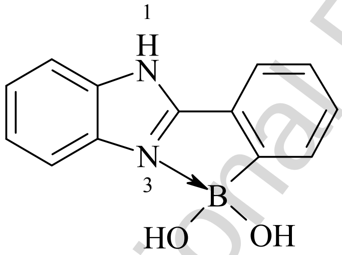


(*N*–*B*)-1-aza-5-borabicyclo[3.3.3]undecane (PIN)

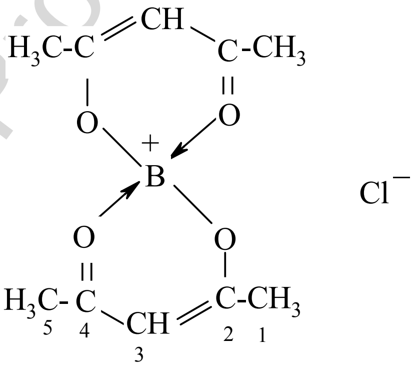
Note: If the structure is shown as a charged system, it is named as a zwitterion (see P-74.1.1)



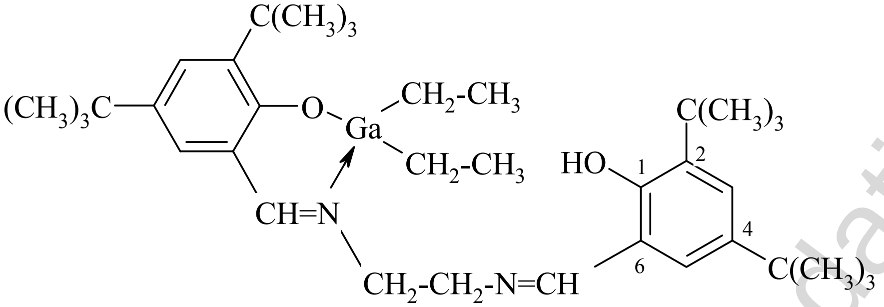
(*O*–*B*)-*O*-(difluoroboranyl)-*N*-methyl-*N*-nitrosohydroxylamine (PIN)



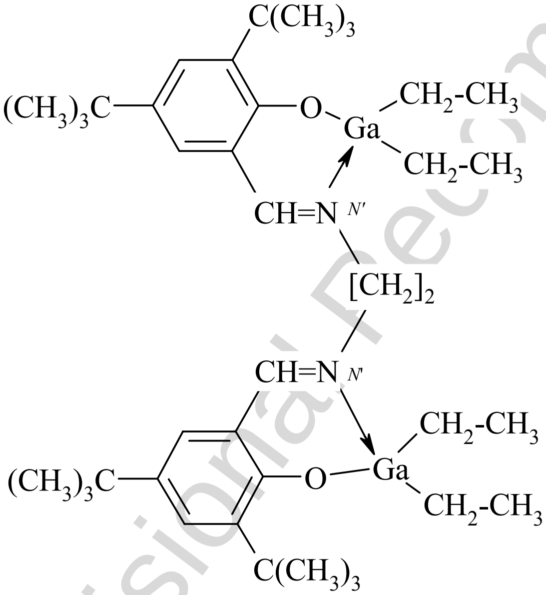
(3-*N*–*B*)-2-[(1*H*-benzimidazol-2-yl)phenyl]boronic acid (PIN)
(not (N^3–*B*)-2-[2-(dihydroxyboranyl)phenyl]benzimidazole)



[2(*O*–*B*)]-bis[(4-oxopent-2-en-2-yl)oxy]boranylium chloride (PIN)



2,4-di-*tert*-butyl-6-[({2-[({(*N*–*B*)-3,5-di-*tert*-butyl-2-[(diethylgallanyl)-oxy]phenyl}methylidene)amino]ethyl}imino)methyl]phenol (PIN)



N,*N*′-ethane-1,2-diylbis[(*N*–*Ga*){3,5-di-*tert*-butyl-2-[(diethylgallanyl)oxy]phenyl}methanimine] (PIN)

P-68.2 Nomenclature of compounds of Group 14

P-68.2.0 Introduction

The nomenclature of carbon compounds as the basis for organic compounds, has been described in previous chapters. It is not exemplified in this Section, unless comparisons with other compounds are needed.

With the exception of silicic acid, a retained name for $Si(OH)_4$ (formerly orthosilic acid), all Si, Ge, Sn, and Pb compounds are named in accordance with the principles, rules and conventions of substitutive nomenclature.

Suffixes and prefixes are used in accordance with the seniority of classes (see P-41). This is a modification to the traditional system that used suffixes and prefixes for silicon compounds, but only prefixes for germanium, tin and lead compounds. Functional class nomenclature is used only to denote esters and anhydrides derived from orthosilicic acid.

P-68.2.1 Si, Ge, Sn, and Pb parent hydrides
P-68.2.2 Substituent groups derived from parent hydrides
P-68.2.3 Modification of the degree of hydrogenation
P-68.2.4 Silicic acid as parent structure
P-68.2.5 Substitution compounds denoted by suffixes
P-68.2.6 Substitution compounds denoted by prefixes

P-68.2.1 Si, Ge, Sn, and Pb parent hydrides

P-68.2.1.1 Mononuclear and acyclic parent hydrides
P-68.2.1.2 Cyclic parent hydrides

P-68.2.1.1 Mononuclear and acyclic parent hydrides

Names of acyclic parent hydrides are formed in accordance with the general rules described in Section P-21. They are preselected names.

Examples:

$\overset{13}{H_3Sn}\text{-}[SnH_2]_{11}\text{-}\overset{1}{SnH_3}$

tridecastannane (preselected name)

$\overset{5}{H_3Ge}\text{-}\overset{4}{Se}\text{-}\overset{3}{GeH_2}\text{-}\overset{2}{Se}\text{-}\overset{1}{GeH_3}$

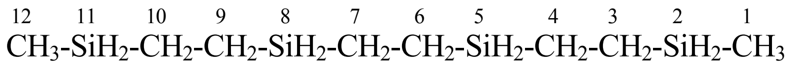
trigermaselenane (preselected name)

$\overset{22}{H_3Si}\text{-}[O\text{-}SiH_2]_{20}\text{-}\overset{2}{O}\text{-}\overset{1}{SiH_3}$

docosasiloxane (preselected name)

$\overset{3}{H_3Pb}\text{-}\overset{2}{Te}\text{-}\overset{1}{PbH_3}$

diplumbatellurane (preselected name)



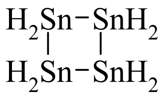
$$\overset{12}{CH_3}\text{-}\overset{11}{SiH_2}\text{-}\overset{10}{CH_2}\text{-}\overset{9}{CH_2}\text{-}\overset{8}{SiH_2}\text{-}\overset{7}{CH_2}\text{-}\overset{6}{CH_2}\text{-}\overset{5}{SiH_2}\text{-}\overset{4}{CH_2}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{SiH_2}\text{-}\overset{1}{CH_3}$$

2,5,8,11-tetrasiladodecane (PIN)
ethylenebis[2-(methylsilyl)ethylsilane]

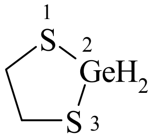
P-68.2.1.2 Cyclic parent hydrides

Names and preferred IUPAC names of cyclic parent hydrides are formed in accordance with the rules described in Sections P-23 to P-29. Those with no carbon atoms have preselected names.

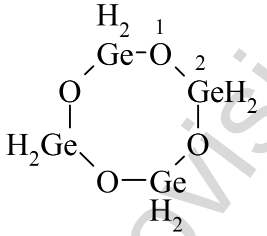
Examples:



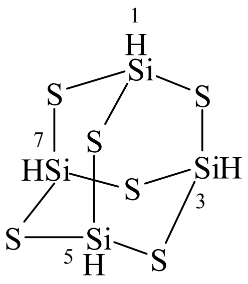
tetrastannetane (preselected name, Hantzsch-Widmnan name)
cyclotetrastannane



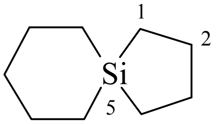
1,3,2-dithiagermolane (PIN)



1,3,5,7,2,4,6,8-tetraoxatetragermocane (preselected name, Hantzsch-Widman name)
cyclotetragermoxane



2,4,6,8,10-pentathia-1,3,5,7-tetrasilaadamantane (preselected name)



5-silaspiro[4.5]decane (PIN)

P-68.2.2 Substituent groups derived from parent hydrides

Names of substituent groups $-XH_3$, $=XH_2$, and $\equiv XH$ derived from mononuclear parent hydrides where X = Si, Ge, Sn, and Pb are formed by the specific method described in P-29.2.1; all other substituent groups are named by using the general method described in P-29.2.2.

Examples:

$-SiH_3$

silyl (preselected name)

$-GeH_3$

germyl (preselected name)

$-SnH_3$

stannyl (preselected name)

$-PbH_3$

plumbyl (preselected name)

$=SiH_2$

silylidene (preselected name)

$=PbH_2$

plumylidene (preselected name)

$\equiv GeH$

germylidyne (preselected name)

$\equiv SnH$

stannylidyne (preselected name)

$-SiH=$

silanylylidene (preselected name)

$=Ge=$

germanediylidene (preselected name)

$-SiH<$

stannanetriyl (preselected name)

$>Pb<$

plumbaneterayl (preselected name)

$H_3Si\text{-}SiH_2-$

disilanyl (preselected name)
(not disilyl)

$\overset{3}{H_3Ge}\text{-}\overset{2}{GeH_2}\text{-}\overset{1}{GeH_2}=$

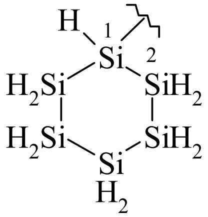
trigerman-1-ylidene (preselected name)

$-\overset{1}{H_2Si}-\overset{2}{SiH_2}-$

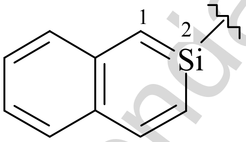
disilane-1,2-diyl (preselected name)

$\overset{2}{SiH_3}-\overset{1}{SiH}<$

disilane-1,1-diyl (preselected name)



hexasilinanyl (preselected name)
cyclohexasilanyl



2-benzosilin-2-yl (PIN)

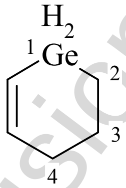
P-68.2.3 Modification of the degree of hydrogenation

Double bonds are denoted by the ‘ene’ ending, as described in Section P-31.1, and ‘hydro’ prefixes as indicated in P-33.2.

Examples:

$HGe{=}GeH$

digermene (preselected name)



1,2,3,4-tetrahydrogermine (PIN)

P-68.2.4 Silicic acid as functional parent

The nomenclature of silicic acid (formerly orthosilicic acid) has been discussed in Section P-67.1.2.1. Silicic acid is modified by prefixes only to denote functional replacement by chalcogen atoms. Functional replacement by other atoms or groups is not recommended. Names of salts, esters and anhydrides are derived from the retained name. Names of amides and hydrazides are based on the name ‘silicic acid’.

Names of substituent groups derived from silicic acid are formed on the basis of the parent hydride ‘silane’ (see P-67.1.4.4).

Examples:

$(HO)_3Si–$

trihydroxysilyl (preselected name)

$(HS)(HO)_2Si–$

dihydroxy(sulfanyl)silyl (preselected name)

$Si(NH_2)_4$

silicic tetramide (preselected name)
(not silanetetramine)

P-68.2.5 Substitutive nomenclature: suffix mode

Traditionally, silicon compounds were denoted suffixes or prefixes; germanium, tin and lead compounds were denoted by prefixes only. Full systematization is recommended to use suffixes, when available, to generate preferred names, in accordance with the seniority order of suffixes, and the seniority of suffixes over prefixes.

Examples:

$CH_3\text{-}Si(NH_2)_3$

methylsilanetriamine (PIN)

$(CH_3)_2Si(OH)_2$

dimethylsilanediol (PIN)

$CH_3\text{-}NH\text{-}Si(OH)_3$

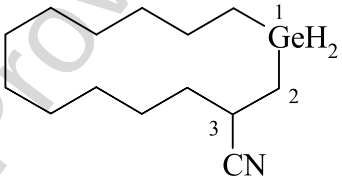
(methylamino)silanetriol (PIN)
N-methylsilicamidic acid

$(CH_3)_3Si\text{-}COOH$

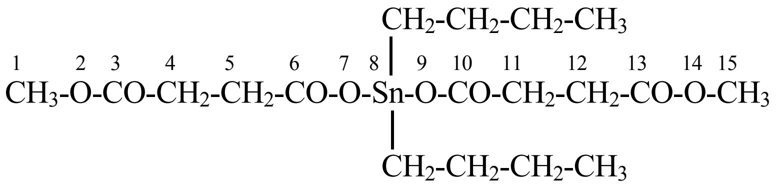
trimethylsilanecarboxylic acid (PIN)

$CH_3\text{-}GeH_2\text{-}SH$

methylgermanethiol (PIN)



1-germacyclotetradecane-3-carbonitrile (PIN)



$$\mathrm{\overset{1}{CH_3}\text{-}\overset{2}{O}\text{-}\overset{3}{CO}\text{-}\overset{4}{CH_2}\text{-}\overset{5}{CH_2}\text{-}\overset{6}{CO}\text{-}\overset{7}{O}\text{-}\underset{\displaystyle CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3}{\overset{\displaystyle CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_3}{\overset{8}{Sn}}}\text{-}\overset{9}{O}\text{-}\overset{10}{CO}\text{-}\overset{11}{CH_2}\text{-}\overset{12}{CH_2}\text{-}\overset{13}{CO}\text{-}\overset{14}{O}\text{-}\overset{15}{CH_3}}$$

8,8-dibutyl-2,7,9,14-tetraoxa-8-stannapentadecane-3,6,10,13-tetrone (PIN)
dimethyl stannanediyl dibutanedioate

P-68.2.6 Prefix nomenclature

Prefixes are used as recommended for substitutive nomenclature in two ways.

P-68.2.8.1 Prefixes added to parent hydrides;
P-68.2.6.2 Prefixes derived from parent hydrides.

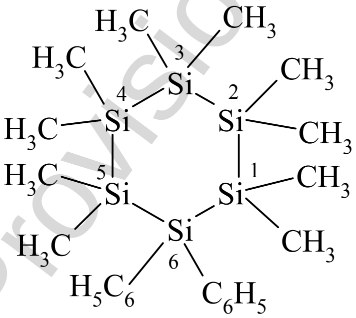
When required, parent structures and prefixes are chosen in accordance with the seniority of classes.

P-68.2.6.1 Substituted parent hydrides

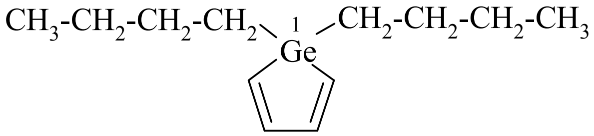
Examples:

$\mathrm{H_3\overset{5}{Si}\text{-}\overset{4}{N}H\text{-}\overset{3}{Si}H(CH_3)\text{-}\overset{2}{N}H\text{-}\overset{1}{Si}H_3}$

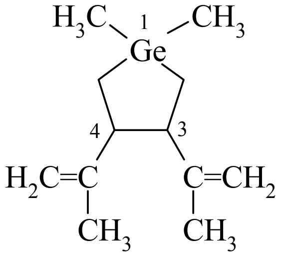
3-methyltrisilazane (PIN)
(not *N*,*N′*-disilyl-*Si*-methylsilanediamine)



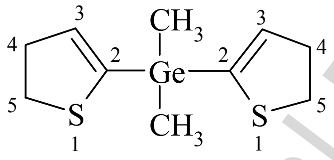
1,1,2,2,3,3,4,4,5,5-decamethyl-6,6-diphenylhexasilinane (PIN; Hantzsch-Widman name)
1,1,2,2,3,3,4,4,5,5-decamethyl-6,6-diphenylcyclohexasilane



1,1-dibutyl-1*H*-germole (PIN)
(note the indicated hydrogen atom)



1,1-dimethyl-3,4-di(prop-1-en-2-yl)germolane (PIN)
1,1-dimethyl-3,4-diisopropenylgermolane



bis(4,5-dihydrothiophen-2-yl)dimethylgermane (PIN)
(Ge is senior to S)

P-68.2.6.2 Substituent groups derived from parent hydrides

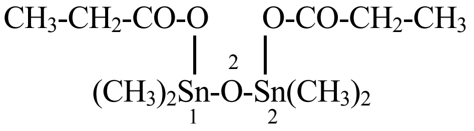
Examples:

$\mathrm{OHC{-}CH_2{-}CH_2{-}\overset{1}{Ge}(CH_3)_2{-}\overset{2}{Ge}(CH_3)_2{-}CH_2{-}CH_2{-}CHO}$

3,3′-(1,1,2,2,-tetramethyldigermane-1,2-diyl)dipropanal (PIN)

$\mathrm{(CH_3{-}CH_2{-}O)_3Ge\ \overset{3}{C}H_2{-}\overset{2}{C}H_2{-}\overset{1}{C}OO{-}CH_3}$

methyl 3-(trimethoxygermyl)propanoate (PIN)

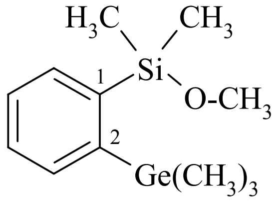


$$\begin{array}{ccc} \mathrm{CH_3{-}CH_2{-}CO{-}O} & & \mathrm{O{-}CO{-}CH_2{-}CH_3} \\ | & & | \\ \mathrm{(CH_3)_2\underset{1}{Sn}} & \mathrm{{-}\overset{2}{O}{-}} & \mathrm{\underset{2}{Sn}(CH_3)_2} \end{array}$$

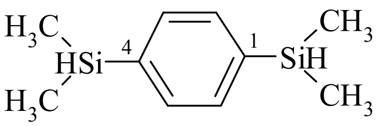
1,1,3,3-tetramethyldistannoxane-1,3-diyl dipropanoate (PIN)

$H_3Pb\text{-}CH_2\text{-}PbH_2\text{-}CH_2\text{-}PbH_3$

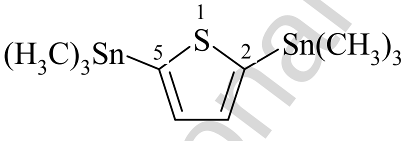
[plumbanediylbis(methylene)]bis(plumbane) (PIN)
bis(plumbylmethyl)plumbane



[(2-(trimethylgermyl)phenyl]methoxydimethylsilane (PIN)
(Si is senior to Ge)



1,4-phenylenebis(dimethylsilane) (PIN)



2,5-bis(trimethylstannyl)thiophene (PIN)
(S preferred to Sn)

$[(CH_3)_3Si]_2CH\text{-}SnH(OH)\text{-}CH[Si(CH_3)_3]_2$

[(hydroxystannediyl)dimethanetriyl]tetrakis(trimethylsilane) (PIN)
(Si preferred to Sn)

P-68.3 Nomenclature of compounds of Group 15

P-68.3.0 Introduction.

For the purposes of nomenclature, compounds of Group 15 are divided into three sub-groups:

(a) Nitrogen compounds, named as amines and imines (see P-62), amides, hydrazides, imides, amidines, amidrazones, hydrazidines, nitriles and cyanides, as described in Section P-66, or substitutively on the basis of parent hydrides, such as hydrazine and triazane or functional parent compounds, such as hydroxylamine. This last aspect is covered in P-68.3.2. For reasons of similarity, azonic, $HN(OH)_2$ and azinic acids, $H_2N(OH)$, are discussed in Section P-67 along with P, As, and Sb oxoacids.

(b) Phosphorus, arsenic and antimony compounds are discussed together in P-68.3.3 because of the importance of functional class nomenclature based on acids used as functional parents. Other compounds are named substitutively on the basis of parent hydrides.

(c) Bismuth compounds are all named by substitution of parent hydrides, such as BiH_3, in P-68.3.4.

P-68.3.1 Nitrogen compounds

P-68.3.1.0 Introduction

Many acyclic nitrogen compounds have retained names or functional class names. These names are retained for use in general nomenclature, but for most acyclic nitrogen compounds preferred IUPAC names are formed systematically. Hydroxylamine, urea, guanidine, and formazan are retained as preferred IUPAC names. Other retained names have been inserted into systematic substitutive nomenclature. Oxime is a retained functional class.

P-68.3.1.1 Hydroxylamines, oximes, nitrolic and nitrosolic acids

Several nitrogen compounds having one nitrogen atom belong to the identified classes: hydroxylamines, oximes, nitrolic and nitrosolic acids. The methodology for naming them is illustrated here. Nitro and nitroso compounds, isocyanates and isonitriles were discussed in Section P-61.

The class name ‘hydroxylamine’, a preselected PIN, is also used as a functional parent and the class name ‘oxime’ is used as a functional class modifier, respectively. Nitrolic and nitrosolic acids are named as oximes of pseudoketones.

P-68.3.1.1.1 Hydroxylamines

P-68.3.1.1.1.1 Substitution on the nitrogen atom

The retained name ‘hydroxylamine’ is a preselected PIN and designates the structure H_2N-OH. It is a functional parent compound allowing full substitution even, as an exception, on the oxygen atom. Substitution on the nitrogen or the oxygen atom of hydroxylamine may create a function senior to amine, justifying a systematic name based on a higher class to denote this new function.

Substituted hydroxylamines of the type R-NH-OH or RR′N-OH are named by prefixing the name(s) of the substituent group(s) together with the locant *N* to the functional parent compound name 'hydroxylamine'.

Examples:

CH_3-NH-OH

N-methylhydroxylamine (PIN)

$(CH_3)_2$N-OH

N,*N*-dimethylhydroxylamine (PIN)

H_3Si-NH-OH

N-silylhydroxylamine
(preselected name)

H_2B-NH-OH

N-borylhydroxylamine
(preselected name)

Substitution by acyl groups generate hydroxamic acids that are named as *N*-hydroxyamides (see P-65.1.3.4).

Examples:

CH_3-CO-NH-OH

N-hydroxyacetamide (PIN)
(not acetohydroxamic acid)

CH_3-SO_2-NH-OH

N-hydroxymethanesulfonamide (PIN)

CH_3-CH_2-CO-NH-OH

N-hydroxypropanamide (PIN)
(no longer propanohydroxamic acid;
or propionohydroxamic acid)

P-68.3.1.1.1.2 Substitution on the oxygen atom

Substitution on the oxygen atom by hydrocarbyl groups or acyl groups is expressed as *O*-substitution. Names such as 'alkyloxyamines' are not recommended and the class peroxyamide has never been recognized.

Examples:

H_2N-O-CH_3

O-methylhydroxylamine (PIN)
(not methoxyamine)

H_2N-O-C_6H_5

O-phenylhydroxylamine (PIN)
(not phenoxyamine)

H_2N-O-CH_2-CH_2-O-NH_2

O,*O*′-ethane-1,2-diylbis(hydroxylamine) (PIN)

$H_2N\text{-}O\text{-}CO\text{-}C_6H_5$

O-benzoylhydroxylamine (PIN)

$H_2N\text{-}O\text{-}SO\text{-}CH_3$

O-methanesulfinylhydroxylamine (PIN)

O-Substitution by –NHR or –NRR′ leads to derivatives of dioxazane (see P-21.2.3.1)

Example:

$H_2\overset{3}{N}\text{-}\overset{2}{O}\text{-}\overset{1}{N}H\text{-}CH_3$

1-methyldiazoxane (PIN)

P-68.3.1.1.1.3 Substitution on both nitrogen and oxygen atoms

Substitution on both nitrogen and oxygen atom is expressed by:

(1) the corresponding *N*-(hydrocarbyloxy)amines, and

(2) *N*,*O*-substituted hydroxylamines.

Method (1) leads to preferred IUPAC names since an amine, expressed by the suffix -amine, is senior to the parent structure 'hydroxylamine' (see P-41).

Examples:

$CH_3\text{-}NH\text{-}O\text{-}CH_3$

N-methoxymethanamine (PIN)
N,*O*-dimethylhydroxylamine

$C_6H_5\text{-}NH\text{-}O\text{-}CH_2\text{-}CH_3$

N-ethoxyaniline (PIN)
O-ethyl-*N*-phenylhydroxylamine

P-68.3.1.1.1.4 Substitution by characteristic groups expressed as suffixes

Hydroxylamine is a functional parent to which suffixes expressing characteristic groups, such as acids, amides, etc., can be attached to the oxygen atom; for exceptional use of suffixes with functional parent compounds see P-46.2.3.1. In names, the locant *O* is placed in front of the suffix. Attachment of characteristic groups to the nitrogen atom generally leads to compounds of higher function.

Examples:

$H_2N\text{-}O\text{-}SO_2\text{-}OH$

hydroxylamine-*O*-sulfonic acid
(preselected name)

$H_2N\text{-}O\text{-}COOH$

hydroxylamine-*O*-carboxylic acid (PIN)

$H_2N\text{-}O\text{-}CONH_2$

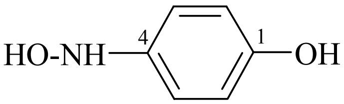
hydroxylamine-*O*-carboxamide (PIN)

P-68.3.1.1.1.5 Hydroxylamine expressed as prefix

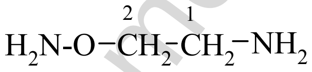
In the presence of a characteristic group having priority for citation as suffix or of a senior parent hydride, the appropriate complex or compound prefixes are used:

−NH-OH	hydroxyamino- (preselected name)
−O-NH_2	aminooxy- (preselected name) (note that there is no elision of the final letter ‘o’ in amino)

Examples:



4-(hydroxyamino)phenol (PIN)



$$H_2N\text{-}O-\overset{2}{C}H_2-\overset{1}{C}H_2-NH_2$$

2-(aminooxy)ethan-1-amine (PIN)

H_2N-NH-CH_2-O-NH_2

[(aminooxy)methyl]hydrazine (PIN)

P-68.3.1.1.1.6 Chalcogen analogues of hydroxylamine

Chalcogen analogs of hydroxylamine are denoted by the appropriate functional replacement prefix ‘thio’, ‘seleno’ and ‘telluro’. Parentheses are sometimes required to avoid the possibility of ambiguity. Substitution follows the principles of hydroxylamine.

Examples:

H_2N-SH

thiohydroxylamine (preselected name)

CH_3-NH-SH

N-methyl(thiohydroxylamine)

CH_3-CO-NH-SH

N-sulfanylacetamide (PIN)

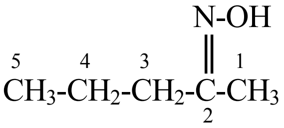
H_2N-S-CH_3

S-methyl(thiohydroxylamine)

P-68.3.1.1.2 Oximes

Compounds having the general structure R-CH=N-OH or RR′C=N=OH have the class name ‘oxime’ and have been further classified as ‘aldoximes’ and ‘ketoximes’ respectively. For general nomenclature they are named according to the principles of functional class nomenclature by placing the class name ‘oxime’ as a separate word after the name of the aldehyde or ketone. Preferred IUPAC names are formed substitutively as ‘ylidene’ derivatives of hydroxylamine. Compounds containing the group =N-OR are named substitutively as alkoxy substituted imines. In the presence of a characteristic group having priority for citation as a suffix, in substitutive nomenclature oximes are designated by the prefix ‘hydroxyimino’.

Examples:

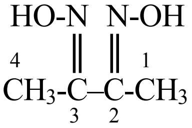


$\overset{5}{C}H_3\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\underset{2}{\overset{\overset{\text{N-OH}}{\|}}{C}}\text{-}\overset{1}{C}H_3$

pentan-2-ylidenehydroxylamine (PIN)
pentan-2-one oxime

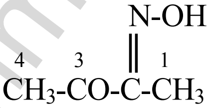
$\overset{3}{C}H_3\text{-}\overset{2}{C}H_3\text{-}\overset{1}{C}H\text{=}\overset{N}{N}\text{-O-}CH_2\text{-}CH_3$

N-ethoxypropan-1-imine (PIN)
propanal *O*-ethyloxime



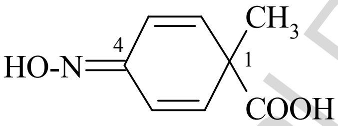
$\overset{4}{C}H_3\text{-}\underset{3}{\overset{\overset{\text{HO-N}}{\|}}{C}}\text{–}\underset{2}{\overset{\overset{\text{N-OH}}{\|}}{C}}\text{-}\overset{1}{C}H_3$

butane-2,3-diylidenebis(hydroxylamine) (PIN)
butane-2,3-dione dioxime

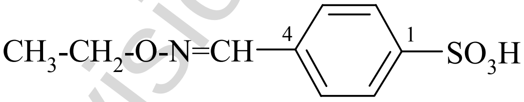


$\overset{4}{C}H_3\text{-}\overset{3}{C}O\text{-}\overset{\overset{\text{N-OH}}{\|}}{C}\text{-}\overset{1}{C}H_3$

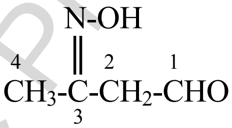
3-(hydroxyimino)butan-2-one (PIN)
butane-2,3-dione oxime



4-(hydroxyimino)-1-methylcyclohexa-2,5-diene-1-carboxylic acid (PIN)

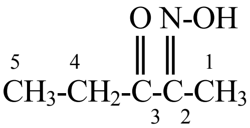


4-[(ethoxyimino)methyl)]benzene-1-sulfonic acid (PIN)



$\overset{4}{C}H_3\text{-}\underset{3}{\overset{\overset{\text{N-OH}}{\|}}{C}}\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}HO$

3-(hydroxyimino)butanal (PIN)



$\overset{5}{C}H_3\text{-}\overset{4}{C}H_2\text{-}\underset{3}{\overset{\overset{\text{O}}{\|}}{C}}\text{-}\underset{2}{\overset{\overset{\text{N-OH}}{\|}}{C}}\text{-}\overset{1}{C}H_3$

2-(hydroxyimino)pentan-3-one (PIN)
pentane-2,3-dione 2-oxime

P-68.3.1.1.3 Nitrolic and nitrosolic acids

Compounds having the general structure R-C(=NOH)-NO_2 and R-C(=NOH)-NO are called ‘nitrolic acids’ and ‘nitrosolic acids’, respectively. They are named substitutively for general nomenclature as oximes of pseudoketones. Preferred IUPAC names are formed as described above for ‘oximes’ (see p-68.3.1.1.3). Traditionally, they were named by functional class nomenclature as oximes of aldehydes substituted in position 1 by a nitro or nitroso group.

Examples

$\overset{3}{\mathrm{C}}\mathrm{H_3}\text{-}\overset{2}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{1}{\mathrm{C}}(=\overset{N}{\mathrm{N}}\mathrm{OH})\text{-}\mathrm{NO_2}$

(1-nitropropylidene)hydroxylamine (PIN)
1-nitropropan-1-one oxime
(not 1-nitropropanal oxime)

$\overset{2}{\mathrm{C}}\mathrm{H_3}\text{-}\overset{1}{\mathrm{C}}(=\overset{N}{\mathrm{N}}\mathrm{OH})\text{-}\mathrm{NO}$

(1-nitrosoethanylidene)hydroxylamine (PIN)
1-nitrosoethan-1-one oxime
(not 1-nitrosoacetaldehyde oxime)

P-68.3.1.2 Hydrazine and related compounds: hydrazones, azines, semicarbazides, semicarbazones, and carbonohydrazides

P-68.3.1.2.1 Hydrazine and derivatives

Hydrazine is a retained name describing the structure $\mathrm{H_2N\text{-}NH_2}$ that is the preferred IUPAC name; it is preferred to the systematic name ‘diazane’.

Substituent groups derived from hydrazine are named systematically:

$\mathrm{H_2N\text{-}NH}–$	hydrazinyl (preselected PIN) diazanyl (not hydrazino)
$\mathrm{H_2N\text{-}N}=$	hydrazinylidene (preselected PIN) diazanylidene (not hydrazono)
$=\mathrm{N\text{-}N}=$	hydrazinediylidene (preselected PIN) diazanediylidene (not azino)
$–\mathrm{NH\text{-}NH}–$	hydrazine-1,2-diyl (preselected PIN) diazane-1,2-diyl (not hydrazo)

As a parent hydride, hydrazine is numbered by numerical locants, 1 and 2, not *N* and *N'*. Hydrazine is substituted by hydrocarbyl groups and characteristic groups expressed by suffixes and prefixes.

Examples:

$(\mathrm{CH_3})_2\overset{1}{\mathrm{N}}\text{-}\overset{2}{\mathrm{N}}\mathrm{H_2}$

1,1-dimethylhydrazine (PIN)

$\mathrm{C_6H_5\text{-}NH\text{-}NH_2}$

phenylhydrazine (PIN)

$H_2N\text{-}NH\text{-}\overset{1}{C}H_2\text{-}\overset{N}{N}H_2$

1-hydrazinylmethanamine (PIN)
(see also P-62.2.1.1.2)

$H_2N\text{-}NH\text{-}COOH$

hydrazinecarboxylic acid (PIN)
(not carbazic acid)

$F_2N\text{-}NF_2$

tetrafluorohydrazine (preselected name)

$H_2N\text{-}NH\text{-}CH_2\text{-}CN$

hydrazinylacetonitrile (PIN)

$H_2N\text{-}CO\text{-}CH_2\text{-}\overset{3}{C}H_2\text{-}NH\text{-}NH\text{-}\overset{3'}{C}H_2\text{-}CH_2\text{-}CO\text{-}NH_2$

3,3′-(hydrazine-1,2-diyl)dipropanamide (PIN)
(not 3,3′-hydrazodipropanamide)

P-68.3.1.2.2 Hydrazones

Compounds having the general structure $RCH{=}N\text{-}NH_2$ or $RR'C{=}N\text{-}NH_2$ are called ‘hydrazones’ and are named in two ways.

(1) substitutively as derivatives of the parent hydride ‘hydrazine’, $H_2N\text{-}NH_2$;

(2) by functional class nomenclature using the class name ‘hydrazone’.

Method (1) generates preferred IUPAC names

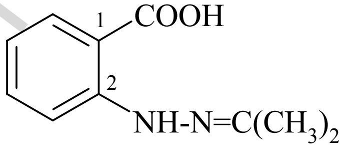
Examples:

$CH_3\text{-}CH_2\text{-}CH{=}N\text{-}NH_2$

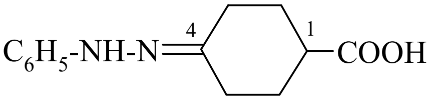
propylidenehydrazine (PIN)
propanal hydrazone

$(CH_3)_2\overset{1}{N}\text{-}\overset{2}{N}{=}C(CH_3)_2$

1,1-dimethyl-2-(propan-2-ylidene)hydrazine (PIN)
1.1-dimethyl-2-(1-methylethylidene)hydrazine
acetone dimethylhydrazone



2-[2-(propan-2-ylidene)hydrazinyl]benzoic acid (PIN)
2-[2-(1-methylethylidene)hydrazinyl]benzoic acid



4-(phenylhydrazinylidene)cyclohexane-1-carboxylic acid (PIN)

P-68.3.1.2.3 Azines

P-68.3.1.2.3.1 Compounds having the general structure R-CH=N-N=CH-R or RR′C=N-N=RR′ are called ‘azines’ and are named in two ways.

(1) substitutively, as derivatives of hydrazine;

(2) by functional class nomenclature using the class name ‘azine’.

Method (1) leads to preferred IUPAC names.

Example:

$$(CH_3)_2C{=}\overset{1}{N}{-}\overset{2}{N}{=}C(CH_3)_2$$

1,2-di(propan-2-ylidene)hydrazine (PIN)
1,2-bis(1-methylethanylidene)hydrazine
acetone azine

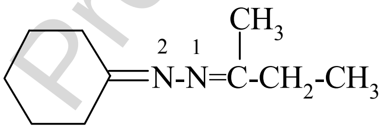
P-68.3.1.2.3.2 Azines are symmetrical derivatives of hydrazine. When this condition is not fulfilled, compounds having the structures R-CH=N-N=CH-R′ or RRC=N-N=CR′R′, are named in two ways.

(1) as unsymmetrical derivatives of hydrazine;

(2) as ‘ylidenehydrazones’ of the preferred ketone or aldehyde

Method (1) generates preferred IUPAC names.

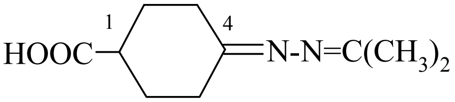
Example:



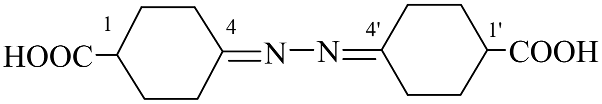
1-(butane-2-ylidene)-2-cyclohexylidenehydrazine (PIN)
2-cyclohexylidene-1-(1-methylpropylidene)hydrazine
cyclohexanone butan-2-ylidenehydrazone

P-68.3.1.2.3.3 In presence of functions having seniority, the prefix ‘hydrazinylidene’ is used. The prefix ‘hydrazinediylidene’ is used in multiplicative nomenclature.

Examples:



4-(propan-2-ylidenehydrazinylidene)cyclohexane-1-carboxylic acid (PIN)
4-[(1-methylethylidene)hydrazinylidene]cyclohexane-1-carboxylic acid



4,4′-hydrazinediylidenedi(cyclohexane-1-carboxylic acid) (PIN)
4,4′-azinodi(cyclohexane-1-carboxylic acid)

P-68.3.1.2.4 Semicarbazides

Semicarbazide is the amide of ‘hydrazinecarboxylic acid’. As acids and amides expressed by suffixes are senior to acids or amides modified by functional replacement, these names are senior to ‘carbonohydrazidic acid’ and ‘carbonohydrazidic’ amide.

H_2N-NH-COOH	hydrazinecarboxylic acid
H_2N-NH-CO-NH_2	hydrazinecarboxamide

Semicarbazide is the traditional name for the compound H_2N-NH-CO-NH_2, systematically named ‘hydrazinecarboxamide’ The systematic name is the preferred IUPAC name. The usual numbering for amides is recommended for the systematic name; special numbering is characteristic for the name semicarbazide.

$\overset{2}{H_2N}\text{-}\overset{1}{NH}\text{-CO-}\overset{N}{NH_2}$

hydrazinecarboxamide (PIN)

$\overset{1}{H_2}\overset{2}{N}\text{-}\overset{}{NH}\text{-}\overset{3}{CO}\text{-}\overset{4}{NH_2}$

semicarbazide

Examples:

$\overset{2}{H_2N}\text{-}\overset{1}{NH}\text{-CO-}\overset{N}{NH}\text{-}C_6H_5$

N-phenylhydrazinecarboxamide (PIN)
4-phenylsemicarbazide

$\overset{2}{H_2N}\text{-}\overset{1}{N}(CH_3)\text{-CO-}\overset{N}{NH}\text{-}CH_3$

N,1-dimethylhydrazinecarboxamide (PIN)
2,4-dimethylsemicarbazide

As a prefix, the −HN-NH-CO-NH_2 group is called ‘semicarbazido’ or ‘2-carbamoylhydrazin-1-yl’ or ‘2-(aminocarbonyl)hydrazine-1-yl’. The systematic name ‘2-carbamoylhydrazin-1-yl’ is the preferred IUPAC name.

Example:

$H_2N\text{-}CO\text{-}NH\text{-}NH\text{-}\overset{3}{C}H_2\text{-}CH_2\text{-}CN$

3-(2-carbamoylhydrazinyl)propanenitrile (PIN)

Chalcogen analogues are named systematically as described for amides or by functional replacement nomenclature using the class term ‘semicarbazide’ modified by the replacement prefixes ‘thio-’, ‘seleno-’, and ‘telluro’, for example, ‘thiosemicarbazide’.

$H_2\overset{2}{N}\text{-}\overset{1}{N}H\text{-}CSe\text{-}\overset{N}{N}H_2$

hydrazinecarboselenoamide (PIN)

$H_2\overset{1}{N}\text{-}\overset{2}{N}H\text{-}\overset{3}{C}Se\text{-}\overset{4}{N}H_2$

selenosemicarbazide

P-68.3.1.2.5 Semicarbazones

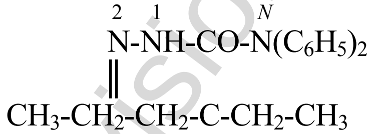
Compounds having the structure R-CH=N-NH-CO-NR′R″ or RR′C=N-NH-CO-NR″R‴ are generically called ‘semicarbazones’. They are named in two ways.

(1) substitutively by using the parent hydride ‘hydrazinecarboxamide’;

(2) by the class modifier ‘semicarbazone’ placed after the name of the corresponding aldehyde or ketone.

Method (1) yields preferred IUPAC names.

Examples:



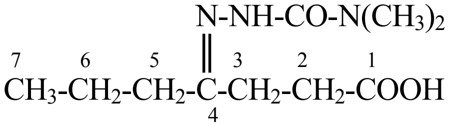
$$CH_3\text{-}CH_2\text{-}CH_2\text{-}\overset{\overset{2}{N}\text{-}\overset{1}{N}H\text{-}CO\text{-}\overset{N}{N}(C_6H_5)_2}{\overset{\|}{C}}\text{-}CH_2\text{-}CH_3$$

2-(hexan-3-ylidene)-*N,N*-diphenylhydrazinecarboxamide (PIN)
2-(1-ethylbutanylidene)-*N,N*-diphenylhydrazinecarboxamide
hexan-3-one 4,4-diphenylsemicarbazone

The compound prefix ‘2-carbamoylhydrazinylidene’ is used as a prefix in the presence of a characteristic group that is preferred for citation as a suffix. This prefix is preferred to the traditional name ‘semicarbazono’, whose structure is numbered as follows:

$=\overset{1}{N}\text{-}\overset{2}{N}H\text{-}\overset{3}{C}O\text{-}\overset{4}{N}H_2$

Example:



$$\overset{7}{\mathrm{CH_3}}\text{-}\overset{6}{\mathrm{CH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\underset{4}{\overset{\overset{\mathrm{N\text{-}NH\text{-}CO\text{-}N(CH_3)_2}}{\|}}{\mathrm{C}}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{COOH}}$$

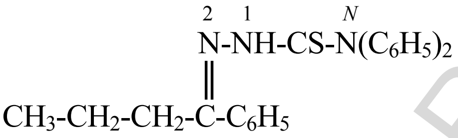
4-[2-(dimethylcarbamoyl)hydrazinylidene]heptanoic acid (PIN)
4-(4,4-dimethylsemicarbazono)heptanoic acid

Chalcogen analogues are named systematically as described for amides to give preferred IUPAC names, or by functional replacement nomenclature using the class terms ‘semicarbazone’ modified by the replacement prefixes ‘thio-’, ‘seleno-’, and ‘telluro’, for example, ‘thiosemicarbazone’. The prefix ‘2-carbamothioylhydrazinylidene’ is preferred to the traditional prefix ‘thiosemicarbazono’.

$\overset{2}{\mathrm{H_2N}}\text{-}\overset{1}{\mathrm{NH}}\text{-CS-}\overset{N}{\mathrm{NH_2}}$ $\qquad$ $\overset{1}{\mathrm{H_2N}}\text{-}\overset{2}{\mathrm{NH}}\text{-}\overset{3}{\mathrm{CS}}\text{-}\overset{4}{\mathrm{NH_2}}$

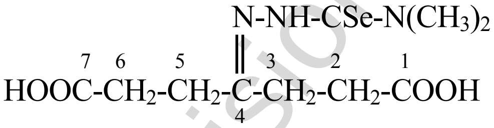
hydrazinecarbothioamide (PIN) $\qquad$ thiosemicarbazide

Examples:



$$\mathrm{CH_3\text{-}CH_2\text{-}CH_2\text{-}\overset{\overset{\overset{2}{N}\text{-}\overset{1}{NH}\text{-}CS\text{-}\overset{N}{N}(C_6H_5)_2}{\|}}{C}\text{-}C_6H_5}$$

N,N-diphenyl-2-(1-phenylbutylidene)hydrazine-1-carbothioamide (PIN)
1-phenylbutan-1-one 4,4-diphenylthiosemicarbazone



$$\overset{7}{\mathrm{HOOC}}\text{-}\overset{6}{\mathrm{CH_2}}\text{-}\overset{5}{\mathrm{CH_2}}\text{-}\underset{4}{\overset{\overset{\mathrm{N\text{-}NH\text{-}CSe\text{-}N(CH_3)_2}}{\|}}{\mathrm{C}}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{2}{\mathrm{CH_2}}\text{-}\overset{1}{\mathrm{COOH}}$$

4-[2-(dimethylcarbamoselenoyl)hydrazinylidene]heptanedioic acid (PIN)
4-[4,4-dimethyl(selenosemicarbazono)]heptanedioic acid

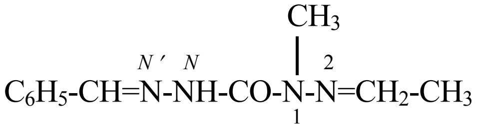
P-68.3.1.2.6 Hydrazinecarbohydrazide and derivatives

P-68.3.1.2.6.1 The compound $\mathrm{H_2N\text{-}NH\text{-}CO\text{-}NH\text{-}NH_2}$ is named ‘hydrazinecarbohydrazide’ systematically;it is the preferred IUPAC name. The name ‘carbonic dihydrazide’ is also recommended, but for general use only; the names ‘carbonohydrazide’, ‘carbohydrazide’, and ‘carbazide’ are not recommended. Systematic numbering is applied to the systematic name; a special numbering is assigned to the retained name, as follows:

$\overset{2}{\mathrm{H_2N}}\text{-}\overset{1}{\mathrm{NH}}\text{-CO-}\overset{N}{\mathrm{NH}}\text{-}\overset{N'}{\mathrm{NH_2}}$ $\qquad$ $\overset{N'''}{\mathrm{H_2N}}\text{-}\overset{N''}{\mathrm{NH}}\text{-CO-}\overset{N}{\mathrm{NH}}\text{-}\overset{N'}{\mathrm{NH_2}}$

hydrazinecarbohydrazide (PIN) $\qquad$ carbonic dihydrazide

Example:



$$C_6H_5\text{-CH=}\overset{N'}{\text{N}}\text{-}\overset{N}{\text{NH}}\text{-CO-}\underset{1}{\overset{CH_3}{\text{N}}}\text{-}\overset{2}{\text{N}}\text{=CH}_2\text{-CH}_3$$

N′-benzylidene-2-ethylidene-1-methylhydrazine-1-carbohydrazide (PIN)
(the twice substituted chain is the principal chain; in alphanumerical order, *N* ′ is senior to 2)
5-benzyl-1-ethylidene-2-methylcarbonohydrazide
(the set of locants 1,2,5 is lower than 1,4,5)

P-68.3.1.2.6.2 As prefixes, the groups −NH-NH-CO-NH-NH_2 and =N=NH-CO-NH-NH_2 are called ‘2-hydrazinecarbonylhydrazin-1-yl’ and ‘2-hydrazinecarbonylhydrazinylidene’, respectively; these names are preferred IUPAC names.

Example:

H_2N-NH-CO-NH-NH-CH_2-CH_2-COOH

3-(2-hydrazinecarbonylhydrazin-1-yl)propanoic acid (PIN)

P-68.3.1.3 Compounds derived from diazene

P-68.3.1.3.1 Azo compounds (R-N=N-R′)
P-68.3.1.3.2 Azoxy compounds (R-N=N(O)-R′)
P-68.3.1.3.3 Diazenecarbohydrazides (HN=N-CO-NH-NH_2)
P-68.3.1.3.4 Formazan and its derivatives (H_2N-N=CH-N=NH)
P-68.3.1.3.5 Carbonylbis(diazene) (HN=N-CO-N=NH)
P-68.3.1.3.6 Isodiazenes (R_2N^+=N^-)

P-68.3.1.3.1 Azo compounds, R-N=N-R′

Compounds with the general structure R-N=N-R′, where R and R′ may be alike or different, are known generically as ‘azo compounds’. They are named in two ways:

(1) substitutively using the parent ‘diazene’, HN=NH;

(2) by using the prefix ‘azo’ in the traditional manner.

Examples: Method (1) leads to preferred IUPAC names.

Rules for naming azo compounds using the azo prefix were quite complex. Two sets of rules were recommended, the so called ‘old method’ (Rule C-911) and the Chemical Abstracts Service rules (C-912). The old method must be totally discarded since some examples do not follow the basic rules developed in the 1979 organic nomenclature rules, especially with respect to the treatment of suffixes. In 1993, a new approach was recommended that was based on the use of the parent ‘diazene’ [Method (1), above]. It brought simplicity and rationalization to the field. It is the method chosen to generate preferred names in these recommendations. The CAS method is given as an acceptable alternative.

Azo compounds are divided into monoazo compounds, having one −N=N− group, bis(azo) compounds, having two −N=N− groups, and so on.

P-68.3.1.3.1.1 Symmetrical monoazo compounds, R-N=N-R, are named:

(1) by substituting the parent diazene, HN=NH, by the appropriate substituent groups;

(2) by adding 'azo' to the name of the parent hydride, RH; substituents are denoted in the usual way by prefixes, the two RH parents being distinguished by unprimed and primed locants. Attachment of the azo group has priority for lowest available numbers.

Method (1) gives preferred IUPAC names.

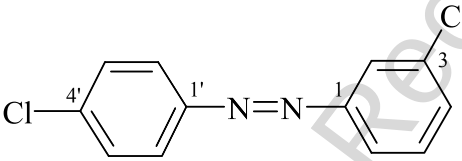
Examples:

CH_3-N=N-CH_3

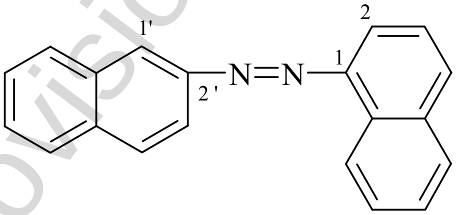
dimethyldiazene (PIN)
azomethane

C_6H_5-N=N-C_6H_5

diphenyldiazene (PIN)
azobenzene



(3-chlorophenyl)(4-chlorophenyl)diazene (PIN)
3,4′-dichloroazobenzene
(numbering shown)



naphthalen-1-yl(naphthalen-2-yl)diazene (PIN)
1,2′-azonaphthalene
(numbering shown)

P-68.3.1.3.1.2 Unsymmetrical monoazo compounds are named in two ways:

(1) substitutively, by prefixing, in alphabetical order, the names of the appropriate substituent groups before the parent hydride name diazene;

(2) by inserting 'azo' between the names of the parent hydrides RH and R′H; the principal chain or the senior ring or ring system is cited first and is assigned plain locants, the other parent hydride being given primed locants; when locants are required to denote the

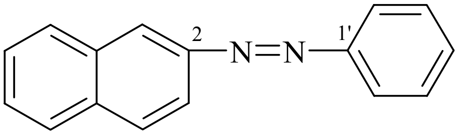
points of attachment of the parent hydrides, they are placed immediately before or after the prefix ‘azo’, respectively.

Method (1) leads to preferred IUPAC names.

Examples:

$CH_2=CH-N=N-CH_3$

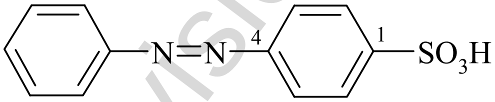
ethenyl(methyl)diazene (PIN)
methyl(vinyl)diazene
etheneazomethane



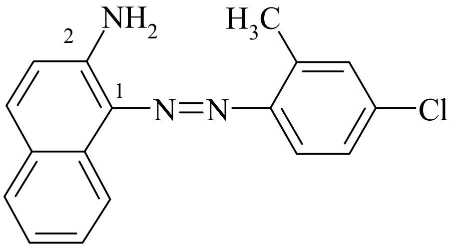
naphthalen-2-yl(phenyl)diazene (PIN)
naphthalene-2-azobenzene
(numbering shown)

Monoazo compounds with the general structure R-N=N-R′ in which R is substituted by a principal characteristic group is named on the basis of the parent hydride, RH, substituted by an organyl diazenyl group, R′-N=N−. If both R and R′ are substituted by the same number of the principal characteristic group, a multiplicative name is preferred to a substitutive name.

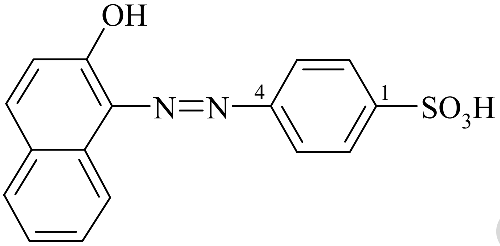
Examples:



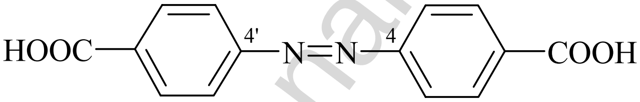
4-(phenyldiazenyl)benzene-1-sulfonic acid (PIN)
4-(phenylazo)benzene-1-sulfonic acid



1-[(4-chloro-2-methylphenyl)diazenyl]naphthalen-2-amine (PIN)
[not 2-aminonaphthalene-1-azo-(4′-chloro-2′-methylbenzene) (see C-911.2, ref. 1); the principal characteristic group, the amine must be denoted by a suffix]



4-[(2-hydroxynaphthalen-1-yl)diazenyl]benzene-1-sulfonic acid (PIN)
4-[(2-hydroxy-1-naphthyl)azo]benzenesulfonic acid)



4,4′-diazenediyldibenzoic acid (PIN)
(traditionally 4,4′-azodibenzoic acid)

P-68.3.1.3.1.3 Bis(azo) compounds and more complex analogues, in the absence of a characteristic group having seniority to be cited as suffix, are named:

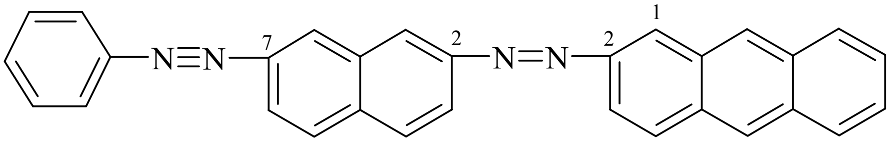
(1) on the basis of ‘diazene’, as described in 68.3.1.3.1.1 above; the first cited substituent being chosen on the basis of the principle of alphanumerical order;

(2) by using the prefix ‘azo’, as described in 68.3.1.3.1.1;

(3) by using the prefix ‘azo’, after choosing the principal parent hydride and substituting the other components as ‘organylazo’ groups.

Method (1) generates preferred IUPAC names.

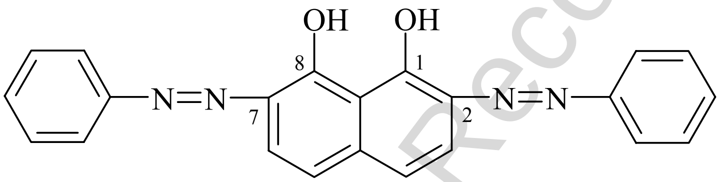
Example:



(1) anthracen-2-yl[(7-phenyldiazenyl)naphthalen-2-yl]diazene (PIN)
(not [7-(anthracene-2-yldiazenyl)naphthalen-2yl]phenyldiazene; in alphanumerical order 'anthracen-2-yl' precedes 'anthracen-2-yldiazenyl'; numbering shown)
(2) anthracene-2-azo-2′-naphthalene-7′-azobenzene)
(3) 2-{[7-(phenylazo)naphthalen-2-yl]azo}anthracene

When characteristic groups that have priority for citation as suffixes are present, the usual substitutive operations based on priority of suffixes are carried out. Names based on the prefix 'diazenyl' are preferred to those using 'azo' for generating preferred IUPAC names.

Example:



2,7-bis(phenyldiazenyl)naphthalene-1,8-diol (PIN)
2,7-bis(phenylazo)naphthalene-1,8-diol

P-68.3.1.3.2 Azoxy compounds, R-N=N(O)-R′

P-68.3.1.3.2.1 *N*-Oxides of azo compounds having the general structure R-N_2(O)-R′ (R = R′ or R ≠ R′) are known generically as 'azoxy compounds'. Their nomenclature was revised in 1993 (ref. 2) and is used in these recommendations. Azoxy compounds are named in two different ways.

(1) by adding the term 'oxide' to the name of the corresponding azo compound, preceded by a locant 1 or 2;

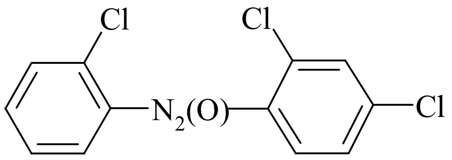
(2) in the traditional way of replacing the prefix 'azo' by 'azoxy' and using the locants *NNO* and *ONN* to indicate the parent hydride associated with the =N→O group. In the general structure R-N(O)N-R′, the symbol *NNO* specifies that the oxygen atom is attached to the nitrogen atom next to the R′ group. The symbol *ONN* specifies that the oxygen atom is attached to the nitrogen atom next to the R group. When the point of attachment is not known, the symbol *NON* is used.

Method (1) leads to preferred IUPAC names. Azoxy compounds could also be named by using the λ-convention or as zwitterions; these methods are not recommended.

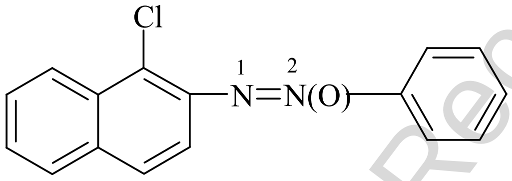
Examples:

C_6H_5-N=N(O)-C_6H_5

(1) diphenyldiazene oxide (PIN)
(2) azoxybenzene
[not 1-oxo-1,2-diphenyl-$1\lambda^5$-diazene)
[not (1,2-diphenyldiazanium-1-yl)oxidanide]



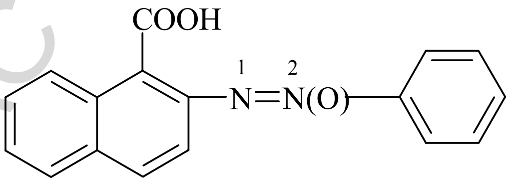
(2-chlorophenyl)(2,4-dichlorophenyl)diazene oxide (PIN)
2,2′,4′-trichloroazoxybenzene
(the absence of locants indicates that the points of attachment are not known)



1-(1-chloronaphthalen-2-yl)-2-phenyldiazene 2-oxide (PIN)
1-chloro-2-(phenyl-*ONN*-azoxy)naphthalene

P-68.3.1.3.2.2 An azoxy compound, according to the general seniority given to zwitterions over suffixes expressing characteristic groups, is preferably named as a derivative of diazene oxide, unless some other priority is given to another radical or ionic group. In general nomenclature, the traditional method for naming azoxy compounds is maintained. An azoxy compound in which the general structure is R-N=N(O)-R′ or R′-N=N(O)-R, in which R is substituted by a principal characteristic group is named on the basis of the parent hydride, RH, substituted by the R′-azoxy group in which the position of the oxygen atom is denoted by the prefix *NNO*-, *ONN*-, or *NON*-, as appropriate.

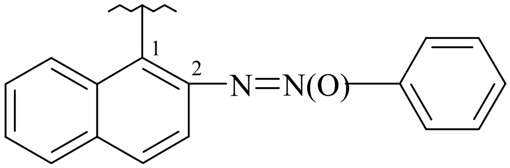
Example:



1-(1-carboxynaphthalen-2-yl)-2-phenyldiazene 2-oxide (PIN)
2-(phenyl-*ONN*-azoxy)naphthalene-1-carboxylic acid
(not 2-(phenyl-*ONN*-azoxy)-1-naphthoic acid; no substitution allowed on naphthoic acid)

When the azoxy compound has to be expressed by a prefix, substitutive nomenclature using the λ-convention is preferred (see Section 74.1.1).

Example:



(1-phenyl-1-oxo-1λ^5-diazen-2-yl)naphthalen-1-yl (PIN)
2-(2-oxido-2-phenyldiazen-2-ium-1-yl)naphthalen-1-yl

P-68.3.1.3.3 Derivatives of diazenecarbohydrazide, $HN{=}N\text{-}CO\text{-}NH\text{-}NH_2$

The hydrazide of ‘diazenecarboxylic acid, $HN{=}N\text{-}CO\text{-}NH\text{-}NH_2$, is named systematically diazenecarbohydrazide; it is the preferred IUPAC name. The name ‘carbazone’ is not recommended. Chalcogen analogues are named by using the infixes and the prefixes ‘thio’, ‘seleno’ and ‘telluro’.

$\mathrm{H}\overset{2}{\mathrm{N}}{=}\overset{1}{\mathrm{N}}\text{-CO-}\overset{N}{\mathrm{N}}\mathrm{H}\text{-}\overset{N'}{\mathrm{N}}\mathrm{H}_2$

diazenecarbohydrazide (PIN)

$\mathrm{H}\overset{2}{\mathrm{N}}{=}\overset{1}{\mathrm{N}}\text{-CS-}\overset{N}{\mathrm{N}}\mathrm{H}\text{-}\overset{N'}{\mathrm{N}}\mathrm{H}_2$

diazenecarbothiohydrazide (PIN)

Examples:

$\mathrm{C_6H_5}\text{-}\overset{2}{\mathrm{N}}{=}\overset{1}{\mathrm{N}}\text{-CO-}\overset{N}{\mathrm{N}}\mathrm{H}\text{-}\overset{N'}{\mathrm{N}}\mathrm{H}\text{-}\mathrm{C_6H_5}$

N′,2-diphenyldiazenecarbohydrazide (PIN)

$\mathrm{C_6H_5}\text{-}\overset{2}{\mathrm{N}}{=}\overset{1}{\mathrm{N}}\text{-CS-}\overset{N}{\mathrm{N}}\mathrm{H}\text{-}\overset{N'}{\mathrm{N}}\mathrm{H}\text{-}\mathrm{C_6H_5}$

N′,2-diphenyldiazenecarbothiohydrazide (PIN_

As a prefix, the group $-HN\text{-}NH\text{-}CO\text{-}N{=}NH$ is named ‘2-diazenecarbonylhydrazin-1-yl’ or ‘diazenecarbohydrazido’; the preferred IUPAC name is ‘2-diazenecarbonylhydrazin-1-yl’. The name ‘carbazono’ is not recommended.

The group $H_2N\text{-}NH\text{-}CO\text{-}N{=}NH-$ is named ‘2-hydrazinecarbonyldiazen-1-yl’.

Example:

$HN{=}N\text{-}CO\text{-}NH\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}COO\text{-}CH_2\text{-}CH_3$

ethyl 3-(2-diazenecarbonylhydrazin-1-yl)propanoate (PIN)

P-68.3.1.3.4 Formazan, $H_2N\text{-}N{=}CH\text{-}N{=}NH$, and its derivatives

The hydrazone of diazenecarbaldehyde, $H_2N\text{-}N{=}CH\text{-}N{=}NH$, has the preferred IUPAC retained name ‘formazan’; it is numbered in a special manner. It can also be named substitutively as a derivative of the parent hydride ‘diazene’; its derivatives are named accordingly.

$\overset{5}{H_2N}\text{-}\overset{4}{N}{=}\overset{3}{CH}\text{-}\overset{2}{N}{=}\overset{1}{NH}$

formazan (PIN)

$H_2N\text{-}N{=}CH\text{-}\overset{1}{N}{=}\overset{2}{NH}$

(hydrazinylidenemethyl)diazene

P-68.3.1.3.4.1 Derivatives of formazan

Preferred names are constructed systematically as derivatives of formazan or by using parent names denoting characteristic groups expressed as suffix.

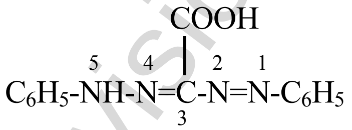
Examples:

$\overset{5}{H_2N}\text{-}\overset{4}{N}{=}\overset{3}{C}(C_6H_5)\text{-}\overset{2}{N}{=}\overset{1}{N}\text{-}C_6H_5$

1,3-diphenylformazan (PIN)
[hydrazinylidene(phenyl)methyl]phenyldiazene

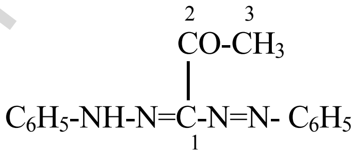
$C_6H_5\text{-}\overset{5}{N}H\text{-}\overset{4}{N}{=}\overset{3}{C}(C_6H_5)\text{-}\overset{2}{N}{=}\overset{1}{N}H$

3,5-diphenylformazan (PIN)
[phenyl(phenylhydrazinylidene)methyl]diazene



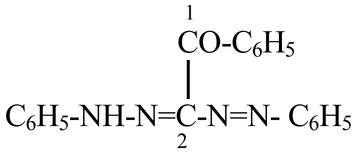
$C_6H_5\text{-}\overset{5}{N}H\text{-}\overset{4}{N}{=}\underset{3}{\overset{COOH}{C}}\text{-}\overset{2}{N}{=}\overset{1}{N}\text{-}C_6H_5$

1,5-diphenylformazan-3-carboxylic acid (PIN)
(phenyldiazenyl)(phenylhydrazinylidene)acetic acid



$C_6H_5\text{-}NH\text{-}N{=}\underset{1}{\overset{\overset{2}{C}O\text{-}\overset{3}{C}H_3}{C}}\text{-}N{=}N\text{-}C_6H_5$

1-(phenyldiazenyl)-1-(phenylhydrazinylidene)propan-2-one (PIN)
3-acetyl-1,5-diphenylformazan



$$C_6H_5\text{-}NH\text{-}N{=}\underset{2}{\overset{\overset{\textstyle 1}{CO\text{-}C_6H_5}}{\overset{|}{C}}}\text{-}N{=}N\text{-}C_6H_5$$

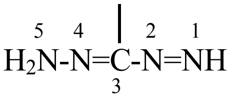
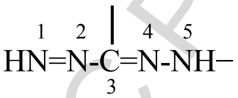
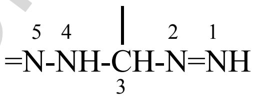
1-phenyl-2-(phenyldiazenyl)-2-(phenylhydrazinylidene)ethan-1-one (PIN)
3-benzoyl-1,5-diphenylformazan

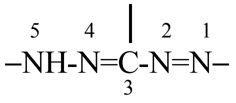
$$CH_3\text{-}CO\text{-}\overset{\mathit{N}}{N}H\text{-}\overset{\mathit{N}'}{N}{=}CH\text{-}N{=}N\text{-}C_6H_5$$

N'-[(phenyldiazenyl)methylidene]acetohydrazide (PIN)

P-68.3.1.3.4.2 Prefixes derived from formazan for substitutive nomenclature

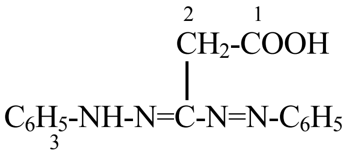
Substituent groups derived from formazan are as follows; retained names lead to preferred IUPAC names.

	Retained name	Systematic name
$H_2\overset{5}{N}\text{-}\overset{4}{N}{=}\overset{3}{C}H\text{-}\overset{2}{N}{=}\overset{1}{N}-$	formazan-1-yl (PIN)	(hydrazinylidenemethyl)diazenyl
$H\overset{1}{N}{=}\overset{2}{N}\text{-}\overset{3}{C}H{=}\overset{4}{N}\text{-}\overset{5}{N}H-$	formazan-5-yl (PIN)	(diazenylmethylidene)hydrazinyl
 $H_2\overset{5}{N}\text{-}\overset{4}{N}{=}\underset{3}{\overset{\mid}{C}}\text{-}\overset{2}{N}{=}\overset{1}{N}H$	formazan-3-yl (PIN)	diazenyl(hydrazinylidene)methyl
$-H\overset{5}{N}\text{-}\overset{4}{N}{=}\overset{3}{C}H\text{-}\overset{2}{N}{=}\overset{1}{N}-$	formazan-1,5-diyl (PIN)	
 $H\overset{1}{N}{=}\overset{2}{N}\text{-}\underset{3}{\overset{\mid}{C}}{=}\overset{4}{N}\text{-}\overset{5}{N}H-$	formazan-3,5-diyl (PIN)	
$=\overset{5}{N}\text{-}\overset{4}{N}{=}\overset{3}{C}H\text{-}\overset{2}{N}{=}\overset{1}{N}-$	formazan-1-yl-5-ylidene (PIN)	
 $=\overset{5}{N}\text{-}\overset{4}{N}H\text{-}\underset{3}{\overset{\mid}{C}}H\text{-}\overset{2}{N}{=}\overset{1}{N}H$	formazan-3-yl-5-ylidene (PIN)	



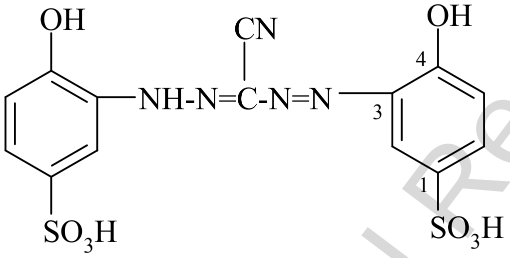
$-\overset{5}{\mathrm{N}}\mathrm{H}\text{-}\overset{4}{\mathrm{N}}=\underset{3}{\overset{|}{\mathrm{C}}}\text{-}\overset{2}{\mathrm{N}}=\overset{1}{\mathrm{N}}-$ formazan-1,3,5-triyl (PIN)

Examples:



$\mathrm{C_6H_5\text{-}NH\text{-}N}=\underset{3}{\overset{\overset{2}{\mathrm{C}}\mathrm{H_2}\text{-}\overset{1}{\mathrm{C}}\mathrm{OOH}}{\overset{|}{\mathrm{C}}}}\mathrm{\text{-}N{=}N\text{-}C_6H_5}$

3-(phenyldiazenyl)-3-(phenylhydrazinylidene)propanoic acid (PIN;
propanoic acid preferred to acetic acid)
(1,5-diphenylformazan-3-yl)acetic acid



(3-cyanoformazan-1,5-diyl)bis(4-hydroxybenzene-1-sulfonic acid) (PIN)
3-({cyano[(2-hydroxy-5-sulfonophenyl)hydrazinyl]methyl}diazenyl)-4-hydroxy-benzenesulfonic acid

P-68.3.1.3.5 1,1′-carbonylbis(diazene), HN=N-CO-N=NH

The compound HN=N-CO-N=NH is named 1,1′-carbonylbis(diazene); its hydrocarbyl derivatives are named substitutively. Such names are preferred IUPAC names over those denoted by the retained name ‘carbodiazone’, which can be used in general nomenclature with full substitution according to a special numbering. Chalcogen analogues are named by using the infixes and the prefixes ‘thio’, ‘seleno’ and ‘telluro’ for naming the chalcogen analogs of the hydrazide and the carbazone. The corresponding prefix is named systematically.

$\mathrm{H\overset{2}{N}{=}\overset{1}{N}\text{-}CO\text{-}\overset{1'}{N}{=}\overset{2'}{N}H}$

carbonylbis(diazene) (PIN)

$\mathrm{\overset{1}{H}N{=}\overset{2}{N}\text{-}\overset{3}{C}O\text{-}\overset{4}{N}{=}\overset{5}{N}H}$

carbodiazone

HN=N-CS-N=NH

1,1′-carbonothioylbis(diazene) (PIN)
thiocarbodiazone

$\mathrm{HN{=}N\text{-}CO\text{-}\overset{2}{N}{=}\overset{1}{N}-}$

diazenecarbonyldiazenyl (PIN)

Example:

C_6H_5-N=N-CO-N=N-C_6H_5

carbonylbis(phenyldiazene) (PIN)
1,5-diphenylcarbodiazone

P-68.3.1.3.6 Isodiazenes, $R_2N^+= N^-$

Compounds with the general structure R_2N-N**:** ↔ $R_2N^+= N^-$ are generically called 'isodiazenes' and named substitutively on the basis of the parent radical 'hydrazinylidene, H_2N-N**:**. This method leads to preferred IUPAC names rather than the parent hydride name 'isodiazene'.

Example:

$(CH_3)_2$N-N:

dimethylhydrazinylidene (PIN)
dimethylisodiazene

P-68.3.1.4 Polyazanes

P-68.3.1.4.1 Acyclic polyazanes are saturated chains composed of nitrogen atoms; hydrazine is the IUPAC preferred retained name for diazane, H_2N-NH_2. Names are formed by prefixing the mononuclear parent hydride name 'azane' with an appropriate numerical prefix and numbered in the same way as hydrocarbons. The parent hydrides are preselected IUPAC names (see P-12)

Examples:

$\overset{}{CH_3}$-$\overset{1}{N}$H-$\overset{2}{N}$H-$\overset{3}{N}H_2$

1-methyltriazane. (PIN)

CH_3-$\overset{1}{N}$H-$\overset{2}{N}(CH_3)$-$\overset{3}{N}$H-$\overset{4}{N}H_2$

1,2-dimethyltetraazane (PIN)

The corresponding prefixes are named according to the general method described in P-29. The traditional names 'triazano' and 'triazeno' are names of bridges in bridged fused ring names and must not be used as substituent groups.

Examples:

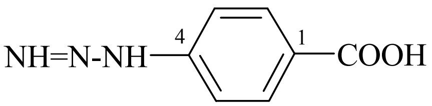
$H_2\overset{3}{N}$-$\overset{2}{N}$H-$\overset{1}{N}$H–

triazan-1-yl- (preselected name)
(not triazano)

H$\overset{3}{N}$=$\overset{2}{N}$-$\overset{1}{N}$H–

triaz-2-en-1-yl- (preselected name)
(not 2-triazeno)

Examples:



4-(triaz-2-en-1-yl)benzoic acid (PIN)
(not 4-triazenobenzoic acid)

$H_2\overset{4}{N}\text{-}\overset{3}{N}H\text{-}\overset{2}{N}H\text{-}\overset{1}{N}H\text{-}CH_2\text{-}CO\text{-}O\text{-}CH_2\text{-}CH_3$

ethyl (tetrazan-1-yl)acetate (PIN)
(not ethyl tetrazanoacetate)

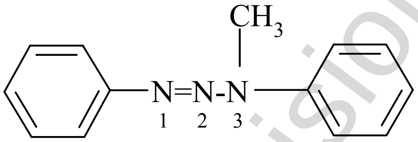
P-68.3.1.4.2 Diazoamino compounds

Compounds having the structure R-N=N-NR$_2$ are classified as ‘diazoamino compounds’, when the same substituent group is located at each end of the chain. They are named substitutively, on the basis of parent hydride name ‘triazene’. The prefix ‘diazoamino’ is no longer recommended.

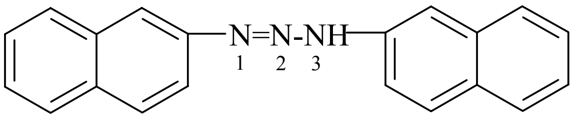
Examples:

$C_6H_5\text{-}\overset{1}{N}\text{=}\overset{2}{N}\text{-}\overset{3}{N}H\text{-}C_6H_5$

1,3-diphenyltriaz-1-ene (PIN)
(formerly diazoaminobenzene)



3-methyl-1,3-diphenyltriaz-1-ene (PIN)
(formerly *N*-methyldiazoaminobenzene)



1,3-di(naphthalen-2-yl)triaz-1-ene (PIN)
(formerly 2,2′-diazoaminonaphthalene)

P-68.3.2 Phosphorus, arsenic and antimony compounds

P-68.3.2.1 General methodology

Preferred names of acyclic phosphorus, arsenic and antimony compounds are functional class names (see P-67) derived from mononuclear and polynuclear acids, such as phosphoric acid, H_3PO_4, arsonous acid, $HAs(OH)_2$, stibinic acid, $H_2Sb(O)(OH)$, diphosphonic acid, HO-HP(O)-O-P(O)H-OH, rather than substitutive names based on parent hydrides.

Other preferred names of acyclic and cyclic compounds are substitutive names, in accordance with the seniority of classes (see P-41).

This subsection includes the description of functional class nomenclature and substitutive nomenclature.

P-68.3.2.2 Parent hydrides
P-68.3.2.3 Substitutive nomenclature

P-68.3.2.2 Parent hydrides

Parent hydrides are formed by the methods described in Chapter 2. They are mononuclear and acyclic polynuclear and cyclic and are preselected names (see P-12) The λ-convention is used to denote pentavalent phosphorus and arsenic atoms. Retained names for use only in general nomenclature are phosphine, phosphorane, arsine, arsorane, stibine, stiborane, and bismuthine.

Preferred names are selected as indicated in Chapter 2.

Examples:

PH_3

phosphane (preselected name)
phosphine

AsH_5

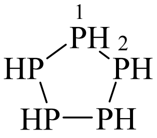
λ^5-arsane (preselected name)
arsorane

$\overset{2}{H_2P}\text{-}\overset{1}{PH_2}$

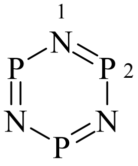
diphosphane (preselected name)
diphosphine

$\overset{5}{H_2As}\text{-}\overset{4}{AsH}\text{-}\overset{3}{AsH}\text{-}\overset{2}{AsH}\text{-}\overset{1}{AsH_2}$

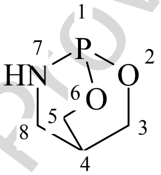
pentaarsane (preselected name)



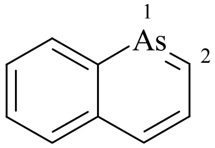
pentaphospholane (preselected name)
cyclopentaphosphane



1,3,5,2,4,6-triazatriphosphinine (preselected name)
cyclotriphosphazene



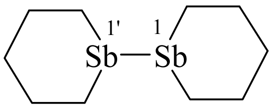
2,6-dioxa-7-aza-1-phosphabicyclo[2.2.2]octane (PIN)



arsinoline (PIN)

$\overset{7}{CH_3}\text{-}\overset{6}{CH_2}\text{-}\overset{5}{O}\text{-}\overset{4}{PH}\text{-}\overset{3}{O}\text{-}\overset{2}{SiH_2}\text{-}\overset{1}{CH_3}$

3,5-dioxa-4-phospha-2-silaheptane (PIN)



1,1′-bistibinane (PIN)

P-68.3.2.3 Substitutive nomenclature

Compounds not named in accordance with the previous section, P-68.3.2.3, are named substitutively on the basis of acyclic and cyclic parent hydrides, using suffixes and prefixes to designate characteristic groups.

P-68.3.2.3.1 Substitutive nomenclature, suffix mode

Suffixes are used to denote characteristic groups present as principal groups, with the exception of acids having retained names and their derivatives, as described in P-68.3.2.3. This method produces preferred IUPAC names over those formed by functional class nomenclature where =O, =S, =Se, =Te, =NH are denoted by the class names oxide, sulfide, selenide, telluride, and imide added to the name of the parent hydride.

Examples:

$H_2P\text{-}COOH$

phosphanecarboxylic acid (PIN)

$H_2P\text{-}CO\text{-}NH_2$

phosphanecarboxamide (PIN)

$C_6H_5\text{-}P{=}O$

phenylphosphanone (PIN)
[not oxo(phenyl)phosphane]

$(C_6H_5)_3P{=}O$

triphenyl-λ^5-phosphanone (PIN)
triphenylphosphane oxide
triphenylphosphine oxide

$HP{=}N\text{-}CH_3$

N-methylphosphanimine (PIN)
[not (methylimino)phosphane]

$(CH_3)_3As{=}Te$

trimethyl-λ^5-arsanetellone (PIN))
trimethylarsane telluride

$C_6H_5\text{-}As{=}S$

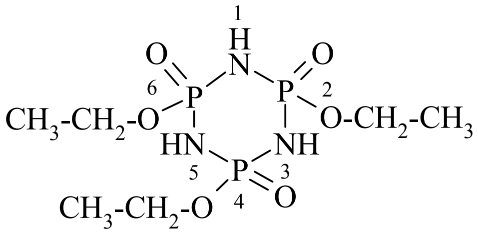
phenylarsanethione (PIN)
[not phenyl(sulfanylidene)arsane]

$(CH_3)_3As{=}NH$

trimethyl-λ^5-arsanimine (PIN)
trimethylarsane imide

$(CH_3)_2\overset{3}{P}\text{-}\overset{2}{P}(OH)\text{-}\overset{1}{P}(CH_3)_2$

1,1,3,3-tetramethyltriphosphan-2-ol



2,4,6-triethoxy-1,3,5-triaza-2λ^5,4λ^5, 6λ^5-triphosphinane-2,4,6-trione (PIN)

P-68.3.2.3.2 Substitutive nomenclature, prefix mode

The seniority of classes must be applied in the following order: classes expressed by suffixes, then classes in order of the senior class, in the order N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl > O > S > Se > Te, and C.

P-68.3.2.4.2.1 Substitution of phosphanes, arsanes and stibanes by organyl groups

Alkyl, aryl, etc. groups and groups derived from parent hydrides containing O, S, Se, and Te atoms are always denoted by prefixes. Halides and pseudohalides are not expressed by prefixes when attached directly to a P, As or Sb atom, because functional replacement of parent acids having retained names is senior for naming them as acid halides and pseudohalides (see P-67).

Examples:

$(C_6H_5)_3P$

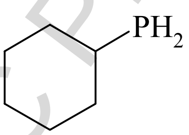
triphenylphosphane (PIN)
triphenylphosphine

CH_3-CH_2-AsH_2

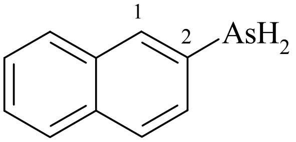
ethylarsane (PIN)
ethylarsine

$P(OCH_3)_5$

pentamethoxy-λ^5-phosphane (PIN)
(formerly pentamethyl holophosphate)



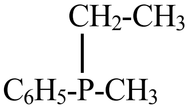
cyclohexylphosphane (PIN)
cyclohexylphosphine



naphthalen-2-ylarsane (PIN)
naphthalen-2-ylarsine
2-naphthylarsane

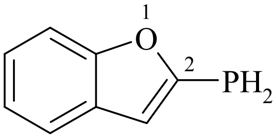
$ClCH_2$-CH_2-AsH-CHCl-CH_3

(1-chloroethyl)(2-chloroethyl)arsane (PIN)
(1-chloroethyl)(2-chloroethyl)arsine

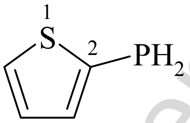


$$\overset{\displaystyle CH_2\text{-}CH_3}{C_6H_5\text{-}P\text{-}CH_3}$$

ethyl(methyl)phenylphosphane (PIN)
ethyl(methyl)phenylphosphine



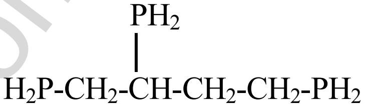
1-benzofuran-2-ylphosphane (PIN)
1-benzofuran-2-ylphosphine



thiophen-2-ylphosphane (PIN)
thiophen-2-ylphosphine

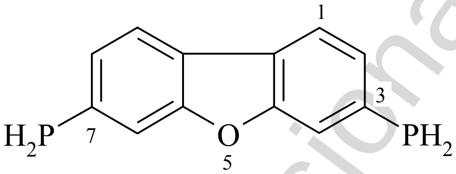
$(CH_3)_2P$-CH_2-CH_2-$P(CH_3)_2$

ethane-1,2-diylbis(dimethylphosphane) (PIN)
ethane-1,2-diylbis(dimethylphosphine)

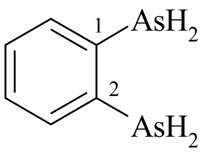


$$H_2P\text{-}CH_2\text{-}\overset{\displaystyle PH_2}{CH}\text{-}CH_2\text{-}CH_2\text{-}PH_2$$

butane-1,2,4-triyltris(phosphane) (PIN)
butane-1,2,4-triyltris(phosphine)



dibenzofuran-3,7-diylbis(phosphane) (PIN)
dibenzofuran-3,7-diylbis(phosphine)



1,2-phenylenebis(arsane) (PIN)
1,2-phenylenebis(arsine)

P-68.3.2.4.2.2 Phosphanes, arsanes and stibanes expressed as substituent groups

Substituent groups are formed by the general method described in Section P-29, by adding the suffixes ‘yl’, ‘ylidene’ and ‘ylidyne’ to the name of the parent hydride with elision of the final letter ‘e’. When required, the order of classes is applied, as indicated in Section P-41. The traditional names phosphino, arsino and stibino are no longer recommended.

$-PH_2$

phosphanyl (preselected name)
(not phosphino)

$-As=$

arsanylylidene (preselected name)

$-H_2P\text{-}PH_2-$

phosphane-1,2-diyl (preselected name)

$-As<$

arsanetriyl (preselected name)

AsH_2

arsanyl (preselected name)
(not arsino)

$-SbH_2$

stibanyl (preselected name)
(not stibino)

$-PH_4$

λ⁴-phosphanyl (preselected name)
phosphoranyl

$-SbH\text{-}SbH_2$

distibanyl (preselected name)

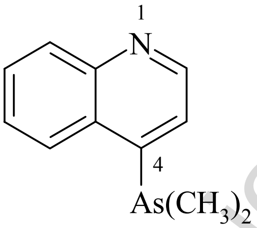
Examples:

$H_2P\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H_2\text{-}NH_2$

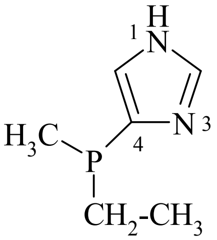
2-phosphanylethanamine (PIN)

$H_2As\text{-}CH_2\text{-}P(C_6H_5)_2$

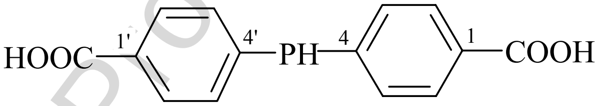
(arsanylmethyl)diphenylphosphane (PIN)



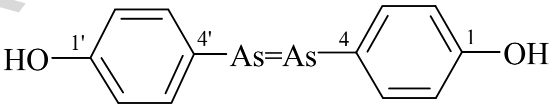
4-(dimethylarsanyl)quinoline (PIN)



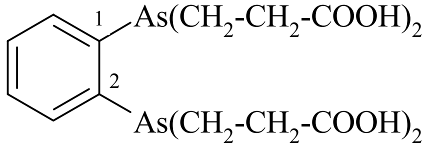
4-[ethyl(methyl)phosphanyl]imidazole (PIN)



4,4′-phosphanediyldibenzoic acid (PIN)



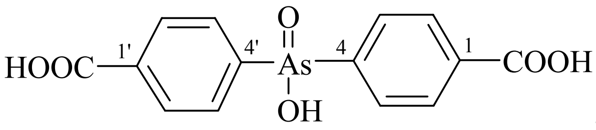
4,4′-diarsenediyldiphenol (PIN)



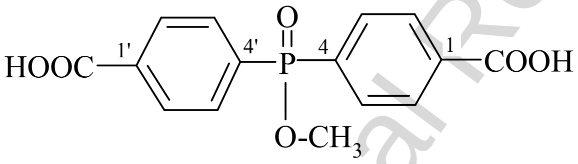
3,3′,3′′,3′′′-[1,2-phenylenebis(arsanetriyl)]tetrapropanoic acid (PIN)

$(HO)_2As(O)-CH_2-COOH$

arsonoacetic acid (PIN)



4,4′-(hydroxyarsoryl)dibenzoic acid (PIN)
4,4′-arsinicodibenzoic acid



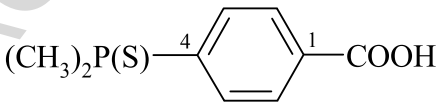
4,4′-(methoxyphosphoryl)dibenzoic acid (PIN)

$Cl_2P(O)-CH_2-CO-Cl$

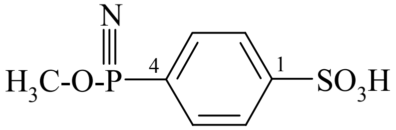
phosphorodichloridoylacetyl chloride (PIN)
(dichlorophosphoryl)acetyl chloride

$(CH_3O)_2P(=NH)-CH_2-CO-O-CH_3$

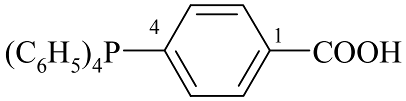
methyl (dimethoxyphosphorimidoyl)acetate (PIN)



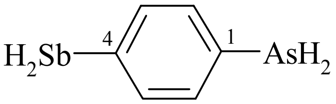
4-(dimethylphosphinothioyl)benzoic acid (PIN)



4-(methoxyphosphoronitridoyl)benzene-1-sulfonic acid (PIN)



4-(tetraphenyl-λ^5-phosphanyl)benzoic acid (PIN)
4-(tetraphenylphosphoranyl)benzoic acid



(4-stibanylphenyl)arsane (PIN)

P-68.3.3 Bismuth compounds

Bismuth compounds are named substitutively on the basis of parent hydrides named in accordance with the rules described in Chapter 2. Suffixes and prefixes are used as indicated for substitutive nomenclature. There are no acids having retained names subject to functional class nomenclature. Substitutive nomenclature is preferred to functional nomenclature to designate oxides, sulfides, selenides, tellurides, and imides. Preferred and preselected names are chosen as for P, As and Sb parents and prefixes.

Examples:

BiH_3

bismuthane (preselected name)
bismuthine

BiH_5

λ^5-bismuthane (preselected name)
bismuthorane

$H_2Bi\text{-}BiH_2$

dibismuthane (preselected name)

H_2Bi-

bismuthanyl (preselected name)
(not bismuthino)

$H_3Bi=$

λ^5-bismuthanylidene (preselected name)

$-HBi\text{-}BiH-$

dibismuthane-1,2-diyl (preselected name)

Examples:

$Bi(CH{=}CH_2)_3$

triethenylstibane (PIN))
trivinylstibane

$Bi(CH_3)_3$

trimethylbismuthane (PIN)

$(C_6H_5)_3Bi{=}O$

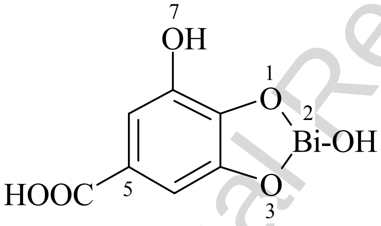
triphenyl-λ^5-bismuthanone (PIN)
triphenylbismuthane oxide

$(C_6H_5)_3Bi{=}NH$

triphenyl-λ^5-bismuthanimine (PIN)
triphenylbismuthane imide

$O{=}\overset{5}{Bi}\text{-}\overset{4}{O}\text{-}\overset{3}{C}O\text{-}\overset{2}{O}\text{-}\overset{1}{Bi}{=}O$

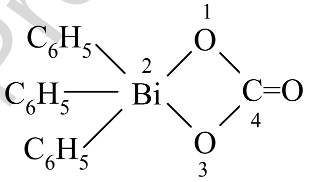
2,4-dioxa-1,5-dibismapentane-1,3,5-trione (PIN)



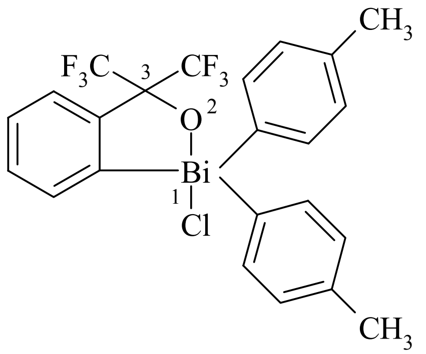
2,7-dihydroxy-2*H*-1,3,2-benzodioxabismole-5-carboxylic acid (PIN)

$(C_6H_5)_3BiCl_2$

dichloro(triphenyl)-λ^5-bismuthane (PIN)
dichloro(triphenyl)-λ^5-bismuthorane



2,2,2-triphenyl-1,3,2λ^5-dioxabismetan-4-one (PIN)



1-chloro-1,1-bis(4-methylphenyl)-3,3-bis(trifluoromethyl)-1,3-dihydro-2,1λ^5-benzoxabismole (PIN)

P-68.4 Nomenclature of elements of Group 16

P-68.4.0 Introduction

The nomenclature of compounds containing chalcogen atoms depends on the number and kind of chalcogen atoms present. When one or two contiguous chalcogen atoms are present, chalcogen atoms are not used as parent hydrides unless there is no other alternative. To the contrary, when three or more contiguous identical chalcogen atoms are present these chalcogen atoms are treated as parent hydrides in the normal way.

Compounds having one or two contiguous chalcogen atoms have been described in previous sections. They are briefly recalled in this introduction, for comparison purposes with compounds having three or more contiguous chalcogen atoms. See P-63.1 for hydroxy compounds, P-63.4 for hydroperoxy compounds, P-63.2 for ethers and P-63.3 for peroxy compounds, and chalcogen analogues. Sulfoxides and sulfones are also included in this type of nomenclature (see P-63.6).

P-68.4.1 Compounds with three or more contiguous chalcogen atoms.

P-68.4.1.1 Compounds with three or more contiguous identical chalcogen atoms are treated as parent hydrides in substitutive nomenclature.

Examples:

HO-O-OH
trioxidane (preselected name)

CH_3-S-S-SH
methyltrisulfane (PIN)

CH_3-O-O-O-CH_3
dimethyltrioxidane (PIN)

CH_3-S-S-S-CH_3
dimethyltrisulfane (PIN)

C_6H_5-Se-Se-Se-CH_3

1-methyl-3-phenyltriselane (PIN)
methyl(phenyl)triselane

C_6H_5-Se-Se-Se-C_6H_5

1,3-diphenyltriselane (PIN)
(not triselanediyldibenzene)

$\text{HO-SO}_2\text{-}\overset{1}{\text{Te}}\text{-}\overset{2}{\text{Te}}\text{-}\overset{3}{\text{Te}}\text{-SO}_2\text{-OH}$

tritellanedisulfonic acid (PIN)
tritelluropentathionic acid
(traditional name)

HO-SO_2-S-S-S-SO_2-OH

trisulfanedisulfonic acid (PIN)
pentathionic acid
(traditional name)

CH_3-SeSeSe-O-SH

methyltriselane-*OS*-thioperoxol (PIN)

H-TeTeTe-SeSe-H

tritellane(diselenoperoxol) (PIN)

C_6H_5-SSS-OH

phenyltrisulfanol (PIN)

CH_3-TeTeTeTe-SH

methyltetratellanethiol (PIN)

P-68.4.1.2 Multiplicative nomenclature is used if conditions are fulfilled. Central substituent groups are derived from the general method for generating divalent substituent groups.

–O-O-O–

trioxidanediyl (preselected name)

–S-S-S-S–

tetrasulfanediyl (preselected name)

Examples:

HS-S-S-CH_2-S-S-SH

methylenebis(trisulfane) (PIN)

4,4′-triselanediyldibenzoic acid (PIN)

P-68.4.1.3 If the chain of identical chalcogen atoms is terminated by one or two acyl groups the compound is named as a pseudoketone on the basis of the preferred carbonyl component. Multiplicative nomenclature is used if the principles for its use are met. When there is a choice between names of a pseudoketone and of a pseudoester, the compound is named as a pseudoketone and not as a pseudoester if that leads to fragmenting the homogeneous chain.

Examples:

CH_3-CH_2-CO-O-O-OH

1-trioxidanylpropan-1-one (PIN)

CH_3-CH_2-CO-S-S-S-CO-CH_2-CH_3

1,1′-trisulfanediyldi(propan-1-one) (PIN)

CH_3-CH_2-CO-Se-Se-Se-CH_3

1-(methyltriselanyl)propan-1-one (PIN; a pseudoketone)
(not *Se*-methyldiselanyl propaneselenoate, a pseudoester; formation of the pseudoester would require the fragmentation of a homogeneous chain)

CH_3-CH_2-CO-S-S-S-S-S-CO-CH_3

1-(acetylpentasulfanyl)propan-1-one (PIN)

P-68.4.2 Compounds with three heterogeneous contiguous chalcogen atoms

P-68.4.2.1 Compounds of the type a(ba)$_x$ are parent hydrides; they are discussed in P-21.2.3.1. Other compounds containing three or more heterogeneous contiguous chalcogen atoms are named on the basis of appropriate mononuclear, dinuclear and polynuclear, as appropriate, chalcogen parent hydrides with the exception of oxidane..

Examples:

HS-O-SH

dithioxane (preselected name)

CH_3-S-O-SH

methyldithioxane (PIN)

CH_3-S-O-S-CH_3

dimethyldithioxane (PIN)

C_6H_5-S-O-S-CH_3

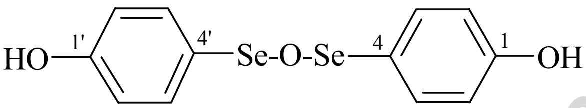
1-methyl-3-phenyldithioxane (PIN)

HS-O-S-OH

dithioxanol (preselected name)
(sulfanyloxy)sulfanol
(not hydroxysulfane-*OS*-peroxol)

HO-S-O-S-OH

dithioxanediol (preselected name)
(not oxydisulfanol)



4,4′-diselenoxanediyldiphenol (PIN)

P-68.4.2.2 Mono, di and polynuclear parent hydride names, except for oxidane, itself, are used for compounds with contiguous chalcogen atoms terminated by hydrogen atoms.

Examples:

HS-OH

sulfanol (preselected name)
(not oxidanethiol)

HO-S-OH

sulfanediol (preselected name)
(not oxidane-*OS*-peroxol)

HSe-Te-SeH

tellanediselenol (preselected name)
(not sellane-*TeSe*-selenotelluroperoxol)

H-OO-S-OH

(hydroperoxy)sulfanol (preselected name)
(not dioxidane-*SO*-peroxol)

H-OO-SS-H

disulfaneperoxol (preselected name)
[(not dioxidane(dithioperoxol)]

P-68.4.2.3 Compounds with an organic group at one or both ends of a heterogeneous chalcogen chain of atoms are named substitutively on the basis of the preferred organic group.

Substituting groups may be made up of individual units or formed by functional replacement nomenclature based on tri or tetraoxide, etc., substituting groups. The latter method is not used if the compound is a pseudoketone or a pseudoester. Multiplicative or skeletal replacement ('a') nomenclature is used if the requirements for either are met.

Examples:

$\mathrm{CH_3\text{-}OO\text{-}SH}$

(sulfanylperoxy)methane (PIN)
(*SOO*-thiohydrotrioxy)methane
(not methyldioxidanethiol)

$\mathrm{CH_3\text{-}SS\text{-}OH}$

(hydroxydisulfanyl)methane (PIN)
(*OSS*-dithiohydrotrioxy)methane
(not methyldisulfanol)

$\mathrm{CH_3\text{-}O\text{-}S\text{-}O\text{-}CH_3}$

[(methoxysulfanyl)oxy]methane (PIN)
(methyl-*OSO*-thiotrioxy)methane
dimethoxysulfane

$\mathrm{CH_3\text{-}OO\text{-}S\text{-}CH_3}$

[(methylperoxy)sulfanyl)]methane (PIN)
methyl(methylsulfanyl)dioxidane
(methyl-*OOS*-thiotrioxy)methane
(methyl-*SSO*-dithiotrioxy)ethane

$\mathrm{CH_3\text{-}S\text{-}S\text{-}O\text{-}CH_2\text{-}CH_3}$

[(methyldisulfanyl)oxy]ethane (PIN)
[methyl(dithiohydroperoxy)oxy]ethane
ethoxy(methyl)disulfane

$\mathrm{C_6H_5\text{-}O\text{-}S\text{-}O\text{-}C_6H_5}$

[sulfanediylbis(oxy)]dibenzene (PIN)
OSO-thiotrioxydibenzene

$\mathrm{CH_3\text{-}O\text{-}S\text{-}Se\text{-}C_6H_5}$

[(methoxysulfanyl)selanyl]benzene (PIN)
methyl-*OSSe*-selenothiotrioxybenzene

$\mathrm{CH_3\text{-}S\text{-}O\text{-}Se\text{-}\overset{1}{C}O\text{-}\overset{2}{C}H_2\text{-}\overset{3}{C}H_3}$

1-{[(methylsulfanyl)oxy]selanyl}propan-1-one (PIN)

$\mathrm{\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}O\text{-}O\text{-}S\text{-}CO\text{-}CH_3}$

[(acetylsulfanyl)peroxy]propan-1-one (PIN)

$\mathrm{\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}O\text{-}O\text{-}S\text{-}S\text{-}O\text{-}\overset{1'}{C}O\text{-}CH_2\text{-}CH_3}$

1,1′-[disulfanediylbis(oxy)]dipropan-1-one (PIN)
1,1′-[dithioperoxybis(oxy)]dipropan-1-one

$\overset{1}{CH_3}\text{-}\overset{2}{CH_2}\text{-}\overset{3}{O}\text{-}\overset{4}{Se}\text{-}\overset{5}{S}\text{-}\overset{6}{O}\text{-}\overset{7}{CO}\text{-}\overset{8}{CH_2}\text{-}\overset{9}{CH_3}$

3,6-dioxa-5-thia-4-selenanonan-7-one (PIN)

P-68.4.3 Chalcogen parent compounds with bonding numbers other the standard bonding number.

Many chalcogen compounds are designated by class names that were used as parent structures to name their derivatives. In these recommendations, in conformity with the principle that substitutive names are preferred, derivatives named on the basis of class names are retained for general use only.

P-68.4.3.1 Sulfanes and similar chalcogen compounds;
P-68.4.3.2 Sulfones and sulfoxides, polysulfones, polysulfoxides, and similar chalcogen compounds: R-EO$_2$-R′, R-EO-R′, R-EO$_2$-EO$_2$-R′, etc. (E = S, Se, and Te).
P-68.4.3.3 Sulfimides, H$_2$E=NH (E = S), and similar chalcogen compounds (E = Se, Te):
P-68.4.3.4 Sulfinylamines, RN=E=O (E = S), and sulfonylamines, RN=E(=O)$_2$ (E = S), and similar chalcogen compounds: (E = Se, Te).
P-68.4.3.5 Sulfonediimines, RE(=NH)$_2$R′ (E = S), and similar chalcogen compounds. (E = Se, Te).
P-68.4.3.6 Sulfoximides, R$_2$E(=O)=NR′ (E = S), and similar chalcogen compounds (E = Se, Te)
P-68.4.3.7 Sulfur dimides, HN=E=NH (E = S),and similar chalcogen compounds (E = Se, Te)
P-68.4.3.8 Sulfur triimides, E(=NH)$_3$ (E = S), and similar chalcogen compounds (E = Se, Te)

P-68.4.3.1 Sulfanes, selanes, and tellanes.

Sulfanes, selanes, and tellanes, that have a nonstandard bonding number are named on the basis of parent hydrides such as λ^4-sulfane, λ^6-sulfane, and λ^4-selane, according to the λ-convention.

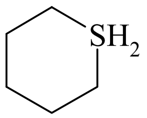
Example:

$CH_2=S(CH_3)_2$

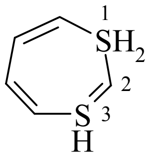
dimethyl(methylidene)-λ^4-sulfane (PIN)

$(CH_3\text{-}O)_4S$

tetramethoxy-λ^4-sulfane (PIN)
(trimethoxy-λ^4-sulfanyl)methane
(formerly tetramethyl orthosulfurite)
(formerly dimethyl sulfoxylate)



λ^4-thiane (PIN)



1H-1λ^4,3λ^4-dithiepine (PIN)

P-68.4.3.2 Di- and polysulfoxides, polysulfones, and selenium and tellurium analogues

Compounds with the general structures R-[SO]$_n$-R′ and R-[SO$_2$]$_n$-R′, in which $n \geq 2$, have the class name ‘disulfoxides’, ‘trisulfoxides’, ‘disulfones’, etc. They are named in two ways. Selenium and tellurium analogues are named in the same manner.

(1) substitutively by adding the suffix ‘one’ to the name of the appropriate parent hydride, λ^4 or λ^6 disulfane, diselane, ditellane, etc.;

(2) by functional class nomenclature, using class names such as ‘disulfoxide’, ‘disulfone’, ‘diselenoxide’, ‘diselenone’, etc.

Method (1) generates preferred IUPAC names and is also used to name mixed sulfoxide-sulfones.

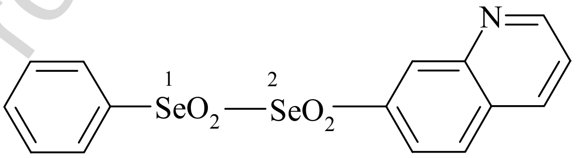
Examples:

$CH_3\text{-}\overset{1}{S}(=O)\text{-}\overset{2}{S}(=O)\text{-}CH_3$

dimethyl-1λ^4,2λ^4-disulfane-1,2-dione (PIN)
dimethyl disulfoxide

$CH_3\text{-}CH_2\text{-}\overset{1}{S}O_2\text{-}\overset{2}{S}O_2\text{-}CH_3$

ethyl(methyl)-1λ^6,2λ^6-disulfane-1,1,2,2-tetrone (PIN)
ethyl methyl disulfone



1-phenyl-2-(quinolin-7-yl)-1λ^6,2λ^6-diselane-1,1,2,2-tetrone (PIN)
phenyl quinolin-7-yl diselenone

$CH_3\text{-}CH_2\text{-}\overset{1}{S}eO_2\text{-}\overset{2}{S}e(O)\text{-}CH_2\text{-}CH_3$

diethyl-1λ^6,2λ^4-diselane-1,1,2-trione (PIN)

P-68.4.3.3 Sulfimides, $H_2E{=}NH$ (E = S), and chalcogen compounds where E = Se, Te.

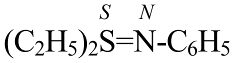
Compounds with the general structures, $H_2S{=}NH$, have the class name ‘sulfimides’ (CAS calls them sulfilimines). They are named in two ways.

(1) substitutively by adding the suffix ‘imine’ to the name of the parent hydride such as, λ^4-sulfane;

(2) by functional class nomenclature, using the class name ‘sulfimide’.

Method (1) generates preferred IUPAC names.

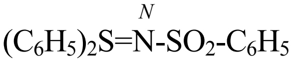
Example:


$(C_2H_5)_2\overset{S}{S}{=}\overset{N}{N}\text{-}C_6H_5$

S,*S*-diethyl-*N*-phenyl-λ^4-sulfanimine (PIN)
S,*S*-diethyl-*N*-phenylsulfimide

N and/or *S* substitution by groups that are not hydrocarbyl groups, may create senior parent structures that become the basis for the name.

Example:


$(C_6H_5)_2S{=}\overset{N}{N}\text{-}SO_2\text{-}C_6H_5$

N-(diphenyl-λ^4-sulfanylidene)benzenesulfonamide (PIN)
S,*S*-diphenyl-*N*-benzenesulfonylsulfimide

P-68.4.3.4 Sulfinylamines, $RN{=}E{=}O$, (E = S), sulfonylamines, $RN{=}E({=}O)_2$ (E = S), and chalcogen analogues where E = Se, Te.

Compounds with the general structures, $R\text{-}N{=}S{=}O$ and $R\text{-}N{=}S({=}O)_2$, have the class names ‘sulfinylamines’ and ‘sulfonylamines’, respectively. They are named substitutively on the basis of the parent hydrides λ^4-sulfane or λ^6-sulfane.

Examples:

$C_5H_5\text{-}N{=}S{=}O$	$CH_3\text{-}N{=}S({=}O)_2$
(phenylimino)-λ^4-sulfanone (PIN) (not *N*-sulfinylaniline)	(methylimino)-λ^6-sulfanedione (PIN) (not *N*-sulfonylmethanamine)

$(CH_3)_2S(O){=}N\text{-}SO_2\text{-}C_6H_5$

(benzenesulfonylimino)dimethyl-λ^6-sulfanone (PIN)

P-68.4.3.5 Sulfonediimines, RE(=NH)$_2$R′ (E = S), and chalcogen analogues where E = Se, Te.

Compounds with the general structures, RE(=NH)$_2$R′, have the class name ‘sulfonediimines’. Preferred IUPAC names are formed substitutively on the basis of the parent hydride λ^6-sulfane. Names based on the the class name ‘sulfonediimine’ are not recommended.

Example:

$(C_6H_5)_2S(=NH)_2$

diphenyl-λ^6-sulfanediimine (PIN)
(not diphenyl sulfonediimine)

P-68.4.3.6 Sulfoximides, R$_2$E(=O)=NR′ (E = S), and chalcogen analogues where (E = Se, Te).

Compounds with the general structure, R$_2$E(=O)=NR′ , have the class name ‘sulfoximides’ (CAS calls them sulfoximines). Preferred IUPAC names are formed substitutively on the basis of the parent hydride λ^6-sulfane. Functional class names are based on the class name ‘sulfoximide’.

Example:

$(CH_3)_2S(=O)=N\text{-}C_6H_5$

dimethyl(phenylimino)-λ^6-sulfanone (PIN)
S,*S*-dimethyl-*N*-phenylsulfoximide

P-68.4.3.7 Sulfur dimides, HN=E=NH (E = S), and chalcogen analogues where E = Se, Te.

Compounds with the general structure, HN=S=NH, have the class name ‘sulfur diimides’. Preferred IUPAC names are formed substitutively on the basis of the parent hydride λ^4-sulfane. Functional class names are based on the class name ‘sulfur diimide’.

Example:

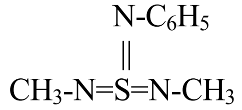
$CH_3\text{-}N=S=N\text{-}CH_2\text{-}CH_3$

ethyl(methyl)-λ^4-sulfanediimine (PIN)
ethylmethylsulfur diimide

P-68.4.3.8 Sulfur triimides, E(=NH)$_3$ (E = S), and chalcogen analogues where E = Se, Te.

Compounds with the general structure, S(=NH)$_3$, have the class name ‘sulfur triimides’. Preferred IUPAC names are formed substitutively on the basis of the parent hydride λ^6-sulfane. Functional class names are based on the class name ‘sulfur triimide’.

Example:



$$CH_3\text{-}N{=}\overset{\overset{\displaystyle N\text{-}C_6H_5}{\|}}{S}{=}N\text{-}CH_3$$

dimethyl(phenyl)-λ^6-sulfanetriimine (PIN)
dimethylphenylsulfur triimide

P-68.5 Nomenclature of compounds of Group 17

P-68.5.0 Substitutive nomenclature

In substitutive nomenclature, halogen atoms are denoted only by specific prefixes (see P-61.3), by their class names in functional class nomenclature (see P-65.3) and by prefixes and infixes in functional replacement nomenclature (see P-35).

Examples:

$CH_3\text{-}Cl$
chloromethane (PIN)

$CH_3\text{-}CH_2\text{-}NH\text{-}Cl$
N-chloroethanamine (PIN)

$C_6H_5\text{-}ClO$
chlorosylbenzene (PIN)

$CH_3\text{-}CH_2\text{-}CO\text{-}Br$
propanoyl bromide (PIN)

$CH_3\text{-}CH_2\text{-}SO_2\text{-}Cl$
ethanesulfonyl chloride (PIN)

$C_6H_5\text{-}P(O)Cl_2$
phenylphosphonic dichloride (PIN)

$CH_3\text{-}BCl_2$
dichloro(methyl)borane (PIN)

$CH_3P(Cl)(S\text{-}C_2H_5)$
ethyl methylphosphonochloridothioite (PIN)
(not ethyl methanephosphonochloridothioite)

P-68.5.1 Nomenclature based on halogen parent hydrides

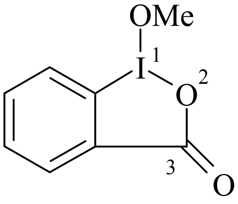
For cyclic and acyclic parent hydrides the lambda convention is used to indicate nonstandard bonding numbers.

Examples:

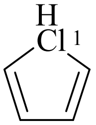
$C_6H_5\text{-}I(OH)_2$
phenyl-λ^5-iodanediol (PIN)

$CH_3\text{-}ICl_2$
dichloro(methyl)-λ^3-iodane (PIN)

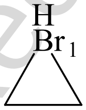
$(CH_3\text{-}CO)_2I$–	bis(acetyloxy)-λ^3-iodanyl (not diacetoxyiodo)
$(HO)_2I$–	dihydroxy-λ^3-iodanyl (not dihydroxyiodo)



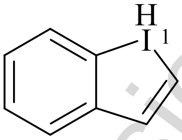
1-methoxy-1λ^3,2-benziodoxol-3(1*H*)-one (PIN)



1λ^3-chlorole (PIN)



1λ^3-bromirane (PIN)



1λ^3-benzoiodole (PIN)

P-68.5.2 Nomenclature of halogen acids

The halogen acids HO-Cl, hypochlorous acid, HO-ClO, chlorous acid, HO-ClO_2, chloric acid, and HO-ClO_3, perchloric acid, and similar acids where Br, F, and I take the place of Cl, are discussed in P-67.1.1. They form esters (see P-67.1.3.1), such as ‘methyl chlorite’, CH_3-O-ClO, and anhydrides (see P-67.1.3.2), such as ‘benzoic hypochlorous anhydride’, C_6H_5-CO-O-Cl.

Substituent groups derived from the halogen acids, such as chlorosyl, -ClO, bromyl, -BrO_2, and periodyl, -IO_3, are discussed in P-67.1.4.5 and exemplified in P-61.3.2.

P-69 Nomenclature of organometallic compounds

P-69.0 Introduction

This Section is partly an application of the principles, rules, and conventions established in previous Chapters, and partly an extension of these principles, rules, and conventions to reconcile the nomenclatures of organic and inorganic compounds (see ref 14) to name organometallic compounds.

Organometallic compounds traditionally are compounds having bonds between one or more metal atoms and one or more carbon atoms of an organic residue. In addition to the traditional metals and semimetals, some compounds containing elements such as boron, silicon, arsenic and selenium have sometimes been considered to be organometallic.

Metals and semimetals are divided into three categories: (1) those belonging to Groups 1 and 2, (2) those belonging to Goups 3-12 (transition metals) and (3) metals and semimetals of Groups 13 through 16. Thus a great part of nomenclature of organometallic compounds is outside the scope of this book covering organic compounds; it follows the principles, rules and conventions of the nomenclature of inorganic compounds described in the Nomenclature of Inorganic Chemistry (Red Book), in particular, Chapter I-10.9 (ref. 14).

All organometallic compounds can be named by a type of additive nomenclature conveniently called coordination nomenclature, a system in which the names of compounds are formed by adding the name(s) of (a) ligand(s), in alphanumerical order if there is more than one, to that of a central atom. (ref. 14., Chapters I-7, I-9). In formulas for compounds named by coordination nomenclature, the whole coordination entity of a neutral coordination compound is enclosed in brackets.

In this Chapter, only organometallic compounds involving the metal atoms of Groups 13, 14, 15, and 16 are considered, and preferred IUPAC names are noted for these. Organometallic compounds of the transition elements included in this Section are restricted to those with ligands attached through one or more carbon atoms; organometallic compounds with other ligating atoms are not a part of the discussion. Metallacycles and ‘ocene’ compounds are included. For organometallic compounds of the transition elements, preferred IUPAC names are not noted; neither are preselected names given (see P-12). This determination will await consideration by a task group on organometallic nomenclature.

P-69.1 Organometallic compounds of Groups 13, 14, 15, and 16

Organometallic compounds derived from elements of Groups 13, 14, 15, and 16 are named substitutively by prefixing the appropriate substituent names to the name of a parent hydride; they are the preferred IUPAC names.

Examples:

$Al(CH_2\text{-}CH_3)_3$

triethylalumane (PIN; substitutive name)
triethylaluminium (additive, coordination-type name)

$Pb(CH_2\text{-}CH_3)_4$

tetraethylplumbane (PIN; substitutive name)
tetraethyllead (additive, coordination-type name)

$BrSb(CH=CH_2)_2$

bromodiethenylstibane (PIN; substitutive name)
bromidodiethenidoantimony (coordination-type name)

$HIn(CH_3)_2$

dimethylindigane (PIN; sbstitutive name)
hydridodimethanidoindium (coordination-type name)

P-69.2 Organometallic compounds of elements in Groups 3 through 12

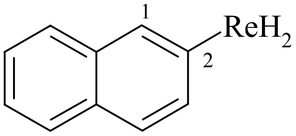
P-69.2.1 Coordination nomenclature is the main nomenclature method used to name organometallic compounds containing elements of Groups 3-12. It is described in *Nomenclature of Inorganic Chemistry* (ref. 14, Chapter 10) and in ‘Nomenclature of organometallic compounds of the transition elements’ (ref 24) It is discussed briefly and exemplified in this Section. The metal is always the central atom.

Linear formulae are composed of the symbol of the central atom, followed by the ligands, in alphabetical order if more than one is present. [This is a change from that described in the 1990 Inorganic Nomenclature recommendations (ref 14)]**.** In a line formula, a coordination entity is always placed in square brackets. No brackets are indicated when the structure is based on developed organic formulas.

P-69.2.2 Compounds consisting solely of individual metal atoms joined to a carbon atom of one or more organyl substituent groups and/or to one or more hydrogen atoms are named by citing the names of such organic groups or hydrogen in alphanumerical order, followed by the name of the metal. The presence of hydrogen attached to a metal atom must always be indicated by the prefix ‘hydrido’.

Examples:

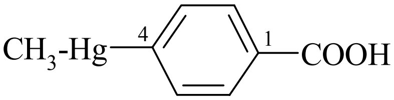
$[Hg\text{-}CH_3]^+$	$[Zn(CH_3)_2]$
methylmercury(1+)	dimethylzinc



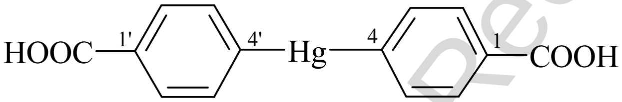
dihydrido(naphthalen-2-yl)rhenium

$[Cu\text{-}C{\equiv}C\text{-}CH_3]$

(prop-1-yn-1yl)copper



(4-carboxyphenyl)methylmercury

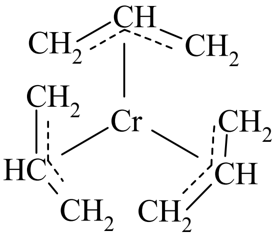


bis(4-carboxyphenyl)mercury

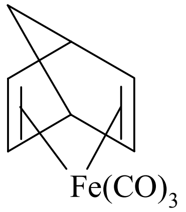
P-69.2.3 Organometallic groups with multicenter bonding to carbon atoms

In order to indicate multicenter bonding to carbon atoms, for example in an unsaturated system, the name of the ligand is preceded by the prefix η (eta) A right superscript is added to the symbol η to indicate the number of atoms that bind to the metal. When it is necessary to indicate that all unsaturation sites are not bonded to the metal, numerical locants are added in front of the symbol η. It may also be necessary to denote a single atom in the ligand that is directly attached to the metal; in this case, the symbol κ (kappa) is cited before the element symbol that indicate the specific position that is bonded to the metal. See ref 12a, Sections 9.2.4 and 10.2.5 for a complete discussion on the use of η and κ symbols in additive nomenclature.

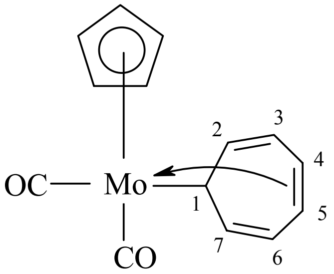
Examples:



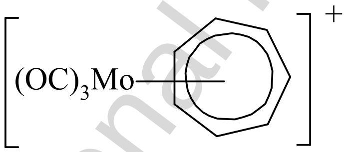
. tris(η^3-allyl)chromium



(η^4-bicyclo[2.2.1]hepta-2,5-diene)tricarbonyliron



dicarbonyl[(4,5-η,κC^1)-cyclohepta-2,4,6-dien-1-yl](η^5-cyclopentadienyl)molybdenum

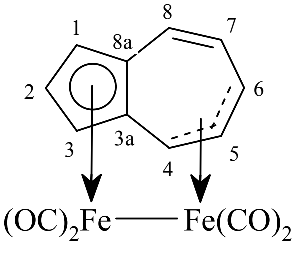


tricarbonyl(η^7-cycloheptatrienylium)molybdenum(1+)

P-69.2.4 Bridging organometallic groups with multicenter bonding to carbon atoms.

The prefix ‘μ’(see I-10.8.2, ref 2) is added to the name of organometallic groups to indicate bridging between two metal atoms. Locants for the ‘η’ positions are separated by the colon and direct bonding between metal atoms is indicated as described in I-10.8.3.1.

Example:

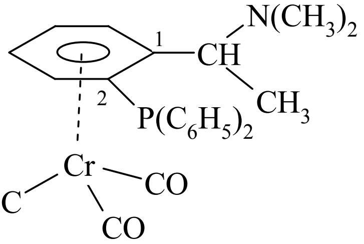


[μ-(1,2,3,3a,8a-η:4,5,6-η)-azulene]-pentacarbonyldiiron (*Fe–Fe*)

P-69.2.4 Organometallic comploupnc with unsaturated molecules and substituent groups

Organic molecules used as ligands are named substitutively in accordance with principles, rules and conventions of substitutive nomenclature and cited in the name of the organometallic compound with the appropriate hapto symbols. This method is preferred to that consisting of using prefixes only to denote characteristic groups in the organic part of the organometallic compound.

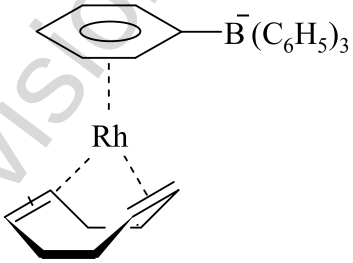
Example:



tricarbonyl{1-[2-(diphenylphosphanyl)-η^6-phenyl]-*N*,*N*-dimethylethanamine}chromium
tricarbonyl{[1-[1-(dimethylamino)ethyl)]-2-(diphenylphosphanyl)-η^6-benzene}chromium
(in the second name, the benzene ring is treated as the principal group because it is the part of the ligand attached to the metal; this method as yet has not official sanction)

In zwitterionic complexes, in which a noncoordinated atom of the ligand carries a charge which is offset by the opposite charge at the metal atom, the charge of the ligand is indicated by the appropriate ligand name ending, while the charge of the central atom is not indicated.

Example:

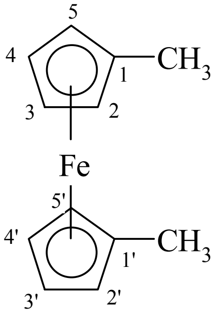


(η^4-cycloocta-1,5-diene)[(η^6-phenyl)triphenylboranuide]rhodium
(η^4-cycloocta-1,5-diene)[(triphenylboranuidyl)-η^6-phenyl]rhodium

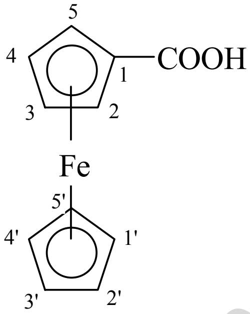
P-69.2.5 "Ocenes"

"Ocenes" are bis(η^5-cyclopentadienyl) complexes of certain metals. The names ferrocene, ruthenocene, osmocene, nickelocene, chromocene, cobaltocene and vanadocene are names for compounds corresponding to 'bis(η^5-cyclopentadienyl)metal', where the metal atom is Fe, Ru, Os, Ni, Cr, Co, and V. These names are substituted in accordance with the principles, rules and conventions of substitutive nomenclature, using suffixes or prefixes to denote characteristic groups.

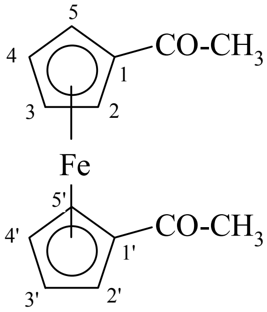
Examples:



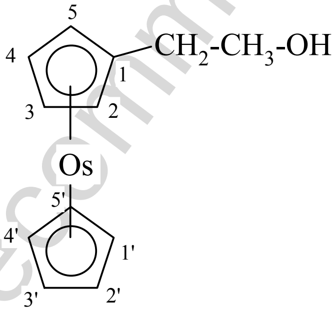
1,1′-dimethylferrocene



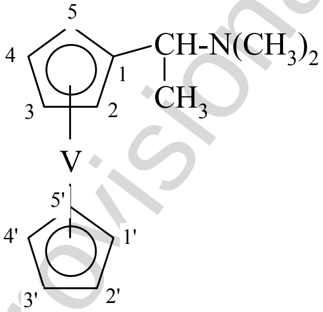
ferrocenecarboxylic acid
carboxyferrocene



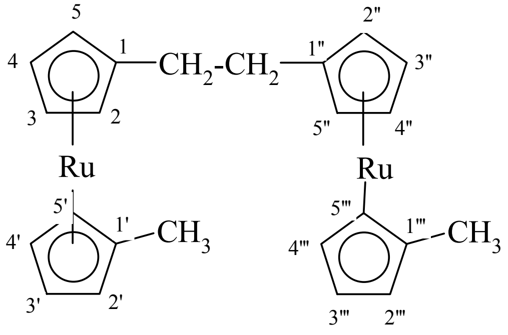
1,1′-(ferrocene-1,1′-diyl)di(ethan-1-one)
1,1′-diacetylferrocene



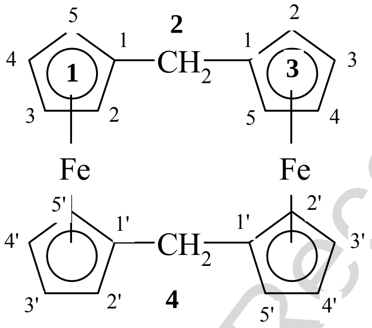
2-(osmocen-1-yl)ethanol
osmocene-2-ethanol



N,*N*-dimethyl(vanadocen-1-yl)ethan-1-amine
1-[1-(dimethylamino)ethyl]vanadocene



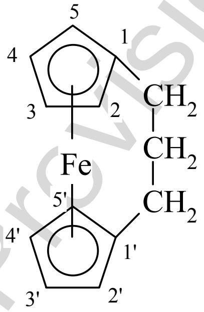
1,1″-(ethane-1,2-diyl)bis(1′-methylruthenocene)



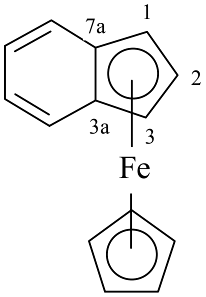
1(1,1′),3(1,1′)-diferocenacylotetraphane

Bridging and fusion principles may also be useful in naming ocene compounds.

Examples:



1,1′-propanoferrocene
1(1,1′)-ferrocenacyclotetraphane

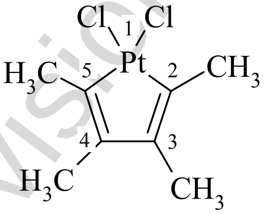


benzoferrocene
(η^5-cyclopentadienyl)[(1,2,3,3a,7a)-η^5-indenyl]iron

P-69.2.6 Metallacycles

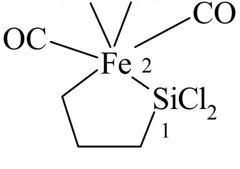
Metallacycles are organic heterocycles in which one or more heteroatoms is (are) metal atoms other than the metals normally included in the nomenclature systems for heteromonocycles (see P-22.2). They are named by extending the Hantzsch-Widman system to include the metallic elements other than those in Groups 13-16, but with a '0' standard valence and the stems 'ine' and 'inane' for unsaturated and saturated six-membered heterocycles, respectively; or by selecting a parent hydrocarbon ring or ring system and replacing one or more carbon atoms by a metal atom from Groups 2-12 using a nondetachable skeletal replacement ('a') prefix to create the metallacyclic parent hydride. The name is adjusted to conform with the observed formula by substitutions using detachable prefixes on the ring and appropriate ligand names to describe atoms or groups attached to the metal atom.

Examples

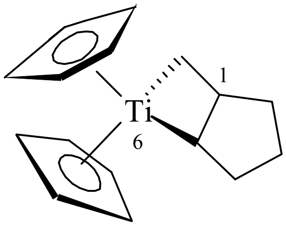


1,1-dichloro-2,3,4,5-tetramethylplatinole Hantzsch-Widman name)
1,1-dichloro-2,3,4,5-tetramethyl-1-platinacyclohexa-2,4-diene (skeletal replacement name)

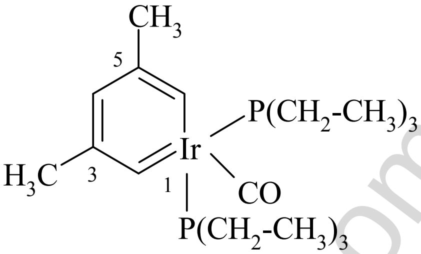
:



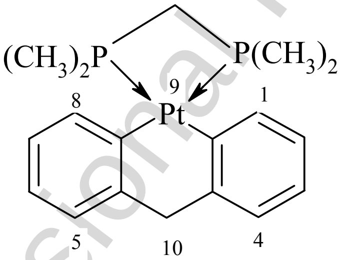
2,2,2,2-tetracarbonyl-1,1-dichloro-1,2-silaferrole (Hantzsch-Widman name)
2,2,2,2-tetracarbonyl-1,1-dichloro-1-sila-2-ferracyclopentane



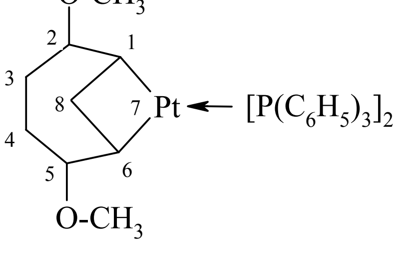
6,6-(η^5-cyclopentadienyl)-6-titanabicyclo[3.2.0]heptane



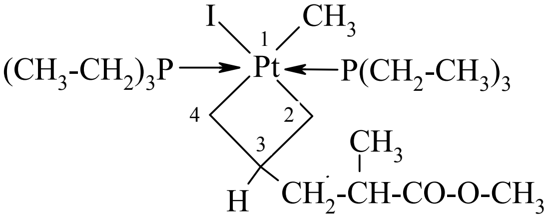
1-carbonyl-3,5-dimethyl-bis(triethylphosphane)iridin (Hantzsch-Widman name)
1-carbonyl-3,5-dimethyl-bis(triethylphosphane)-1-iridabenzene



9,9-[methylenebis(dimethylphosphane)-*P*,*P'*]-10*H*-9-platinaanthracene



2,5-dimethoxy-7,7-bis(triphenylphosphane-*P*)-7-platinabicyclo[4.1.1]octane



methyl 3-[1-iodo-1-methyl-1,1-bis(triethylphosphane-*P*)platinetan-3-yl]-2-methylpropanoate (Hantzsch-Widman name)

methyl 3-[1-iodo-1-methyl-1,1-bis(triethylphosphane-*P*)-1-platinacyclobutyl]-2-methylpropanoate

P-69.3 Order of seniority for organometallic compounds

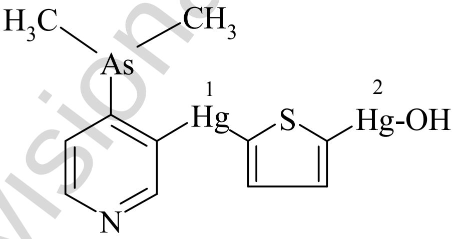
When two different metals are present in an organometallic compound, one must be chosen as the basis of the name. Metals are classifed into:

(1) metals of Groups 1 through 12; and

(2) metals (semimetals) of Groups 13 through 16.

P-69.4.1 Compounds having two identical or different metal atoms belonging to the first class are named additively using the methodology described in Section IR-9.2.5 of ref 12a, and the order of seniority of the Element Sequence Table beginning at Zn, i.e. Zn > Cd > Hg >.....Li > Na > K > Rb > Cs > Fr (see Table IV, ref. 11)

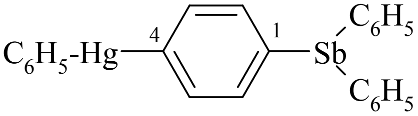
Example:



1-[4-(dimethylarsanyl)pyridin-3-yl]-2-hydroxido-μ-thiophene-2,5-diyl-dimercury

P-69.4.2 Compounds having one metal atom of class (1) and another atom of class (2) are named additively using the metal atom of class (1) as central atom, as in P-69.6.1; the other metal atom is named as a substituent group in substitutive nomenclature or as a neutral ligand.

Example:



[(4-diphenylstibanyl)phenyl]phenylmercury (PIN)

P-69.4.3 For organometallic compounds having two metal atoms belonging to class (2), substitutive nomenclature is used, as described in Section P-68. The order of priority to select the parent hydride is described in Section P-41: N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl > S > Se > Te > C.

Example:

$(C_6H_5)_2Bi\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}Pb(C_2H_5)_3$

diphenyl[3-(triethylplumbyl)propyl]bismuthane (PIN)

$H_2Bi\text{-}GeH_3$

germylbismuthane

$Pb(SnH_3)_4$

plumbanetetrayltetrakisstannane

CHAPTER 7 RADICALS, IONS, AND RELATED SPECIES

P-70 Introduction

P-70.1 General Methodology

The nomenclature for radicals, ions and related species is described in this Chapter. Its rules are based on the same principles as those of organic compounds defined in the Chapters 1 to 6. The nomenclature was revised in 1993 (ref. 3).

P-70.2 Seniority of radicals and ions

As classes, radicals and ions are senior to acids and other classes in the following order:

(1) radicals;
(2) anions;
(3) cations.

P-70.3 Name formation

Substitutive names and functional class names denote radicals and ions and related compounds. Parent hydrides and parent compounds are selected and modified by use of specific suffixes (called cumulative suffixes) and prefixes; traditional endings are used to describe anions derived from acids and related compounds (see Table 7.1). The nomenclature of di- and trivalent radicals does not indicate nor imply an elctronic structure or spin multiplicity.

P-70.3.1 The following suffixes, prefixes and endings are also described in Table 3.2. They are as follows:

The suffixes 'elide' and 'elium' are recommended to denote modification of a parent hydride by the addition or the subtraction of one electron to a parent hydride, respectively.

Radicals formed by	Suffix or Ending	Prefix
loss of H•	yl	ylo
loss of 2 H•		
from one atom	ylidene	
from different atoms	diyl	

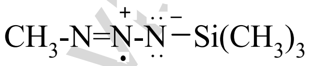
loss of 3 H•	
from one atom	ylidyne
from different atoms	triyl or ylylidene
addition of H•	hydryl
Anions formed by	
loss of H^+	ide ate, ite (endings)
addition of $H^−$	uide
addition of an electron	elide
Cations formed by	
loss of $H^−$	ylium
addition of H^+	ium
loss of an electron	elium

P-70.3.2 Basic multiplying prefixes are used to denote multiplicity of the suffixes ‘yl’, ‘ylidene’, ‘ylidyne’, ‘ide’, ‘uide’, ‘ium’ and of the prefix ‘ylo’. Multiplying prefixes ‘bis’, ‘tris’, etc., are used at the front of the suffix ‘ylium’ and before compound suffixes, such as ‘aminium’, ‘olate’, etc.

P-70.3.3 In names, suffixes and endings are cited in a specific order as described below.

P-70.3.3.1 When two or more cumulative suffixes are present in a name, the order of citation is the reverse of the order of seniority of radicals and ions, i.e.,‘ium’, ‘ylium’, ‘ide’, ‘uide’, ‘yl’, ‘ylidene’, ‘ylidyne’.

Example:



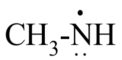
$CH_3\text{-}N{=}\overset{+}{\underset{\bullet}{N}}\text{-}\overset{..\;-}{\underset{..}{N}}{-}Si(CH_3)_3$

3-methyl-1-(trimethylsilyl)triaz-2-en-2-ium-1-id-2-yl (PIN)_

P-70.3.3.2 When functional and cumulative suffixes are present, the order of citation is prescribed by specific rules.

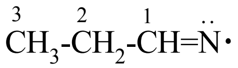
(a) a cumulative suffix is added to a functional suffix to form a compound suffix (see P-71.3.2):

Examples:



$CH_3\text{-}\overset{\bullet}{\underset{..}{N}}H$

methanaminyl (PIN)
methylazanyl
(traditionally: methylamino)

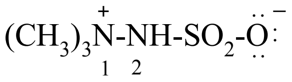


$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H{=}\overset{..}{N}\bullet$

propan-1-iminyl (PIN)
propylideneazanyl

(b) in zwitterionic compounds, the cumulative suffixes precede functional suffixes and have seniority for lowest locants:

Example:



$$(CH_3)_3\underset{1}{\overset{+}{N}}\text{-}\underset{2}{N}H\text{-}SO_2\text{-}\ddot{\underset{..}{O}}{:}^{-}$$

1,1,1-trimethylhydrazin-1-ium-2-sulfonate (PIN)

P-70.4 General rules for the selection of preferred names

The concept of preferred IUPAC names as applied to radicals and ions is based on the following principles.

(1) some names are retained, for example ‘onium cations’, such as ammonium and sulfonium, carbene, CH_2**:**, and amide, NH_2^-, that are used only in general nomenclature.

(2) substitutive nomenclature based on carbane and heterane nomenclatures and a set of suffixes and prefixes designed to express the formal operations needed to generate radicals and ions are systematically used to generate preferred IUPAC names.

(3) when there is a choice, preference is given to names including the largest parent, expressed by means of a functional suffix, for example, methanaminide is preferred to methylamide, for CH_3-CH_2-NH^-**.**

(4) Functional class nomenclature is used to name radicals and ions. These names can be used in general nomenclature, but systematically constructed names are preferred IUPAC names, for example, ‘methylium’ is preferred to ‘methyl cation’, for CH_3^+.

P-71 Radicals

P-71.1 General methodology

All radicals are named by modifying a parent hydride name to signal the subtraction or addition of one or more hydrogen atoms, H•. The modification to signal the addition of hydrogen atoms is recommended for the first time. These two operations are expressed by suffixes.

The suffixes ‘yl’ (− H•), ‘ylidene’ (− 2H•), ‘ylidyne’ (− 3H•) correspond to the subtractive operation, i.e., the removal of hydrogen atoms. The suffix ‘hydryl’ corresponds to the additive operation, i.e., the addition of hydrogen atoms .

The prefix ‘ylo’ is used to indicate the removal of H• from a substituent prefix.

P-71.2 Radicals derived from parent hydrides

P-71.2.1 Monovalent radicals.

P-71.2.1.1 A radical formally derived by the removal of one hydrogen atom from a mononuclear parent hydride of an element of Group 14, or from a terminal atom of an unbranched acyclic hydrocarbon, or from any position of a monocyclic saturated hydrocarbon ring is named by replacing the ‘ane’ ending of the systematic name of the parent hydride by ‘yl’.

Examples:

$\dot{C}H_3$

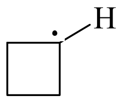
methyl (PIN)

$CH_3\text{-}CH_2\text{-}\dot{C}H_2$

propyl (PIN)

$\dot{G}eH_3$

germyl (preselected name)



cyclobutyl (PIN)

P-71.2.1.2 A radical formally derived by the removal of one hydrogen atom from any position of a parent hydride other than those described by P-71.2.1.1, above, is named by adding the suffix ‘yl’ to the name of the parent hydride, eliding the final letter ‘e’ of the name of the parent hydride, if any. As exceptions, the names of the radicals HO• and HOO• are ‘hydroxyl’ and ‘hydroperoxyl’, repectively. They must not be used when substituted, for example, CH_3-O• is named ‘methyloxidanyl’, not ‘methylhydroxyl’.

Examples:

$H\underset{..}{\ddot{S}}\cdot$

sulfanyl (preselected name)

$H\ddot{N}\cdot$

azanyl (preselected name)
aminyl
(traditional name: amino)

$HB\cdot$

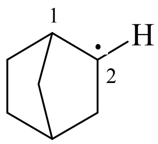
boranyl (preselected name)
(not boryl)

$\underset{3}{SiH_3}\text{-}\underset{2}{\dot{S}iH}\text{-}\underset{1}{SiH_3}$

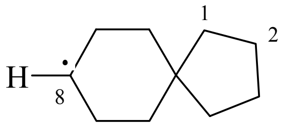
trisilan-2-yl (preselected name)

$(CH_3)_3C\text{-}O\text{-}\dot{P}(C_6H_5)_3$

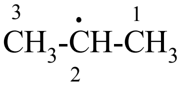
tert-butoxytriphenylphosphoranyl (PIN)
[(2-methylpropan-2-yl)oxy]triphenyl-λ^5-phosphanyl
(1,1-dimethylethoxy)triphenyl-λ^5-phosphanyl



bicyclo[2.2.1]heptan-2-yl (PIN)

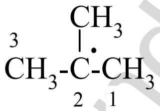


spiro[4.5]decan-8-yl (PIN)



$\overset{3}{C}H_3\text{-}\underset{2}{\overset{\bullet}{C}}H\text{-}\overset{1}{C}H_3$

propan-2-yl (PIN)
1-methylethyl
isopropyl

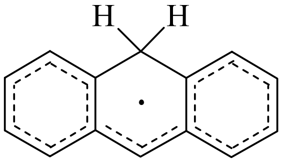


$\overset{3}{C}H_3\text{-}\underset{2}{\overset{\overset{CH_3}{|}\,\bullet}{C}}\text{-}\underset{1}{C}H_3$

2-methylpropan-2-yl (PIN)
1,1-dimethylethyl
tert-butyl

P-71.2.1.3 The suffix ‘hydryl’ is used to indicate the addition of H• when the position of the hydrogen atom is to be specified:

Example:



anthracene-9-hydryl (PIN)

P-71.2.2 Divalent and trivalent radicals.

The names of divalent and trivalent radicals are formed substitutively using the suffixes ‘ylidene’ and ‘ylidyne’ in two ways:

(1) replacing the ending ‘ane’ of a mononuclear parent hydride of an element of Group 14, or from a terminal atom of an unbranched acyclic hydrocarbon, or from any position of a monocyclic saturated hydrocarbon ring by the appropriate suffix (corresponds to P-71.2.1.1)

(2) adding the appropriate suffix to the name of any position of a parent hydride other than those described by P-71.2.1.1, is named by adding the appropriare suffix ‘yl’ to the name of the parent hydride, eliding the final letter ‘e’ of the name of the parent hydride, if any (corresponds to P-71.2.1.2).

These systematic names are preferred to retained names which may be used in general nomenclature.

P-71.2.2.1 Specific method and retained names

A radical formally derived by the removal of two hydrogen atom from one position of a mononuclear parent hydride of an element of Group 14, or from a terminal atom of an unbranched acyclic hydrocarbon, or from one position of a monocyclic saturated hydrocarbon ring is named by replacing the ‘ane’ ending of the systematic name of the parent hydride by the suffix ‘ylidene’. The suffix ‘ylidyne’ is used to name radicals formally derived by the removal of three hydrogen atoms from a mononuclear parent hydride of an element of Group 14 or from a terminal atom of an unbranched acyclic hydrocarbon.

Systematic names are the preferred IUPAC names; the retained names carbene or methylene, nitrene or aminylene, silylene, and carbyne, can be used in general nomenclature, with full substitution.

The use of the systematic or retained names does not imply a specific electronic configuration. If needed, such a distinction could be made by using a separate word such as singlet or triplet, or a descriptive phrase.

Exampes:

$H_2\overset{\bullet}{\underset{\bullet}{C}}$ and/or $H_2C{:}$

methylidene (PIN)
carbene
methylene

$H_2\overset{\bullet}{\underset{\bullet}{Si}}$ and/or $H_2Si{:}$

silylidene (preselected name))
silylene

$H_2\overset{\bullet}{\underset{\bullet}{C}}\cdot$ and/or $H_2\overset{\bullet}{C}{:}$

methylidyne (PIN)
carbyne

$(C_6H_5)_2\overset{\bullet}{\underset{\bullet}{C}}$ and/or $(C_6H_5)_2C{:}$

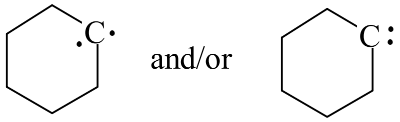
diphenylmethylidene (PIN)
diphenylcarbene
diphenylmethylene

$C_6H_5\text{-}CH_2\text{-}\overset{\bullet}{\underset{\bullet}{Si}}H$ and/or $C_6H_5\text{-}CH_2\text{-}\overset{\bullet\bullet}{Si}H$

benzylsilylidene (PIN)
benzylsilylene

$CH_3\text{-}\overset{\bullet}{\underset{\bullet}{C}}\cdot$ and/or $CH_3\text{-}\overset{\bullet}{C}{:}$

ethylidyne (PIN)
(not methylcarbyne)



cyclohexylidene (PIN)

P-71.2.2.2 General method

With the exception of the radicals named in P-71.2.2.1, the names of the divalent and trivalent radicals derived by the removal of two hydrogen atoms from one position of a parent hydride are formed by adding the suffixes ‘ylidene’ or ‘ylidyne’ to the name of the parent hydride, with elision of the final letter ‘e’, if present. The name azanylidene is the preferred IUPAC name; nitrene or aminylene are retained names for use in general nomenclature.

Examples:

$H\underset{\bullet}{\dot{N}}{:}$ and/or $H\ddot{N}{:}$

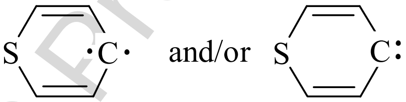
azanylidene (preselected name)
aminylene
nitrene

$H_2N\text{-}\underset{\bullet}{\dot{N}}{:}$ and/or $H_2N\text{-}\ddot{N}{:}$

hydrazinylidene (preselected name)
diazanylidene
(traditional name: hydrazono)
(not aminonitrene)

$H_2P\text{-}\underset{\bullet}{\dot{P}}{:}$ and/or $H_2P\text{-}\ddot{P}{:}$

diphosphanylidene (preselected name)

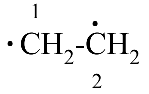


thiopyran-4-ylidene (PIN)

P-71.2.3 Multiple radical centers (Polyradicals)

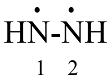
Polyradicals containing two or more radicals centers, formally derived by the removal of two or more hydrogen atoms from each of two or more different skeletal atoms of a parent hydride, are named by adding to the name of the parent hydride combinations of the suffix ‘yl’ for a monovalent radical center, ‘ylidene’ for a divalent radical center, and ‘ylidyne’ for a trivalent radical center, together with the appropriate numerical prefixes indicating the number of each kind of radical center. The final letter ‘e’ of the name of the parent hydride, if present, is elided when followed by ‘y’.

Examples:



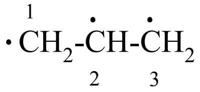
$\cdot\overset{1}{\mathrm{C}}\mathrm{H}_2\text{-}\underset{2}{\dot{\mathrm{C}}}\mathrm{H}_2$

ethane-1,2-diyl (PIN)
(traditional name: ethylene)



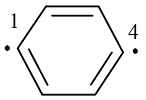
$\mathrm{H}\underset{1}{\dot{\mathrm{N}}}\text{-}\underset{2}{\dot{\mathrm{N}}}\mathrm{H}$

hydrazine-1,2-diyl (preselected name)
diazane-1,2-diyl

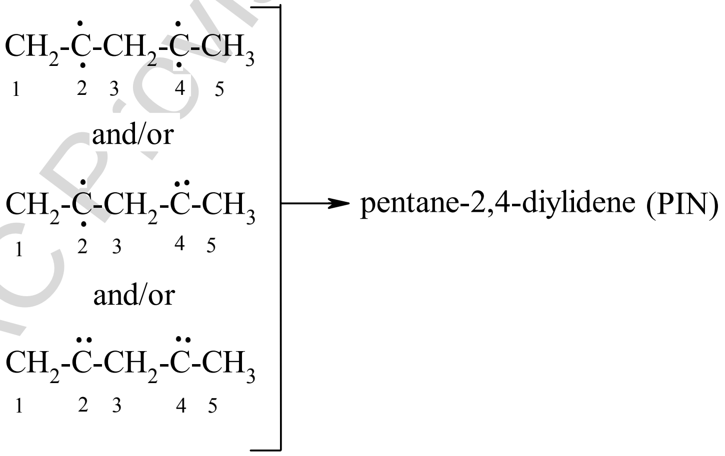


$\cdot\overset{1}{\mathrm{C}}\mathrm{H}_2\text{-}\underset{2}{\dot{\mathrm{C}}}\mathrm{H}\text{-}\underset{3}{\dot{\mathrm{C}}}\mathrm{H}_2$

propane-1,2,3-triyl (PIN)



benzene-1,4-diyl)PIN)
(traditional name: *p*-phenylene or 1,4-phenylene)



pentane-2,4-diylidene (PIN)

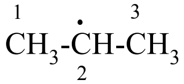
P-71.2.4 Acyclic radicals derived by the removal of one or more hydrogen atoms from nonterminal chain positions are named

(a) by citing the locant of the nonterminal position of the chain, or

(b) by substituting a parent radical that has the free valence(s) at the end of a chain.

Method (a) generates preferred IUPAC names. The principal chain is chosen, if necessary, by the method indicated in Section P-44 for substituent groups.

Examples:

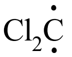
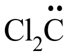

$\overset{1}{C}H_3\text{-}\underset{2}{\overset{\bullet}{C}}H\text{-}\overset{3}{C}H_3$

propan-2-yl (PIN)
1-methylethyl

P-71.2.5 The λ-convention

Divalent and trivalent radical centers in a parent hydride formally derived by the removal of two or three hydrogen atoms from the same skeletal atom in its standard valence state may be described by the λ-convention. Locants for the radical centers are followed by the symbol λ^n, where ‘*n*’ is the bonding number of the skeletal atom (see P-14.1). This method is only for general nomenclature.

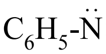
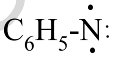
Examples:


$Cl_2\overset{\bullet}{\underset{\bullet}{C}}$ and/or 
$Cl_2\ddot{C}$

dichloro-λ^2-methane
methylidene (PIN)


$F\overset{\bullet}{\underset{\bullet}{C}}\bullet$ and/or 
$F\dot{C}:$

fluoro-λ^1-methane
fluoromethylidyne (PIN)

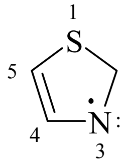

$C_6H_5\text{-}\ddot{N}:$ and/or 
$C_6H_5\text{-}\overset{\bullet}{\underset{\bullet}{N}}:$

phenyl-λ^1-azane
phenylazanylidine (PIN)

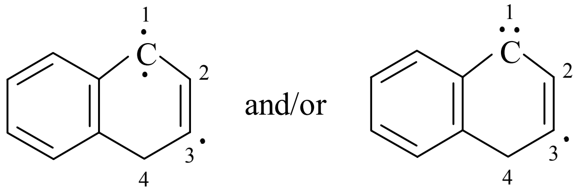
P-71.2.6 Hydro prefixes *vs*. added hydrogen

A radical center at a position in a mancude parent hydride where there is an insufficient number of hydrogen atoms to apply directly the recommendations for the use of ‘yl’ or ‘ylidene’ given in P-71.2.1 and P-71.2.2 is derived formally from a dihydro derivative of the cyclic parent hydride. Such a radical can also be described by applying the principle of ‘added hydrogen’ (see P-14.6). In this method the ‘hydro’ derivative is described by specifying the hydrogen atom of a dihydro pair that remains after the radical center is created by citing in italic capital *H* and the locant of the skeletal atom to which the hydrogen atom resides, both enclosed in a set of parentheses and inserted into the name of the corresponding parent hydride immediately after the locant for the radical center. Names formed by the ‘added hydrogen’ method are preferred.

Examples:



1,3-thiazol-3(2*H*)-yl (PIN)
2,3-dihydro-1,3-thiazol-3-yl



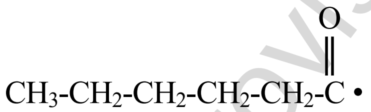
naphthalen-3-yl-1(4*H*)-ylidene (PIN)
1,4-dihydronaphthalen-3-yl-1-ylidene

P-71.3 Radical centers on characteristic groups

P-71.3.1 Acyl radicals

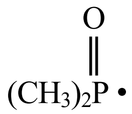
Acyl radicals, i.e., radicals with at least one chalcogen or nitrogen atom attached to a radical center by a (formal) double bond, which may be considered to be formally derived by the removal of a hydroxy group from acid characteristic groups, are named by replacing the ‘ic acid’ or ‘carboxylic acid’ ending of the name of the acid with ‘oyl’or ‘yl’, or ‘carbonyl’, according to the method for forming names of acyl groups (see P-65.1.8). Substituent groups denoted by prefixes such as ‘oxo’, ‘thioxo’, ‘sulfanylidene’, are not recommended for naming acyl radicals.

Examples:



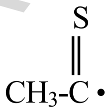
$CH_3\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}\overset{\overset{\displaystyle O}{\|}}{C}\,\bullet$

hexanoyl (PIN)
(not 1-oxohexyl)



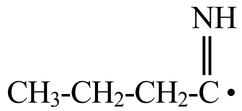
$(CH_3)_2\overset{\overset{\displaystyle O}{\|}}{P}\,\bullet$

dimethylphosphinoyl (PIN)
P-methylmethanephosphinoyl
dimethyloxo-λ^5-phosphanyl



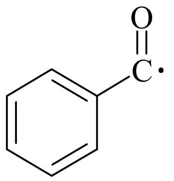
$CH_3\text{-}\overset{\overset{\displaystyle S}{\|}}{C}\,\bullet$

thioacetyl (PIN)
(not sulfanylideneethyl)

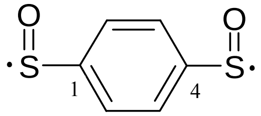


$CH_3\text{-}CH_2\text{-}CH_2\text{-}\overset{\overset{\displaystyle NH}{\|}}{C}\,\bullet$

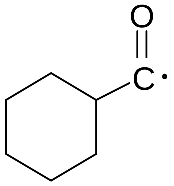
butanimidoyl (PIN)
(not 1-iminobutyl)



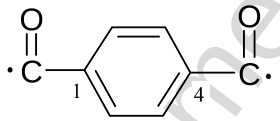
benzoyl (PIN)
phenyl(oxo)methyl



benzene-1,4-disulfinyl (PIN)
1,4-phenylenebis(oxo-λ^4-sulfanyl)



cyclohexanecarbonyl (PIN)
cyclohexyl(oxo)methyl



1,4-phenylenebis(carbonyl) (PIN)
terephthaloyl
[not 1,4-phenylenebis(oxomethyl)]

P-71.3.2 A radical derived formally by the removal of one hydrogen atom from an **amine, imine,** or **amide** characteristic group is named by adding the corresponding compound suffix formed by adding the suffix 'yl' to the basic suffix:

$-NH_2$	amine (preselected name)	$-\overset{\bullet}{\underset{\cdot\cdot}{N}}H$	aminyl (preselected name)
$=NH$	imine (preselected name)	$=\overset{\cdot\cdot}{N}\cdot$	iminyl(preselected name)
$-(C)O\text{-}NH_2$	amide (PIN)	$-(C)O\text{-}\overset{\bullet}{\underset{\cdot\cdot}{N}}H$	amidyl (PIN)
$-CO\text{-}NH_2$	carboxamide (PIN)	$-CO\text{-}\overset{\bullet}{\underset{\cdot\cdot}{N}}H$	carboxamidyl (PIN)

Examples:

$\overset{1}{C}H_3\text{-}\underset{N}{\overset{\cdot\cdot}{N}}H\cdot$

methanaminyl (PIN)
methylazanyl
(traditionally: methylamino)

$\overset{3}{C}H_3\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}H=\overset{\cdot\cdot}{N}\cdot$

propan-1- iminyl (PIN)
propylideneazanyl

$C_6H_5\text{-}\overset{\bullet}{\underset{\cdot\cdot}{N}}H$

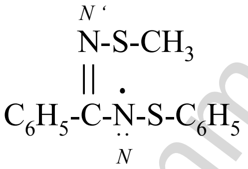
anilinyl (PIN)
benzenaminyl
(not anilino)
(traditionally: phenylamino)
(removal of a hydrogen atom from the benzene ring generates a radical named, for example, 4-aminophenyl)

$(CH_3)_3P{=}\overset{\cdot\cdot}{N}\cdot$

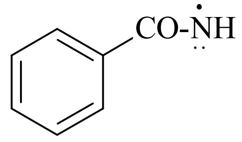
trimethyl-λ^5-phosphaniminyl (PIN)
(trimethylphosphoranylidene)azanyl
trimethylphosphane imidyl

$HCO\text{-}\overset{\bullet}{\underset{\cdot\cdot}{N}}H$

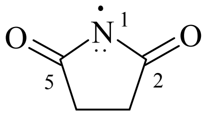
formamidyl (PIN)


$$\begin{array}{l} \qquad\quad\; N' \\ \qquad\quad\; N\text{-}S\text{-}CH_3 \\ \qquad\quad\; \| \\ C_6H_5\text{-}C\text{-}\overset{\bullet}{\underset{\cdot\cdot}{N}}\text{-}S\text{-}C_6H_5 \\ \qquad\qquad\quad N \end{array}$$

N'-(methylsulfanyl)-*N*-(phenylsulfanyl)benzenecarboximidamidyl (PIN)



pyridine-2-carboxamidyl (PIN)



2,5-dioxopyrrolidin-1-yl (PIN)
succinimidyl

P-71.3.3 Divalent radical centers

A radical derived formally by the removal of two hydrogen atoms from an amine or amide characteristic group is named by substituting the parent radical ‘azanylidene’ by the appropriate substituent groups. Azanylidene is the preferred IUPAC name; the names nitrene and aminylene are retained for usein general nomenclature.

Examples:

$C_6H_5\text{-}\overset{\bullet}{\underset{\bullet}{N}}\!:$ and/or $C_6H_5\text{-}\overset{\cdot\cdot}{N}\!:$

phenylazanylidene (PIN)
phenylnitrene
phenylaminylene

$CH_3\text{-}CO\text{-}\overset{\bullet}{\underset{\bullet}{N}}\!:$ and/or $CH_3\text{-}CO\text{-}\overset{\cdot\cdot}{N}\!:$

acetylazanylidene (PIN)
acetylnitrene
acetylaminylene

P-71.3.4 Polyamide, polyamine and polyimine radicals

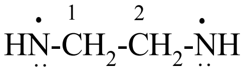
Polyradicals with radical centres identically derived but located on two or more amine, imine, or amide characteristic groups are named in two ways.

(a) by using the compound suffixes (see P-71.3.2) denoting the presence of one electron on each characteristic group and the multiplying prefixes 'bis-', 'tris-', etc. or

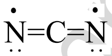
(b) by multiplicative nomenclature based on the parent radical 'azanyl '.

In order to avoid any confusion, the name 'aminyl' is reserved for denoting the suffix in substitutive nomenclature; the parent radical 'azanyl' (not 'aminyl') is used in multiplicative nomenclature. Method (a) leads to preferred IUPAC names.

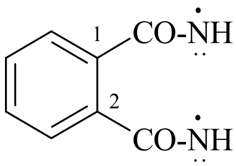
Examples:


$H\dot{N}-\overset{1}{C}H_2-\overset{2}{C}H_2-\dot{N}H$

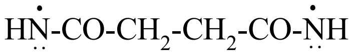
ethane-1,2-bis(aminyl) (PIN)
(ethane-1,2-diyl)bis(azanyl)


$\dot{N}=C=\dot{N}$

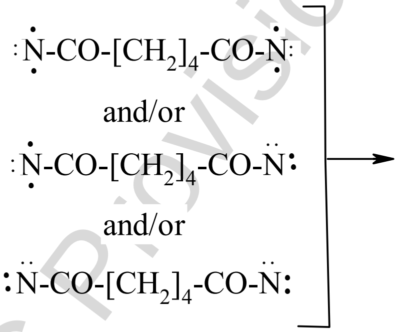
methanebis(iminyl) (PIN)
methanediylidenebis(azanyl)



benzene-1,2-bis(carboxamidyl) (PIN)


$H\dot{N}-CO-CH_2-CH_2-CO-\dot{N}H$

butanediamidyl (PIN)
butanedioylbis(amidyl)



hexanedioylbis(azanylidene) (PIN)
hexanedioylbis(nitrene)
hexanedioylbis(aminylene)

P-71.3.5 A radical derived formally by the removal of the hydrogen atom of a hydroxy group (or chalcogen analog) of an acid or hydroxy characteristic group is named in two ways.

(a) by substituting the parent radicals HO•, 'oxidanyl (preselected name)', or HOO•., 'dioxidanyl' (preselected name), by the appropriate substituent groups;

(b) by using the term 'oxyl' or 'peroxyl' instead of the preselected systematic names 'oxidanyl' and 'dioxidanyl',.

The names methoxyl, ethoxyl, propoxyl, butoxyl and aminoxyl are retained and may be used in general nomenclature; systematic names are preferred. Method (a) generates preferred IUPAC names.

Examples:

$CH_3\text{-}\ddot{\underset{\cdot\cdot}{O}}\cdot$

methyloxidanyl (PIN)
methoxyl

$Cl\text{-}CH_2\text{-}CO\text{-}\ddot{\underset{\cdot\cdot}{O}}\cdot$

(chloroacetyl)oxidanyl (PIN)
chloroacetoxyl

$(Cl\text{-}CH_2)_2N\text{-}\ddot{\underset{\cdot\cdot}{O}}\cdot$

bis(chloromethyl)amino]oxidanyl (PIN)
bis(chloromethyl)aminoxyl

$CH_3\text{-}[CH_2]_4\text{-}CO\text{-}O\text{-}\ddot{\underset{\cdot\cdot}{O}}\cdot$

hexanoyldioxidanyl (PIN)
hexanoylperoxyl

$CH_3\text{-}[CH_2]_3\text{-}\ddot{\underset{\cdot\cdot}{O}}\cdot$

butyloxidanyl (PIN)
butoxyl

Chalcogen analogs are named on the basis of preselected parent radical names, such as ‘sulfanyl’, ‘selanyl,’ ‘disulfanyl’, etc.

Examples:

$C_6H_5\text{-}\ddot{\underset{\cdot\cdot}{S}}\cdot$

phenylsulfanyl (PIN)
(not benzenesulfenyl;
sulfenic acids are no
longerrecognized)

$CH_3\text{-}CO\text{-}\ddot{\underset{\cdot\cdot}{S}}\cdot$

acetylselanyl (PIN)

$CH_3\text{-}C(CH_3)_2\text{-}S\text{-}\ddot{\underset{\cdot\cdot}{S}}\cdot$

tert-butyldisulfanyl (PIN)
(2-methylpropan-2-yl)disulfanyl

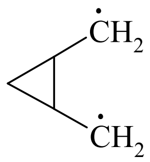
$Cl\text{-}CH_2\text{-}CS\text{-}\ddot{\underset{\cdot\cdot}{S}}\cdot$

[chloro(thioacetyl)]sulfanyl (PIN)

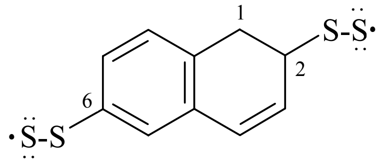
P-71.4 Assemblies of parent radicals

Polyradicals with radical centers identically derived from the same parent hydride or the same characteristic group (except for polyacyl or polyimide radicals) but located in different parts of the structure are named, if possible, according to the principles for nomenclature of assemblies of identical units.

Examples:



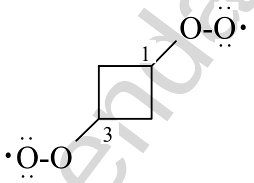
cyclopropane-1,2-diyldimethyl (PIN)



naphthalene-2,6-diylbis(disulfanyl) (PIN)

$^{\bullet}\underset{\cdot\cdot}{\ddot{O}}\text{-C(CH}_3)_2\text{-CH}_2\text{-C(CH}_3)_2\text{-}\underset{\cdot\cdot}{\ddot{O}}^{\bullet}$

2,4-dimethylpentane-2,4-diylbis(oxidanyl) (PIN)
1,1,3,3-tetramethylpropane-1-3-diylbis(oxidanyl)

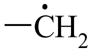


cyclobutane-1,3-diylbis(dioxidanyl) (PIN)

P-71.5 Prefixes denoting radicals

The presence of a radical center in a substituent that is to be cited as a prefix is expressed by the prefix ‘ylo’, indicating the removal of a hydrogen atom. This prefix is a nondetachable prefix, attached to the parent substituent prefix, which is formed by usual methods. The removal of two or more hydrogen atoms from a substituent cited as prefix is indicated by the appropriate multiplying prefix ‘di’, ‘tri’, etc. The prefix ‘ylo’ is also combined with prefixes used additively, such as oxy and carbonyl.

Examples:

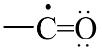


$\text{—}\dot{C}H_2$

ylomethyl (PIN)

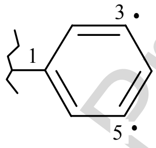
$\text{—}\underset{\cdot\cdot}{\ddot{O}}^{\bullet}$

ylooxy (preselected name)
(not ylohydroxy)



$\text{—}\dot{C}\text{=}\underset{\cdot\cdot}{\ddot{O}}$

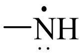
ylocarbonyl (PIN)



3,5-diylophenyl (PIN)

$\text{—CO-}\underset{\cdot\cdot}{\ddot{O}}^{\bullet}$

(ylooxy)carbonyl (PIN)
(not ylocarboxy)



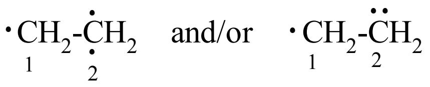
$\text{—}\underset{\cdot\cdot}{\dot{N}}H$

yloamino (preselected name)

P-71.6 Order of citation and seniority of suffixes ‘yl’, ‘ylidene’, and ‘ylidyne’

The suffixes ‘yl’, ‘ylidene’, and ‘ylidyne’ are cited in that order in a name, if applicable; lowest locants are assigned to radicals as a set, then in the order ‘yl’, ‘ylidene’and ‘ylidyne’. The order of citation is identical to that used for naming substituent groups (see P-28.2).

Example:



$\cdot\underset{1}{C}H_2\text{-}\underset{2}{\overset{\cdot}{\underset{\cdot}{C}}}H_2$ and/or $\cdot\underset{1}{C}H_2\text{-}\underset{2}{\ddot{C}}H_2$

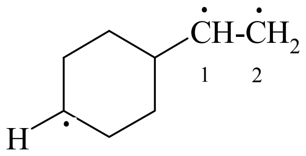
ethan-1-yl-2-ylidene (PIN)

P-71.7 Choice of parent structure

When a choice of a parent radical is necessary, the following criteria are applied, in the order given, until a decision is reached.

(a) Maximum number of radical centers of any kind in a single parent structure:

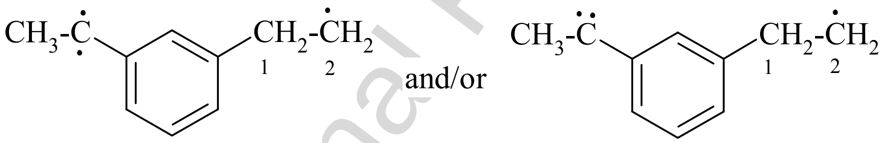
Example:



1-(4-ylocyclohexyl)ethane-1,2-diyl (PIN)

(b) Maximum number of -yl, then -ylidene radical centers;

Example:



2-[3-(1,1-diyloethyl)phenyl]ethyl (PIN)

(c) Maximum number of radical centers at the skeletal atom first cited in the seniority order classes: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > C > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;

Example:

$\cdot CH_2\text{-}C(CH_3)_2\text{-}\overset{..}{\underset{..}{O}}\cdot$

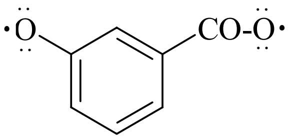
(2-methyl-1-ylopropan-2-yl)oxidanyl (PIN)
(1,1-dimethyl-2-yloethyl)oxidanyl

(d) Further choice, if necessary, is made by applying the general criteria for chains and rings given in Chapters 1 to 6 for neutral compounds.

Examples:

(1) maximum number of radical centers according to the order of suffixes.

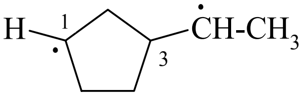
Example:



[3-(ylooxy)benzoyl]oxidanyl (PIN)

(2) rings are senior to chains

Example:



3-(1-yloethyl)cyclopentyl (PIN)

P-72 Anions

P-72.1 General methodology

Anions are named in two ways.

(1) by using suffixes and endings, and

(2) by functional class nomenclature.

Method (1) leads to preferred IUPAC names. Some names and some contracted names are retained as preferred IUPAC names and for use in general nomenclature.

The following suffixes are used:

‘ide’ (corresponding to removal of a hydron, H^+),

‘uide’ (corresponding to the addition of a hydride, H^-),

‘elide’ (corresponding to the addition of an electron)

The endings ‘ate’ and ‘ite’ are used to indicate removal of a proton from a –OH group of acids and hydroxy compounds.

Functional class nomenclature is based on the class name ‘anion’ in association with the name of the corresponding radical (not necessarily the name of the corresponding substituent group).

P-72.2 Anions formed by removal of hydrons

P-72.2.1 Functional class nomenclature

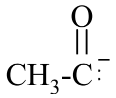
Functional class nomenclature can be used, in general nomenclature, to describe anionic compounds. An anion that can be considered as derived formally by adding an electron to a radical may also be named by adding the class name ‘anion’ as a separate word to the name of the substituent group. The names are formed by using the names of corresponding radicals (not necessarily the name of substitutent groups) and the class name ‘anion’ as a separate word. The multiplying prefixes ‘di’, ‘tri’, etc., are added to the class name to denote multiple anions.

This type of nomenclature is limited to anions having the anionic centers in a same structure. Systematic names (see P-72.2.2) are preferred IUPAC names.

Examples:

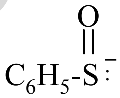
$H_3C\colon^{-}$

methyl anion
methanide (PIN)



$CH_3\text{-}C(=O)\colon^{-}$

acetyl anion
1-oxoethanide(PIN)



$C_6H_5\text{-}S(=O)\colon^{-}$

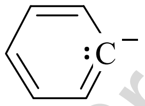
benzenesulfinyl anion
oxophenyl-λ^4-sulfanide (PIN)

$CH_3\text{-}\ddot{\underset{\cdot\cdot}{N}}H^{-}$

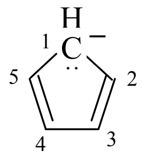
methanaminyl anion
methanaminide (PIN)

$(C_6H_5)_2\ddot{\underset{\cdot\cdot}{C}}^{2-}$

diphenylmethylidene dianion
diphenylmethanide (PIN)



phenyl anion
benzenide (PIN)



cyclopenta-2,4-dien-1-yl anion
cyclopenta-2,4-dien-1-ide (PIN)

P-72.2.2 Systematic nomenclature

P-72.2.2.1 Anions derived from parent hydrides

An anion derived formally by the removal of one or more hydrons from any position of a neutral parent hydride is preferably named by using the suffix '-ide', with elision of the final letter 'e' of the parent hydride, if any. Numerical prefixes 'di', 'tri', etc. are use to denote multiplicity; locants identify positions of the negative charges..

The retained names 'amide' and 'imide' for the anions H_2N^- and HN^{2-}, respectively, can be used in general nomenclature. The systematic names 'azanide' and 'azanediide', respectively, are preselected names.

The retained names hydroxide, for HO^-, and hydroperoxide, for HOO^-, are preselected names but cannot be substituted; thus, the preferred IUPAC names for $CH_3\text{-}O^-$ and $CH_3\text{-}OO^-$ are methyloxidanyl and methyldioxidanyl, respectively

The name 'acetylide', for $^-C{\equiv}C^-$, is retained for general use only.

Examples:

$(NC)_3\ddot{C}^-$

tricyanomethanide (PIN)

$(C_6H_5)_2\underset{..}{\ddot{C}}^{2-}$

diphenylmethanediide (PIN)

$CH_3\text{-}\underset{..}{\ddot{N}}H^-$

methylazanide
methylamide
methanamide (PIN, see P-72.2.3)

$C_6H_5\text{-}\underset{..}{\ddot{N}}\!:^{2-}$

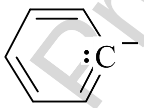
phenylazanedide
phenylimide
benzenaminediide (PIN, see P-72.2.3)

$(CH_3)_2\underset{..}{\ddot{P}}^-$

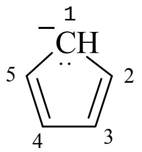
dimethylphosphanide (PIN)
dimethylphosphinide

$HC{\equiv}\ddot{Si}^-$

methylidynesilanide (PIN)



benzenide (PIN)

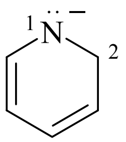


cyclopenta-2,4-dien-1-ide (PIN)

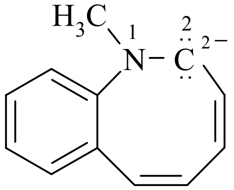
P-72.2.2.1.1 Hydro prefixes *vs*. added hydrogen

An anionic center at a position in a mancude parent hydride where there is an insufficient number of hydrogen atoms to apply directly recommendations for the use of 'ide' given in P-72.2.1 is derived formally from a dihydro derivative of the cyclic parent hydride. Such a radical can also be described by applying the principle of 'added hydrogen' (see P-14.6). In this method the 'hydro' derivative is described by specifying the hydrogen atom of a dihydro pair that remains after the anionic center is created by citing in italic capital *H* and the locant of the skeletal atom to which the hydrogen atom resides, both enclosed in a set of parentheses and inserted into the name of the corresponding parent hydride immediately after the locant for the radical center. Names formed by the 'added hydrogen' method are preferred IUPAC names.

Examples:



pyridin-1(2*H*)-ide (PIN)
1,2-dihydropyridine-1-ide



1-methyl-1-benzazocine-2,2(1*H*)-diide (PIN)
1-methyl-1,2-dihydro-1-benzoazocine-2,2-diide

P-72.2.2.2 Anions derived from characteristic groups

Anions derived from characteristic groups are named in two ways;

(1) directly for acids, alcohols and amines, by modifying the suffix normally used in substitutive nomenclature:

(a) the endings 'ate' or 'ite' to name anions derived from acids;

(b) the ending 'ate' to name anions derived from alcohols,

(c) the suffix 'aminide' (formed by combining the two suffixes 'amin(e) + ide') to name anions derived from amines where the negative charge is on the nitrogen atom;

(2) by using the appropriate preselected anionic parent names in the case of other characteristic groups, such as 'azanide' for NH_2^-, 'azanediide' for NH^{2-}, 'oxidanide' for HO^-. Amides, hydrazides and imides are not named directly by the method (1), as are amines and imines; the reason being that there could be real ambiguity to have the suffix 'ide' used at the end of names such as amide, hydrazides, etc; furthermore, the name 'amide' may be used in general nomenclature to designate the parent NH_2^-. The use of parents azanide and azanediide eliminates all possible ambiguity.

P-72.2.2.2.1 Anions derived from acids

P-72.2.2.2.1.1 An anion formed by the removal of a hydron from the chalcogen atom of an acid characteristic group or functional parent compound is named by replacing the 'ic acid' or 'ous acid' ending of the acid name by 'ate' or 'ite', respectively. Names of acids are described in Section P-65.1.

Examples:

$CH_3\text{-}CO\text{-}\ddot{\underset{..}{O}}{:}^-$

acetate (PIN)

$CH_3\text{-}CH_2\text{-}CO\text{-}O\text{-}\ddot{\underset{..}{O}}{:}^-$

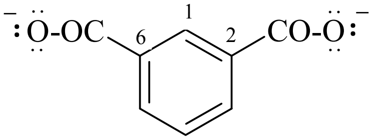
propaneperoxoate (PIN)

$C_6H_5\text{-}SO_2\text{-}\ddot{\underset{..}{O}}{:}^-$

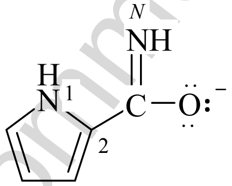
benzenesulfonate (PIN)

$(C_6H_5\text{-}CH_2)_2P\text{-}\ddot{\underset{..}{O}}{:}^-$

dibenzylphosphinite (PIN)



pyridine-2,6-dicarboxylate (PIN)



1*H*-pyrrole-2-carboximidate (PIN)

P-72.2.2.2.1.2 The method of 'hydrogen salts' is used to name partially ionized acids and their esters. The name of the anion is preceded, in order, by the name of the cation, the hydrocarbyl group, and finally the word hydrogen. If necessary, lowest locants are assigned in the same order. The resulting names are preferred IUPAC names; they are preferred to those formed substitutively (see P-65.5.1).

Examples:

$HOOC\text{-}[CH_2]_4\text{-}CO\text{-}\ddot{\underset{..}{O}}{:}^-$

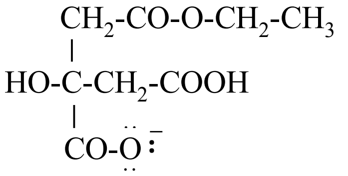
hydrogen hexanedioate (PIN)
5-carboxypentanoate

$C_6H_5\text{-}P(O)(OH)\text{-}\ddot{\underset{..}{O}}{:}^-$

hydrogen phenylphosphonate (PIN)
hydrogen benzenephosphonate
(not hydroxy(phenyl)phosphinate;
phosphonic acid is senior to
phosphinic acid

$CH_3\text{-}CH_2\text{-}O\text{-}CO\text{-}CH_2\text{-}CH_2\text{-}CO\text{-}\ddot{\underset{..}{O}}\cdot$

ethyl hydrogen butanedioate (PIN)
ethyl hydrogen succinate



$$\begin{array}{l} \quad CH_2\text{-}CO\text{-}O\text{-}CH_2\text{-}CH_3 \\ \quad | \\ HO\text{-}C\text{-}CH_2\text{-}COOH \\ \quad | \\ \quad CO\text{-}\ddot{\underset{\cdot\cdot}{O}}{:}^{-} \end{array}$$

4-ethyl 2-(carboxymethyl)-2-hydroxybutanedioate (PIN)
3-ethyl 1-hydrogen citrate
4-hydrogen 2-(2-methoxy-2-oxoethyl)-2-hydroxybutanedioate
(alphanumerical order makes the first name senior to the third name and also preferred to the second name)

P-72.2.2.2.2 Anions derived from hydroxy compounds

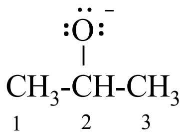
An anion formed by subtracting a hydron from the chalcogen atom of a hydroxy characteristic group, or a chalcogen analog, that can be expressed by a suffix such as ‘ol’, ‘thiol’, ‘-peroxol’, etc., is preferably named by using complex suffixes ‘olate’, ‘thiolate’, ’peroxolate’, etc., formed by addition of the ending ‘ate’ to the suffixes ‘ol’, ‘thiol’, ‘peroxol’, etc. The multiplying prefixes ‘bis’, ‘tris’, etc. are used before compound suffixes, to avoid any ambiguity.

The traditional names methoxide, ethoxide, proproxide, butoxide, isopropoxide, *tert*-butoxide, phenoxide, and aminoxide, for $CH_3\text{-}O^-$, $C_2H_5\text{-}O^-$, $C_3H_7\text{-}O^-$, $C_4H_9\text{-}O^-$, $(CH_3)CH\text{-}O^-$, $(CH_3)_3C\text{-}O^-$, $C_6H_5\text{-}O^-$, and $H_2N\text{-}O^-$ are retained for use in general nomenclature.

Examples:

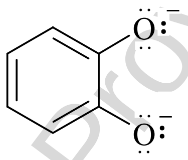
$CH_3\text{-}\ddot{\underset{\cdot\cdot}{O}}{:}^{-}$

methanolate (PIN)
methoxide

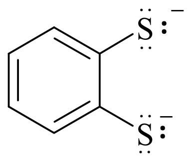


$$\begin{array}{l} \quad\ {:}\ddot{O}{:}^{-} \\ \qquad | \\ CH_3\text{-}CH\text{-}CH_3 \\ {\scriptstyle 1}\qquad {\scriptstyle 2}\qquad {\scriptstyle 3} \end{array}$$

propan-2-olate (PIN)
isopropoxide



benzene-1,2-bis(olate) (PIN)
(not pyrocatecholate)



benzene-1,2-bis(thiolate) (PIN)

P-72.2.2.2.3 Anions derived from amines and imines

Amines and imines having one negative charge on the nitrogen atom are named by using the compound suffixes ‘aminide’and ‘iminide’, formed by the addition of the suffix ‘ide’ to the suffix ‘amine’ or ‘imine’, respectively. The resulting names are preferred IUPAC names; for names acceptable in general nomenclature, see P-77.2.2.1. The name ‘anilinide’ is recommended as a retained IUPAC preferred name.

Examples:

$CH_3\text{-}\underset{\cdot\cdot}{\overset{\cdot\cdot}{N}}H^-$

methanaminide (PIN)

$C_6H_5\text{-}\underset{\cdot\cdot}{\overset{\cdot\cdot}{N}}H^-$

anilinide (PIN)
benzenaminide

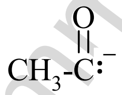
P-72.2.2.2.4 Anionic centers on other characteristic groups

Anionic centers generated formally by the removal of hydrons from atoms of characteristic groups other than those considered in P-72.2.2.1, are named on the basis of the corresponding anionic parent hydrides.

Examples:

$(CH_3)_3C\text{-O-O-}\underset{\cdot\cdot}{\overset{\cdot\cdot}{O}}\colon^-$

tert-butyltrioxidanide (PIN)
(2-methylpropan-2-y)loxidanide
(1,1-dimethylethyl)oxidanide



$CH_3\text{-}\overset{\overset{\displaystyle O}{||}}{C}\colon^-$

1-oxoethanide (PIN)

$CH_3\text{-O-}\underset{\cdot\cdot}{\overset{\cdot\cdot}{O}}\colon^-$

methyldioxidanide (PIN)

$CH_3\text{-}CH_2\text{-S-}\underset{\cdot\cdot}{\overset{\cdot\cdot}{O}}\colon^-$

(ethylsulfanyl)oxidanide (PIN)
(not benzenesulfenate; sulfenic acids
are no longer recognized)

$CH_3\text{-CS-O-}\underset{\cdot\cdot}{\overset{\cdot\cdot}{O}}\colon^-$

(ethanethioyl)dioxidanide (PIN)
(thioacetyl)dioxidanide

$CH_3\text{-CO-O-}\underset{\cdot\cdot}{\overset{\cdot\cdot}{S}}\colon^-$

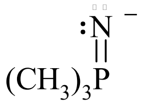
(acetyloxy)sulfanide (PIN)
(not acetoxysulfanide)

$CH_3\text{-CO-}\underset{\cdot\cdot}{\overset{\cdot\cdot}{N}}H^-$

acetylazanide (PIN)
acetylamide

$CH_3\text{-CO-}\overset{2}{N}H\text{-}\overset{1}{\underset{\cdot\cdot}{\overset{\cdot\cdot}{N}}}\colon^{2-}$

acetylhydrazine-1,1-diide (PIN)
acetyldiazane-1,1-diide



$(CH_3)_3P{=}\ddot{N}{:}^{-}$

(trimethyl-λ^5-phosphanylidene)azanide (PIN)

P-72.3 Anions formed by addition of a hydride

Two methods are used to name anions formally formed by adding a hydride ion, H$^-$.

(1) an anion formally derived by adding a hydride ion, H$^-$, to a parent hydride is named by the suffix 'uide', preceded by the multiplying prefixes 'di', 'tri' etc. to indicate multiplicity;

(2) by using the suffix 'ide' with a parent hydride in which the bonding number is expressed by the λ-convention, thus subtracting a hydron, H$^+$, as described in Section P-72.2.

Method (1) leads to preferred IUPAC names.

Examples:

$CH_3\text{-}SiH_4^{-}$

methylsilanuide (PIN)

$(CH_3)_4B^{-}$

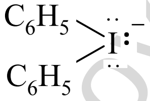
tetramethylboranuide (PIN)

$(CH_3)_4\ddot{P}^{-}$

tetramethylphosphanuide (PIN)
tetramethyl-λ^5-phosphanide
tetramethylphosphoranide

$C_6H_5\text{-}\underset{\cdot\cdot}{\ddot{S}}F_2^{-}$

difluoro(phenyl)sulfanuide (PIN)
difluoro(phenyl)- λ^4-sulfanide



$(C_6H_5)_2\underset{\cdot\cdot}{\ddot{I}}{:}^{-}$

diphenyliodanuide (PIN)
diphenyl-λ^3-iodanide

$F_6\ddot{I}^{-}$

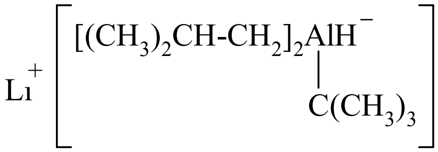
hexafluoro-λ^5-iodanuide (preselected name)
hexafluoro-λ^7-iodanide

F_8Te^{2-}

octafluoro-λ^6-tellanediuide (preselected name)
octafluoro-λ^{10}-tellanediide

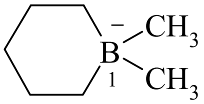
$\mathrm{Na}^{+}\ (\mathrm{CH_3})_3\mathrm{BH}^{-}$

sodium trimethylboranuide (PIN)

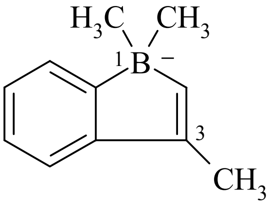


$$\mathrm{Li}^{+}\left[\begin{array}{r}[(\mathrm{CH_3})_2\mathrm{CH\text{-}CH_2}]_2\mathrm{AlH}^{-}\\ |\ \ \\ \mathrm{C(CH_3)_3}\end{array}\right]$$

lithium *tert*-butylbis(3-methylbutyl)alumanuide (PIN)



1,1-dimethylborinan-1-uide (PIN)



1-methoxy-1,3-dimethyl-1-benzoborol-1-uide

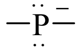
P-72.4 Skeletal replacement nomenclature

Anionic centers in parent hydrides are named by two methods using the principles of skeletal replacement (‘a’) nomenclature described in Section P-15.4.

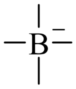
(1) by forming the name of the neutral compound according to skeletal replacement (‘a’) nomenclature and using the suffixes ‘ide’ and ‘uide’ to describe the anionic centers`;

(2) by adding the anionic skeletal replacement (‘a’) prefixes formed by adding the suffixes ‘ida’ and ‘uida’ to the name of the corresponding mononuclear parent hydride, with elision of the final letter ‘e’; these replacement prefixes indicate an anionic center having a bonding number one lower or one higher, respectively, than the bonding number of the corresponding neutral mononuclear parent hydride.

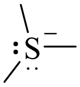
Examples:



phosphanida (PIN)
(preselected name)



boranuida (PIN)
(preselected name)

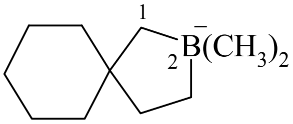


sulfanuida (preselected name)
λ^4-sulfanida

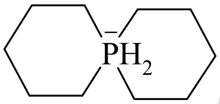
Method (1) results in preferred IUPAC names. Furthermore, names that do not require designation of skeletal heteroatoms in nonstandard valence states using the λ-convention are preferred (see P-72.5).

Skeletal replacement (‘a’) prefixes ending in ‘ata’, for example ‘borata’, are no longer recognized.

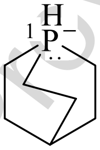
Examples:



2,2-dimethyl-2-boraspiro[4.5]decan-2-uide (PIN)
2,2-dimethyl-2-boranuidaspiro[4.5]decane
(not 2,2-dimethyl-2-borataspiro[4.5]decane)



$6\lambda^5$-phosphaspiro[5.5]undecan-6-uide (PIN)
$6\lambda^5$-phosphanuidaspiro[5.5]nonane
(not 6-phosphataspiro[5.5]nonane)



1-phosphabicyclo[2.2.2]octan-1-uide (PIN)
1-phosphanuidabicyclo[2.2.2]octane
$1\lambda^5$-phosphabicyclo[2.2.2]octan-1-ide
$1\lambda^5$-phosphanidabicyclo[2.2.2]octane

P-72.5 Multiple anionic centers

Multiple anionic centers are named by several methods in accordance with the previous rules.

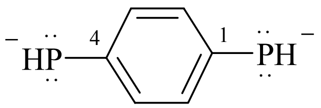
- P-72.5.1 Assemblies of parent anions
- P-72.5.2 'Ide' and 'uide' centers in the same parent hydride
- P-72.5.3 Anionic characteristic groups on anionic parent hydrides
- P-72.5.4 Anionic centers in both parent compounds and substituent groups

P-72.5.1 Assemblies of parent anions

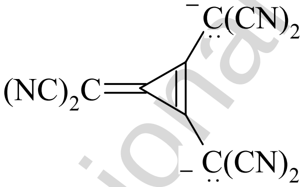
P-72.5.1.1 Assemblies derived from parent anions

Anionic compounds with anionic centers derived from the same parent hydride, but located in different parts of a structure, are named, if possible, according to the principles of multiplicative nomenclature (see P-15.3), using the multiplying prefixes 'bis', 'tris', etc. where necessary.

Examples:



1,4-phenylenebis(phosphanide) (PIN)

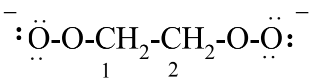


[3-(dicyanomethylidene)cycloprop-1-ene-1,2-diyl]bis(dicyanomethanide) (PIN)

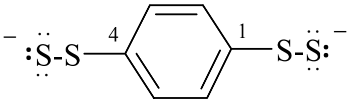
P-72.5.1.2 Polyanions derived from characteristic groups

Anions derived from diacids and polyacids, from diols and polyols, including phenols, and their chalcogen analogues, and also from diamines and polyamines are named substitutively as indicated in P-72.2.2.1. Other characteristic groups are named in accordance with the principles of multiplicative nomenclature, using the multiplying prefixes 'bis', 'tris', etc.

Examples:



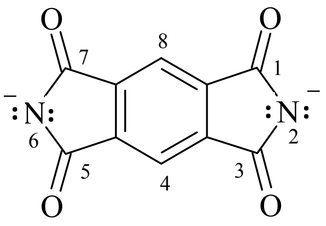
ethane-1,2-diylbis(dioxidanide) (PIN)



1,4-phenylenebis(disulfanide) (PIN)

$^{-}\mathrm{H}\underset{\cdot\cdot}{\ddot{\mathrm{N}}}\text{-CO-CH}_2\text{-CH}_2\text{-CO-}\underset{\cdot\cdot}{\ddot{\mathrm{N}}}\mathrm{H}^{-}$

butanedioylbis(azanide) (PIN)
butanedioylbis(amide)

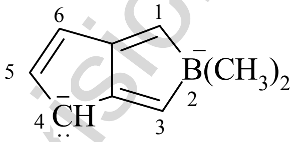


1,3,5,7-tetraoxo-5,7-dihydropyrrolo[3,4-*e*]isoindole-2,6(1*H*,3*H*)-diide (PIN)
(not 1,3,5,7-tetraoxo-5,7-dihydrobenzo[1,2-*c*:4,5-*c'*]dipyrrole-2,6(1*H*,3*H*)-diide)

P-72.5.1.3 'Uide' and 'ide' centers in the same parent hydride

Anionic compounds with two or more anionic centers in the same parent hydride structure, at least one of which is derived formally by removal of a hydron from a skeletal position and one by adding a hydride ion at another position, are named by adding the suffix '-ide', then the suffix '-uide' to the name of the parent hydride, with elision of the final letter 'e' of the parent hydride and of the suffix '-ide'. Each suffix is preceded, where necessary, by the appropriate multiplying prefix. Where there is a choice, low locants of the parent hydride are assigned first to the anionic centers regardless of the kind and then to '-uide' anionic centers.

Example:

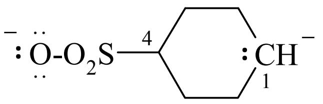


2,2-dimethyl-2,4-dihydrocyclopenta[*c*]borol-4-id-2-uide (PIN)

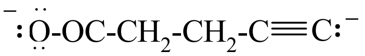
P-72.5.1.4 Anionic characteristic groups on anionic parent hydrides

Polyanions with anionic centers both in the parent hydride part of the structure and on a characteristic group that may be expressed as an anionic suffix are named by adding the anionic suffix to the name of a parent anion formed according to Rules P-72.2.2.1 and P-72.2.3. Where there is a choice, low locants are assigned to the anionic skeletal atoms.

Examples:



cyclohexan-1-ide-4-sulfonate (PIN)



$^{-}:\!\ddot{O}\text{-OC-CH}_2\text{-CH}_2\text{-C}\equiv\text{C}:^{-}$

pent-1-yn-1-id-5-oate (PIN)

P-72.6 Anionic centers in both parent compounds and substituent groups

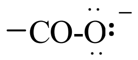
When anionic centers are not in the same parent structure, one anion is chosen as the parent anion and the other expressed as anionic substituent group(s).

P-72.6.1 Prefixes for anionic centers derived from acid characteristic groups
P-72.6.2 Prefixes for anionic centers derived from hydroxy compounds
P-72.6.3 Systematically derived prefixes other than those cited in P-72.6.1 and P-72.6.2
P-72.6.4 Choice of parent anionic struture

P-72.6.1 Prefixes for anionic centers derived from acid characteristic groups

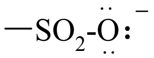
Substituent anions derived from acid characteristic groups by removal of a hydron from all hydroxy, thiol, etc. groups or a chalcogen analogue, and that are attached to the parent structure by a single bond are named by prefixes formed by changing the ending 'ate' in the name of the anionic suffix to 'ato'.

Examples:



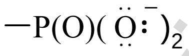
$-\text{CO-}\ddot{O}:^{-}$

carboxylato (PIN)



$-\text{SO}_2\text{-}\ddot{O}:^{-}$

sulfonato (preselected name)



$-\text{P(O)(}\ddot{O}:^{-}\text{)}_2$

phosphonato (preselected name)

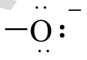
$-\text{As(O)(}\ddot{O}:^{-}\text{)}_2$

arsonato (preselected name)

P-72.6.2 Prefixes for anionic chalcogen atoms

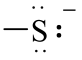
These prefixes are derived from the names oxide, sulfide, selenide, and telluride by changing the final letter 'e', to 'o'.

Examples:



$-\ddot{O}:^{-}$

oxido (preselected name)



$-\ddot{S}:^{-}$

sulfido (preselected name))

P-72.6.3 Systematically formed prefixes that include anionic center(s)

These prefixes are formed by adding the cumulative suffixes ‘yl’ or ‘ylidene’ to the name of the parent anion, with elision of the final letter ‘e’ in the name of the parent anion. Multiplying prefixes ‘di’, tri’, etc, are used to denote multiplicity of free valences. Where there is a choice, low locants are assigned to the free valences.

Examples:

$-\ddot{C}H_2^-$

methanidyl (PIN)

$-\underset{\cdot\cdot}{\ddot{N}}H^-$

azanidyl (preselected name)
amidyl

$-\underset{\cdot\cdot}{\ddot{N}}\!:^{2-}$

azanediidyl (preselected name

$-BH_3^-$

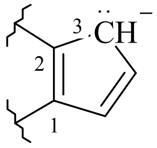
boranuidyl (preselected name)

$=\underset{\cdot\cdot}{\ddot{N}}^-$

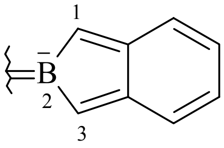
azanidylidene (preselected name)
amidylidene

$-S\text{-}\underset{\cdot\cdot}{\ddot{S}}\!:^-$

disulfanidyl (preselected name)



cyclopenta-1,4-dien-3-ide-1,2-diyl (PIN)



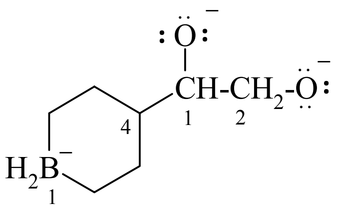
2*H*-2-benzoborol-2-uid-2-ylidene (PIN)

P-72.7 Choice of an anionic parent structure

When necessary, a parent anionic structure must be chosen by applying the following criteria in order until a definitive choice is achieved.

(a) maximum number of anionic centers on characteristic groups of any kind, including anionic suffixes;

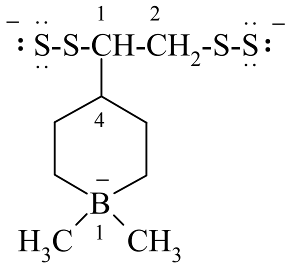
Example:



1-(borinan-1-uid-4-yl)ethane-1,2-bis(olate) (PIN)

(b) maximum number of anionic centers ‘uide’ and ‘ide’;

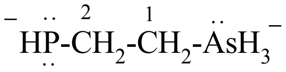
Example:



(1,1-dimethylborinan-1-uide-4-yl)ethane-1,2-diylbis(disulfanide) (PIN)

(c) Maximum number of ‘uide’ centers;

Example:

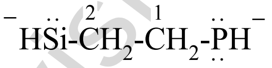


$^{-}\mathrm{H}\ddot{\mathrm{P}}\text{-}\overset{2}{\mathrm{C}}\mathrm{H}_2\text{-}\overset{1}{\mathrm{C}}\mathrm{H}_2\text{-}\ddot{\mathrm{As}}\mathrm{H}_3^{-}$

(2-phosphanidylethyl))arsanuide (PIN)

(d) Maximum number of senior anionic centers, according to the nature of anionic atoms, in the same order as the corresponding replacement prefixes: F > Cl > Br > I > O > S > Se > Te > N > P > As > Sb > Bi > C > Si > Ge > Sn > Pb > B > Al > Ga > In > Tl;

Example:

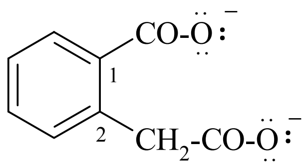


$^{-}\mathrm{H}\ddot{\mathrm{Si}}\text{-}\overset{2}{\mathrm{C}}\mathrm{H}_2\text{-}\overset{1}{\mathrm{C}}\mathrm{H}_2\text{-}\ddot{\mathrm{P}}\mathrm{H}^{-}$

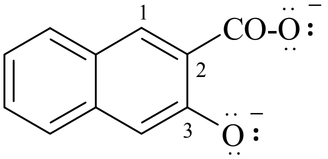
(2-silanidylethyl)phosphanide (PIN)

(e) Further choice, if necessary, is made by giving priority to corresponding suffixes and by using general priorities.

Examples:



2-(carboxylatomethyl)benzoate (PIN)
(ring senior to a chain)



3-oxidonaphthalene-2-carboxylate (PIN)

P-73 Cations

P-73.0 Introduction

For the purpose of organic nomenclature a cation is a molecular entity carrying at least one unit of positive charge formally derived from a parent hydride or parent compound by adding one or more hydrons, by the removal of one or more hydride ions, or a combination of these operations. An atom where a positive charge is considered to reside is called a cationic center. Cations with two or more cationic centers in the same structure are called dications, trications, etc.

73.1 Cationic compounds with cationic centers derived formally by the addition of hydrons

P-73.1.1 Cations centers in parent hydrides

P-73.1.1.1 Retained names of monocationic mononuclear parent cations of Groups 15, 16, and 17

A parent ion derived formally by adding one hydron to a mononuclear parent hydride of the nitrogen, chalcogen and halogen families, in its standard bonding state is named by adding the term ‘onium’ to a root for the element as indicated in Table 7.1. These cations are parent compounds; they can thus be substituted, but are used only in general nomenclature. For preferred IUPAC names see P-73.1.1.2.

Table 7.1 Retained preselected names of mononuclear parent cations of Groups 15, 16, and 17

H_4N^+	ammonium	H_3O^+	oxonium	H_2F^+	fluoronium
H_4P^+	phosphonium	H_3S^+	sulfonium	H_2Cl^+	chloronium
H_4As^+	arsonium	H_3Se^+	selenonium	H_2Br^+	bromonium
H_4Sb^+	stibonium	H_3Te^+	telluronium	H_2I^+	iodonium
H_4Bi^+	bismuthonium				

Examples:

$(CH_3)_4N^+$

tetramethylammonium
tetramethylazanium
N,*N*,*N*-trimethylmethanaminium (PIN)

$Cl(CH_3)_3P^+$

chloro(trimethyl)phosphonium
chloro(trimethyl)phosphanium (PIN)

$(CH_3)_2\overset{+}{S}H$

dimethylsulfonium
dimethylsulfanium (PIN)

$CH_3\text{-}C{\equiv}O^+$

ethylidyneoxonium
ethylidyneoxidanium(PIN)

$(C_6H_5)_2I^+$

diphenyliodonium
diphenyliodanium (PIN)

$CH_3\text{-}\overset{+}{F}\text{-}Cl$

chloro(methyl)fluoronium
chloro(methyl)fluoranium (PIN)

P-73.1.1.2 General rule for systematically naming cationic centers in parent hydrides

A cation derived formally by adding one or more hydrons to any position of a neutral parent hydride (listed in Chapter 2), or whose degree of hydrogenation has been modified (see P-31) is named by replacing the final letter ‘e’ of the parent hydride name, if any, by the suffix ‘ium’, preceded by multiplying locants ‘di’, ‘tri’, etc., to denote the multiplicity of identical cationic centres. These names for mononuclear cations derived from the mononuclear parent hydrides of Groups 15, 16, and 17, are preferred IUPAC names; these are the preferred IUPAC names and not those given in Table 7.1

Examples:

$[CH_5]^+$

methanium (PIN)

$[C_6H_7]^+$

benzenium (PIN)

H_4N^+

azanium (preselected name)
ammonium

H_4P^+

phosphanium (preselected name)
phosphonium

H_3S^+

sulfanium (preselected name)
sulfonium

H_2Cl^+

chloranium (preselected name)
chloronium

$CH_3\text{-}\overset{+}{S}F_4$

tetrafluoro(methyl)-λ^4-sulfanium (PIN)
tetrafluoro(methyl)-λ^4-sulfonium;

$(CH_3)_2N\text{-}\overset{+}{N}(CH_3)_3$

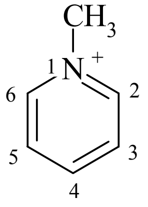
pentamethylhydrazinium (PIN)
pentamethyldiazanium

$CH_3\text{-}S\text{-}\overset{+}{S}(CH_3)\text{-}S\text{-}CH_3$

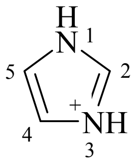
1,2,3-trimethyltrisulfan-2-ium (PIN)

$Cl_2P\text{-}\overset{+}{P}(CH_3)_3$

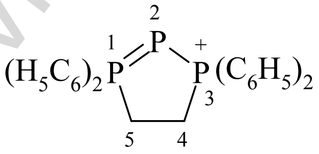
2,2-dichloro-1,1,1-trimethyldiphosphan-1-ium (PIN)



1-methylpyridin-1-ium (PIN)



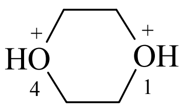
1*H*-imidazol-3-ium (PIN)



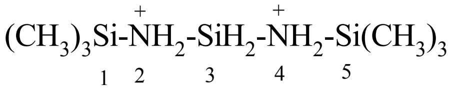
1,1,3,3-tetraphenyl-4,5-dihydro-3*H*-1λ^5,2,3-triphosphol-3-ium (PIN)

$(CH_3)_2\underset{1}{\overset{+}{N}}=\underset{2}{\overset{+}{N}}(CH_3)_2$

tetramethyldiazen-1,2-diium (PIN)



1,4-dioxan-1,4-diium (PIN)



$$(CH_3)_3\underset{1}{Si}\text{-}\underset{2}{\overset{+}{N}}H_2\text{-}\underset{3}{Si}H_2\text{-}\underset{4}{\overset{+}{N}}H_2\text{-}\underset{5}{Si}(CH_3)_3$$

1,1,1,5,5,5-hexamethyltrisilazane-2,4-diium (PIN)

P-73.1.2 Cationic centers on characteristic groups

The principle applied in the naming of cationic centers on characteristic groups is to use the largest neutral parent possible. It is applied particularly in the case of neutral compounds expressed by suffixes containing nitrogen and in the case of oxoacids. Other classes are named on the basis of the largest cationic parent hydride.

P-73.1.2.1 Cationic compounds derived from neutral compounds expressed by suffixes are named in two ways.

(1) Cationic suffixes expressing oxoacids and functional groups containing nitrogen (amide, imide, nitrile, amine, and imine) are formed by adding the suffix ‘ium’ to the neutral suffix, as indicated in Table 7.2. These cationic suffixes are used as normal suffixes, with the multiplying prefixes ‘bis’, ‘tris’, etc., are used to denote multiplicity. Retained names, used as preferred IUPAC names or in general nomenclature, are modified in the same way.

Table 7.2 Suffixes for cationic characteristic groups

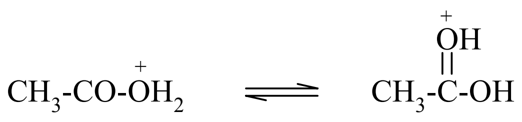
Neutral characteristic group suffix	Cationic characteristic group suffix
ic acid (oxoacids only)	ic acidium
amide, carboxamide	amidium, carboxamidium
imide, carboximide	imidium, carboximidium
nitrile, carbonitrile	nitrilium, carbonitrilium
amine	aminium
imine	iminium

When retained names of amides and nitriles used in general nomenclature imply the presence of two characteristic groups, for example succinonitrile, the corresponding cationic suffix denotes the addition of one hydron to each of the characteristic groups.

(2) By substituting cationic parent hydrides described in P-73.1.1.

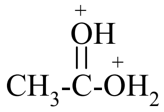
Method (1) is used to generate preferred IUPAC names

Examples:



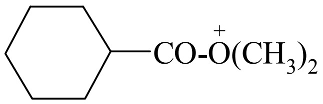
$CH_3\text{-}CO\text{-}\overset{+}{O}H_2 \rightleftharpoons CH_3\text{-}\overset{\overset{+}{O}H}{\overset{||}{C}}\text{-}OH$

acetic acidium

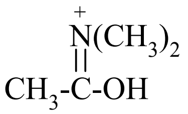


$CH_3\text{-}\overset{\overset{+}{O}H}{\overset{||}{C}}\text{-}\overset{+}{O}H_2$

acetic acidodiium (PIN)



O,*O*-dimethylcyclohexanecarboxylic acidium (PIN)
(cyclohexanecarbonyl)dimethyloxonium



$CH_3\text{-}\overset{\overset{+}{N}(CH_3)_2}{\overset{||}{C}}\text{-}OH$

N,*N*-dimethylacetimidic acidium (PIN)
(1-hydroxyethylidene)dimethylammonium

$(CH_3)_4N^+$

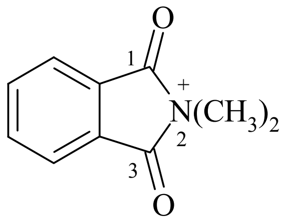
N,*N*,*N*-trimethylmethanaminium (PIN)
tetramethylammonium

$C_6H_5\text{-}CO\text{-}\overset{+}{N}(CH_3)_3$

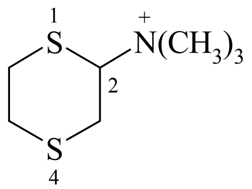
N,*N*,*N*-trimethylbenzamidium (PIN)
benzoyltrimethylammonium

$(CH_3)_3\overset{+}{N}\text{-}OC\text{-}CH_2\text{-}CO\text{-}\overset{+}{N}(CH_3)_3$

N,*N*,*N*,*N*′,*N*′,*N*′-hexamethylpropanebis(amidium) (PIN)
N,*N*,*N*,*N*′,*N*′,*N*′-hexamethylmalonamidium



2,2-dimethyl-1,3-dioxo-2,3-dihydro-1*H*-isoindol-2-ium (PIN)
N,*N*-dimethylphthalimidium



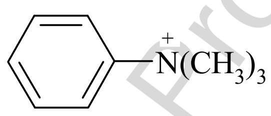
N,*N*,*N*-trimethyl-1,4-dithian-2-aminium (PIN)
(1,4-dithian-2-yl)trimethylammonium

$C_6H_5\text{-}C{\equiv}\overset{+}{N}H$

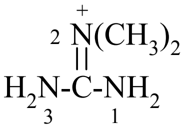
benzonitrilium (PIN)
benzylidyneammonium
benzylidyneazanium

$H\overset{+}{N}{\equiv}C\text{-}CH_2\text{-}CH_2\text{-}C{\equiv}\overset{+}{N}H$

butanebis(nitrilium) (PIN)
butanediylidynebis(ammonium)
butanediylidynebis(azanium)



N,*N*,*N*-trimethylanilinium (PIN)



$$\overset{2\ \overset{+}{N}(CH_3)_2}{\underset{3}{H_2N}\text{-}\overset{\|}{C}\text{-}\underset{1}{NH_2}}$$

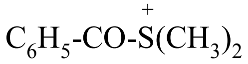
2,2-dimethylguanidinium (PIN)

$CH_3\text{-}CH{=}\overset{+}{O}H$

ethylideneoxidanium (PIN)
ethylideneoxonium

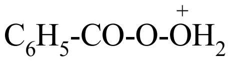
$(CH_3)_2C{=}\overset{+}{O}\text{-}CH_2\text{-}CH_3$

ethyl(propan-2-ylidene)oxidanium (PIN)
ethyl(propan-2-ylidene)oxonium



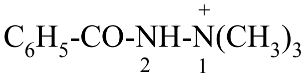
$C_6H_5\text{-CO-}\overset{+}{S}(CH_3)_2$

S,*S*-dimethylbenzenecarbothioic acidium (PIN)
benzoyldimethylsulfonium
benzoyldimethylsulfanium



$C_6H_5\text{-CO-O-}\overset{+}{O}H_2$

benzoyldioxidanium (PIN)
peroxybenzoic *OO*-acidium



$C_6H_5\text{-CO-}\underset{2}{N}H\text{-}\underset{1}{\overset{+}{N}}(CH_3)_3$

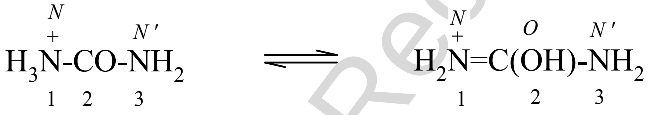
N,N-dimethylbenzenecarbohydrazid-1-ium (PIN)
2-benzoyl-1,1,1-trimethylhydrazinium
2-benzoyl-1,1,1-trimethyldiazanium

$CH_3\text{-CO-}\overset{+}{Cl}\text{-}CH_3$

acetyl(methyl)chloronium (PIN)

P-73.1.2.2 Uronium ions and chalcogen analogs

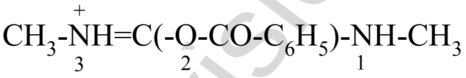
Cations derived formally by adding a hydron to urea (or isourea) are named on the basis of the parent cation ‘uronium’, representing the following tautomeric structures:



$$H_3\underset{1}{\overset{\overset{N}{+}}{N}}\text{-}\underset{2}{C}O\text{-}\underset{3}{\overset{N'}{N}}H_2 \rightleftharpoons H_2\underset{1}{\overset{\overset{N}{+}}{N}}\text{=}\underset{2}{C}(\overset{O}{O}H)\text{-}\underset{3}{\overset{N'}{N}}H_2$$

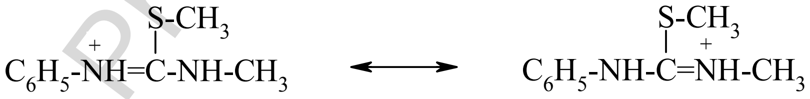
Locants follow those used for urea and isourea. Chalcogen analogues are named on the basis of parent cations, such as ‘thiouronium’, etc. When a choice between two or more tautomeric structures cannot be made, the locants *N*, *N* ‘, and *O*, *S*, etc. are used.

Examples:



$CH_3\text{-}\underset{3}{\overset{+}{N}}H\text{=}C(\text{-}\underset{2}{O}\text{-CO-}C_6H_5)\text{-}\underset{1}{N}H\text{-}CH_3$

1,3-dimethyl-2-phenyluronium



N-phenyl-*N'*,*S*-dimethylthiouronium

P-73.2 Cations formed by the removal of hydride ions

P-73.2.1 Functional class names

Cationic compounds that can be considered as being derived formally by removal of electrons from the corresponding radical may be named by adding the class name ‘cation’ as a separate word after the name of the radical . Polycations are indicated by adding the multiplying prefixes ‘di’, ‘tri’, etc., as appropriate, to the class name. Systematic names formed by using the suffix ‘ylium’ are preferred (see P-73.2.2).

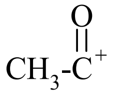
Examples:

CH_3^+

methyl cation
methylium (PIN)

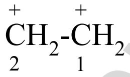
$[C_6H_5]^+$

phenyl cation
benzenylium (PIN)



$CH_3\text{-}\overset{\overset{\Large O}{||}}{C}{}^+$

acetyl cation
1-oxoethylium



$\overset{+}{C}H_2\text{-}\overset{+}{C}H_2$ (locants 2, 1)

ethane-1,2-diyl dication
ethane-1,2-bis(ylium)

P-73.2.2 Cationic centers in parent hydrides

The following recommendations follow closely those for naming radicals, for which see P-71.

P-73.2.2.1 Cationic centers in parent hydrides
P-73.2.2.2 Cationic centers on characteristic groups

P-73.2.2.1 Cationic centers in parent hydrides

P-73.2.2.1.1 Specific method

Cations formed formally by the removal of a hydride ion, H^-, from a terminal atom of a saturated unbranched acyclic hydrocarbon, a saturated monocyclic hydrocarbon, or a mononuclear parent hydride belonging to Group 14, i.e., methane, CH_4, silane, SIH_4, germane, GeH_4, stannane, SnH_4, and plumbane, PbH_4, are named by replacing the ‘ane’ ending in the name of the parent hydride by the suffix ‘ylium’.

Examples:

CH_3^+

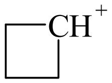
methylium (PIN)

$(C_6H_5)_3Si^+$

triphenylsilylium (PIN)

$CH_3\text{-}CH_2\text{-}CH_2^+$

propylium (PIN)



cyclobutylium (PIN)

P-73.2.2.1.2 General method

According to the general method, cations formally derived by the removal of one hydride ion, H^-, from any position of a parent hydride are named by adding the suffix '-ylium' to the name of the parent hydride, with elision of the final 'e' in the name of the parent hydride, if present'. Di- and polycations formally derived by the removal of two or more hydride ions from the parent hydride are named by using the suffix 'ylium' and the multiplying prefixes 'bis', 'tris', etc. Preferred IUPAC names for the parent hydrides are used, as indicated in Chapters 2 and 5. In the examples that follow, preferred IUPAC names are indicated when traditional names are used in general nomenclature.

Examples:

$H_2\ddot{N}{}^+$

azanylium (preselected name)
aminylium
nitrenium

$C_6H_5\text{-}\underset{..}{\ddot{S}}{}^+$

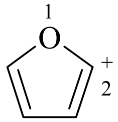
phenylsulfanylium (PIN)

$CH_3\text{-}\underset{3}{NH}\text{-}\underset{2}{N}=\underset{1}{\ddot{N}}{}^+$

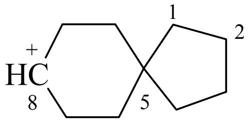
3-methyltriaz-1-en-1-ylium (PIN)

$(CH_3)_3\underset{3}{Si}\text{-}\underset{2}{\overset{+}{Si}}(CH_3)\text{-}\underset{1}{Si}(CH_3)_3$

heptamethyltrisilan-2-ylium (PIN)



furan-2-ylium (PIN)



spiro[4.5]decan-8-ylium (PIN)

$\underset{3}{\overset{+}{CH_2}}\text{-}\underset{2}{CH_2}\text{-}\underset{1}{\overset{+}{CH_2}}$

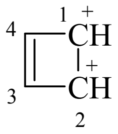
propane-1,3-bis(ylium) (PIN)

$(CH_3)_2\underset{2}{N}\text{-}\underset{1}{\ddot{N}}{}^{2+}$

2,2-dimethylhydrazine-1,1-bis(ylium) (PIN)
2,2-dimethyldiazane-1,1-bis(ylium)

$\underset{3}{CH_3}\text{-}\underset{2}{\overset{2+}{C}}\text{-}\underset{1}{CH_3}$

propane-2,2-bis(ylium) (PIN)
1-methylethane-1,1-bis(ylium)

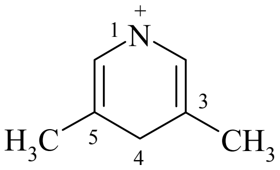


cyclobut-3-ene-1,2-bis(ylium) (PIN)

P-73.2.2.2 Hydro prefixes *vs*. added hydrogen

A cationic center at a position in a mancude parent hydride where there is an insufficient number of hydrogen atoms to apply directly recommendations for the use of 'ylium' as given in P-73.2.2.1.2 is derived formally from a dihydro derivative of the cyclic parent hydride. Such a radical can also be described by applying the principle of 'added hydrogen' (see P-14.6). In this method the 'hydro' derivative is described by specifying the hydrogen atom of a dihydro pair that remains after the cationic center is created by citing an italic capital *H* and the locant of the skeletal atom at which the hydrogen atom resides, both enclosed in a set of parentheses and inserted into the name of the corresponding parent hydride immediately after the locant for the radical center. Names formed by the 'added hydrogen' method are preferred IUPAC names.

Example:



3,5-dimethylpyridin-1(4*H*)-ylium (PIN)
3,5-dimethyl-1,4-dihydropyridin-1-ylium

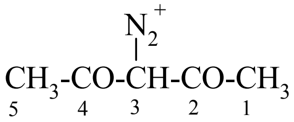
P-73.2.2.3 Diazonium ions

Cations containing a $-N_2^+$ group attached to a parent hydride are traditionally named according to the principles of substitutive nomenclature by using the suffix 'diazonium' and the multiplying prefixes 'bis', 'tris', etc. to denote multiplicity. Diazonium ions may also be named on the basis of the parent cation 'diazenylium', $HN=N^+$. The use of the suffix 'diazonium' yields preferred IUPAC names.

Examples:

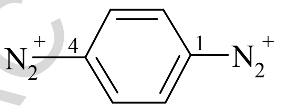
$CH_3\text{-}N_2^+$

methanediazonium (PIN)
methyldiazenylium



$$\underset{5}{CH_3}\text{-}\underset{4}{CO}\text{-}\underset{3}{\overset{\overset{N_2^+}{|}}{CH}}\text{-}\underset{2}{CO}\text{-}\underset{1}{CH_3}$$

2,4-dioxopentane-3-diazonium (PIN)
(2,4-dioxopentan-3-yl)diazenylium



benzene-1,4-bis(diazonium) (PIN)
1,4-phenylenebis(diazenylium)

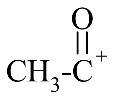
P-73.2.3 Cationic groups on characteristic groups

P-73.2.3.1 Acylium ions
P-73.2.3.2 Cationic groups expressed by suffixes
P-73.2.3.3 Cationic groups expressed as derivatives of parent cations

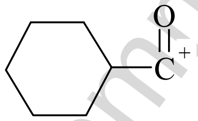
P-73.2.3.1 Acylium cations

Cations formally derived by the removal of all the hydroxy groups as hydroxide ions from acids having systematic or retained names are named by replacing the ‘oic acid’ or ‘ic acid’ ending by the suffix ‘oylium’ or ‘ylium’, or the ‘carboxylic acid’ ending by ‘carbonylium’, in accordance with the rules for naming neutral acyl groups (see P-65.1.8). These names are preferred IUPAC names.

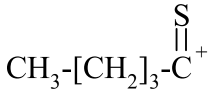
Examples:


$CH_3\text{-}\overset{O}{\overset{\|}{C}}{}^{+}$

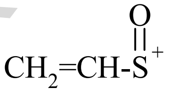
acetylium (PIN)
acetyl cation



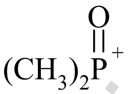
cyclohexanecarbonylium (PIN)
cyclohexanecarbonyl cation


$CH_3\text{-}[CH_2]_3\text{-}\overset{S}{\overset{\|}{C}}{}^{+}$

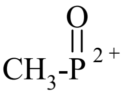
pentanthioylium (PIN)


$CH_2\text{=}CH\text{-}\overset{O}{\overset{\|}{S}}{}^{+}$

ethenesulfinylium (PIN)


$(CH_3)_2\overset{O}{\overset{\|}{P}}{}^{+}$

dimethylphosphinoylium (PIN)

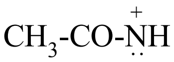

$CH_3\text{-}\overset{O}{\overset{\|}{P}}{}^{2+}$

methylphophonoylium (PIN)

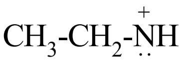
P-73.2.3.2 Cationic groups expressed by suffixes

Mono- and polycationic centers formally derived by the removal of a hydride ion from the nitrogen atom of an amide, imide, amine, and imine characteristic group are named by using the appropriate suffixes for neutral groups modified by the addition of the suffix ‘ylium’, with elision of the final ‘e’ of the neutral suffix. Multiplying prefixes ‘bis’, ‘tris-’, etc., are used to denote the multiplicity of these suffixes. These names are the preferred IUPAC names; they are preferred to those formed by substitution of the appropriate parent cation.

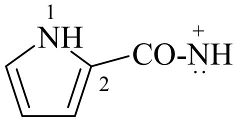
Examples:


$CH_3\text{-}CO\text{-}\overset{+}{\underset{..}{N}}H$

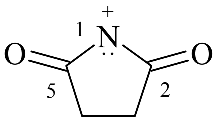
acetamidylium (PIN)


$CH_3\text{-}CH_2\text{-}\overset{+}{\underset{..}{N}}H$

ethanaminylium (PIN)



1*H*-pyrrole-2-carboxamidylium (PIN)



2,5-dioxopyrrolidin-1-ylium (PIN)
succinimidylium

P-73.2.3.3 Cationic groups expressed as substituted parent cations

P-73.2.3.3.1 Cationic centers on oxygen atoms of acids, peroxy acids, hydroxy and hydroperoxy characteristic groups

Cationic centers that are formed by the removal of a hydride ion from an acid, peroxy acid, hydroxy and hydroperoxy characteristic groups are named by substitutive nomenclature on the basis of the corresponding parent cations ‘oxidanylium’ and ‘dioxidanylium’. These are preselected names; a less preferred method uses the terms ‘oxylium’ and peroxylium’, respectively.

The names methoxylium, ethoxylium, propoxylium, butoxylium, phenoxylium, and aminoxylium are retained for use in general nomenclature.

Examples:

$CH_3\text{-}\ddot{\underset{\cdot\cdot}{O}}{}^{+}$

methoxylium (PIN)
methyloxidanylium

$(CH_3)_3C\text{-}O\text{-}\ddot{\underset{\cdot\cdot}{O}}{}^{+}$

tert-butyldioxidanylium (PIN)
tert-butylperoxylium

$Cl\text{-}CH_2\text{-}CO\text{-}\ddot{\underset{\cdot\cdot}{O}}{}^{+}$

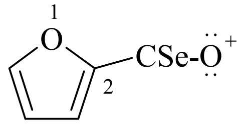
(chloroacetyl)oxidanylium (PIN)
chloracetoxylium

$CH_3\text{-}CS\text{-}\ddot{\underset{\cdot\cdot}{O}}{}^{+}$

(thioacetyl)oxidanylium (PIN)
(thioacetyl)oxylium

$(CH_3)_2N\text{-}\ddot{\underset{\cdot\cdot}{O}}{}^{+}$

(dimethylamino)oxidanylium (PIN)
dimethylaminoxylium



furan-2-carboselenoyloxidanylium (PIN)
furan-2-carboselenoyloxylium

P-73.2.3.3.2 Cationic centers on other characteristic groups

All other cationic centers are named by substituting the appropriate parent cation. The use of the terms ‘thiylium’ and ‘perthiylium’ is not recommended in the case of sulfur cationic centers.

Examples:

$Cl_2C\text{-}CH_2\text{-}\ddot{\underset{\cdot\cdot}{S}}{}^{+}$

(2,2-dichloroethyl)sulfanylium (PIN)
[not 2,2-dichloro(ethylthiylium)]

$CH_3\text{-}CO\text{-}\ddot{\underset{\cdot\cdot}{S}}{}^{+}$

acetylsulfanylium (PIN)
(not acetylthiylium)

$C_6H_5\text{-}S\text{-}\ddot{\underset{\cdot\cdot}{S}}{}^{+}$

phenyldisulfanylium (PIN)
(not phenylperthiylium)

$CH_3\text{-}CH_2\text{-}S\text{-}\ddot{\underset{\cdot\cdot}{O}}{}^{+}$

(ethylsulfanyl)oxidanylium (PIN)
ethyl(sulfanyloxylium)

$CH_3\text{-}CH_2\text{-}\ddot{N}{}^{2+}$

ethylazanebis(ylium) (PIN)

$C_6H_5\text{-}CO\text{-}\ddot{N}{}^{2+}$

benzoylazanebis(ylium) (PIN)

$C_6H_5\text{-}CO\text{-}\underset{2}{NH}\text{-}\underset{1}{\overset{+}{\underset{\cdot\cdot}{N}}}H$

2-benzoylhydrazin-1-ylium (PIN)
2-benzoyldiazane-1-ylium

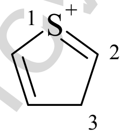
$CH_3\text{-}CH_2\text{-}O\text{-}\ddot{\underset{\cdot\cdot}{Te}}{}^{+}$

ethoxytellanylium (PIN)

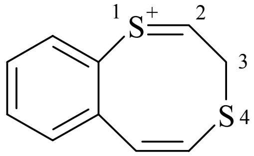
P-73.3 Application of the λ-convention with the suffix 'ylium'

P-73.3.1 A cationic heterocycle having a cationic center on a heteroatom that has one more skeletal bonds than it has in the corresponding neutral heterocycle is named by adding the suffix 'ylium' to the name of the neutral parent hydride for which the λ-convention has been used to describe a nonstandard bonding state of the heteroatom and that heteroatom has at least one hydrogen atom in the neutral heterocycle on which the 'ylium' suffix can operate. Indicated hydrogen (see P-14.6) is used as needed.

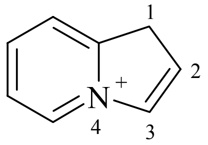
Examples:



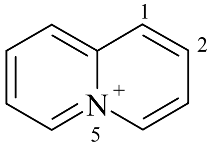
$3H$-1λ^4-thiophen-1-ylium (PIN)



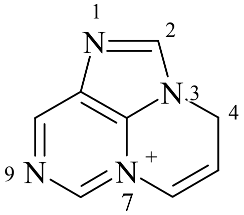
$3H$-1λ^4,4-benzodithiocin-1-ylium (PIN)
$3H$-1λ^4-benzo[*e*][1,4]dithiocin-1-ylium



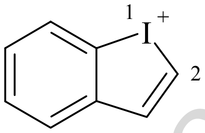
1*H*-4λ^5-indolizin-4-ylium (PIN)



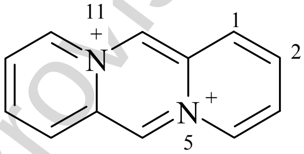
5λ^5-quinolizin-5-ylium (PIN)



4*H*-7λ^5-pyrimido[1,2,3-*cd*]purin-7-ylium (PIN)



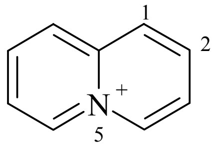
1λ^3-benzoiodol-1-ylium (PIN)



5λ^5,11λ^5-dipyrido[1,2-*a*:1’,2’-*d*]pyrazine-5,11-bis(ylium) (PIN)

For certain cationic heterocycles of this type, especially those with cationic centers on heteroatoms from the second period elements, it might seem more acceptable to use replacement nomenclature (see P-73.4) or to derive the name by removal of two hydrogen atoms from a cation formed by addition of a hydron using the prefix ‘didehydro’, for example ‘4a-azonianaphthalene’ or ‘2,5-didehydro-2*H*-quinolizin-5-ium’ for the cation also known as quinolizinium.

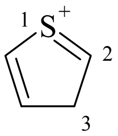
Example:



$5\lambda^5$-quinolizin-5-ylium (PIN)
4a-azonianaphthalene
2,5-didehydro-2*H*-quinolizin-5-ium

The ‘dehydro’ method, however, can become quite cumbersome requiring both ‘hydro’ and ‘dehydro’ prefixes in some cases.

Example:

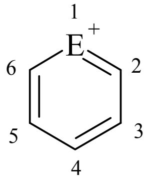
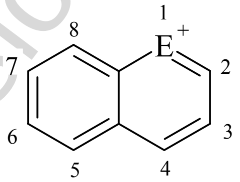
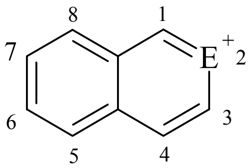
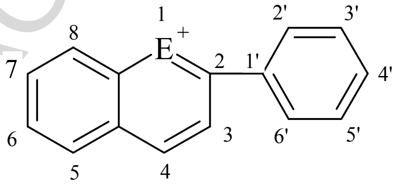
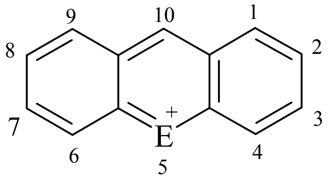


3*H*-$1\lambda^4$-thiophen-1-ylium (PIN)
1,2-didehydro-2,3-dihydrothiophen-1-ium

P-73.3.2 Retained names

The contracted and traditional names listed in Table 7.3 are retained as preferred IUPAC names and for use in general nomenclature.

Table 7.3 Retained names of ‘ylium’ cationic parent compounds

 E=O: pyrylium (PIN) E=S: thiopyrylium (PIN)	 E=O: chromenylium (PIN) E=S: thiochromenylium (PIN)	 E=O: isochromenylium (PIN) E=S: isothiochromenylium (PIN)
 E=O: flavylium (PIN) E=S: thioflavylium (PIN)	 E=O: xanthylium (PIN) E=S: thioxanthylium (PIN)	

P-73.4 Skeletal replacement (‘a’) nomenclature for cations

Two methods are used to name cationic centers by skeletal replacement (‘a’) nomenclature.

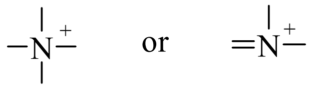
(1) name the compound using neutral skeletal replacememt (‘a’) prefixes and then describe the cationic centers by the appropriate suffix ‘ium’ and ‘ylium’.

(2) using cationic skeletal replacement (‘a’) prefixes.

Cationic skeletal replacement (‘a’) prefixes are formed, except for bismuth, by replacing the ‘a’ ending of the normal skeletal replacement (‘a’) prefixes’ by ‘onia’; and, except for carbon, by ‘ylia’, to indicate a cationic center having a boinding order one higher and one lower, respectively, than the bonding number of the corresponding neutral mononuclear hydride. The cationic skeletal replacement (‘a’) prefix corresponding to ‘bismuthonium’ is ‘bismuthonia’.

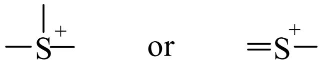
Cationic skeletal replacement (‘a’) prefixes are used in the same way neutral replacement prefixes

Examples:



$-\overset{|}{\underset{|}{\text{N}}}{}^{+}-$ or $=\overset{|}{\text{N}}{}^{+}-$

azonia (preselected name)



$-\overset{|}{\text{S}}{}^{+}-$ or $=\text{S}^{+}-$

thionia (preselected name)

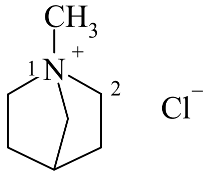
$-\text{I}^{+}-$ iodonia (preselected name)

$-\text{N}^{+}-$ azanylia (preselected name)

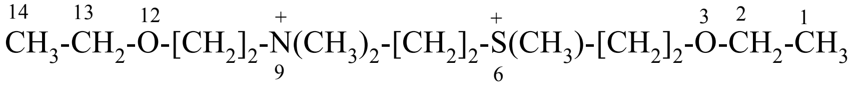
$-\text{B}^{+}-$ boranylia (preselected name)

Method (1) gives preferred IUPAC names. Furthermore, names that do not require designation of skeletal in nonstandard valence state by the λ-convention are preferred (see P-73.1 and P-73.2).

Examples:

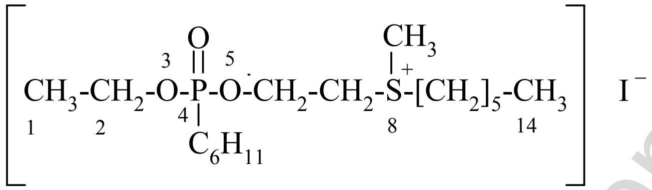


1-methyl-1-azabicyclo[2.2.1]heptan-1-ium chloride (PIN)
1-methyl-1-azoniabicyclo[2.2.1]heptane chloride



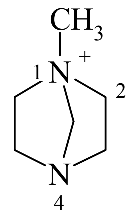
$$\overset{14}{CH_3}-\overset{13}{CH_2}-\overset{12}{O}-[CH_2]_2-\underset{9}{\overset{+}{N}}(CH_3)_2-[CH_2]_2-\underset{6}{\overset{+}{S}}(CH_3)-[CH_2]_2-\overset{3}{O}-\overset{2}{CH_2}-\overset{1}{CH_3}$$

6,9,9-trimethyl-3,12-dioxa-6-thia-9-azatetradecane-6,9-diium (PIN)
6,9,9-trimethyl-3,12-dioxa-6-thionia-9-azoniatetradecane

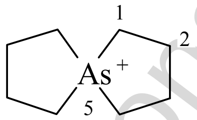


$$\left[\underset{1}{CH_3}-\underset{2}{CH_2}-\overset{3}{O}-\underset{\underset{C_6H_{11}}{|}}{\overset{\overset{O}{\|}}{\underset{4}{P}}}-\overset{5}{O}-CH_2-CH_2-\underset{8}{\overset{\overset{CH_3}{|}}{\overset{+}{S}}}-[CH_2]_5-\underset{14}{CH_3}\right]\ I^-$$

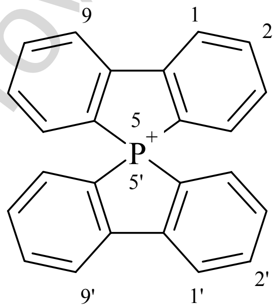
4-cyclohexyl-8-methyl-4-oxo-3,5-dioxa-8-thia-4λ^5-phosphatetradecan-8-ium iodide (PIN)
4-cyclohexyl-8-methyl-4-oxo-3,5-dioxa-8-thionia-4λ^5-phosphatetradecane iodide



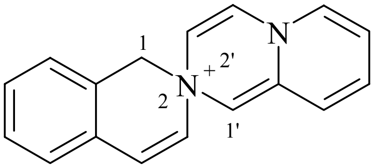
1-methyl-1,4-diazabicyclo[2.2.1]heptan-1-ium (PIN)



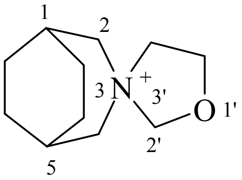
5λ^5-arsaspiro[4.4]nonan-5-ylium (PIN)
5-arsoniaspiro[4.4]nonane



5λ^5,5′-spirobi[benzo[*b*]phosphindole]-5-ylium (PIN)
9-phosphonia-9,9′-spirobi[fluorene]
(for construction of the name for the neutral, noncationic compound, see P-24.8.4)



1H-2λ^5-spiro[isoquinoline-2,2′-pyrido[1,2-*a*]pyrazin]-2-ylium (PIN)



2′H-3λ^5-spiro[3-azabicyclo[3.2.2]nonane-3,3′-[1,3]oxazol]-3-ylium (PIN)

P-73.5 Multiple cationic centers

Cationic compounds with multiple cationic centers are named by several methods in accordance with previous rules.

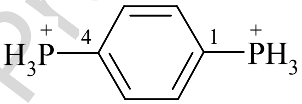
P-73.5.1 Assemblies of parent cations
P-73.5.2 ‘Ium’ and ‘ylium’ centers in the same parent hydride
P-73.5.3 Cationic characteristic groups on parent cations
P-73.5.4 Cationic centers in both parent compounds and substituent groups

P-73.5.1 Assemblies of parent cations

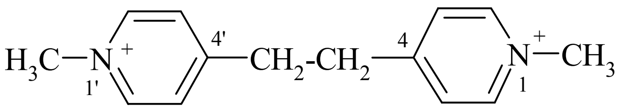
P-73.5.1.1 Assemblies derived from parent cations

Cationic compounds with cationic centers derived from the same parent hydride, but located in different parts of a structure, are named, if possible, according to the principles of multiplicative nomenclature (see P-15.3), using the multiplying prefixes ‘bis-’, ‘tris-’, etc. where necessary.

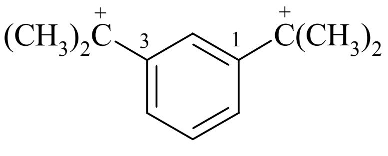
Examples:



1,4-phenylenebis(phosphanium) (PIN)
1,4-phenylenebis(phosphonium)



4,4′-ethane-1,2-diylbis(1-methylpyridin-1-ium) (PIN)
1,1′-dimethyl-4,4′-ethane-1,2-diyldipyridin-1-ium

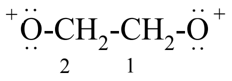


benzene-1,3-diyldi(propan-2-ylium) (PIN)
1,3-phenylenedi(propan-2-ylium)

P-73.5.1.2 Polycations with cationic centers on characteristic groups

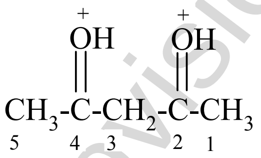
With the exception of di- and polyamides, di- and polyamines, di- and polyimines, and di- and polyimides, which are named by using direct substitutive nomenclature, polycations with cationic centers on characteristic groups are named by multiplicative nomenclature provided the requirements for the use of multiplicative nomenclature are met.

Examples:



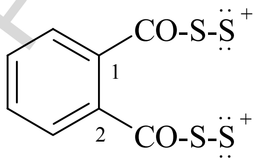
$$^{+}\overset{..}{\underset{..}{O}}\text{-}\underset{2}{CH_2}\text{-}\underset{1}{CH_2}\text{-}\overset{..}{\underset{..}{O}}{}^{+}$$

ethane-1,2-diylbis(oxidanylium) (PIN)

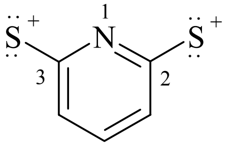


$$\underset{5}{CH_3}\text{-}\underset{4}{\overset{\overset{+}{O}H}{\overset{\|}{C}}}\text{-}\underset{3}{CH_2}\text{-}\underset{2}{\overset{\overset{+}{O}H}{\overset{\|}{C}}}\text{-}\underset{1}{CH_3}$$

pentane-2,4-diylidenebis(oxonium) (PIN)



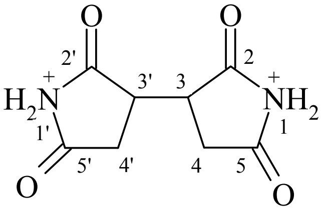
benzene-1,2-diyldicarbonylbis(disulfanylium) (PIN)
benzene-1,2-dicarbonylbis(disulfanylium)



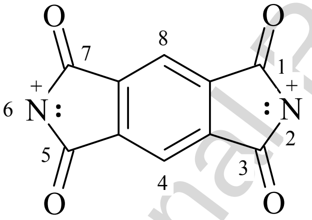
pyridine-2,6-diylbis(sulfanylium) (PIN)

P-73.5.1.3 Polycations derived from cyclic diimides and polyimides are named on the basis of the heterocyclic structure of the imides.

Examples:



2,2′,5,5′-tetraoxo[3,3′-bipyrrolidine]-1,1′-diium (PIN)



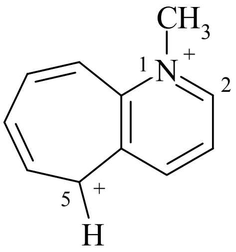
1,3,5,7-tetraoxo-5,7-dihydropyrrolo[3,4-*e*]isoindole-2,6(1*H*,3*H*)-bis(ylium) (PIN)
[not 1,3,5,7-tetraoxo-5,7-dihydrobenzo[1,2-*c*:4,5-*c'*]dipyrrole-2,6(1*H*,3*H*)-bis(ylium)]

P-73.5.2 'Ium' and 'ylium' centers in the same parent hydride

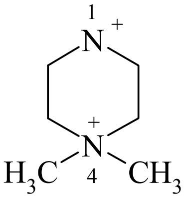
Cyclic compounds with two or more cationic centers in the same parent hydride structure, at least one being denoted by 'ium' and another by 'ylium' suffixes, are named by placing the 'ium' and 'ylium' suffixes, in that order, after the name of the parent hydride, preceded by the appropriate multiplying numerical prefixes and locants, where required.

When there is a choice, low locants are assigned first to the cationic centers irrespective of their kind, then to 'ylium' centers.

Examples:



1-methyl-5*H*-cyclohepta[*b*]pyridin-1-ium-5-ylium (PIN)
(not 1-methyl-5*H*-1-azoniabenzo[7]annulen-5-ylium; a skeletal replacement (‘a’) name is not recommended when fusion names are available)

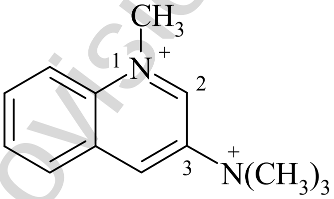


4,4-dimethylpiperazin-4-ium-1-ylium (PIN)

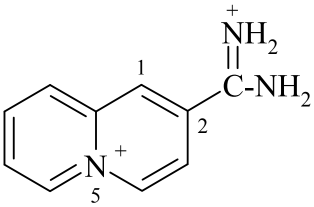
P-73.5.3 Cationic characteristic groups on parent cations

Cationic compounds with cationic centers both in the parent hydride part of the structure and on a characteristic group expressed as a cationic suffix are named by citing both cationic centers, in the order cumulative suffix and cationic suffix.

Examples:



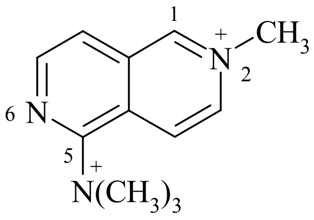
N,*N*,*N*,1-tetramethylquinolin-1-ium-3-aminium (PIN)



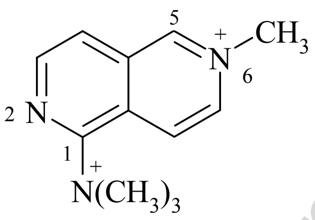
5λ^5-quinolizin-5-ylium-2-carboximidamidium (PIN)

Where there is a choice, low locants for skeletal cationic centers are determined before considering locants for cationic suffixes.

Example:



not



N,*N*,*N*,2-tetramethyl-2,6-naphthyridin-5-aminium-2-ium (PIN)
(not *N*,*N*,*N*,6-tetramethyl-2,6-naphthyridin-1-aminium-6-ium)

P-73.6 Cationic prefix names

A polycation in which all cationic centers cannot be included in the cationic parent hydride or cationic parent compound is named by selecting one part of the structure as the parent cation and citing the other part(s) as cationic substituent prefixes. The selection of the parent cation is achieved by using the criteria for selecting the cationic parent structure. In zwitterions and in radical cations, the cationic part is always substituted into the anionic portion or into the part including a radical, in accordance with the seniority of anions and radicals over cations.

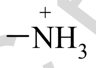
Two methods are used to name substituent structural units containing cationic centers.

(1) all prefix names are formed by adding to the cation name the suffixes ‘yl’, ‘ylidene’, etc. preceded by the multiplying prefixes ‘di’, ‘tri’, etc., to indicate multiplicity, where required. Where required, appropriate locants are used. Where there is a choice for numbering, free valences receive lowest possible locants, the suffix ‘yl’ being senior to ‘ylidene’

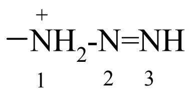
(2) prefixes for expressing a monovalent substituent derived from a mononuclear parent cation denoted by ‘ium’ or by ‘onium’ described in Table 7.1 are formed by changing the ‘onium’ ending of the parent cation to ‘io’ or ‘onio’.

Method (1) leads to preferred IUPAC names.

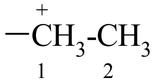
Examples:


$-\overset{+}{N}H_3$

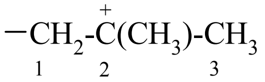
azaniumyl (preselected name)
ammonio


$\underset{1}{-\overset{+}{N}H_2}\text{-}\underset{2}{N}=\underset{3}{N}H$

triaz-2-en-1-ium-1- yl (preselected name)
triaz-2-en-1-io


$-\underset{1}{\overset{+}{C}H_3}\text{-}\underset{2}{CH_3}$

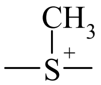
ethan-1-ium-1-yl (PIN)


$-\underset{1}{CH_2}\text{-}\underset{2}{\overset{+}{C}}(CH_3)\text{-}\underset{3}{CH_3}$

2-methylpropan-2-ylium-1-yl (PIN)

$-\overset{+}{S}eH_2$

selaniumyl (preselected name)
selenonio



$-\overset{+}{S}(CH_3)-$

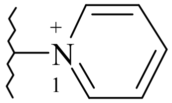
methylsulfaniumdiyl (PIN)
methylsulfoniundiyl

$-\overset{+}{N}{\equiv}N$

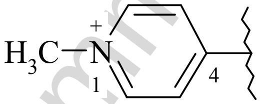
diazyn-1-ium-1-yl (preselected name)

$=\overset{+}{N}(CH_3)_2$

dimethylazaniumylidene (PIN)
(not dimethylammoniumylidene),
(not dimethylimmonio)



pyridin-1-ium-1-yl (PIN)
pyridinio



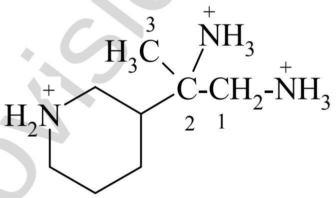
1-methylpyridin-1-ium-4-yl (PIN)

P-73.7 Seniority order of cations and choice of a parent structure

A parent cationic structure is chosen by applying the following criteria in order until a definitive choice is achieved.

(a) maximum number of cationic centers of any kind, including cationic suffix groups, including those derived from characteristic groups:

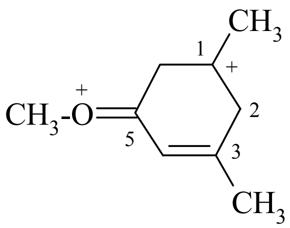
Example:



2-(piperidin-1-ium-3-yl)propane-1,2-bis(aminium) (PIN)

(b) maximum number of 'ylium' cationic centers:

Example:



1,3-dimethyl-5-(methyloxxidaniumylidene)cyclohex-3-en-1-ylium (PIN)

(c) maximum number of senior cationic centers, according to the nature of the cationic atom, in the same order as for the corresponding replacement prefixes: F > Cl > Br > I < O > S > Se > Te > N > P > As > Sb > Bi > Si > Ge > Sn > Pb > B < Al > Ga > In > Tl.

Examples:

$$(CH_3)_3\overset{+}{P}-CH_2-[CH_2]_4-CH_2-\overset{+}{S}(CH_3)_2$$

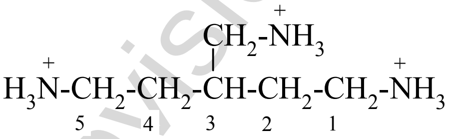
dimethyl[6-(trimethylphosphaniumyl)hexyl]sulfanium (PIN)

$$(CH_3)_3\overset{+}{N}-CH_2-[CH_2]_4-CH_2-\overset{+}{S}(CH_3)_2$$

dimethyl[(6-trimethylazaniumyl)hexyl]sulfanium (PIN)

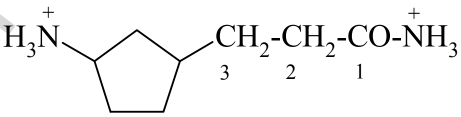
(d) further choice, if necessary, is made by applying the the general criteria, in accordance with the principles, rules and conventions described in Chapters 1 through 6.

Examples:



$$H_3\overset{+}{N}-\underset{5}{C}H_2-\underset{4}{C}H_2-\underset{3}{\overset{\overset{\displaystyle CH_2-\overset{+}{N}H_3}{|}}{C}}H-\underset{2}{C}H_2-\underset{1}{C}H_2-\overset{+}{N}H_3$$

3-(azaniumylmethyl)pentane-1,5-bis(aminium) (PIN)



3-(3-azaniumylcyclopentyl)propanamidium (PIN)

P-74 Zwitterionic compounds or zwitterions

Zwitterionic compounds, or zwitterions, are electrically neutral compounds having an equal number of formal unit charges of opposite sign. The structures in this section are all represented as zwitterionic even though some can be drawn as neutral or ionic structures. This section also includes inner salts and dipolar compounds. Section P-74.1 will cover zwitterionic compounds with the ionic centers on the same parent compound and with ionic centers on different parent structures. Section P-74.2 deals with 1,2- and 1,3-dipolar compounds.

According to the seniority of classes, an anionic center has priority over a cationic center in zwitterions. Thus, in zwitterionic compounds anionic centers are preferred for lower locants and are become the parent structure, into which the cationic part is substituted. For the latter CAS uses the reverse order and name.

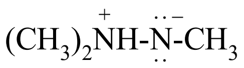
P-74.1 Zwitterionic compounds having equal numbers of anionic and cationic centers on the same parent compound, including ionic centers on characteristic groups expressible as suffixes.

P-74.1.1 Ionic centers in the same parent structure.

Zwitterionic compounds with the ionic centers in the same parent structure may be named by combining appropriate cumulative suffixes at the end of the name of a parent hydride in the order ‘ium’, ‘ylium’, ‘ide’, ‘uide’. This method is preferred to the one using ionic replacement prefixes, as indicated in Sections P-72.4 and P-73.4. In either case anionic suffixes are cited after cationic suffixes in the name, and are given seniority for low locants. The final letter ‘e’ of the name of a parent hydride, or of an ‘ide’ or ‘uide’ suffix, is elided before the letter ‘i’ or ‘y’, or before a cumulative suffix beginning with a vowel. Multiplying prefixes ‘di’, tri’, etc., appropriate for each type of suffix, are added to specify the number of each kind of ionic center. Where there is a choice, lowest locants are given to the ionic centers in the following order, listed in decreasing order of seniority: ‘uide’ (‘uida’), ‘ide’ (‘ida’), ‘ylium’ (‘ylia’), and ‘ium’ (‘onia’).

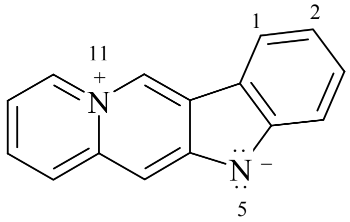
> For nomenclature purposes, zwitterionic compounds having the ionic centers in the same structure are considered as neutral compounds. This concept is important in naming zwitterionic compounds having also a characteristic group denoted by a suffix. These compounds may be named by citing the cumulative suffixes immediately after the name of the parent hydride, in the order given above, and finally the name of the functional suffix denoting the characteristic group, as shown by the last example below.

Examples:

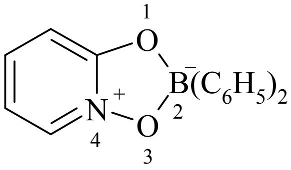


$(CH_3)_2\overset{+}{N}H\text{-}\underset{..}{\overset{..-}{N}}\text{-}CH_3$

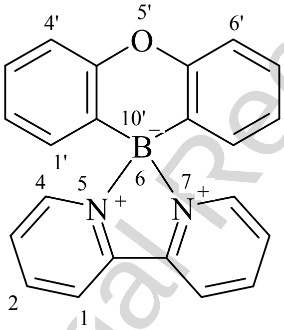
1,2,2-trimethylhydrazin-2-ium-1-ide (PIN)



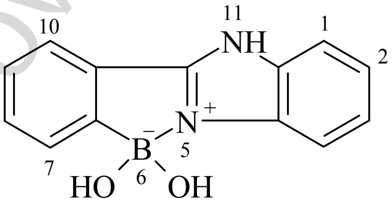
11λ^5-5*H*-indolo[2,3-*b*]quinolizin-11-ylium-5-ide (PIN)



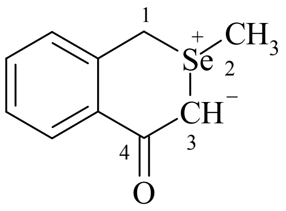
2,2-diphenyl-4λ^5-[1,3,4,2]dioxazaborolo[4,5-*a*]pyridin-4-ylium-2-uide (PIN)



5λ^5,7λ^5-spiro[1,3,2-diazaborolo[3,4-a:5,1-a]dipyridine-6,10′-phenoxaborinine]-5,7-bis(ylium)-6-uide (PIN)
(for the name of a structure drawn as an intramolecular adduct, see P-68.1.6.1.1)



6,6-dihydroxy-6,11-dihydro-5λ^5-benzimidazolo[3,2-b][2,1]benzazaborol-5-ylium-6-uide

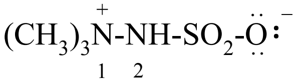


2-methylisoselenochroman-2-ium-3-id-4-one

P-74.1.2 Zwitterionic compounds with at least one ionic center on a characteristic group

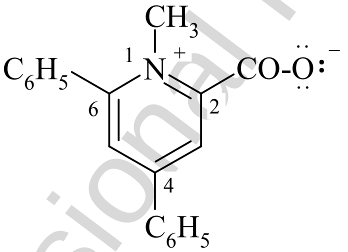
Zwitterionic compounds with at least one ionic center on a characteristic group may be named by adding the appropriate ionic suffix to the name of the ionic parent hydride. In names, cumulative suffixes are cited before functional suffixes. For assignment of lower locants, ionic centers on skeletal atoms of the parent hydride are preferred to the position of attachment of characteristic groups denoted by ionic suffixes.

Examples:

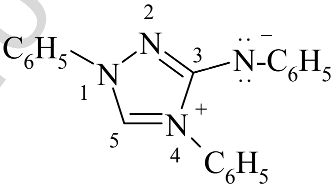


$$(CH_3)_3\underset{1}{\overset{+}{N}}\text{-}\underset{2}{N}H\text{-}SO_2\text{-}\ddot{\underset{..}{O}}\!:^{-}$$

1,1,1-trimethylhydrazin-1-ium-2-sulfonate (PIN)



1-methyl-4,6-diphenylpyridin-1-ium-2-carboxylate (PIN)



N-(1,4-diphenyl-1H-1,2,4-triazole-4-ium-3-yl)anilinide (PIN, see P-72.2.2.2.3)
N,1,4-triphenyl-1*H*-1,2,4-triazol-4-ium-3-aminide

P-74.1.3 Anionic and cationic centers on different parent structures

Zwitterionic compounds with anionic and cationic centers on different parent structures may be named by prefixing the name of the cationic center or the parts of the structure containing the cationic centers to the name of the anionic parent compound.

Examples:

$$(C_6H_5)_2\overset{+}{P}(CH_3)\text{-}CH{=}CH\text{-}\overset{-}{B}(CH_3)_3$$

[(methyldiphenylphosphaniumyl)ethenyl]trimethylboranuide (PIN)

$$(CH_3)_3\overset{+}{N}\text{-}CH_2\text{-}CO\text{-}\overset{..}{\underset{..}{O}}\!:^{-}$$

(trimethylazaniumyl)acetate (PIN)

$$CH_3\text{-}\underset{1}{\overset{-}{B}}H_2\text{-}\underset{2}{\overset{+}{N}}H_2\text{-}\underset{3}{\overset{-}{B}}H_2\text{-}\overset{+}{N}H_2\text{-}CH_3$$

1-methyl-3-(methylazaniumyl)diborazan-2-ium-1,3-diuide (PIN)
(not 2,4-diaza-3,5-diborahexane-2,4-diium-3,5-diide)
(not 3,5-diazonia-2,4-diboranuidahexane)
(Since diborazane is a nonfunctional parent hydride, there are insufficient heterounits to qualify for a skeletal replacement (‘a’) name.

P-74.2 Dipolar compounds

Dipolar compounds are electrically neutral molecules carrying a negative and a positive charge in one of their major canonical descriptions. In most dipolar compounds the charges are delocalized; however the term is also applied to species where this is not the case. 1,2-Dipolar compounds have the opposite charges on adjacent atoms. The term 1,3-dipolar compounds is used for those in which a significant canonical resonance form can be represented by a separation of charge over three atoms.

P-74.2.1 1,2-Dipolar compounds
P-74.2.2 1,3-Dipolar compounds
P-74.2.3 Dipolar substituent groups

P-74.2.1 1,2-Dipolar compounds

P-74.2.1.1 ‘Ylides’

Compounds in which an anionic site Y^- (originally only on carbon, but now including other atoms) is attached directly to a heteroatom X^+ (usually nitrogen, phosphorus, sulfur, selenium) carrying a formal positive charge are 1,2-dipolar species of the type $R_mX^+\text{-}Y^-\text{-}R_n$. If X is a saturated atom of an element from the first row of the periodic system, the ‘ylide’ is commonly represented by a charge separated form; if X is a second, third, etc. row element uncharged canonical forms are available, $R_mX{=}YR_n$.

These ‘ylides’ are subdivided into subclasses: nitrogen ylides, phosphorus ylides, oxygen ylides, sulfur ylides, etc. They may be named in different ways depending on the nature of the atoms X and Y.

(1) as zwitterionic compounds, without breaking a homogeneous chain of heteroatoms;

(2) by applying the λ convention, for X = P, As, S, and Se;

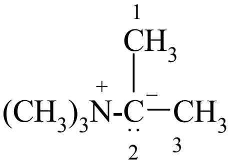
(3) by functional class using the class names oxide, sulfide, imides.

Method (1) is applicable to all ‘ylides’ and leads to preferred IUPAC names.

P-74.2.1.1.1 Nitrogen ylides.

Nitrogen ylides have the general structure $R_3N^+\text{-}C^-R_2$.

Example:



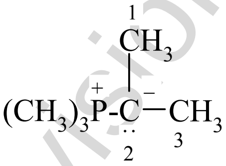
$$(\mathrm{CH_3})_3\overset{+}{\mathrm{N}}\text{-}\overset{\overset{1}{\mathrm{CH_3}}}{\underset{\underset{2}{\cdot\cdot}}{\overset{-}{\mathrm{C}}}}\text{—}\underset{3}{\mathrm{CH_3}}$$

(trimethylazaniumyl)propan-2-ide (PIN)

P-74.2.1.1.2 Phosphorus ylides

Phosphorus ylides have the general structure $R_3P^+\text{-}C^-R_2 \quad \leftrightarrow \quad R_3P{=}CR_2$.

Example:



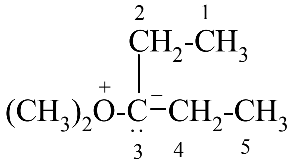
$$(\mathrm{CH_3})_3\overset{+}{\mathrm{P}}\text{-}\overset{\overset{1}{\mathrm{CH_3}}}{\underset{\underset{2}{\cdot\cdot}}{\overset{-}{\mathrm{C}}}}\text{—}\underset{3}{\mathrm{CH_3}}$$

(trimethylphosphaniumyl)propan-2-ide (PIN)
trimethyl(propan-2-ylidene)-λ^5-phosphane
trimethyl(isopropylidene)phosphorane

P-74.2.1.1.3 Oxygen ylides

Oxygen ylides have the general structure $R_2O^+\text{-}C^-R_2$.

Example:



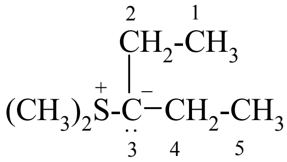
$$\begin{array}{l} \qquad\qquad\;\, \overset{2}{C}H_2-\overset{1}{C}H_3 \\ \qquad\qquad\;\, | \\ (CH_3)_2\overset{+}{O}-\underset{3}{\underset{\cdot\cdot}{\overset{-}{C}}}-\underset{4}{C}H_2-\underset{5}{C}H_3 \end{array}$$

(dimethyloxidaniumyl)pentan-3-ide (PIN)

P-74.2.1.1.4 Sulfur ylides

Sulfur and selenium ylides have the general structure $R_2S^+\text{-}C^-R_2 \leftrightarrow R_2S{=}CR_2$.

Example:



$$\begin{array}{l} \qquad\qquad\;\, \overset{2}{C}H_2-\overset{1}{C}H_3 \\ \qquad\qquad\;\, | \\ (CH_3)_2\overset{+}{S}-\underset{3}{\underset{\cdot\cdot}{\overset{-}{C}}}-\underset{4}{C}H_2-\underset{5}{C}H_3 \end{array}$$

(dimethylsulfaniumyl)pentan-3-ide (PIN)
dimethyl(propan-2-ylidene)-λ⁴-sulfane

This method is also applicable to the analogous selenium compounds.

P-74.2.1.2 Amine oxides, imine oxides, and their chalcogen analogues

Amine oxides and imine oxides have the generic formulae $R_3N^+\text{–}O^-$ and $R_2{=}N^+\text{-}O^-$, respectively; chalcogen analogues are amine sulfides, imine selenides, etc. (where O is replaced by S, Se, or Te). They may be named:

(1) as zwitterionic compounds;

(2) by functional class nomenclature using the functional class name ‘oxide’.

Method (2) leads to preferred IUPAC names provided that the resulting name is unambiguous; otherwise, method (1) gives IUPAC preferred names (see also P-62.5).

Example:

$$(CH_3)_3\overset{+}{N}\text{-}\underset{\cdot\cdot}{\ddot{O}}{:}^-$$

N,*N*-dimethylmethanamine oxide (PIN)
trimethylamine oxide
(trimethylazaniumyl)oxidanide

P-74.2.1.3 Amine imides

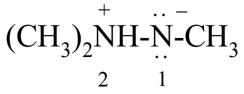
Amine imides (not amine imines) have the generic formula R_3N^+-N^--R. They may be named by two methods.

(1) as a zwitterion based on hydrazine (in order to maintain the nitrogeneous chain);

(2) by functional class nomenclature using the class name imide placed after the name of the amine.

Method (1) leads to preferred IUPAC names.

Example:



$(CH_3)_2\underset{2}{\overset{+}{N}}H\text{-}\underset{1}{\overset{..\,-}{\underset{..}{N}}}\text{-}CH_3$

1,2,2-trimethylhydrazin-2-ium-1-ide (PIN)
1,2,2-trimethyldiazan-2-ium-1-ide
N,*N*-dimethylmethanamine *N*-methylimide
N,*N*,*N*′-trimethylmethanamine imide
trimethylamine *N*-methylimide

P-74.2.1.4 Phosphine oxides and chalcogen analogues

Phosphine oxides have the generic formula R_3P^+-O^- ↔ R_3P=O. Chalcogen analogs are phosphine sulfides, phosphine selenides, and phosphine telluride (where O is replaced by S, Se, and Te, respectively. They may be named by three methods.

(1) as zwitterionic compounds;

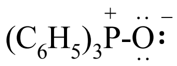
(2) by functional class nomenclature using the class names oxide, sulfide, selenide, and telluride;

(3) substitutively, as heterones, by using the suffix ‘-one’ and λ^5-phosphane as the parent hydride.

Method (2)_leads to preferred IUPAC names provided that the resulting name is unambiguous; otherwise, method (1) gives IUPAC preferred names.

This rule is applied to arsine and stibine oxides, sulfides, etc.

Example:



$(C_6H_5)_3\overset{+}{P}\text{-}\overset{..\,-}{\underset{..}{O}}\colon$

triphenylphosphane oxide (PIN)
triphenylphosphine oxide
(triphenylphosphaniumyl)oxidanide
triphenyl-λ^5-phosphanone

P-74.2.1.5 Phosphine imides

Phosphine imides have the generic structure: $R_3P^+\text{-}N^-\text{-}R \leftrightarrow R_3P{=}N\text{-}R$. They may be named in three ways.

(1) as zwitterionic compounds;

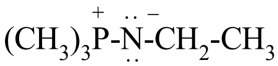
(2) by functional class nomenclature using the class name imide;

(3) as imines of λ^5-phosphane.

Method (1) leads to preferred IUPAC names.

These methods are extended to arsine and stibine imides.

Example:



$$(CH_3)_3\overset{+}{P}\text{-}\overset{\cdot\cdot\;-}{\underset{\cdot\cdot}{N}}\text{-}CH_2\text{-}CH_3$$

ethyl(triphenylphosphaniumyl)azanide (PIN)
triphenylphosphane N-ethylimide
N-ethyl-P,P,P-triphenylphosphane imide
N-ethyl-P,P,P-triphenyl-λ^5-phosphanimine

P-74.2.2 1,3-Dipolar compounds

The term 1,3-dipolar compounds is used for those compounds in which a significant canonical resonance can be represented by a separation of charge over three atoms. The subclasses of 1,3-dipolar compounds include:

P-74.2.2.1 the allyl type
P-74.2.2.2 the propargyl type
P-74.2.2.3 the carbene type

P-74.2.2.1 Allyl type compounds have the delocalized general structure where Y and/or Z = C, N, or O; and X = N or O.

$$Z{=}X^+\text{-}Y^- \leftrightarrow Z^-\text{-}X^+{=}Y \leftrightarrow Z^+\text{-}X\text{-}Y^- \leftrightarrow Z^-\text{-}X\text{-}Y^+,$$

Preferred IUPAC names are based on the first canonical form, although each canonical form can be named, if desired. Names are formed in three different ways.

(1) by substituting a cationic substituent into a parent anion;

(2) by functional class nomenclature using the class names imide, oxide, etc.;

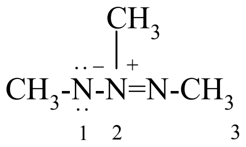
(3) by using the λ convention.

Preferred IUPAC names are those expressing the zwitterionic nature of the compounds. Three exceptions are recognized: (1) heteroatom oxides, such as ‘thial’ oxides; (2) azoxy compounds, which are preferably named as diazene oxides; (3) the name nitro, which is retained for $-NO_2$.

P-74.2.2.1.1 Azo imides, analogous to azoxy compounds, have the delocalized general structure:

$$RN\text{=}N^{+}(R)\text{-}N^{-}\text{-}R \ \leftrightarrow \ RN^{-}\text{-}N^{+}(R)\text{=}NR$$

Example:

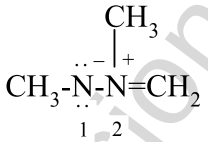

$CH_3\text{-}\ddot{\underset{..}{N}}^{-}\text{-}N^{+}(CH_3)\text{=}N\text{-}CH_3$

1,2,3-trimethyltriaz-2-en-2-ium-1-ide (PIN; the preferred name
is based on the unbroken nitrogen chain)
dimethyldiazene methylimide
trimethyldiazene imide
[methyl(methylimino)ammoniumyl]methanaminide

P-74.2.2.1.2 Azomethine imides have the delocalized general structure:

$$N^{-}\text{-}N^{+}(R)\text{=}CR_2 \ \leftrightarrow \ RN\text{=}N^{+}(R)\text{-}C^{-}R_2$$

Example:

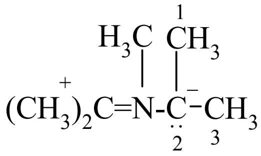

$CH_3\text{-}\ddot{\underset{..}{N}}^{-}\text{-}N^{+}(CH_3)\text{=}CH_2$

1,2-dimethyl-2-methylidenehydrazin-2-ium-1-ide (PIN)
N-methylmethanimine methylimide

P-74.2.2.1.3 Azomethine ylides, have the delocalized general structure:

$$R_2C^{-}\text{-}N^{+}(R)\text{=}CR_2 \ \leftrightarrow \ R_2CN^{+}(R)\text{-}C^{-}R_2$$

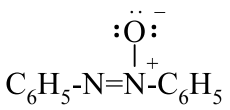
Example:


$\overset{+}{(CH_3)_2}C\text{=}N(CH_3)\text{-}\underset{..}{C}^{-}(CH_3)\text{-}CH_3$

2-[methyl(propan-2-ylidene)azaniumyl]propan-2-ide (PIN)

P-74.2.2.1.4 Azoxy compounds, have the general structure $RN=N^{+}(O^{-})-R$ (see also P-68.3.1.3.2.1)

Example:


$C_6H_5-N=N^{+}(O^{-})-C_6H_5$

diphenyldiazene oxide (PIN)
(1,2-diphenylhydraziniumyl)oxidanide

P-74.2.2.1.5 Carbonyl imides, have the delocalized general structure:

$$R_2C=O^{+}-N^{-}-R \quad \leftrightarrow \quad R_2C^{+}-O-N^{-}-R$$

Example:

$$(CH_3)_2C=\overset{+}{O}-\ddot{N}^{-}-CH_3$$

N-[(propan-2-ylidene)oxidaniumyl]methanaminide (PIN)
propan-2-one methylimide
N-methylpropan-2-one imide

P-74.2.2.1.6 Carbonyl oxides, have the delocalized general structure:

$$R_2C^{-}-O^{+}=O \quad \leftrightarrow \quad R_2C^{-}-O-O^{+}$$

Example:

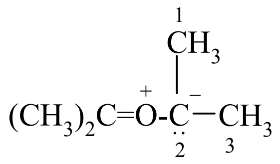
$$(CH_3)_2C=\underset{2}{\overset{+}{O}}-\underset{1}{\ddot{O}}{:}^{-}$$

2-(propan-2-ylidene)dioxidan-2-ium-1-ide (PIN)
propan-2-one oxide

P-74.2.2.1.7 Carbonyl ylides, have the delocalized general structure:

$$R_2C=O^{+}-C^{-}(R)_2 \quad \leftrightarrow \quad R_2C^{+}-OC^{-}(R)_2$$

Example:



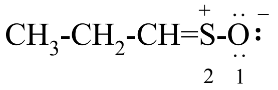
$$(CH_3)_2C{=}\overset{+}{O}\text{-}\underset{2}{\underset{\cdot\cdot}{\overset{-}{C}}}(\overset{1}{CH_3})\text{—}\underset{3}{CH_3}$$

2-[(propan-2-ylidene)oxidaniumyl]propan-2-ide (PIN)

P-74.2.2.1.8 Thioaldehyde S-oxides, thioketone *S*-oxides, and heterone *S*-oxides have the generic structure:

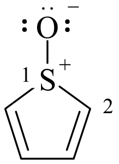
$$RR'C{=}S^+\text{-}O^- \quad \leftrightarrow \quad RR'C{=}S{=}O \quad \text{(where } R' = \text{or} \neq H\text{)}$$

Examples:

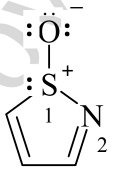


$$CH_3\text{-}CH_2\text{-}CH{=}\underset{2}{\overset{+}{S}}\text{-}\underset{1}{\ddot{\underset{\cdot\cdot}{O}}}{:}^{-}$$

propanethial oxide (PIN)
(propylidenesulfaniumyl)oxidanide
propylidene-λ^4-sulfanone



thiophene oxide (PIN)
(thiophen-1-ium-1-yl)oxidanide
λ^4-thiophen-1-one

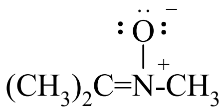


1,2-thiazine 1-oxide (PIN)
1,2-thiazine *S*-oxide

P-74.2.2.1.9 Nitrones have the delocalized general structure:

$$R_2C{=}N^+(O^-)R' \quad \leftrightarrow \quad R_2C^+\text{-}N(O^-)R' \quad \text{where } R' \neq H\text{; compounds where } R' = H \text{ are not included in this class}$$

Example:

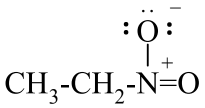


$(CH_3)_2C=\overset{\overset{\ddot{O}^{-}}{|}}{\overset{+}{N}}-CH_3$

N-methylpropan-2-imine oxide (PIN)
[propan-2-ylidene(methyl)azaniumyl]oxidanide

P-74.2.2.1.10 Nitro compounds may be named on the basis of the traditional structure R-NO_2, with the permanent prefix 'nitro' (see also P-61.5.1).

Example:



$CH_3-CH_2-\overset{\overset{\ddot{O}^{-}}{|}}{\overset{+}{N}}=O$

nitroethane (PIN)

P-74.2.2.2 The propargyl type includes compounds having the canonical resonance forms:

$X{\equiv}N^{+}\text{-}Z^{-} \leftrightarrow {}^{-}X{=}N^{+}{=}Z \leftrightarrow {}^{-}X{=}N\text{-}Z^{+} \leftrightarrow X\text{-}N{=}Z$, where X = C or O and Z = C, N or O

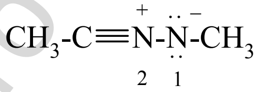
These compounds may be named in different ways:

(1) as zwitterionic compounds, without breaking the longest chain composed of heteroatoms;

(2) by functional class nomenclature using the class names imide, oxide, sulfide, etc.

P-74.2.2.2.1 Nitrile imides. Zwitterionic names generate preferred IUPAC names.

Example:



$CH_3-C\equiv\underset{2}{\overset{+}{N}}-\underset{1}{\ddot{N}^{-}}-CH_3$

2-ethylidyne-1-methylhydrazin-2-ylium-1-ide (PIN)
acetonitrile methylimide
N-methylacetonitrile imide

P-74.2.2.2.2 Nitrile oxides and sulfides. Functional class names are preferred IUPAC names (see also P-66.5.3.1).

Examples:

$$CH_3\text{-}C{\equiv}\overset{+}{N}{-}\overset{..\,-}{\underset{..}{O}}{:}$$

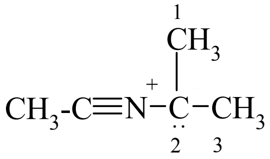
acetonitrile oxide (PIN)_
(ethylidyneazaniumyl)oxidanide

$$CH_3\text{-}C{\equiv}\overset{+}{N}{-}\overset{..\,-}{\underset{..}{S}}{:}$$

acetonitrile sulfide (PIN)
(ethylidyneazaniumyl)sulfanide

P-74.2.2.2.3 Nitrile ylides. Zwitterionic names are preferred IUPAC names.

Example:



$$CH_3\text{-}C{\equiv}\overset{+}{N}{-}\underset{2}{\underset{..}{\overset{\overset{1}{CH_3}}{C}}}{-}\underset{3}{CH_3}$$

(ethylidyneazaniumyl)propan-2-ide

P-74.2.2.2.4 Azides

Azides may be named by two methods.

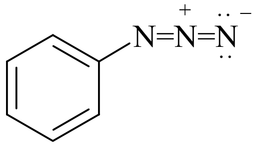
(1) substitutively by using the prefix azido (P-61.6, azido = compulsory prefix)

(2) by functional class nomenclature using the class name azide.

(3) as derivatives of the zwitterionic parent hydride name: triazadien-2-ium-1-ide.

Method (1) yields preferred IUPAC names (see also P-61.6)

Example:



azidobenzene (PIN)
phenyl azide
phenyltriazadien-2-ium-1-ide.

P-74.2.2.2.5 Diazo compounds

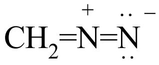
Diazo compounds may be named in two ways:

(1) substitutively by using the prefix diazo.

(2) As derivatives of the zwitterionic parent hydride name diazen-2-ium-1-ide

Method (1) leads to preferred IUPAC names (see also P-61.4).

Example:



$CH_2=\overset{+}{N}=\underset{..}{\overset{..}{N}}{}^{-}$

diazomethane (PIN)
methylidene diazen-2-ium-1-ide

P-74.2.2.3 The carbene type includes compounds having the canonical resonance forms:

:X-C=Z ↔ $^{+}$X=C-Z^{-}, where X = C or N and Z = C, N or O

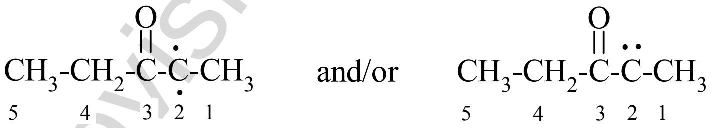
P-74.2.2.3.1 Acyl carbenes have the generic structure acyl-$C^{2\bullet}$-R. In organic chemistry, an unspecified acyl carbene is generally a carbonyl carbene. They may be named in two ways:

(1) by using the longest carbon chain, according to the principles of substitutive nomenclature for radicals (see P-29.3.2), priority being given to the radical to be cited as the suffix; or

(2) substitutively on the basis of the corresponding carbene.

Method (1) generates preferred IUPAC names.

Example:



$\underset{5}{CH_3}\text{-}\underset{4}{CH_2}\text{-}\underset{3}{\overset{\overset{O}{||}}{C}}\text{-}\underset{2}{\underset{\bullet}{\overset{\bullet}{C}}}\text{-}\underset{1}{CH_3}$ and/or $\underset{5}{CH_3}\text{-}\underset{4}{CH_2}\text{-}\underset{3}{\overset{\overset{O}{||}}{C}}\text{-}\underset{2}{\overset{\bullet\bullet}{C}}\text{-}\underset{1}{CH_3}$

3-oxopentan-2-ylidene (PIN)
1-propanoylethylidene

P-74.2.2.3.2 Imidoyl carbenes

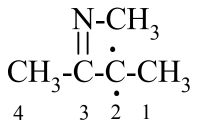
Compounds having the structure RC(=NH)$C^{2\bullet}$-R are imidoyl carbenes. Imidoyl is a shortened but imprecise term for carboximidoyl, RC(=NH)−. These carbenes may be named:

(1) by using the longest carbon chain, according to the principles of substitutive nomenclature for radicals, low locants being assigned to the radical to be cited as suffix;

(2) substitutively on the basis of carbene used as parent structure.

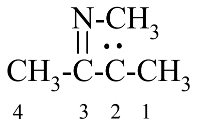
Method (1) leads to preferred IUPAC names.

Example:



$\underset{4}{CH_3}\text{-}\underset{3}{\overset{\overset{N\text{-}CH_3}{||}}{C}}\text{-}\underset{2}{\overset{\bullet}{\underset{\bullet}{C}}}\text{-}\underset{1}{CH_3}$

and/or



$\underset{4}{CH_3}\text{-}\underset{3}{\overset{\overset{N\text{-}CH_3}{||}}{C}}\text{-}\underset{2}{\overset{\bullet\bullet}{C}}\text{-}\underset{1}{CH_3}$

3-(methylimino)butan-2-ylidene (PIN)
1-(dimethylcarbonimidoyl)ethylidene

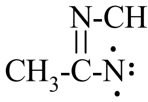
P-74.2.2.3.3 Imidoyl nitrenes

Imidoyl nitrenes have the general structure:

$$RC(=N\text{-}R')N^{2\bullet} \leftrightarrow RC(N^{-}\text{-}R')=N^{+}$$

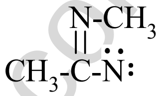
They may be named substitutively using the parent names azanylidene, nitrene, or aminylene.

Example:



$CH_3\text{-}\overset{\overset{N\text{-}CH_3}{||}}{C}\text{-}\overset{\bullet}{\underset{\bullet}{N}}\colon$

and/or



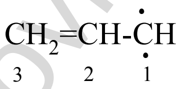
$CH_3\text{-}\overset{\overset{N\text{-}CH_3}{||}}{C}\text{-}\overset{\bullet\bullet}{N}\colon$

(*N*-methylacetimidoyl)azanylidene (PIN)
(*N*-methylacetimidoyl)nitrene
(*N*-methylacetimidoyl)aminylene

P-74.2.2.3.4 Vinyl carbenes

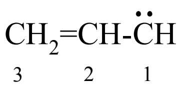
Vinyl carbenes have the structure $RR'=CR''\text{-}C^{2\bullet}\text{-}R'''$. They may be named using the longest carbon chain according to the principles of substitutive nomenclature for radicals, low locants being assigned to the suffix ylidene.

Example:



$\underset{3}{CH_2}=\underset{2}{CH}\text{-}\underset{1}{\overset{\bullet}{\underset{\bullet}{C}}H}$

and/or



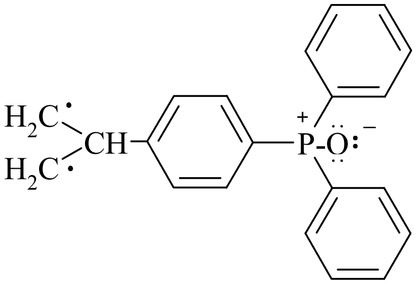
$\underset{3}{CH_2}=\underset{2}{CH}\text{-}\underset{1}{\overset{\bullet\bullet}{C}H}$

prop-2-en-1-ylidene (PIN)

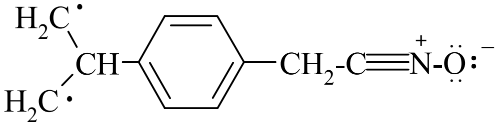
P-74.2.3 Dipolar substituent groups

Names of dipolar substituent groups are formed by using prefixes for naming ions in the substituent group and using the suffixes 'yl', 'ylidene' and 'ylidyne' to designate the free valences.

Examples:



2-[4-(oxidophosphaniumyl)phenyl]propane-1,3-diyl (PIN)



2-[4-[2-(oxidoazaniumyl)ethyl]benzyl}propane-1,3-diyl (PIN)

P-75 Radical Ions

For the purpose of nomenclature of organic chemistry, a radical ion is a molecular entity having at least one radical center and one ionic center, which may be on the same or on different atoms. They are formally classified as:

P-75.1 Radical ions formed by the addition or subtraction of electrons
P-75.2 Radical ions derived from parent hydrides
P-75.3 Radical ions on characteristic groups
P-75.4 Ionic and radical centers in different parent structures

P-75.1 Radical ions formed by the addition or removal of electrons

Radical ions formed by the addition or removal of electrons may be named in two ways.

(1) by using the suffixes ‘elide’ and ‘elium’ in substitutive nomenclature

Radical ions derived formally from a neutral parent hydride, parent compound, or hydro derivative of either, by the addition or removal of electrons may be named by adding the suffixes ‘elide’ or ‘elium’ to the name of the neutral parent. The number of radical centers is denoted by numerical prefixes.

> This new method may be used to indicate a global structure, when the positions of the radical and/or ionic centers are not known, or when it is not necessary, nor desirable, to name a specific structure.

(2) by functional class nomenclature

Radical ions derived formally from a neutral parent hydride, parent compound, or hydro derivative of either by the addition or removal of electrons may be named by adding the terms ‘radical cation’ or ‘radical anion’ as separate words to the name of the neutral parent hydride or parent compound having the same molecular formula. The multiplying prefixes ‘di’, ‘tri’ etc. are used to denote multiple radical or ionic centers. The terms ‘radical ion’ can also be used, followed by a Ewens-Basset number indicating the appropriate charge sign.

The substitutive method , (1), leads to preferred IUPAC names.

Examples:

$[C_6H_5\text{-}C_6H_5]^{(2\bullet)((2-)}$

biphenyldielide (PIN)
biphenyl diradical dianion
biphenyl diradical ion(2-)

$[C_{10}H_8]^{\bullet +}$

azulenelium (PIN)
azulene radical cation
azulene radical ion(1+)

P-75.2 Radical ions derived from parent hydrides

The order of seniority, radicals > anions > cations, is reflected in a preferred IUPAC name. Suffixes assigned to anionic and/or cationic centers are placed first after the name of the parent structure (parent hydride, functional parent hydride, or functionalized parent hydride), followed by suffixes attributed to radical centers.

A radical ion derived formally by the removal of one or more hydrogen atoms from a single skeleton atom or from different skeletal atoms of an ionic or zwitterionic parent hydride is named by adding to its name the suffixes ‘yl’ or ‘ylidene’ with appropriate multiplying prefixes before ‘yl’ or ‘ylidene’, with elision of the final letter ‘e’ of the name of the ionic parent hydride. Skeletal positions with radical centers have preference over those with ionic centers for assignment of low locants.

P-75.2.1 Examples of radical anions:

$H\underset{\cdot\cdot}{\overset{\cdot\cdot}{N}}^{\bullet\,-}$

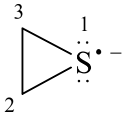
azanidyl (preselected name)

$^{-}\!:\underset{2}{CH_2}\text{-}\underset{1}{\overset{\bullet}{C}H_2}$

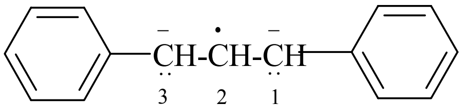
ethan-2-id-1-yl (PIN)

$(CH_3)_2B^{\bullet -}$

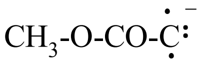
trimethylboranuidyl (PIN)
trimethyl-1λ^5-boranidyl



1λ^4-thiiran-1-id-1-yl (PIN)

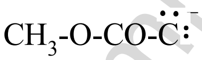


1,3-diphenylpropan-1,3-diid-2-yl (PIN)



$CH_3\text{-O-CO-}\overset{\bullet\,-}{\underset{\bullet}{C}}\colon$

and/or



$CH_3\text{-O-CO-}\overset{\bullet\bullet\,-}{C}\colon$

(methoxycarbonyl)methanidylidene (PIN)

P-75.2.2 Examples of radical cations:

$CH_2^{\bullet +}$

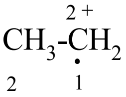
methyliumyl (PIN)

$SiH_4^{\bullet +}$

silaniumyl (preselected name)

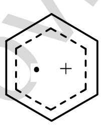
$[CH_3\text{-}CH_2]^{(\bullet)(2+)}$

ethaniumyliumyl (PIN)



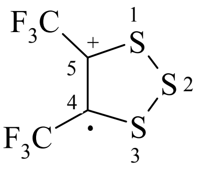
$\underset{2}{CH_3}\text{-}\underset{1}{\overset{2+}{\underset{\bullet}{C}}H_2}$

ethan-1-ium-1-ylium-1-yl (PIN)



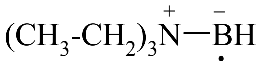
or $[C_6H_6]^{\bullet +}$

benzenelium



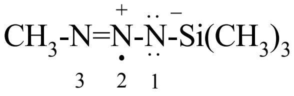
4,5-bis(trifluoromethyl)-1,2,3-trithiolan-5-ylium-4-yl

P-75.2.3 Examples of zwitterionic radical ions:



$(CH_3\text{-}CH_2)_3\overset{+}{N}\text{—}\underset{\bullet}{\overset{-}{B}}H$

(triethylazaniumyl)boranuidyl (PIN)
(triethylazaniumyl)-λ^5-boranidyl



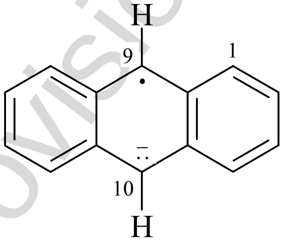
$CH_3\text{-}N\text{=}\underset{\bullet}{\overset{+}{N}}\text{-}\underset{\cdot\cdot}{\overset{\cdot\cdot\;-}{N}}\text{-}Si(CH_3)_3$

3-methyl-1-(trimethylsilyl)triaz-2-en-2-ium-1-id-2-yl

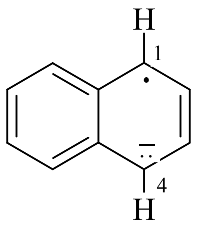
P-75.2.4 Hydro prefixes vs. added hydrogen

Radical and ionic centers at positions in a mancude parent hydride where there is an insufficient number of hydrogen atoms to directly apply recommendations for the use of 'yl, 'ylidene', 'ide' or 'ylium' as given in P-72.1, P-72.2 and P-72.3, respectively are derived formally from a dihydro derivative of the cyclic parent hydride. Radical ions can also be described by applying the principle of 'added hydrogen' (see P-14.6). In this method, the 'hydro' derivative is described by specifying the hydrogen atom of a dihydro pair that remains after the radical center is created by citing in italic capital H and the locant of the skeletal atom to which the hydrogen atom resides, both enclosed in a set of parentheses and inserted into the name of the corresponding parent hydride immediately after the locant for the radical center. The ionic center is created next, by subtraction of a hydron. For clarity of names, the 'added hydrogen' is cited in names. Preferred IUPAC names are formed by the 'added hydrogen' method.

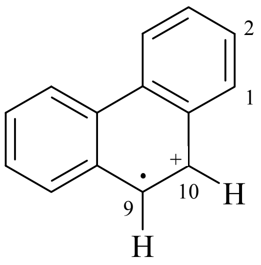
Examples:



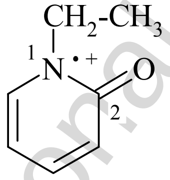
anthracen-10-id-9(10H)-yl (PIN)
9,10-dihydroanthracen-10-id-9-yl
anthracenelide (unspecified)



naphthalen-4-id-1(4H)-yl (PIN)
1,4-dihydronaphthalen-4-id-1-yl



phenanthren-10-ylium-9(10H)-yl (PIN)
9,10-dihydrophenanthren-10-ylium-9-yl
phenanthrenelium (unspecified)



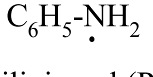
1-ethyl-2-oxopyridin-1-ium-1(2H)-yl (PIN)
1-ethyl-2-oxo-1,2-dihydropyridin-1-ium-1-yl

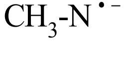
P-75.3 Radical ions on characteristic groups

P-75.3.1 Radical ions on ionic suffix groups

When ions may be named by using modified suffixes (see P-73.121 and P-73.2.3.2), the suffixes denoting radical centers are added to the name of the anionic parent hydride.

Examples:


$C_6H_5\text{-}\overset{+}{\underset{\bullet}{N}}H_2$


$CH_3\text{-}\ddot{N}^{\bullet -}$

anilinium yl (PIN)
benzenaminiumyl

methanaminidyl (PIN)

$CH_3\text{-}CO\text{-}\ddot{N}^{\bullet -}$

acetamidyliumyl(PIN)

$C_6H_5\text{-}C{\equiv}N^{\bullet -}$

benzonitriliumyl (PIN)

P-75.3.2 Radical ions other than those named by using ionic suffix groups

Examples:

$CH_3\text{-}CO\text{-}\overset{\bullet +}{\underset{\cdot\cdot}{O}}\text{-}CH_3$

acetyl(methyl)oxidaniumyl(PIN)

$CH_3\text{-}CH_2\text{-}CH_2\text{-}\overset{\bullet +}{\underset{\cdot\cdot}{O}}H$

propyloxidaniumyl (PIN)

$CH_3\text{-}CO\text{-}\underset{\cdot\cdot}{\ddot{N}}^{\bullet -}$

acetylazanidyl (PIN)

$C_6H_5\text{-}SO_2\text{-}\underset{2}{NH}\text{-}\underset{1}{\underset{\cdot\cdot}{\ddot{N}}}^{\bullet -}$

2-benzenesulfonyldiazan-1-id-1-yl (PIN)

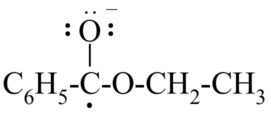
P-75.4 Ionic and radical centers in different parent structures

Radical centers have priority over ionic centers. A radical ion derived formally by the subtraction of one or more hydrogen atom(s) from an ionic or zwitterionic compound in which the ionic and radical centers cannot be included in the same parent structure is named by expressing the ionic center(s), or the part of the structure containing the ionic center(s), by means of substituent prefixes attached to the name of the parent radical.

Examples:

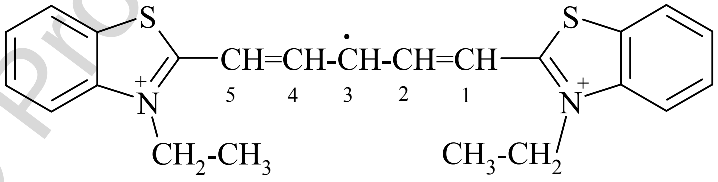
$:\overset{+}{O}{\equiv}\underset{2}{C}\text{-}\underset{1}{\dot{C}}H_2$

2-oxidaniumylidyneethyl(PIN)



$C_6H_5\text{-}\underset{\bullet}{\overset{\overset{\cdot\cdot\,-}{:\!O\!:}\,|}{C}}\text{-}O\text{-}CH_2\text{-}CH_3$

ethoxy(oxido)benzyl (PIN)



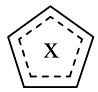
1,5-bis(3-ethyl-1,3-benzothiazol-3-ium-2-yl)penta-1,4-dien-3-yl (PIN)

P-76 Delocalized and non-classical radicals and ions

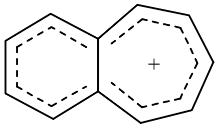
P-76.1 Delocalized radicals and ions

P-76.1.1 Delocalization in names involving one radical or anionic center in an otherwise conjugated double bonds structure is denoted by the appropriate suffix, without locants.

Examples:



x = • : cyclopentadienyl (PIN)
x = + : cyclopentadienylium (PIN)
x = − : cyclopentadienide (PIN)



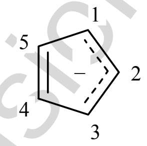
benzo[7]annulenylium (PIN)

$$\mathrm{CH_2}\overset{\text{- - -}}{\text{—}}\mathrm{CH}\overset{\text{- - -}}{\text{—}}\overset{\bullet}{\mathrm{C}}\mathrm{H}\overset{\text{- - -}}{\text{—}}\mathrm{CH}\overset{\text{- - -}}{\text{—}}\mathrm{CH_2}$$

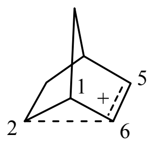
pentadienyl (PIN)

P-76.1.2 Partial delocalization is denoted by the descriptor *deloc* preceded by the locants indicating the extent of delocalization. This descriptor and its locants are cited immediately before the appropriate suffix and enclosed in parentheses.

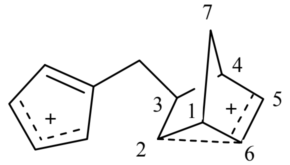
Examples:



cyclopenta-2,4-dien(1,2,3-*deloc*)ide (PIN)



bicyclo[2.2.1]hept-5-en(2,5,6-*deloc*)ylium (PIN)



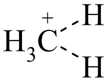
3-{[cyclopenta-2,4-dien(2,3,4-*deloc*)ylium-1-yl]methyl}bicyclo[2.2.1]hept-5-en(2,5,6-*deloc*)ylium

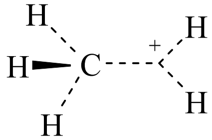
P-76.2 Nonclassical carbocations

A nonclassical carbocation is a structure having cationic center(s) that cannot be represented by the normal valence system. Hypercoordinated and bridged carbocations belong to this class.

P-76.2.1 Hypercoordinated carbocations (ref. 25)

The prototype of a hypercoordinated carbocation is methanium, CH^{5+}, which results from the addition of a proton to methane. It is best represented by a two-electron three-center system involving the carbon atom and two hydrogen atoms, and three normal valences for the remaining three carbon-hydrogen bonds.





methanium (PIN)

P-76.2.2 Bridged carbocations (see ref. 25)

A carbocation (real or hypothetical) in which there are two (or more) carbon atoms that could be designated as carbenium centers in alternative Lewis formulas but which instead is represented by a structure in which a group (a hydrogen atom or a hydrocarbon residue, possibly with substituent in non involved positions) bridges these potential carbenium centers. One may distinguish 'electron-sufficient bridged carbocations' and 'electron-deficient bridged carbocations'.

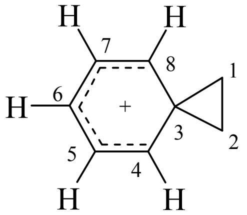
Examples of 'electron-sufficient bridged carbocations' are phenyl-bridged ions (for which the trivial name 'phenonium' has been used), described in P-76.2.2.1. These ions are straightforwardly classified as carbenium ions.

The three types of 'electron-deficient bridged carbocations' described in P-76.2.2.2 necessarily involve three-center bonding. The 'hydrogen-bridge-carbocation' shown in P-76.2.2.2.1 contains a two-coordinate hydrogen atom. The 'bridged carbocations' in P-76.2.2.2.2 contain five-coordinate carbon atoms. Hypercoordination (see P-76.2.1), which includes two-coordination for hydrogen and five- but also higher coordination for carbon, is generally observed in bridged carbocations.

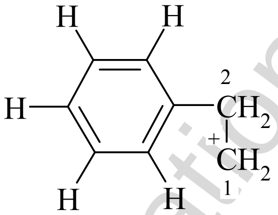
P-76.2.2.1 Phenonium ions (electron-sufficient bridged carbocations)

The class name 'phenonium ion' designates cyclohexadienyl cations (cyclohexadienylium cations) that are spiro-fused with a cyclopropane unit. Individual compounds may be named as carbenium ions of the corresponding spiro compounds, by using the suffix 'ylium'.

Examples:



spiro[2.5]octa-5,7-dien(4,5,6,7,8-*deloc)*ylium (PIN)



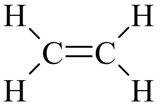
2-phenylethylium (PIN)

P-76.2.2.2 Electron-deficient bridged carbocations

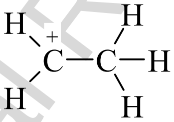
P-76.2.2.2.1 Hydrogen-bridged-carbocations

It is specifically stated in the document Radicals and Ions (RC-82.1.1.2) that specific structures obtained by the addition of a hydron to one end of a double bond resulting in the formation of a tricoordinate carbocation at the other end of the double bond may be named by using the 'ylium' suffix. However, according to the recommendations given herein for naming delocalized cations the name for a delocalized ethylium would be ethen(1,2-*deloc*)ium. The name ethenium would then be used only to describe the formula $[C_2H_5]^+$.

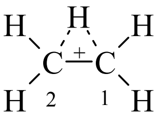
Example:



ethene (PIN)



ethylium(PIN)

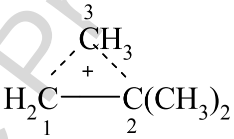


ethen(1,2-*deloc*)ium (PIN)
ethyl(1,2-*deloc*)ylium

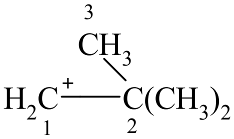
P-76.2.2.2.2 Carbon-bridged carbocations

Locants describing delocalized carbocation systems are cited in names in ascending order following the path of the two delocalized bonds.

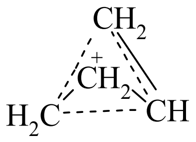
Examples:



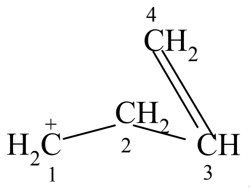
2,2-dimethylpropan(1,3,2-*deloc*)ylium (PIN)



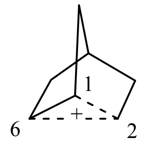
2,2-dimethylpropylium (PIN)



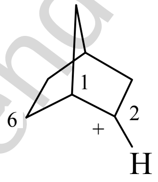
but-3-ene(3,1,4-deloc)ylium (PIN)



but-3-en-1-ylium (PIN)



bicyclo[2.2.1]heptane-(1,2,6-deloc)-2-ylium (PIN)



bicyclo[2.2.1]heptan-2-ylium (PIN)

P-77 Preferred names for radicals, ions, radical ions

Preferred names for radicals, ions, and radical ions are selected either between systematically formed and retained names, or between systematic names.

P-77.1 Selection of preferred names between systematically formed and retained names

Traditional names are retained for naming radicals and ions (see Table 7.3). Most of them are recommended only for use in general nomenclature. Preferred IUPAC names, with a few exceptions, are systematically formed.

Table 7.3 Retained names used as preselected or preferred IUPAC names and in general nomenclature

Structure	Preselected or Preferred IUPAC name	Retained name for general nomenclature
Radicals		
$\mathrm{H_2N}\cdot$	azanyl (preselected)	aminyl
$\mathrm{H_2C}:$	methylidene (PIN)	carbene, methylene
$\mathrm{HC}\vdots$	methylidyne (PIN)	carbyne
$\mathrm{H_2Si}:$	silylidene (preselected)	silylene
$\mathrm{HN}:$	azanylidene (preselected)	nitrene, aminylene
$\mathrm{R\text{-}O}\cdot$	(see P-71.3.3)	

R = CH_3-	methyloxidanyl (PIN)	methoxyl
R = CH_3-CH_2-	ethyloxidanyl (PIN)	ethoxyl
R = CH_3-CH_2-CH_2-	propyloxidanyl (PIN)	propoxyl
R = CH_3-$[CH_2]_2$-CH_2-	butyloxidanyl (PIN)	butoxyl
R = CH_3-CO-	acetyloxidanyl (PIN)	acetoxyl
R = H_2N-	aminooxidanyl (PIN)	aminoxyl
$HO\text{-}O^{\bullet}$	dioxidanyl (preselected)	peroxyl, dioxyl

Anions

H_2N^{-}	azanide (preselected)	amide
$HN{:}^{2-}$	azandiide (preselected)	imide

$R\text{-}O{:}^{-}$

R = CH_3-	methanolate (PIN)	methoxide
R = CH_3-CH_2-	ethanolate (PIN)	ethoxide
R = CH_3-CH_2-CH_2-	propan-1-olate (PIN)	propoxide
R = CH_3-$[CH_2]_2$-CH_2-	butan-1-olate (PIN)	butoxide
R = H_2N-	aminooxidanide (preselected)	aminoxide

Cations

$R\text{-}O^{+}$

R = CH_3-	methyloxidanylium (PIN)	methoxylium
R = CH_3-CH_2-	ethyloxidanylium (PIN)	ethoxylium
R = CH_3-CH_2-CH_2-	propyloxidanylium (PIN)	propoxylium
R = CH_3-$[CH_2]_2$-CH_2-	butyloxidanylium (PIN)	butoxylium
R = CH_3-CO-	acetyloxidanylium (PIN)	acetoxylium
R = H_2N-	aminooxidanylium (preselected)	aminoxylium
$HO\text{-}O^{+}$	dioxidanylium (preselected)	peroxylium, dioxylium
	pyrylium (PIN)	(see P-73.3.2)

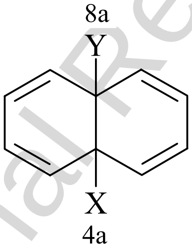
chromenylium (PIN)	(see P-73.3.2)
isochromenylium (PIN)	(see P-73.3.2)
flavylium (PIN)	(see P-73.3.2)
xanthylium (PIN)	(see P-73.3.2)

P-77.2 Preferred systematic names

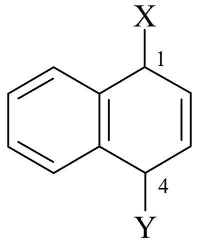
P-77.2.1 Preferred names derived from mancude parent hydrides and fullerenes

Preferred names for radicals, ions and radicals-ions derived from mancude parent hydrides and fullerenes are formed by using the ‘added hydrogen’ method. In general nomenclature, the addition of hydrogen atoms and the creation of radicals and ions by the subtraction of hydrogen atom, hydrons or hydrides as appropriate, is an acceptable method.

Examples:

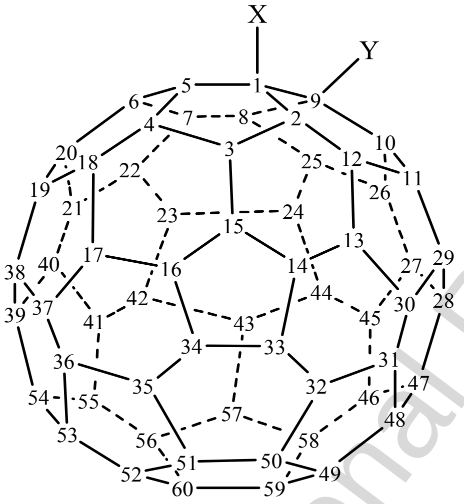


X = • Y = H	naphthalen-4a(8aH)-yl (PIN) 1,4-dihydronaphthalen-1-yl
X = • Y = •	naphthalene-4a,8a-diyl (PIN) 4a,8a-dihydronaphthalene-4a,8a-diyl
X = ⊕ Y = H	naphthalen-4a(8a*H*)-ylium (PIN) 4a,8a-dihydronaphthalen-4a-ylium
X = • Y = ⊕	naphthalen-8a-ylium-4a(8a*H*)-yl (PIN) 4a,8a-dihydro-naphthalen-8a-ylium-4a-yl



X = • Y = – naphthalen-4-id-4(8a*H*)-yl (PIN)
1,4-dihydronaphthalen-4-id-1-yl

X = Y = – naphthalene-1,4-diide (PIN)
1,4-dihydronaphthalen-1,4-diide



I X = • ; Y = H
II X = + ; Y = H
III X = • ; Y = +
IV X = − : Y = H
V X = • ; Y = −
VI X = • ; Y = •

I (C_{60}-I_h)[5,6]fulleren-1(9*H*)-yl (PIN)
1,9-dihydro(C_{60}-I_h)[5,6]fulleren-1-yl

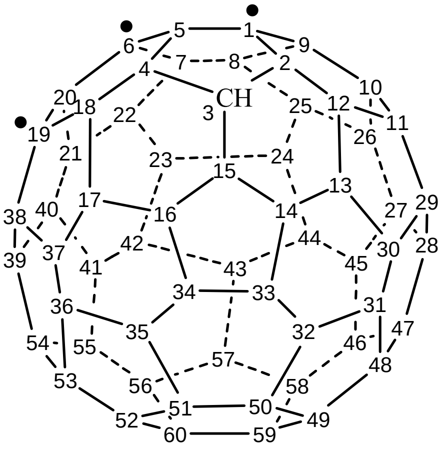
II (C_{60}-I_h)[5,6]fulleren-1(9*H*)-ylium (PIN)
1,9-dihydro(C_{60}-I_h)[5,6]fulleren-1-ylium

III (C_{60}-I_h)[5,6]fulleren-9-ylium-1(9*H*)-yl (PIN)
1,9-dihydro(C_{60}-I_h)[5,6]fulleren-1,9-diyl

IV (C_{60}-I_h)[5,6]fulleren-1(9*H*)-ide ((PIN)
1,9-dihydro(C_{60}-I_h)[5,6]fulleren-1-ide

V (C_{60}-I_h)[5,6]fulleren-9-id-1(9*H*)-yl (PIN)
1,9-dihydro(C_{60}-I_h)[5,6]fulleren-9-id-1-yl

VI (C_{60}-I_h)[5,6]fullerene-1,9-diyl (PIN)
1,9-dihydro(C_{60}-I_h)[5,6]fulleren-9-ylium-1-yl



(C60-Ih)[5,6]fullerene-1,6,19(3H)-triyl (PIN)
1,3,6,19-tetrahydro(C60-Ih)[5,6]fullerene-1,6,19-triyl

P-77.2.2 Anions

P-77.2.2.1 Substitutive names that involve the suffix ‘uide’ are preferred to those that are denoted by the suffix ‘ide’ with the λ-convention.

Examples:

$CH_3\text{-}SiH_4^-$

methylsilanuide (PIN)
methyl-λ^6-silanide

F_6I^-

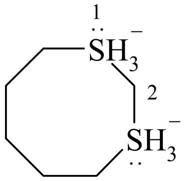
hexafluoro-λ^5-iodanuide (preselected name)
hexafluoro-λ^7-iodanide

P-77.2.2.2 The use of the suffix ‘ide’ is preferred to that of the suffix ‘uide’ added to a parent hydride modified by the λ-convention; the suffix ‘ide’ is also preferred over ‘uide’ when the λ-convention must be used to denote both anionic centers.

Examples:

$H_3C:^-$

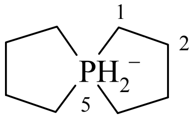
methanide (PIN)
λ^2-methanuide



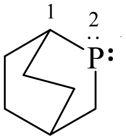
$1\lambda^4$, $3\lambda^4$-dithiocane-1,3-diide (PIN)
$1\lambda^6$, $3\lambda^6$-dithiocane-1,3-diuide
$1\lambda^4$, $3\lambda^6$-dithiocane-3-ide-1-uide

P-77.2.2.3 Names denoted by the suffixes 'uide' or 'ide' added to neutral replacement names of parent hydrides are preferred to those formed by anionic replacement prefixes 'uida' or 'ida' (see P-72.4).

Examples:



$5\lambda^5$-phosphaspiro[4.4]nonan-5-uide (PIN)
$5\lambda^5$-phosphanuidaspiro[4.4]nonane



2-phosphabicyclo[2.2.2]octan-2-ide (PIN)
2-phosphanidabicyclo[2.2.2]octane

P-77.2.3 Cations

P-77.2.3.1 'Onium cations'

Names of mononuclear cations of Groups 15, 16, and 17, formed by adding the suffix 'ium' to the name of the mononuclear parent hydride are preferred to those formed by using the ending 'onium'.

Examples:

NH_4^+	H_3S^+	H_2Br^+
azanium (preselected name) ammonium	sulfanium (preselected name) sulfonium	bromanium (preselected name) bromonium

P-77.2.3.2 Prefixes for denoting cations

Prefixes formed by adding the suffix ‘yl’ to the systematic name of the cation are preferred to those derived from ‘onium cations’, ending with the letter ‘o’.

Examples:

$-PH_3^+$

phosphaniumyl (preselected name)
phosphonio

$-SeH_2^+$

selaniumyl (preselected name)
selenonio

$-IH^+$

iodaniumyl (preselected name)
iodonio

P-77.2.3.3 Preference between ‘ylium’ and ‘ium’ suffixes

P-77.2.3.3.1 The use of the suffix ‘-ylium’ is preferred to that of the suffix ‘-ium’ added to a parent hydride modified by the λ-convention.

Example:

$H_2\ddot{N}^+$

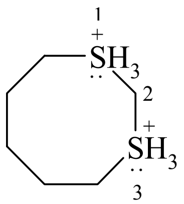
azanylium (preselected name)
λ^1-azanium
aminylium
nitrenium

P-77.2.3.3.2 The use of the suffix ‘ium’ is preferred to that of the suffix ‘ylium’ added to a parent hydride modified by the λ-convention; the suffix ‘ium’ is also preferred over ‘ylium’ when the λ-convention must be used to denote both cationic centers.

Examples:

$\overset{+}{P}H_4$

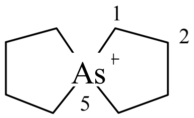
phosphanium (preselected name)
phosphonium
λ^5-phosphanylium



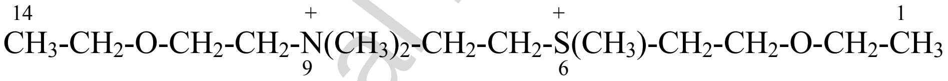
$1\lambda^4$, $3\lambda^4$-dithiocane-1,3-diium (PIN)
λ^6, $3\lambda^6$-dithiocane-1,3-bis(ylium)
$1\lambda^6$, $3\lambda^4$-dithiocane-3-ium-1-ylium

P-77.2.3.3.3 Names denoted by the suffixes ‘ium’ or ‘ylium’ added to neutral replacement names of parent hydrides are preferred to those formed by cationic replacement prefixes (see P-73.4).

Examples:



$5\lambda^5$-arsaspiro[4.4]nonan-5-ylium (PIN)
5-arsoniaspiro[4.4]nonane



$$\overset{14}{C}H_3\text{-}CH_2\text{-}O\text{-}CH_2\text{-}CH_2\text{-}\underset{9}{\overset{+}{N}}(CH_3)_2\text{-}CH_2\text{-}CH_2\text{-}\underset{6}{\overset{+}{S}}(CH_3)\text{-}CH_2\text{-}CH_2\text{-}O\text{-}CH_2\text{-}\overset{1}{C}H_3$$

6,9,9-trimethyl-3,12-dioxa-6-thia-9-azatetradecane-6,9-dium (PIN)
6,9,9-trimethyl-3,12-dioxa-6-thionia-9-azoniatetradecane

P-77.3 Preferred parent structures

Names of radicals and ions are constructed on the basis of functional parents (e.g. acetic acid) or functionalized parents (e.g. methanamine), and on radical and ionic parents derived from parent hydrides (e,g, acetylazanide, methyloxidanyl). Preferred names are based on these two principal types.

Table 7.4 illustrates this dichotomy.

Table 7.4 Preferred IUPAC names for radicals and ions derived from functionalized and functional parents

Type I: Functional and functionalized parents parents		Type II: Derivatives of radical and ionic parents	
Acids			
		(a) CH_3-CO-O•	acetyloxidanyl
(b) CH_3-COO^{-}	acetate		
(c) $[CH_3\text{-}COOH]H^{+}$	acetic acidium	(c) CH_3-CO-($O^{+}H_2$) CH_3-CO-O^{+}	acetyloxidanium acetyloxidanylium
Amides			
(a) CH_3-CO-$N^{\bullet}$H	acetamidyl	(a) CH_3-CO-$N^{2\bullet}$	acetylazanylidene
(b)		(b) CH_3-CO-N^{-}H	acetylazanide
(c) $[CH_3\text{-}CO\text{-}NH_2]H^{+}$	acetamidium	(c) CH_3-CO-$N^{+}H_3$	acetylazanium
CH_3-CO-$N^{+}(CH_3)_3$	*N*,*N*,*N*-trimethyl-acetamidium	CH_3-CO-$N^{+}(CH_3)_3$	acetyltrimethyl azanium
CH_3-CO-N^{+}H	acetamidylium	CH_3-CO-N^{2+}	acetylazanebis(ylium)
Nitriles			
(c) CH_3-C≡N^{+}H	acetonitrilium		
Aldehydes/Ketones		(c) CH_3-CH=O^{+}H	ethylideneoxidanium
Hydroxy compounds			
		(a) CH_3-O•	methyloxidanyl
(b) CH_3-O^{-}	methanolate		

		(c) $CH_3\text{-}O^{+}H_2$	methyloxidanium
		$CH_3\text{-}O^{+}$	methyloxidanylium

Amines - imines

(a) $CH_3\text{-}N^{\bullet}H$	methanaminyl	(a) $CH_3\text{-}N^{2\bullet}$	methylazanylidene
(b) $CH_3\text{-}N^{-}H$	methanaminide	(b) $CH_3\text{-}N^{2-}$	methylazanediide
(c) $CH_3\text{-}N^{+}H_3$	methanaminium		
CH3-N+H	methanaminylium	(c) CH3-N2+	methylazanebis(ylium)

P-77.4 Preferred names for salts of organic bases

P-77.4.1 Preferred names are binary names formed by citing the name of the cation followed by that of the anion.

Examples:

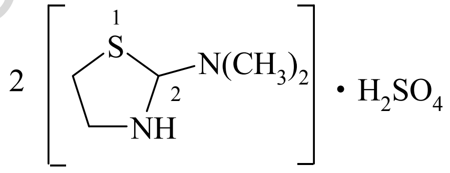
$[C_6H_5\text{-}NH_3]Cl$	anilinium chloride (PIN)
$[CH_3\text{-}NH_3]_2SO_4$	bis(methanaminium) sulfate (PIN)
$[(CH_3\text{-}CH_2)_3NH]HSO_4$	*N*,*N*-diethylethanaminium hydrogen sulfate (PIN)

P-77.4.2 When the above rule cannot be applied, recourse is found in two traditional methods of naming salts of organic bases, namely:

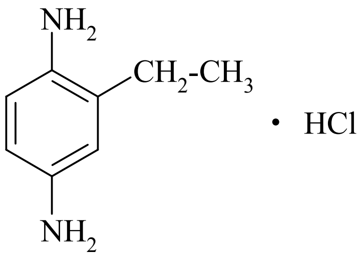
(a) the unaltered name of the base is followed by the name of the anion;

(b) for salts of hydrohalogen acids only, the unaltered name of the base is followed by hydrofluoride, hydrobromide, hydrochloride, or hydroiodide, as the case may be.

Examples:



bis(N,N-dimethyl-1,3-thiazolidin-2-amine) sulfate (PIN)



2-ethylbenzene-1,4-diamine monohydrochloride (PIN)

CHAPTER 8 ISOTOPICALLY MODIFIED COMPOUNDS

P-80 Introduction

This Section describes a general system of nomenclature for organic compounds whose isotopic nuclides composition (ref. 12) deviates from that occurring in nature (for a discussion of the meaning of 'natural composition' see ref. 26). Comparative examples of the application of these rules are given in Table 8.1, page 17). This Chapter is derived from Section H of the 1979 Recommendations (ref. 1).

There is one other general system in use for describing isotopically modified compounds. It is based on an extension of the principles proposed by Boughton (see ref. 27) for designating compounds containing hydrogen isotopes and is used mainly in the Chemical Abstracts Service index nomenclature system (see ref. 28).

The system codified in these recommendations provides for recognition of various types of isotopic modifications and thus was chosen in preference to the system based on the Boughton principles.

P-81 Symbols and Definitions

P-81.1 Nuclide symbols

The symbol for denoting a nuclide in the formula and name of an isotopically modified compound consists of the atomic symbol for the element and an arabic numeral in the left superscript position indicating the mass number of the nuclide (see ref. 14).

P-81.2 Atomic symbols

The atomic symbols used in the nuclide symbol are those given in IUPAC *Nomenclature in Inorganic Chemistry* (see ref. 14). In the nuclide symbol, the atomic symbol is printed in roman type, italicized atomic symbols being reserved for letter locants, as is customary in the nomenclature of organic compounds and described in P-14.3.

For the hydrogen isotopes protium, deuterium and tritium, the nuclides symbols ^{1}H, ^{2}H, and ^{3}H, are used. The symbols D and T for ^{2}H and ^{3}H, respectively, are used, but not when other modifying nuclides are present , because this may cause difficulties in alphabetic ordering of the nuclide symbols in the isotopic descriptor. Although the symbols *d* and *t* have been used and are still used in place of ^{2}H and ^{3}H in names formed according to the Boughton system, in no other cases are lower-case letters used as atomic symbols. Therefore, the use of *d* and *t* in chemical nomenclature outside of the Boughton system is not recommended.

P-81.3 Names for hydrogen atoms and ions

The names of the hydrogen atoms and ions are as follows (see ref. 29):

		^1H	^2H	^3H	natural composition
atom	H	protium	deuterium	tritium	hydrogen
anion	H^-	protide	deuteride	tritide	hydride
cation	H^+	proton	deuteron	triton	hydron

P-81.4 Isotopically unmodified compounds

An isotopically unmodified compound has a macroscopic composition such that its constituent nuclides are present in the proportions occurring in nature. Its formula and name are written in the customary manner.

Examples:

CH_4	CH_3-CH_2-OH
methane (PIN)	ethanol (PIN)

P-81.5 Isotopically modified compounds

An isotopically modified compound has a macroscopic composition such that the isotopic ratio of nuclides for at least one element deviates measurably from that occurring in nature. Isotopically modified compounds may be classified as

(1) isotopically substituted compounds or

(2) isotopically labeled compounds

P-82 Isotopically Substituted Compounds

P-82.0 Introduction

An isotopically substituted compound has a composition such that essentially all the molecules of the compound have only the indicated nuclide at each designated position. For all other positions, the absence of nuclide indication means that the nuclide composition is the natural one.

P-82.1 Formulas

The formula of an isotopically substituted compound is written in the usual way except that appropriate nuclides symbols are used. When different isotopes of the same element are present in the same position, common usage is to write their symbols in order of increasing mass number.

Examples:

$^{14}CH_4$

$^{12}CHCl_3$

$CH_3\text{-}CH^2H\text{-}OH$
(not $CH_3\text{-}C^2HH\text{-}OH$)

P-82.2 Names

P-82.2.1 The name of an isotopically substituted compound is formed by inserting in parentheses the nuclide symbol(s), preceded by any necessary locant(s), letters and/or numerals, before the name or preferably before the denomination of that part of the compound that is isotopically substituted. Immediately after the parentheses there is neither space nor hyphen, except that when the name, or a part of a name, includes a preceding locant, a hyphen is inserted.

When polysubstitution is possible, the number of atoms substituted is always specified as a right subscript to the atomic symbol(s), even in case of monosubstitution.

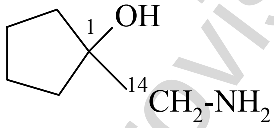
Examples:

$^{14}CH_4$
(^{14}C)methane (PIN)

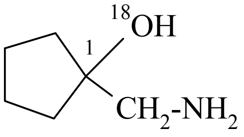
$^{12}CHCl_3$
(^{12}C)chloroform (PIN)

$CH_3{}^2H$
($^2H_1$)methane (PIN)

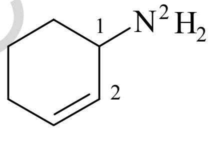
$C^2H_2Cl_2$
dichloro($^2H_2$)methane (PIN)



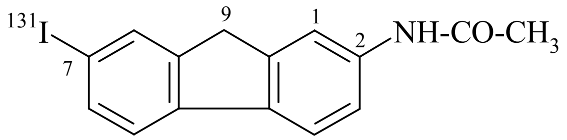
1-[amino(^{14}C)methyl]cyclopentan-1-ol (PIN)



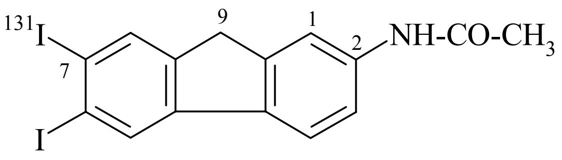
1-(aminomethyl)cyclopentan-1-(^{18}O)ol (PIN)



cyclohex-2-en-1-($^2H_2$)amine (PIN)



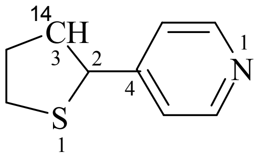
N-[7-(^{131}I)iodo-9*H*-fluoren-2-yl]acetamide (PIN)



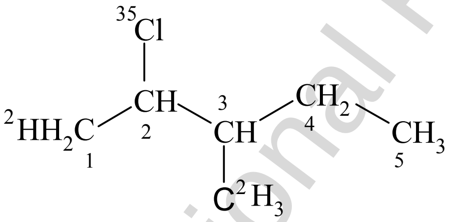
N-[6,7-(7-^{131}I)iodo-9*H*-fluoren-2-yl]acetamide (PIN)

$C_2H_5\text{-O-}\overset{4}{C}O\text{-}{}^{14}\overset{3}{C}H_2\text{-}{}^{14}\overset{2}{C}H_2\text{-}\overset{1}{C}OO^- \; Na^+$

sodium ethyl (2,3-$^{14}C_2$)butanedioate (PIN)
sodium ethyl (2,3-$^{14}C_2$)succinate



4-[(3-^{14}C)thiolan-2-yl]pyridine (PIN)
4-[tetrahydro-(3-^{14}C)-furan-2-yl]pyridine



2-(^{35}Cl)chloro-3-[($^2H_3$)methyl](1-$^2H_1$)pentane (PIN)

P-82.2.2 In a name consisting of two or more words, the isotopic descriptor is placed before the appropriate word or part of the word that includes the nuclide(s), unless unambiguous locants are available or are unnecessary.

Examples:

$\overset{2}{C}H_2{}^2H\text{-}\overset{1}{C}OOH$

(2-$^2H_1$)acetic acid (PIN)

$CH_3\text{-}COO^2H$

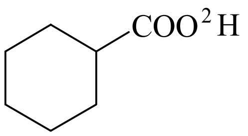
(*O*-^{2}H)acetic acid (PIN)
acetic (^{2}H)acid

$\overset{5}{C}H_3\text{-}\overset{4}{C}H_2\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}{}^{14}\overset{1}{C}OO^3H$

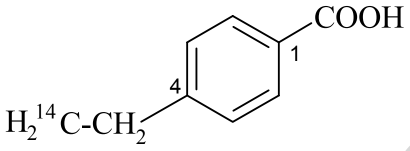
(1-^{14}C)pentan(^{3}H)oic acid (PIN)

$H^{14}COO^- \; Na^+$

sodium (^{14}C)formate (PIN)



cyclohexane(²H)carboxylic acid (PIN)



4-[(2-^{14}C)ethyl]benzoic acid (PIN)

$\mathrm{CH_3\text{-}CH_2\text{-}COO\text{-}\overset{1}{^{14}CH_2}\text{-}\overset{2}{CH_3}}$

(1-^{14}C)ethyl propanoate (PIN)

$\mathrm{\overset{3}{CH_3}\text{-}\overset{2}{^{14}CH_2}\text{-}\overset{1}{COO}\text{-}CH_2\text{-}CH_3}$

ethyl (2-^{14}C)propanoate (PIN)

P-82.2.3 In a retained name or in a semisystematic name (i.e. the name of a stereoparent hydride) consisting of one word, the isotopic descriptor is placed before the name, with an appropriate locant. This method is preferred to that placing the descriptor before the implied name of the characteristic group.

Example:

$\mathrm{\overset{2}{CH_3}\text{-}\overset{1}{CO}\text{-}\overset{\mathit{N}}{N}H^2H}$

(*N*-²H)acetamide (PIN)
acet(²H)amide

P-82.3 Order of nuclide symbols

P-82.3.1 When isotopes of different elements are present as nuclides in a isotopically substituted, their symbols are arranged in alphabetical order if they are appear at the same place in the name.

Example:

$\mathrm{CH_3{}^{18}O^2H}$

methan(²H,^{18}O)ol (PIN)

P-82.3.2 When several isotopes of the same element are present as nuclides, their symbols are arranged in the order of increasing mass number if they are inserted at the same place.

Example:

$\mathrm{\overset{2}{CH_2}{}^2H\text{-}\overset{1}{CH}{}^3H\text{-}OH}$

(2-$^2H_1$,1-$^3H_1$)ethanol (PIN)

P-82.4 Stereoisomeric isotopically substituted compounds

Two types of stereoisomeric isotopically substituted compounds are possible:

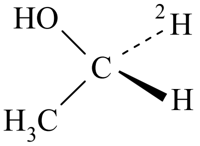
(1) those in which the stereoisomerism results from isotopic modification; and

(2) those whose analogous unmodified compounds are stereoisomers.

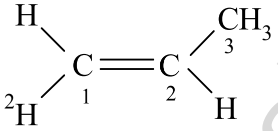
The nomenclature of stereoisomers of isotopically substituted compounds follows the general methods described in Chapter 9.

Stereochemical affixes are cited at the specified place in the name according to the stereochemical rules. When they must be inserted into the name at the same place as isotopic descriptors, the stereochemical affixes are cited first.

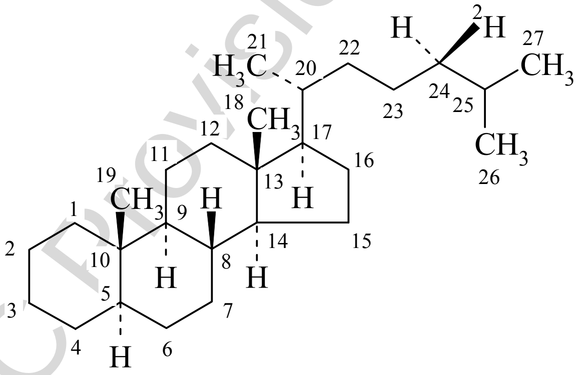
P-82.4.1 Examples in which stereoisomerism results from isotopic substitution



(R)-(1-$^{2}H_{1}$)ethanol (PIN)

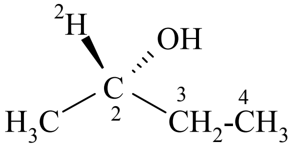


(*E*)-(1-$^{2}H_{1}$)prop-1-ene (PIN)

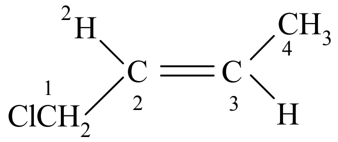


(24*R*)-5α-(24-$^{2}H_{1}$)cholestane (PIN)

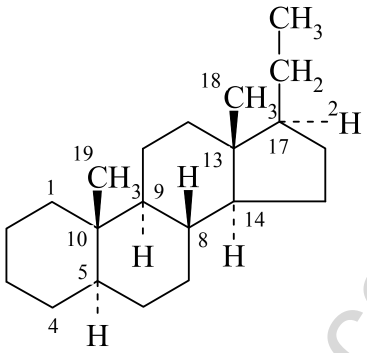
P-82.4.2 Examples of isotopically substituted stereoisomers



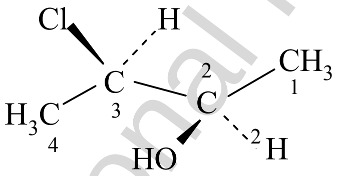
(*S*)-(2-^{2}H)-butan-2-ol (PIN)



(*E*)-1-chloro(2-^{2}H)but-2-ene (PIN)



5α-(17-^{2}H)pregnane (PIN)



(2*R*,3*R*)-2-chloro(3-$^{2}H_{1}$)butan-2-ol (PIN)

P-82.5 Numbering

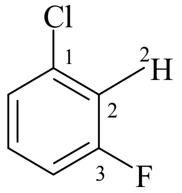
P-82.5.1 Numbering in relation to the unmodified compound

Numbering of an isotopically substituted compound is not changed from that of an isotopically unmodified compound. Among the structural features of a compound to be considered successively for numbering as given by P-14.4, the presence of nuclides is considered last with the exception of chirality arising from isotopic modification.

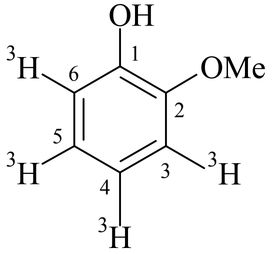
Examples:

$\overset{1}{C}F_3\text{-}\overset{2}{C}H_2{}^2H$

1,1,1-trifluoro(2-$^{2}H_{1}$)ethane (PIN)



1-chloro-3-fluoro(2-^{2}H)benzene (PIN)



2-methoxy(3,4,5,6-$^3H_4$)phenol (PIN)

P-82.5.2 Priority between isotopically substituted and unmodified atoms or groups

When there is a choice between equivalent numberings in an isotopically unmodified compound, the starting point and the direction of numbering of the analogous isotopically substituted compound are chosen so as to give lowest locants to the modified atoms or groups considered together in one series in increasing numerical order. If a choice still remains, precedence for the lowest locants is given to the nuclide of higher atomic number. In the case of different nuclides of the same element, precedence is given to the nuclide of higher mass number.

Examples:

$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{^{14}CH_2}}\text{-}\overset{3}{\mathrm{CH_2}}\text{-}\overset{4}{\mathrm{CH_3}}$

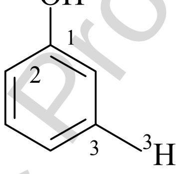
(2-^{14}C)butane (PIN)
[not (3-^{14}C)butane]

$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{C^2H_2}}\text{-}\overset{3}{\mathrm{^{14}CH_2}}\text{-}\overset{4}{\mathrm{CH_3}}$

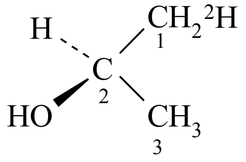
(3-^{14}C,2,2-$^2H_2$)butane (PIN)
[not (2-^{14}C,3,3-$^2H_2$)butane]

$\overset{1}{\mathrm{CH_3}}\text{-}\overset{2}{\mathrm{^{14}CH_2}}\text{-}\overset{3}{\mathrm{CH^2H}}\text{-}\overset{4}{\mathrm{CH_3}}$

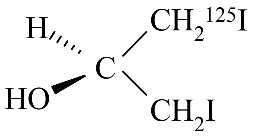
(2-^{14}C,3-$^2H_1$)butane (PIN)
[not (3-^{14}C,2-$^2H_1$)butane]



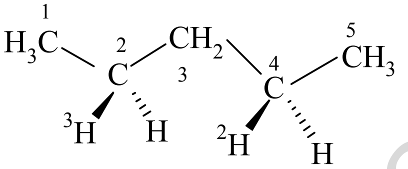
(3-^{3}H)phenol (PIN)



(*R*)-(1-$^2H_1$)propan-2-ol (PIN)



(*R*)-1,3-(1-^{125}I)diiodopropan-2-ol (PIN)



(2*S*,4*R*)-(4-$^{2}H_{1}$,2-$^{3}H_{1}$)pentane (PIN)

P-82.6 Locants

P-82.6.1 Omission of locants

In preferred IUPAC names, locants are omitted if no locants are necessary in unmodified names. In general nomenclature, omission may occur when no ambiguity would result.

Examples:

$C^{2}H_{3}$-CN

($^{2}H_{3}$)acetonitrile (PIN)
(as in trichloroacetonitrile)

CH_{3}-CH_{2}-$O^{2}H$

ethan(^{2}H)ol (PIN)

$CH_{2}{}^{2}H$-O-$C^{2}H_{2}$-S-CH_{2}-OOH

{[($^{2}H_{1}$)methoxy($^{2}H_{2}$)methyl]sulfanyl}methaneperoxol (PIN)

P-82.6.2 Letter and/or numeral locants

When locants are needed, all locants must be cited. Specific positions of nuclides must be indicated in the isotopic descriptor by appropriate locants, letters and/or numerals, preceding the nuclide symbol(s). In preferred names, all locants are placed before the nuclide that is multiplied accordingly.

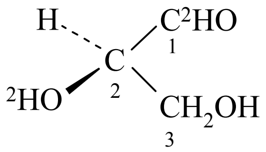
Examples:

CH_{3}-$CH^{2}H$-$O^{2}H$

(*O*,1-$^{2}H_{2}$)ethanol (PIN)
(*O*-^{2}H,1-^{2}H)ethanol

$\overset{1}{C^{2}H_{3}}$-$\overset{2}{CO}$-$\overset{3}{C^{2}H_{2}}$-$\overset{4}{CH_{2}}$-$\overset{5}{CH_{3}}$

(1,1,1,3,3-$^{2}H_{5}$)pentan-2-one (PIN)
(1-^{2}H,1-^{2}H,1-^{2}H,3-^{2}H,3-^{2}H)pentan-2-one

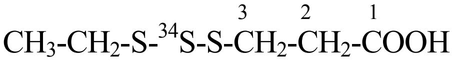


(*R*)-(2-*O*,1-$^{2}\mathrm{H}_2$)glyceraldehyde (PIN)
(*R*)-(2-*O*-^{2}H,1-^{2}H)glyceraldehyde

P-82.6.3 Location of nuclides on positions not normally denoted by locants

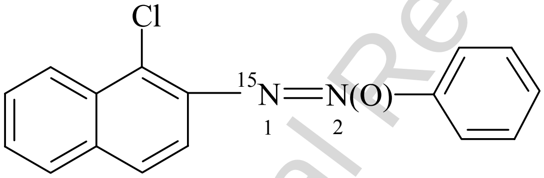
When the nuclide occupies a position that is not normally numbered, or when its position cannot be easily be defined by using the two preceding rules, the nuclide symbol may be included in the entire symbol for the group through which it is linked to the main part of the structure.

Examples:



$$\mathrm{CH_3\text{-}CH_2\text{-}S\text{-}{}^{34}S\text{-}S\text{-}\overset{3}{C}H_2\text{-}\overset{2}{C}H_2\text{-}\overset{1}{C}OOH}$$

3-[ethyl(2-^{34}S)trisulfanyl]propanoic acid (PIN)



1-(1-chloro-naphthalen-2-yl)-2-phenyl(2-^{15}N)diazene 2-oxide (PIN)
2-(1-chloronaphthalen-2-yl)-1-phenyl-(2-^{15}N)-λ^{5}-diazen-1-one
[2-(1-chloronaphthalen-2-yl)-1-phenyl(2-^{15}N)diazen-1-ium-1-yl]oxidanide
1-chloro-2-(phenyl-*ON*^{15}*N*-azoxy)naphthalene

P-82.6.4 Italicized nuclide symbols and/or capital italic letters are used to distinguish between different nuclides of the same element.

Examples:

$\mathrm{CH_3\text{-}CH_2\text{-}CO\text{-}{}^{18}O\text{-}CH_2\text{-}CH_3}$

^{18}*O*-ethyl ($^{18}\mathrm{O}_1$)propanoate (PIN)

$\mathrm{CH_3\text{-}CH_2\text{-}C{}^{18}O\text{-}O\text{-}CH_2\text{-}CH_3}$

O-ethyl ($^{18}\mathrm{O}_1$)propanoate (PIN)

$\mathrm{CH_3\text{-}O\text{-}CO\text{-}{}^{18}O\text{-}CH_2\text{-}CH_3}$

^{18}*O*-ethyl *O*-methyl ($^{18}\mathrm{O}_1$)carbonate (PIN)

$\mathrm{CH_3\text{-}CH_2\text{-}O\text{-}C{}^{18}O\text{-}{}^{18}O\text{-}CH_3}$

O-ethyl ^{18}*O*-methyl ($^{18}\mathrm{O}_2$)carbonate (PIN)

P-83 Isotopically labeled compounds

An isotopically labeled compound is a mixture of isotopically unmodified compound with one or more analogous isotopically substituted compound(s).

Although an isotopically labeled compound is really a mixture as far as chemical identity is concerned (in the same way as is an unmodified compound), for nomenclature purposes, such mixtures are called ‘isotopically labeled’ compounds.

P-83.1 Specifically labeled compounds

An isotopically labeled compound is designated as ‘specifically labeled’ when a unique isotopically substituted compound is formally added to the analogous isotopically unmodified compound. In such a case, both position(s) and number of nuclides are defined.

P-83.1.1 Formulas

The structural formula of a specifically labeled compound is written in the usual way, but with the appropriate nuclide symbol(s) and multiplying subscript enclosed in square brackets, [ ]. The structural formula is written in the same way as that of an isotopically substituted compound.

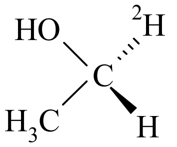
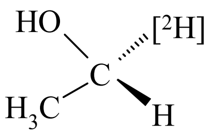
Although the formula for a specifically labeled compound does not represent the composition of the bulk material, which usually consists overwhelmingly of the isotopically unmodified compound, it does indicate the presence of the compound of chief interest, the isotopically substituted compound.

Examples:

Isotopically substituted compound	when added to	Isotopically unmodified compound	gives rise to	Specifically labeled compound
$^{13}CH_4$		CH_4		$[^{13}C]H_4$
$CH_2{}^2H_2$		CH_4		$CH_2[^2H_2]$

All structures of isotopically labeled compounds are identical to those given in Section P-8.2 for isotopically substituted compounds, but include the brackets around the nuclide.

Examples:

Formulas of isotopically substituted compounds	Formulas of specifically labeled compounds
$CH_3\text{-CO-NH}^2H$	$CH_3\text{-CO-NH}[^2H]$
	
$C^2H_3\text{-CO-}C^2H_2\text{-}CH_2\text{-}CH_3$	$C[^2H_3]\text{-CO-}C[^2H_2]\text{-}CH_2\text{-}CH_3$

P-83.1.1 A specifically labeled compound is

(a) singly labeled when the isotopically substituted compound has only one isotopically modified atom.

Example:

$CH_3\text{-}CH[^2H]\text{-}OH$

(b) multiply labeled when the isotopically substituted compound has more than one modified atom of the same element at the same position or at different positions.

Examples:

$CH_3\text{-}C[^3H_2]\text{-}OH$ and $CH_2[^2H]\text{-}CH[^2H]\text{-}OH$

(c) mixed labeled when the isotopically substituted compound has more than one kind of modified atom.

Example:

$CH_3\text{-}CH_2\text{-}[^{18}O][^2H]$

P-83.1.3 Names

The name of a specifically labeled compound is formed by inserting in square brackets, [ ], the nuclide symbol(s) preceded by any necessary locants before the name or preferably before the denomination of that part of the compound that is isotopically modified. When polylabeling is possible, the number of atoms that have been labeled is always specified as a subscript to the atomic symbol(s) even in the case of monolabeling. This is necessary in order to distinguish between a specifically and a selectively or nonselectively labeled compound.

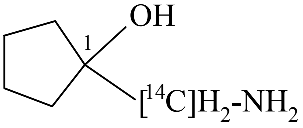
All rules given in P-10.2 to construct names of isotopically substituted compounds are applicable to construct names of specifically labeled compounds, with the exception that parentheses are used around complex prefixes when the isotopic descriptor is placed in brackets.

Examples:

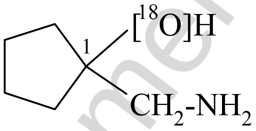
$[^{13}C]H_4$
$[^{13}C]$methane (PIN)

$CH_3[^2H]$
$[^2H_1]$methane (PIN)

$C[^2H_2]Cl_2$
dichloro$[^2H_2]$methane (PIN)



1-(amino$[^{14}C]$methyl)yclopentan-1-ol (PIN)



1-(aminomethyl)cyclopentan-1-$[^{18}O]$ol (PIN)

P-83.2 Selectively labeled compounds

An isotopically labeled compound is designated as selectively labeled when a mixture of isotopically substituted compounds is formally added to the analogous isotopically unmodified compound in such a way that the position(s) but not necessarily the number of each labeling nuclide is defined. A selectively labeled compound may be considered as a mixture of specifically labeled compounds. A selectively labeled compound may be:

(a) multiply labeled when in the unmodified compound there is more than one atom of the same element at the position where the isotopic modification occurs, for example H, in CH_4; or there are several atoms of the same element at different positions where the isotopic modification occurs, for example C, in C_4H_8O;

(b) mixed labeled when there is more than one labeling nuclide in the compound, for example, C and O in CH_3-CH_2-OH.

When there is only one atom of an element that can be modified in a compound, only specific labeling can result.

P-83.2.1 Formulas

P-83.2.1.1 A selectively labeled compound cannot be described by a unique structural formula; therefore it is represented by inserting the nuclide symbol(s) preceded by any necessary locant(s) (letters and/or numbers) but without multiplying subscripts, enclosed in square brackets, [ ], directly before the usual formula or, if necessary, before parts of the formula that have an independent numbering. Identical locants are not repeated. When different nuclides are present, the nuclide symbols are written in alphabetical order according to their symbols, or when the atomic symbols are identical, in order of increasing mass number.

Examples:

Mixture of isotopically substituted compounds	when added to	Isotopically unmodified compound	gives rise to	Selectively labeled compound
$CH_3{}^2H$, $CH_2{}^2H_2$ CH^2H_3, C^2H_4 or any two or more of the above		CH_4		$[^2H]CH_4$
$\overset{4}{CH_3}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH^2H}\text{-}\overset{1}{COOH}$ $\overset{4}{CH_3}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{C^2H_2}\text{-}\overset{1}{COOH}$		$CH_3\text{-}CH_2\text{-}CH_2\text{-}COOH$		$[2\text{-}^2H]\overset{4}{CH_3}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{COOH}$
$\overset{4}{CH_3}\text{-}\overset{3}{^{14}CH_2}\text{-}\overset{2}{^{14}CH_2}\text{-}\overset{1}{COOH}$ $\overset{4}{CH_3}\text{-}\overset{3}{^{14}CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{COOH}$ $\overset{4}{CH_3}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{^{14}CH_2}\text{-}\overset{1}{COOH}$ or any two of the above		$CH_3\text{-}CH_2\text{-}CH_2\text{-}COOH$		$[2,3\text{-}^{14}C]\overset{4}{CH_3}\text{-}\overset{3}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{COOH}$
$\overset{2}{CH_3}\text{-}\overset{1}{^{14}CH_2}\text{-}OH$ $\overset{2}{CH_3}\text{-}\overset{1}{CH_2}\text{-}^{18}OH$ $\overset{2}{CH_3}\text{-}\overset{1}{^{14}CH_2}\text{-}^{18}OH$ or any two of the above		$\overset{2}{CH_3}\text{-}\overset{1}{CH_2}\text{-}OH$		$[1\text{-}^{14}C,^{18}O]\overset{2}{CH_3}\text{-}\overset{1}{CH_2}\text{-}OH$
$^{14}\overset{3}{CH_3}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{COO}\text{-}CH_3$ $\overset{3}{CH_3}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{COO}\text{-}^{14}CH_3$ $^{14}\overset{3}{CH_2}\text{-}\overset{2}{CH_2}\text{-}\overset{1}{COO}\text{-}^{14}CH_3$ or any two of the above		$CH_3\text{-}CH_2\text{-}COO\text{-}CH_3$		$[3\text{-}^{14}C]\underset{3}{\overset{3}{CH_3}}\text{-}\underset{2}{\overset{2}{CH_2}}\text{-}\underset{1}{\overset{1}{COO}}\text{-}^{14}C]CH_3$

P-83.2.1.2 In a selectively labeled compound formally arising from mixing several known isotopically substituted compounds with the analogous isotopically unmodified compound, the number or the possible number of labeling nuclide(s) for each position may be indicated by subscripts to the atomic symbol(s).Two or more subscripts referring to the same nuclide symbol are separated by a semicolon. For a multiply labeled or mixed labeled compound, the subscripts are written successively in the same order as the various isotopically substituted compounds are considered. The subscript zero is used to indicate that one of the isotopically substituted is not modified at the indicated position.

Examples:

Mixture of isotopically substituted compounds	when added to	Isotopically unmodified compound	gives rise to	Selectively labeled compound
$\overset{2}{C}H_2{}^2H\text{-}\overset{1}{C}H_2\text{-}OH$ $\overset{2}{C}H^2H_2\text{-}\overset{1}{C}H_2\text{-}OH$		$CH_3\text{-}CH_2\text{-}OH$		$[2\text{-}{}^2H_{1;2}]\overset{2}{C}H_3\text{-}\overset{1}{C}H_2\text{-}OH$
$\overset{2}{C}H^2H_2\text{-}\overset{1}{C}H_2\text{-}OH$ $\overset{2}{C}H^2H_2\text{-}\overset{1}{C}H_2\text{-}{}^{18}OH$		$CH_3\text{-}CH_2\text{-}OH$		$[2\text{-}{}^2H_{2;2},{}^{18}O_{0;1}]\overset{2}{C}H_3\text{-}\overset{1}{C}H_2\text{-}OH$

P-83.2.2 Names

The name of a selectively labeled compound is formed in the same way as the name of a specifically labeled compound, except that the multiplying subscripts following the atomic symbols are generally omitted. Identical locants corresponding to the same element are not repeated. The name of a selectively labeled compound differs from the name of the corresponding isotopically substituted compound in the use of square brackets, [ ], surrounding the nuclide descriptor rather than parentheses and in the omission of repeated identical locants and multiplying subscripts.

Examples:

Mixture of isotopically substituted compounds	when added to	is named
$CH_3{}^2H$, $CH_2{}^2H_2$ $CH{}^2H_3$, C^2H_4	CH_4	[^{2}H]methane (PIN) (not [$^2H_4$]methane)
$\overset{2}{C}H_3-\overset{1}{C}H{}^2H-OH$ $\overset{2}{C}H_3-\overset{1}{C}{}^2H_2-OH$	CH_3-CH_2-OH	[1-^{2}H]ethanol (PIN) (not [1,1-$^2H_2$]ethanol)
${}^{14}\overset{3}{C}H_3-\overset{2}{C}H_2-\overset{1}{C}OO-CH_2-CH_3$ $\overset{3}{C}H_3-\overset{2}{C}H_2-\overset{1}{C}OO-{}^{14}CH_2-CH_3$	$CH_3-CH_2-COO-CH_2-CH_3$	[1-^{14}C]ethyl [3-^{14}C]propanoate (PIN)
$\overset{2}{C}H_2{}^2H-\overset{1}{C}H_2-OH$ $\overset{2}{C}H{}^2H_2-\overset{1}{C}H_2-OH$	CH_3-CH_2-OH	[2-$^2H_{1;2}$]ethanol (PIN)
$\overset{2}{C}H{}^2H_2-\overset{1}{C}H_2-OH$ $\overset{2}{C}H{}^2H_2-\overset{1}{C}H_2-{}^{18}OH$	CH_3-CH_2-OH	[2-$^2H_{2;2}$,$^{18}O_{0;1}$]ethanol (PIN)

P-83.3 Nonselectively labeled compounds

P-83.3.1 An isotopically labeled compound is designated as nonselectively labeled when the position(s) and the number of the labeling nuclide(s) are both undefined.

When only atoms of an element to be modified are present at the same position in a compound, only specific or selective labeling can result. Nonselective labeling requires that the element to be modified be at different positions in the structure. For example, CH_4 and $CCl_3-CH_2-CCl_3$ can only be specifically or selectively labeled with a hydrogen isotope.

P-83.3.2 Formulas

Nonselective labeling is indicated in a formula by inserting the nuclide symbol, enclosed in brackets, directly before the line formula without locants or subscripts.

Example:

$$[^{13}C]CH_3-CH_2-CH_2-COOH$$

P-83.3.3 Names

The name of a nonselectively labeled compound is formed in the same way as the name of a selectively labeled compound but contains neither locants nor subscripts in the nuclide descriptor.

Examples:

chloro[^{3}H]benzene (PIN)

[^{13}C]glycerol (PIN)

P-83.4 Isotopically deficient compounds

P-83.4.1 An isotopically labeled compound may be designated as isotopically deficient when the isotopic content of one or more element has been depleted, i.e. when one or more nuclide(s) is(are) present in less than the natural ratio.

P-83.4.2 Formulas

Isotope deficiency is denoted in the formula by adding the italicized symbol '*def*' immediately preceding and without a hyphen, the appropriate nuclide symbol.

Example:

[def^{13}C]$CHCl_3$

P-83.4.3 Names

The name of an isotopically deficient compound is formed by adding the italicized symbol *def* immediately preceding and without a hyphen, the appropriate nuclide symbol, both enclosed in brackets and cited before the name or the part of the name that is isotopically modified.

Example:

trichloro[def^{13}C]methane (PIN)
[def^{13}C]chloroform

P-8.4 Comparative Examples of Formulas and Names of Isotopically Modified Compounds

Table 8.1 Comparative examples of Formulas and names of isotopically modified compounds

Types of compounds	Formula	Name
Unmodified	$CH_3\text{-}CH_2\text{-}OH$	Ethanol (PIN)
Isotopically substituted	$\overset{2}{C}{}^2H_3\text{-}\overset{1}{C}H_2\text{-}O^2H$	(2,2,2-$^2H_3$)ethan(^2H)ol (PIN) (*O*,2,2,2-$^2H_4$)ethanol (PIN)
Specifically labeled	$\overset{2}{C}[^2H_2]\text{-}\overset{1}{C}H_2\text{-}O[^2H]$	[2,2,2-$^2H_3$]ethan[^2H]ol (PIN) [*O*,2,2,2-$^2H_4$]ethanol (PIN)
Selectively labeled	$[O,2\text{-}^2H]\overset{2}{C}H_3\text{-}\overset{1}{C}H_2\text{-}OH$	[*O*,2-^2H]ethanol (PIN)
	$[2\text{-}^2H_{2;2},{}^{18}O_{0;1}]\underset{2}{C}H_3\text{-}\underset{1}{C}H_2\text{-}OH$	[2-$^2H_{2;2}$,$^{18}O_{0;1}$]ethanol (PIN)
Nonselectively labeled	$[^2H]CH_3\text{-}CH_2\text{-}OH$	[^2H]ethanol (PIN)
Isotopically deficient	$[def\,^{13}C]CH_3\text{-}CH_2\text{-}OH$	[*def*^{13}C]ethanol (PIN)

CHAPTER 9 SPECIFICATION OF CONFIGURATION AND CONFORMATION

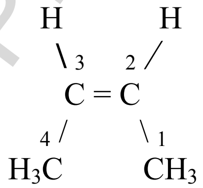
P-90 Introduction

This section is concerned only with the main principles for specification of configuration and conformation of organic compounds. The spatial structure of an organic compound is systematically indicated by one or more affixes added to a name that does not itself prescribe stereochemical configuration or conformation; such affixes are generally called stereodescriptors. Thus stereoisomers, such as *cis*/*trans* isomers and enantiomers, have names that differ only in the stereodescriptors used. By contrast, certain retained names imply their own stereochemical description, for example, maleic acid (recommended only for general nomenclature), cholesterol and other natural products described in Chapter 10 that are used as preferred IUPAC names or recommended only for general nomenclature.

In order to arrive at a non-ambiguous description of stereoisomers, Cahn, Ingold and Prelog (ref. 30, 31, 32) recommended an order of seniority for the atoms and groups attached to carbon and other atoms, which is commonly called the CIP priority system. The priority is established by the application of ‘sequence rules’. As these rules are fundamental to describe both *cis* and *trans* isomers and enantiomers, they are discussed in the first section of this chapter. Their application is then described for stereogenic units, mainly for the most usual compounds, synthetic or natural, encountered in organic chemistry

When different stereodescriptors are recommended to describe *cis* and *trans* isomers, diastereoisomers, and enantiomers, one of them is recommended as a preferred stereodescriptor. This preferred stereodescriptor is used to generate a preferred IUPAC name. Obviously, in general nomenclature, any appropriate descriptor can be used.

Example:

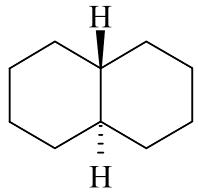


$$\begin{array}{ccc} H & & H \\ \backslash_{3} & & {}_{2}/ \\ & C = C & \\ {}_{4}/ & & \backslash_{1} \\ H_3C & & CH_3 \end{array}$$

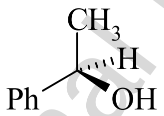
(2*Z*)-but-2-ene (PIN)
cis-but-2-ene

Structural diagrams which depicts tridimensional structures must be prepared with extra care to ensure there is no ambiguity. In general, normal lines depict bonds approximately in the plane of the drawing; bonds to atoms above the plane are shown with a bold wedge ◀ (starting from an atom in the plane of the drawing at the narrow end of the wedge); and bonds to atoms below the plane are shown with a hashed wedge '''''' which is used with the understanding that the narrow end of the wedge begins at the atom in the plane of the drawing. This system is used in the recommendations in this book. A guide to graphic representation of tridimensional structures has been published along with the basic terminology of stereochemistry (ref. 33). In that publication, an alternative to the hashed wedge has been proposed which uses short parallel lines; however, it must be noted that this is not a symbol in many chemical structure drawing programs. A broken line - - - - has been used instead of hashed wedge but this is better reserved for a partial bond, delocalization, or a hydrogen bond. When the configuration of a bond is unknown this can be shown explicitly by a wavy line ∿∿∿ . The use of dots or open circles at a center to show configuration is strongly deprecated.

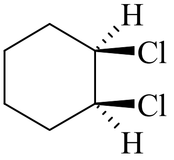
Strict rules for drawing configuration are not possible. In general it is most clear if all rings of an *ortho*-fused ring system (or saturated derivatives) are kept in the plane and bridgehead substituents are shown above or below the plane **(1)**. With an acyclic structure **(2)** or other substituent on a ring **(3)** [(including bridges **(4)**] bonds are shown as above or below the plane. Hydrogen atoms attached to stereochemically designated positions should not be omitted **(3)**.



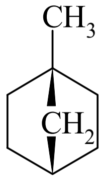
(1)



(2)

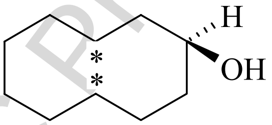


(3)

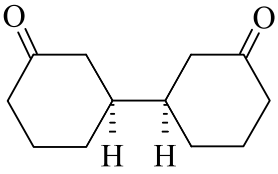


(4)

The configuration due to substituents attached to a ring should not be shown at a reentrant angle(marked with an asterisk on **(5)**, although this is suitable for a carbonyl group or *N*-methyl group). Any bond between two stereochemically designated positions should be left plane **(6)**.

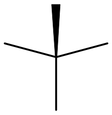


(5)

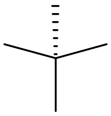


(6)

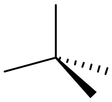
For tetrahedral configuration the following are recommended:



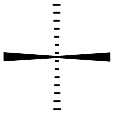
or



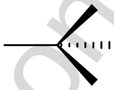
or



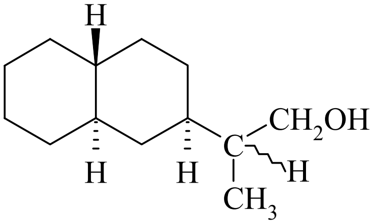
may also be



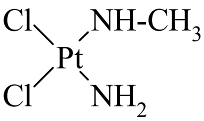
or



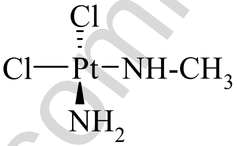
A wavy line can be used to indicate either that the configuration is unknown **(7)** but only one form is present, or if explained in the text that both isomers are present and will be defined when required. If it is intended not to show any configuration it is best to only use plain lines for all bonds. Note that the planar molecule **(8)** can also be drawn as **(9)** or **(10)**.



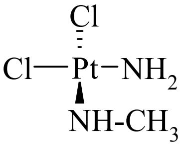
(7)



(8)

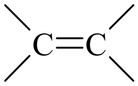


(9)

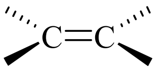


(10)

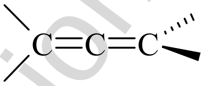
Double bonds should be shown as far as possible with accurate angles (*ca* 120°) when configuration is implied [**(11)**,**(12)**,**(13)**]. To show the absence of any configurational information a linear representation should be used [see **(14)**,**(15)**,**(16)**].



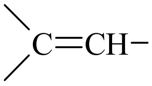
(11)



(12)



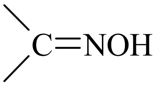
(13)



(14)

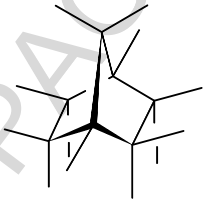
$-HC{=}CH-$

(15)

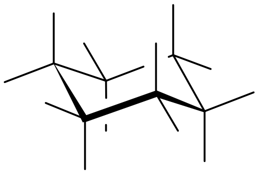


(16)

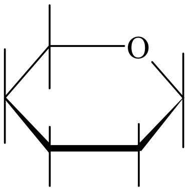
In a perspective drawing it is preferable to indicate which edge of the ring is considered in front by bold or wedge lines as in **(17)**, **(18)**, and **(19)** and 'breaking' the bond at the back when a bond passes in front, as in **(17)** and **(18)**. In this type of configurational representation bonds to substituents should usually be left plain.



(17)



(18)



(19)

P-91 Enantiomers and *cis*-*trans* isomers

P-91.1 Enantiomers: the CIP priority system

P-91.1.1 The CIP priority system

This Section describes the CIP priority system which was developed to deal with all compounds with a bonding number up to six for organic compounds, and for all configurations and conformations of these compounds (ref. 30, 31, 32). Its description for specifying configurations and conformations is discussed herein.

Chirality is the property of an object, thus of a molecular entity, of being non-superposable on its mirror image. If the object (molecular entity) is superposable to its mirror image, it is said to be ‘achiral’.

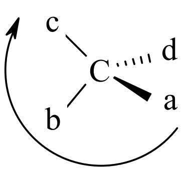
The CIP system is based on rules and a strict hierarchical order of decisions until a single stereodescriptor can be used to describe a given configuration.

For tetrahedral stereogenic atoms having four different atoms or groups, the chirality rule is based on the arrangement of these atoms or groups (including chains and rings) in an order of precedence, often referred to as an order of priority. For discussion this order can conveniently be generalized as ‘a’ > ‘b’ > ‘c’ > ‘d’, where > denotes ‘has priority over’ or ‘has precedence over’. The order of precedence is reached by the application of the sequence rules using specific and hierarchical digraphs as explained below.

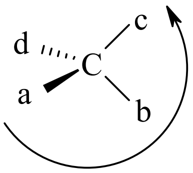
In inorganic terminology, the term ‘ligand’ is defined as ‘the atoms or groups joined to the central atom in an inorganic coordination entity’ (ref. 14). Thus, for organic compounds, the term ligand is inappropriate to describe the atoms or groups attached to an atom of a stereogenic unit. The expression ‘atom or group’ will be used. The terms derived from ‘ligand’ such as ligancy and tetraligancy that are widely used in reference to the CIP system, are replaced by valence and tetravalence.

The chirality rule is expressed by Prelog and Helmchen (ref. 32) as follows: ″Among ligands of highest precedence the path of their sequence is followed from their preferred side of the model, that is, the side remote from the group of lowest precedence, and, depending on whether the path turns to right or left, the chirality unit will be assigned the chiral label *R* or *S*.″

For ‘a’ > ‘b’ > ‘c’ > ‘d’:



R



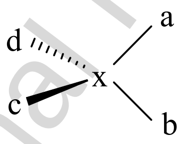
S

P-91.1.1.1 Stereogenic units

A stereogenic unit (i.e. a unit generating stereoisomerism) is a grouping within a molecular entity that may be considered a focus for stereoisomerism. At least one stereogenic unit must be present in every enantiomer; however, conversely, the presence of stereogenic units does not require the corresponding molecular entity to be chiral. Three basic types of stereogenic units in molecular entities involving atoms having not more than four substituents are considered below:

(a) A grouping of atoms consisting of a central atom (X) and distinguishable atoms or groups (‘a’, ‘b’, ‘c’, ‘d’), so that the interchange of any two of the atoms or groups ‘a’, ‘b’, ‘c’, and ‘d’, leads to a stereoisomer. A chirality center, formerly known as an ‘asymmetric atom’, is the classical example of a stereogenic unit.

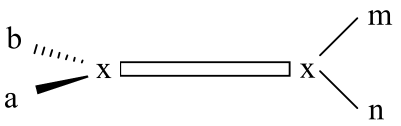
Example:



R for ‘a’ > ‘b’ > ‘c’ > ‘d’

(b) A chain of four noncoplanar atoms (or rigid groups) in a stable arrangement, such that an imaginary or real (restricted) rotation (with a change of sign of torsion angle) about the central bond leads to a stereoisomer.

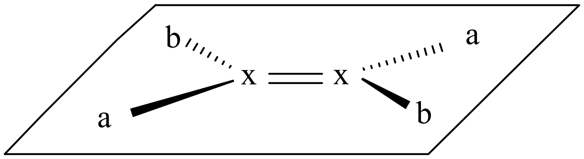
Example:



R_a or *M* for ‘a’ > ‘b’ and ‘m’ > ‘n’ (m and n = or ≠ ‘a’ and ‘b’)

c) A grouping of atoms consisting of a double bond with substituents which give rise to *cis*-*trans* isomerism.

Example:



E for ‘a’ > ‘ b’

P-91.1.1.2 The ‘Sequence Rules’

The following ‘Sequence Rules’ are used (ref. 30, 31, 32) to establish the order of precedence of atoms and groups. A more encompassing set of rules, proposed by Mata, Lobo, Marshall, and Johnson (ref. 34), including amendments by Custer (ref. 35), Hirschmann and Hanson (ref. 36), is used in this Chapter. The rules are hierarchical, i.e., each rule must be exhaustively applied in the order given until a decision is reached:

Rule 1 (a) Higher atomic number precedes lower;

(b) A duplicated atom, with its predecessor node having the same label closer to the root, ranks higher than a duplicated atom, with its predecessor node having the same label farther from the root, which ranks higher than any nonduplicated-atom-node (proposed by Custer, ref. 36)

Rule 2 Higher atomic mass number precedes lower;

Rule 3 *seqcis* Stereogenic units precede *seqtran*s stereogenic units and these precede nonstereogenic units (*seqcis* > *seqtrans* > *nonstereogeni*). (Proposed by Mata, Lobo, Marshall, and Johnson, ref. 34);

> The domain of application of this rule is restricted to geometrically diastereomorphic planar tetravalent atoms and double bonds. All cases involving geometrically diastereomorphic two-dimensional stereogenic units are considered in Rules 4 and 5. (Proposed by Hirschmann and Hanson, ref. 36).

Rule 4 (a) Chiral stereogenic units precede pseudoasymmetric stereogenic units and these precede nonstereogenic units. (Sub-rule originally proposed by Prelog and Helmchen (ref. 32), but their inclusion as first sub-rule of Rule 4 was proposed by Custer, ref. 35). Geometrically enantiomorphic twodimensional stereogenic units precede two-dimensional nonstereogenic units (Proposed by Mata, Lobo, Marshall and Johnson, ref. 34).

(b) When two ligands have different descriptor pairs, then the one with the first chosen *like* descriptor pairs has priority over the one with a corresponding *unlike* descriptor pair.

(i) *Like* descriptor pairs are: ‘*RR*’, ‘*SS*’, ‘*MM*’, ‘*PP*’, ‘*seqCis/seqCis*’, ‘*seqTran/sseqTrans*’, ‘*RseqCis*’, ‘*SseqTrans*’, ‘*MseqCi*s’, ‘*PseqTrans’*.

(ii) *U*nlike discriptor pairs are '*RS*', '*MP*', '*RP*', '*SM*', '*seqCis/seqTrans*', '*RseqTrans*', '*SseqCis*', '*PseqCis*' and '*MseqTrans*'. (the descriptor pairs '*RRe*', '*SSi*', '*ReRe*', '*SiSi*','*ReM*', '*SiP*', '*ReSi*', '*Rsi*', '*ReP*' and '*MSi*' are not included in this rule (proposed by Mata, Lobo, Marshall and Johnson, ref. 34).

Methodology for pairing descriptors:

The descriptor assigned to geometrically enantiomorphic double bonds should be associated in the digraph with the first node corresponding to the atoms involved in the double bond (proposed by Mata, Lobo, Marshall and Johnson, ref. 34).

For each atom or group the descriptor chosen at first (highest ranked descriptor) is paired with all the remaining descriptors. The following characteristics determine the hierarchical rank of the pairs of descriptors:

(i) higher rank of the second descriptor in the pair;

(ii) lower rank of the least common ancestor in the graph (proposed by Custer, ref. 35).

(c) 'r' Precedes 's' and '*p*' precedes '*m*' (proposed by Mata, Lobo, Marshall and Johnson, ref. 34).

Re-inclusion of this subrule in Rule **4** was proposed by Custer (ref. 35).

Rule 5 An atom or group with descriptor '*R*', '*M*' and '*seqCis*' has priority over its enantiomorph '*S*', '*P*' or '*seqTrans*', '*seqCis*' and '*seqTrans*' (proposed by Hirschmann and Hanson, ref. 36)

These rules are based on the hierarchical order of atoms or groups properties, material and topological properties for rules **1** and **2**, geometrical properties for rules **3** and **4**, and topographical properties for rule **5**. The first four properties are reflection-invariant, the fifth is reflection-variant.

Atoms and groups of atoms are monovalent or divalent as exemplified by 'diyl' groups; they can be acyclic or cyclic.

The five 'Sequence Rules' are applied as follows:

(a) each rule is applied exhaustively to all atoms or groups being compared;

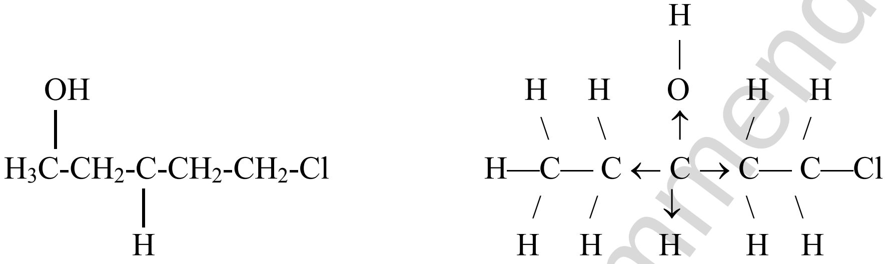
(b) each rule is applied in accordance with a hierachical digraph (see P-91.2)

(c) the atom or group that is found to have precedence (priority) at the first occurrence of a difference in a digraph retains this precedence (priority) regardless of differences that occur later in the exploration of the digraph;

(d) precedence (priority) of an atom in a group established by a rule does not change on application of a subsequent rule.

P-91.1.2 Digraphs

In order to establish the order of precedence of atoms or groups in a stereogenic unit, the atoms of the stereogenic unit are rearranged in a hierarchical diagram, called a ‘digraph’ or a ‘tree-graph’, representing the connectivity (topology) and make-up of atoms; a digraph originates from the core of the stereogenic unit and is developed by indicating the various branches (see section 3, ref. 32) representing atoms or groups of atoms, monovalent or divalent, acyclic or cyclic. A simple example for a stereogenic center follows.



$H_3C\text{-}CH_2\text{-}\overset{OH}{\underset{H}{C}}\text{-}CH_2\text{-}CH_2\text{-}Cl$

a chiral compound and its corresponding digraph

P-91.1.3 Exploration of a hierarchical digraph

Digraphs are constructed to show the ranking of atoms according to the topological distance i.e., number of bonds, from the core of the stereogenic unit (i.e., center) and their evaluation by the sequence rules (see section 3.3, ref. 34).

(a) Atoms lie in spheres and atoms of equal distance from the core of the stereogenic unit are in the same sphere; spheres are identified as **I**, **II**, **III**, and **IV**, as shown in **Fig. 1**. The first sphere is occupied by the ‘proximal atoms’, ‘p’ and ‘p′’. Those in the sphere **II** are numbered 1,2,3 and 1′,2′,3′. Those in sphere **III** are numbered 11, 12, 13, 21, 22, 23,… 11′,12′,13′... and so on for each further sphere. Indicated branches may not be present in all molecules.

(b) Atoms in the n^{th} sphere have precedence over those in the (n + 1)th sphere. (Ranking Rule **1**).

(c) The ranking of each atom in the n^{th} sphere depends in the first place on the ranking of atoms of the same branch in (n − 1)th sphere, and then by the application of the Sequence Rules to it; the smaller the number, the higher the relative ranking. (Ranking Rule **2**).

(d) Those atoms in the n^{th} sphere which are of equal rank to those in the (n − 1)th sphere in the same branch are ranked by means of the sequence rules, first by the exhaustive application of Sequence Rule **1**; if no decision is reached, Sequence Rule **2** is exhaustively applied, and so on.

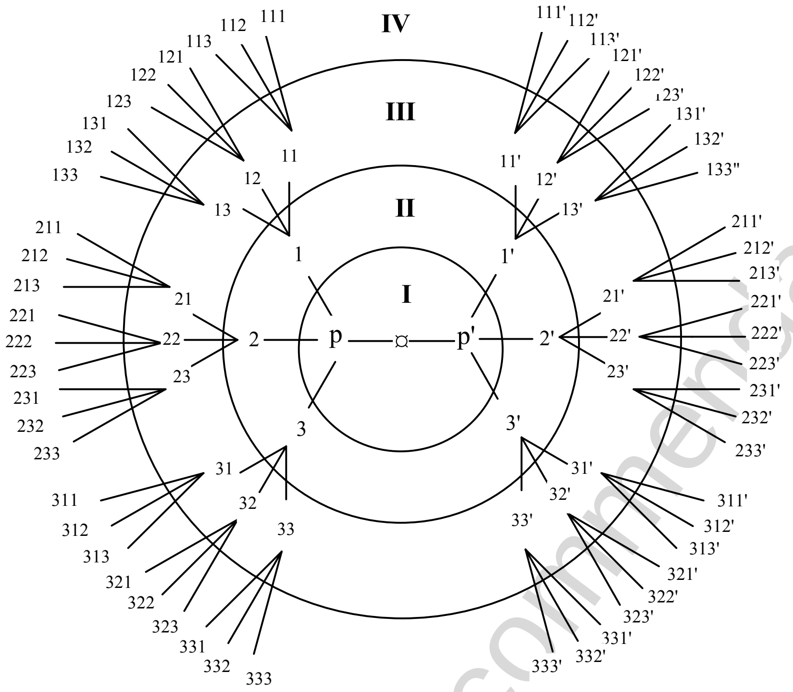


Fig. 1 Ranking order of two ligands

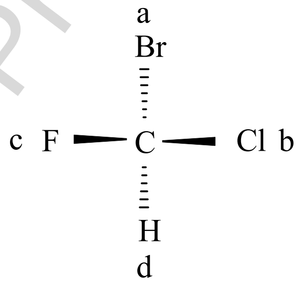
P-91.1.4 Application of Sequence Rule 1 to tetravalent systems

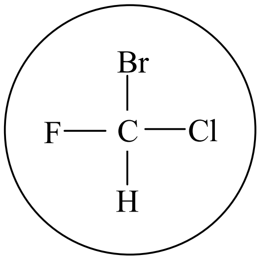
P-91.1.4.1 Sequence Rule **1** is expressed as follows: atoms or groups are arranged in order of decreasing atomic number.

Atoms or groups ‘a’, ‘b’, ‘c’, and ‘d’ are ranked stepwise, by a procedure called the ‘ranking procedure’ that always starts at the atom to be specified and proceeds further away until a decision is reached. The comparison of atoms starts at sphere **I** and proceeds to sphere **II** if a decision is not reached, and so on.

P-91.1.4.1.1 Analysis of sphere I

In the compound HCBrClF, below, all atoms are included in sphere I.





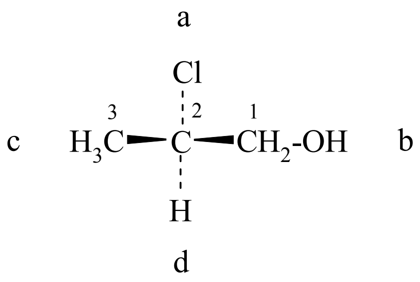
The order ‘a’ > ‘b’ > ‘c’ > ‘d’ is, in accordance with Sequence Rule **1**, i.e, Br > Cl > F > H.

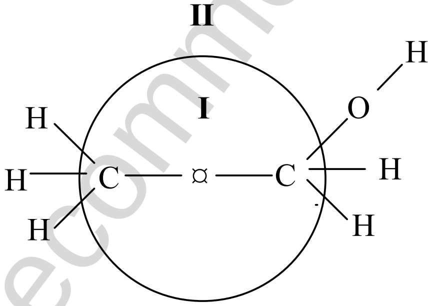
P-91.4.1.2 Analysis of spheres **I** and **II**

When atoms attached to the stereogenic unit are identical, precedence is established by the atoms in turn that are directly attached to the identical atoms. When the molecule contains several atoms and branches, it is convenient to number it, either by using the numbering system recommended in nomenclature or by applying an arbitrary system to properly identify all atoms appearing in the digraph.

Example 1:

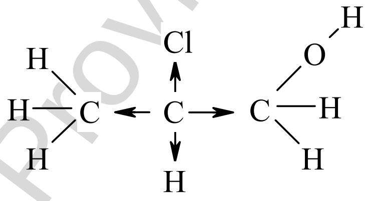
In the compound H_3C-CHCl-CH_2OH, below, the order of seniority for 'a' > 'b' > 'c' > d is Cl > C and C > H. No decision is attained in sphere **I**, as the two proximate atoms are identical.



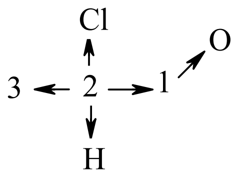


In sphere **II**, however, the atoms attached to the two carbon atoms are (O,H,H) and (H,H,H), respectively, and, as O > H, the order of precedence is 'b' > 'c' and hence the group –CH_2OH is 'b' and the group –CH_3 is 'c'.

Different types of digraphs may be used, the so called complete hierarchical digraph and the simplified hierarchical digraph based on the numbering of the structure. For the compound 2-chloropropan-1-ol, below, the complete hierarchical digraph and the simplified hierarchical digraph are shown:

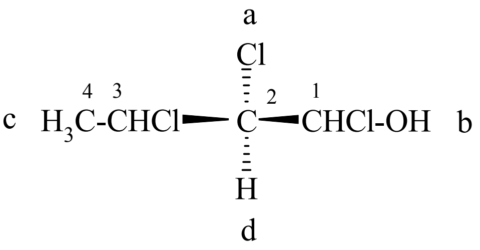


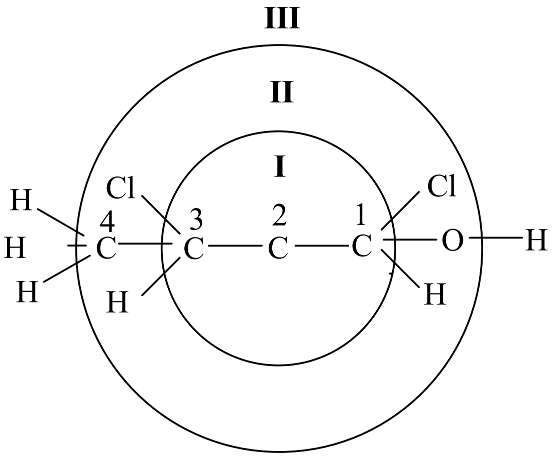
the complete hierarchical digraph

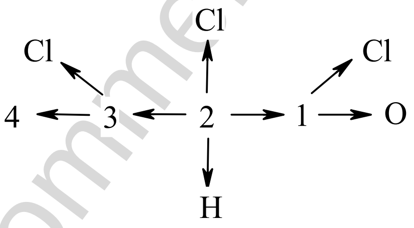


a simplified hierarchical digraph

Example 2:





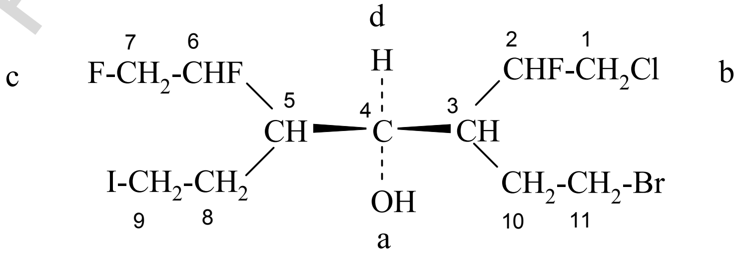


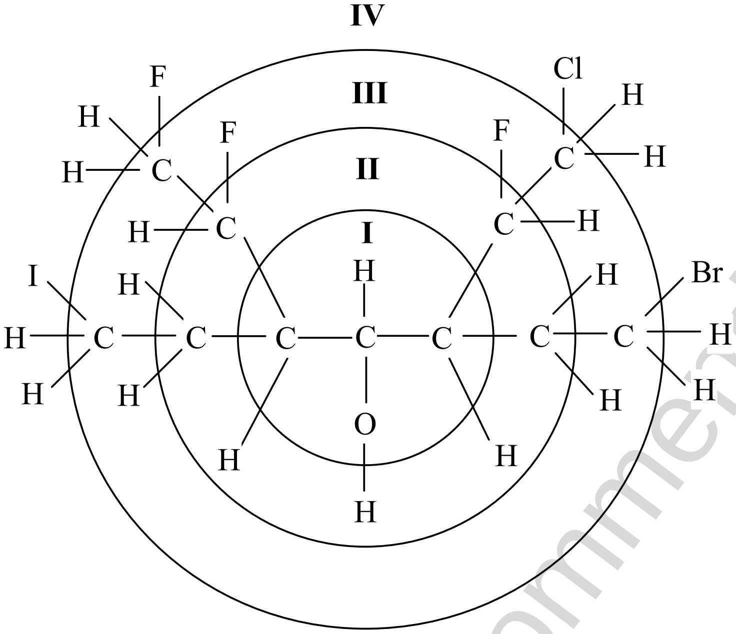
In this example, Sequence Rule **1** establishes the seniority order Cl > C > C > H in sphere **I**; but no decision between ‘b’ and ‘c’ can reached. However, in sphere **II**, the atoms attached to the carbon atoms 1 and 3 are (Cl,O,H) and (Cl,C,H), respectively. The comparison of the two senior atoms in each set, Cl atoms, does not permit a choice to be made; however, comparison of the two second atoms in the set O and C, respectively, establishes the order O > C and thus the group –CHCl-OH is ‘b’ and the group $-CHCl-CH_3$ is ‘c’.

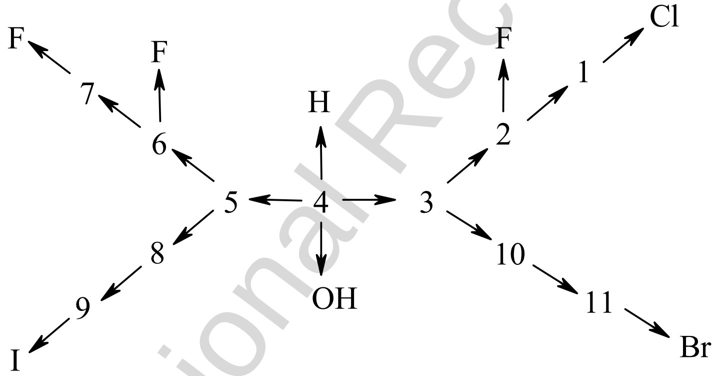
P-91.1.4.1.3 Analysis of spheres I, II, III and IV

When choices remain after evaluating the second level, the exploration procedure is continued farther away from the stereogenic center.

Example:







The first level of the exploration, sphere **I**, leads to O > C and C > H, but no decision can be made between the carbon atoms. And, in sphere **II**, still no decision can be made, because of the two identical sets of (C,C,H) atoms attached to carbon atoms. In sphere **III**, the two branches on the left hand side are ranked (F,C,H) > (C,H,H); on the right hand side, the two branches are ranked (F,C,H) > (C,H,H). However, still no decision can be made, but the two branches can be ranked giving precedence to the branches denoted by (F,C,H) over (C,H,H). Then, in sphere **IV**, the two branches having precedence are examined and a decision is reached, because (Cl,H,H) has precedence over (F,H,H). Accordingly, the branch on the right hand side is assigned the priority ‘b’ and the branch on the left gets priority ‘c’. The fact that, in the branches of lower precedence in sphere **III**, the iodine and Br atoms have priority over Cl and F are not taken into consideration, because a decision has already been reached.

P-91.1.4.1.4 Higher levels

After the fourth level, exploration is continued in the same manner until a decision can be made.

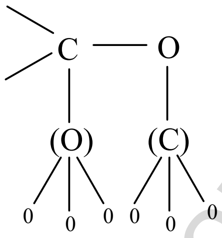
P-91.1.4.2 Duplicate atoms and phantom atoms

There is no difficulty in the expression of the connectivity between the various atoms used in a digraph.of atoms or groups when they are monovalent. A special interpretation is necessary to treat multiple bonds, saturated and mancude rings and ring systems, and lone pairs of electrons in order to maintain the tetravalency indispensable to the application of the sequence rules.

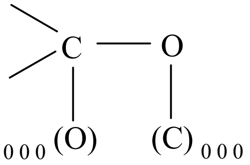
P-91.1.4.2.1 Treatment of double and triple bonds
P-91.1.4.2.2 Treatment of saturated rings and ring systems
P-91.1.4.2.3 Treatment of mancude rings and ring systems
P-91.1.4.2.4 Treatment of tetrahedral systems including a pair of electrons

P-91.1.4.2.1 Treatment of double and triple bonds

When double and triple bonds have to be considered, as in the groups >C=O and −C≡N, the multiple bonds are split into two and three single bonds respectively. A >C=O group is treated as

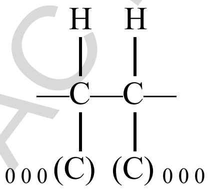


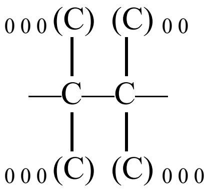
or

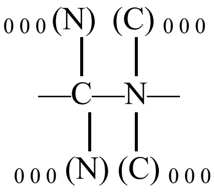


where the (O) and (C) are duplicate representations of the atoms at the other end of the double bond. Each real atom, except for hydrogen, and each duplicated atom is converted to single bond tetracovalency by adding ‘phantom atoms’, i.e. imaginary atoms having an atomic number of zero. Duplicate atoms are denoted in parentheses; ‘phantom atoms’ are denoted by the cipher zero, which often is shown as a subscript.

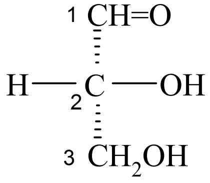
Similarly, −CH=CH–, −C≡C–, and −C≡N are treated as follows, respectively:

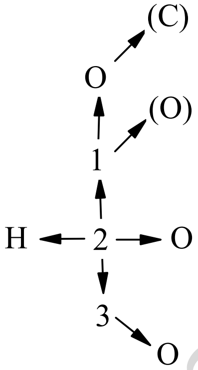






Example:

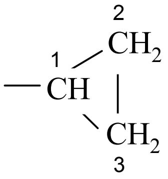


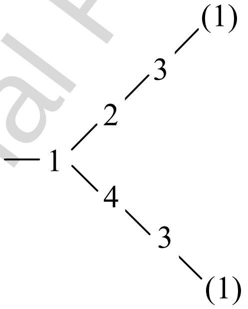


The priority order is O > C and C > H in accordance with Sequence Rule **1**. The priority order is (O,O,H) for the –CH=O group and (O,H,H) for the $–CH_2OH$ group; thus, –CH=O > $–CH_2OH$.

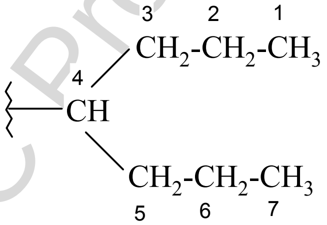
P-91.1.4.2.2 Treatment of saturated rings and ring systems

Saturated rings are opened and treated as branched chains. In order to arrive at a decision, the ranking operation is pursued until an atom already involved in the exploration is reached. This atom is considered as a 'duplicate atom' to which 'phantom atoms' are attached. In the examples, the symbol '>' means 'has precedence over' in Sequence Rule terminology.

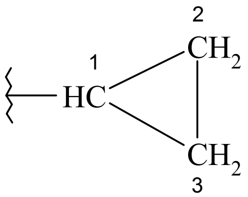


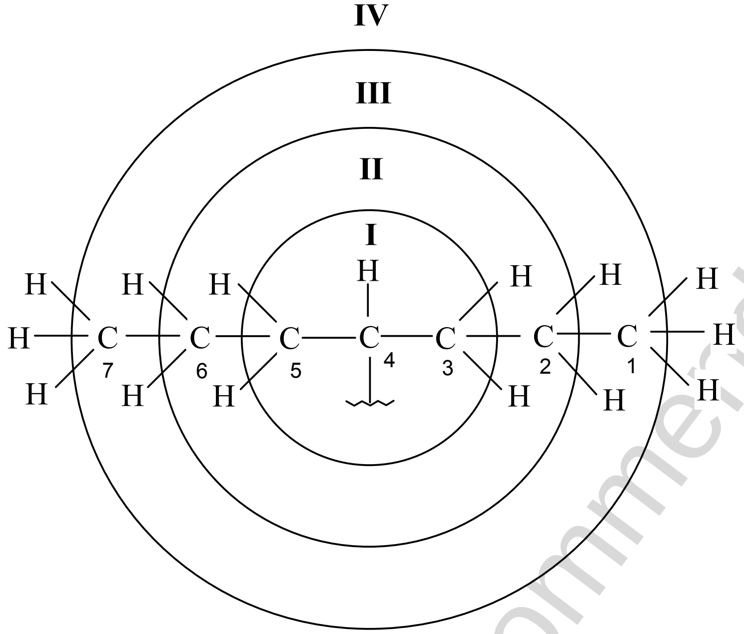


Example 1:

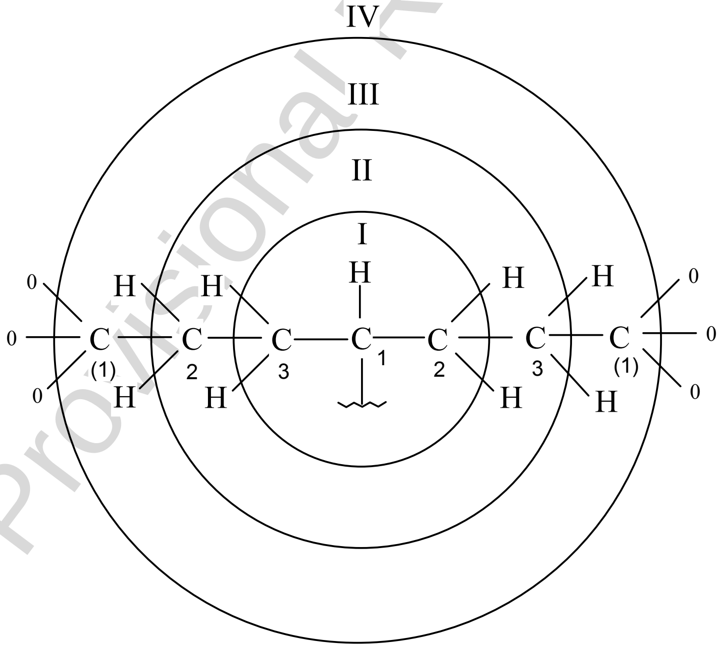


>





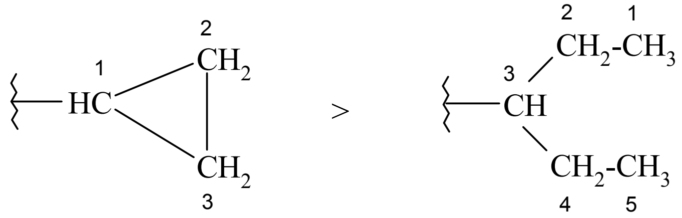
Digraph of heptan-4-yl showing the hydrogen atoms in sphere IV

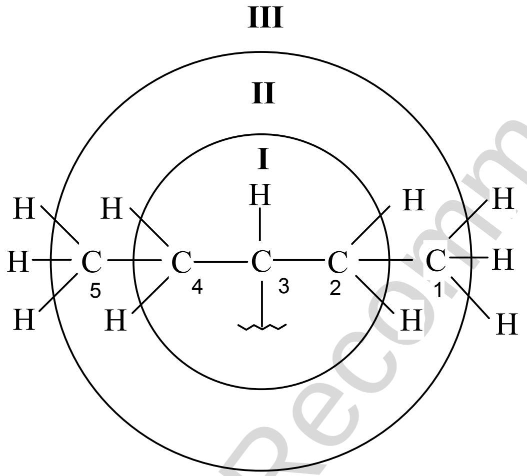


Digraph of cyclopropyl showing phantom atoms in sphere IV

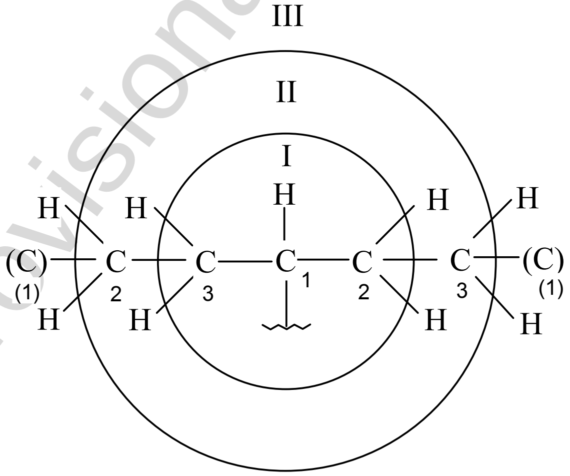
Since real hydrogen atoms have priority over phantom atoms, heptan-4-yl has Sequence Rule precedence over cyclopropyl.

Example 2:





Digraph of pentan-3-yl showing the hydrogen atoms in sphere III

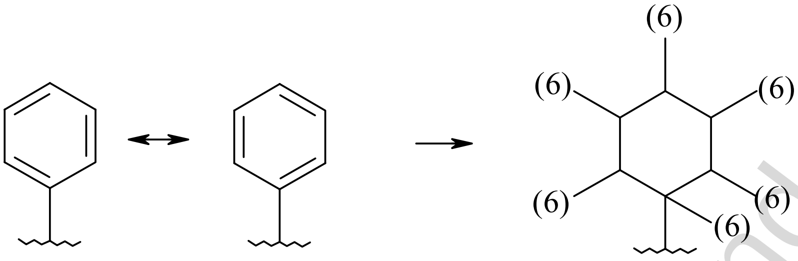


Digraph of cyclopropyl showing duplicate carbon atoms in sphere III

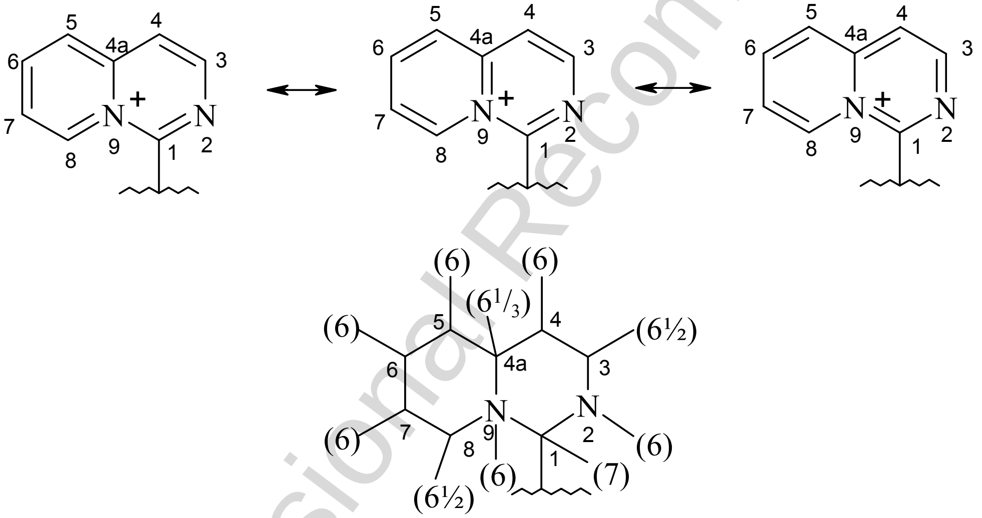
P-91.1.4.2.3 Treatment of mancude rings and ring systems

Mancude rings, i.e., rings or ring systems having the maximum number of noncumulative double bonds, are treated as Kekulé structures. For mancude hydrocarbons, it is immaterial which

Kekulé structure is used because 'splitting' the double bonds give the same result in all cases. The atomic number 6 is always present, as exemplified for a phenyl group:



For mancude heterocycles, each duplicate atom is given an atomic number that is the mean of what it would have if the double bonds were located at each of the possible positions. A complete case is illustrated.

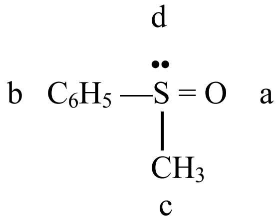


Explanation: C-1 is doubly bonded to one or the other of their nitrogen atoms and never to carbon, so its added duplicate atom has an atomic number '7' (that of nitrogen). C-3 is doubly bonded either to C-4 (atomic number 6) and to N-2 (atomic number 7); so its added duplicate atom has an atomic number of '6½'; as it is for C-8. But C-4a may be doubly bonded to C-4, C-5 and N-9; so its added duplicate atom has an atomic number of '$6^1/_3$'.

P-91.1.4.2.4 Treatment of tetrahedral systems having a pair of electrons

A lone pair of electrons on an atom such as nitrogen or sulfur has the fictitious atomic number of zero. It is thus ranked lower than a hydrogen atom.

Example:



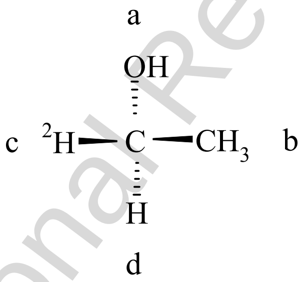
$C_6H_5{-}\overset{\bullet\bullet}{S}(CH_3){=}O$

Explanation: The ranking order ‘a’ > ‘b’ > ‘c’ > ‘d’ is O > $-C_6H_5$ > $-CH_3$ > lone pair of electrons (atomic number = zero). The ‘double bond’ S=O is not duplicated; it is part of the tetrahedral structure that includes the nonbonded electron pair.

P-91.1.5 Sequence Rule **2**

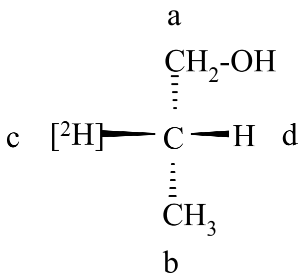
When isotopes are present in a chiral center, Sequence Rule **1** is first applied ignoring isotopic differences between otherwise identical atoms or groups; no decision can be reached. Isotopes are then taken into consideration; they are arranged in decreasing order of their atomic mass, i.e. ^3H > ^2H > ^1H (or H).

Example 1:



The ranking order, ‘a’ > ‘b’ > ‘c’ > ‘d’, after application of Sequence Rule **1** followed by Sequence rule **2**, is O > C > ^2H > H

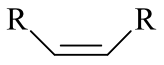
Example 2:



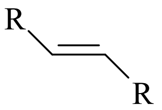
The ranking order ‘a’ > ‘b’ > ‘c’ > ‘d’, after application of Sequence Rules **1** followed by Sequence Rule **2**, is CH_2-OH > CH_3 < [^2H] > H

P-91.2 *cis*/*trans*-Isomers

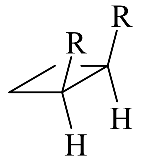
cis/trans-Stereoisomerism is the relationship between isomers which differ in the position of atoms or groups relative to a reference plane: in the *cis*-isomer the atoms or groups are on the same side of the reference plane, in the *trans*-isomer they are on opposite sides. This type of isomerism is encountered in double bonds and in cycloalkanes and their hetero analogues.



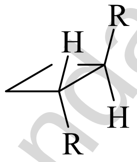
cis



trans



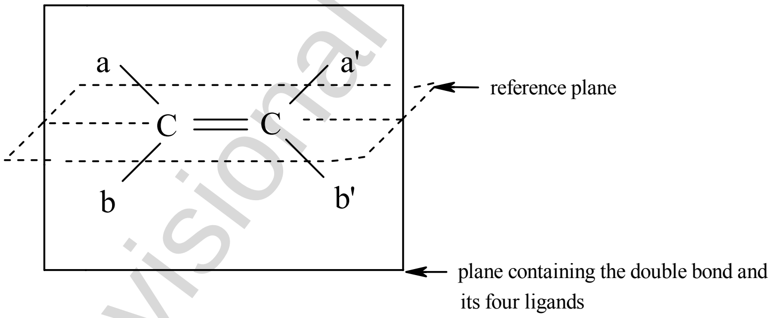
cis



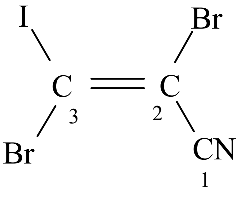
trans

P-91.2.1 ‘*E*’ and ‘*Z*’ descriptors.

The descriptors ‘*E*’ and ‘*Z*’ are used to describe *cis/trans*-isomers at double bonds. The sequence rule atom or group having precedence attached to one of a doubly bonded pair of atoms are compared with the sequence rule atom or group having precedence attached to the other atom; if the atoms or groups having precedence are on the same side of the reference plane, the italic capital letter ‘*Z*’ is used as a stereodescriptor; if the atoms or groups having precedence are on opposite sides, the italic capital letter ‘*E*’ is used. These stereodescriptors have been coined from German, ‘*Z*’ is derived from ‘zusammen’ (together) and ‘*E*’ from ‘entgegen’ (opposite).



Example:



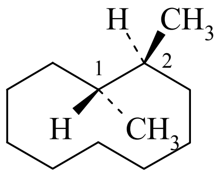
(2*Z*)-2,3-dibromo-3-iodoprop-2-enenitrile (PIN)

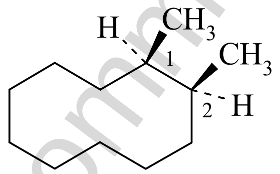
In this compound, application of Sequence Rule **1** described in P-91.1.l.2 gives precedence to I over Br in position 3; similarly, in position 2, Br precedes the C of the CN group. Thus the configuration of the double bond is ‘Z’, the atoms I in position 3 and Br in position 2 being compared

P-91.2.2 *cis*/*trans*-Isomerism in rings

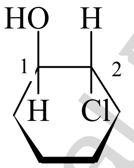
The stereodescriptors '*cis*' and '*trans*' are used to show the relationship (relative configuration) between two atoms or groups attached to separate atoms that are contained in a ring. The two atoms or groups are said to be located 'cis' to each other if they lie on the same side of a pseudo plane. If they are on opposite sides, their relative position is described as 'trans'. The pseudo plane is the mean plane of the ring(s) (the ring being in a conformation , real or assumed, without reentrant angles at the two substituted atoms)

The structures below look like *cis/trans*-isomers, but are actually different conformations of the same *cis*-stereoisomer. In the conformation on the left hand side, the stereogenic center at C-1 is located on a reentrant angle.





Example:



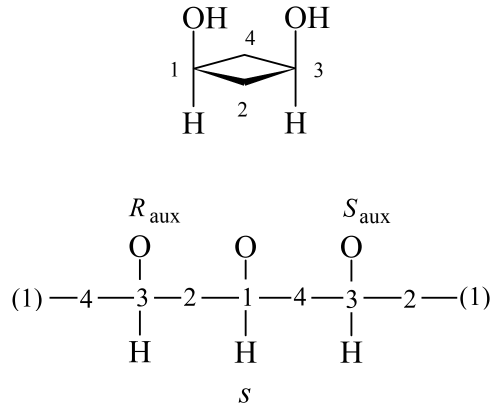
(1*R*,2*R*)- 2-chlorocyclohexan-1-ol (absolute configuration) (PIN)
trans-2-chlorocyclohexan-1-ol (relative configuration)

In this example, the compound is chiral and the hydroxy group and the Cl atom are *trans*. The absolute configuration is expressed by the stereodescriptors '*R*' and '*S*' (see P-92.1.1). The relative configuration may be described by using the stereodescriptor '*trans*'; in this case the compound may be the isomer shown or its enantiomer.

P-91.3 Auxiliary stereodescriptors

Auxiliary stereodescriptors have been recommended by Prelog and Helmchen (Section 6.2.1, ref. 32) to permit the assignment of stereodescriptors to stereogenic units that could not be described by using the recommended methodology for determining '*R*' and '*S*' configuration (see P-92.1.1.2). These descriptors are temporary descriptors that do not appear in the final stereodescriptor. It is recommended that the subscript 'aux' be added in digraphs to clearly indicate their temporary status and function.

Example:



(1*s*,3*s*)-cyclobutane-1,3-diol (PIN)
cis-cyclobutane-1,3-diol (see P-91.2)

Explanation: In order to specify the configuration of the achiral cyclic diol, the configuration of the pseudoasymmetric centers at C-1 and C-3 cannot be specified directly. In the digraph of the cyclic system the configuration at C-3 can be specified as '*R*' in the left branch, and as '*S*' in the right branch, thus permitting the use of Sequence Rule **5**, '*R*' precedes '*S*', to determine the configuration '*s*' at C-1; by the same method, the configuration '*s*' is determined for C-3. For use of auxiliary descriptors, see P-92.1.1.2, P-92.1.4, P-92.1.6.2.1, and examples in P-93.

P-92 Definition and use of configurational stereodescriptors

P-92.0 Introduction
P-92.1 CIP Stereodescriptors
P-92.2 Non-CIP stereodescriptors

P-92.0 Introduction

The steric structure of a compound is denoted by an affix or affixes to the name that does not prescribe the configuration. Such affixes do not change the name and the numbering of the compound, except in certain cases where stereochemical relations are used to decide between alternative names and numbering (see for example P-92.5.4 and P-92.7.3).

The CIP stereodescriptors are described in this section, with the methodology used to generate them. Two or three simple examples are given. In Section 93, examples are described and the use of non-CIP stereodescriptors are discussed.

P-92.1.1 Absolute configuration. Stereodescriptors '*R*' and '*S*'
P-92.1.2 Relative configuration. Stereodescriptors '*rel*', '*R**', and '*S**'
P-92.1.3 Racemates and meso compounds. Stereodescriptors '*rac*', '*RS*', and '*SR*'
P-92.1.4 Pseudo-asymmetric carbon atom. Stereodescriptors '*r*' and '*s*'

P-92.1.5 Helicity, axial and planar chirality. Stereodescriptors ‘*M*’, ‘*P*’, ‘R_a’, ‘S_a’, ‘R_p’, and ‘S_p’
P-92.1.6 Pseudo-asymmetric axes. Stereodescriptors ‘r_a’, ‘s_a’, ‘*m*’, and ‘*p*’
P-92.1.7 *cis*/*trans*-Isomerism. Stereodescriptors ‘*E*’ and ‘*Z*’
P-92.1.8 *cis/trans*-Isomerism. ‘*r*’, ‘*c*’, and ‘*t*’ Stereodescriptors
P-92.1.9 Nontetrahedral configurations. Stereodescriptors ‘*TPY*-3’, ‘*TS*-3’, ‘*SS*-4’, ‘*TBPY*-3’, ‘*TBPY*-4’, ‘*YBPY*-5’, ‘*TPY*-5’, ‘*OC*-6’, ‘*A*’, ‘*C*’

P-92.1.1 Absolute configuration. Stereodescriptors ‘*R*’ and ‘*S*’

Chiral compounds in which the absolute configuration is known are described by the stereodescriptors ‘*R*’ and ‘*S*’ assigned by the sequence rule procedure (ref. 30,31,32). For carbon (and other atoms) to which four different atoms or groups are attached in the system, Cabcd may be depicted as follows, where ‘a’ > ‘b’ > ‘c’ > ‘d’.

(*R*) (*S*)

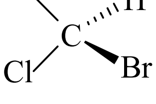
When the model is viewed from the carbon atom along the axis C → ‘d’, the path from ‘a’ to ‘b’ to ‘c’ traces a clockwise direction, and the system has the ‘*R*’ configuration. If passing from ‘a’ to ‘b’ to ‘c’ traces an anticlockwise direction, the configuration is ‘*S*’.

The sequence rules (1) and (2) described in P-91.1.4 and P-91.1.5, respectively, are used to establish the seniority ‘a’ > ‘b’ > ‘c’ > ‘d’, when four different atoms or groups are present.

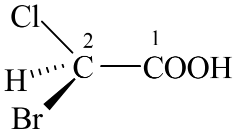
P-92.1.1.1 Name formation

In names, a single stereodescriptor, ‘*R*’ or ‘*S*’, related to the parent structure is cited at the front of the name of the compound, preceded by the appropriate locants and enclosed in parentheses. In preferred IUPAC names, locants that denote chiral centers are repeated before the stereodescriptors ‘*R*’ and ‘*S*’; when no locant is used in the name of the compound, none is necessary before the stereodescriptor.

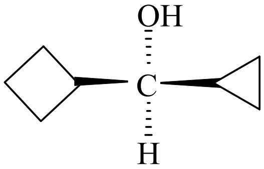
Examples:



(*R*)-bromochlorofluoromethane (PIN)



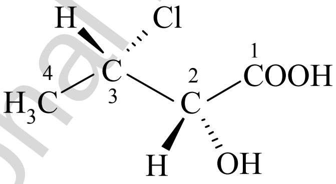
(2*R*)-2-bromo-2-chloroacetic acid (PIN)



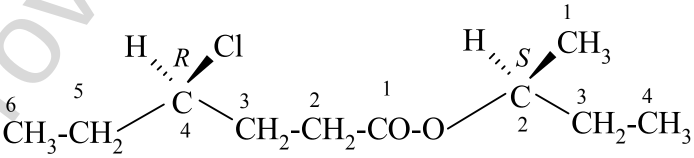
(*S*)-cyclobutyl(cyclopropyl)methanol (PIN)
(α*S*)-α-cyclopropylcyclobutanemethanol

When a molecule contains more than one chiral centre, the above mentioned procedure is applied to each chiral center, and the configuration of the parent structure is expressed as a set of '*R*/*S*' symbols. In names of compounds, the symbols '*R*' and '*S*', with locants if needed, are written in parentheses and separated by a comma, followed by a hyphen, at the front of the complete name or appropriate substituent.

Examples:



(2*S*,3*S*)-3-chloro-2-hydroxybutanoic acid (PIN)

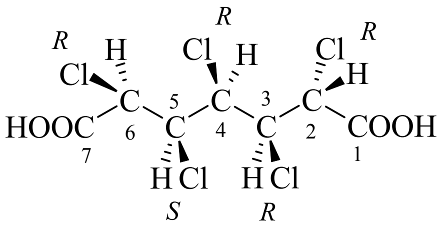


(2*S*)-butan-2-yl (4*R*)-4-chlorohexanoate (PIN)

P-92.1.1.2 Compounds with polychiral centers denoted by '*R*' and '*S*' stereodescriptors

When the use of Sequence Rules **1** and **2** does not permit the determination of the configuration of all chirality centers of a molecule, Sequence Rules **3**, **4** and **5** are applied as described by the following examples.

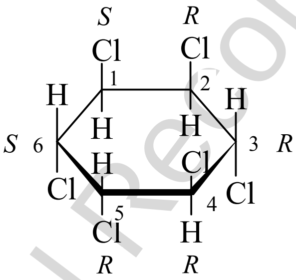
Example 1:



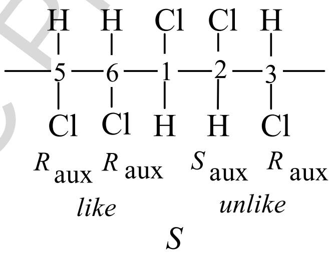
(2*R*,3*R*,4*R*,5*S*,6*R*)-2,3,4,5,6-pentachloroheptanedioic acid (PIN)

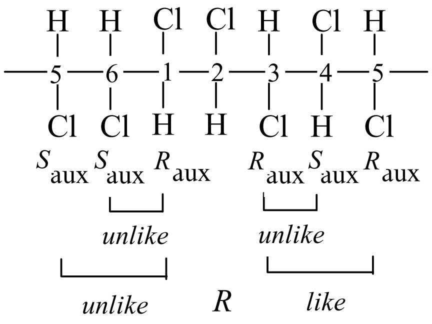
In this example, the configuration at C-4 is determined by comparing the two pairs of configurations denoted by '*RR*' on one side (C-2 and C-3) and '*SR*' on the other side (C-5 and C-6). Since like descriptor pairs precede unlike descriptor pairs [(sequence rule (4)], the order 'a > b > c > d' corresponds to OH > *RR* > *SR* > H; thus, the configuration at C-4 is '*R*'

Example 2:



(1*S*,2*R*,3*R*,4*R*,5*R*,6*S*)-1,2,3,4,5,6-hexachlorocyclohexane (PIN)
(not 1L-*chiro*-1,2,3,4,5,6-hexachlorocyclohexane; the use of such configurational prefixes is not recommended for preferred IUPAC names)
(not 1,2,3,4,5,6-hexachloro-1,2,3,4,5,6-hexachloro-1L-*chiro*-inositol; replacement of –OH groups in inositols by monovalent atoms or groups is limited to three, see I-7.1, ref. 44)



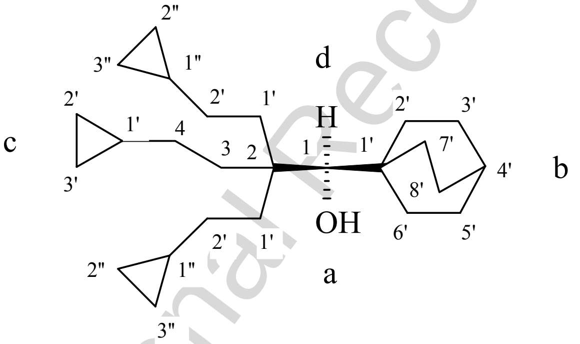


Explanation: *cis/trans*-Pairs of chlorine atoms are present in hexachlorocyclohexanes. For example, in the above compound, starting from C-1, atoms at C-2 and C-3 are in a '*trans*' arrangement and atoms at C-5 and

C-6 are in a '*cis*' arrangement. This difference is used to determine the chirality at C-1, by applying sequence rule (4) that gives precedence to *like* pairs of descriptor*s* over *unlike* pairs of descriptors. For C-1, the priority order 'a' > 'b' > 'c' > 'd' is Cl > C-6 > C-2 > H; this order generates a '*S*' configuration. The determination of the configuration at C-2 is not possible using the pairs C-3/C-4 and C-6/C-5 which are both described as *unlike* pairs of descriptors. A difference, however, is found when the pairs C-2/C-4 and C-6/C-4 are determined and compared: C-2 and C-4 are described as *like*, C-6 and C-4 are described as *unlike*, leading to the configuration '*R*' for C-2. The configuration of the six chirality centers are determined in the same way.

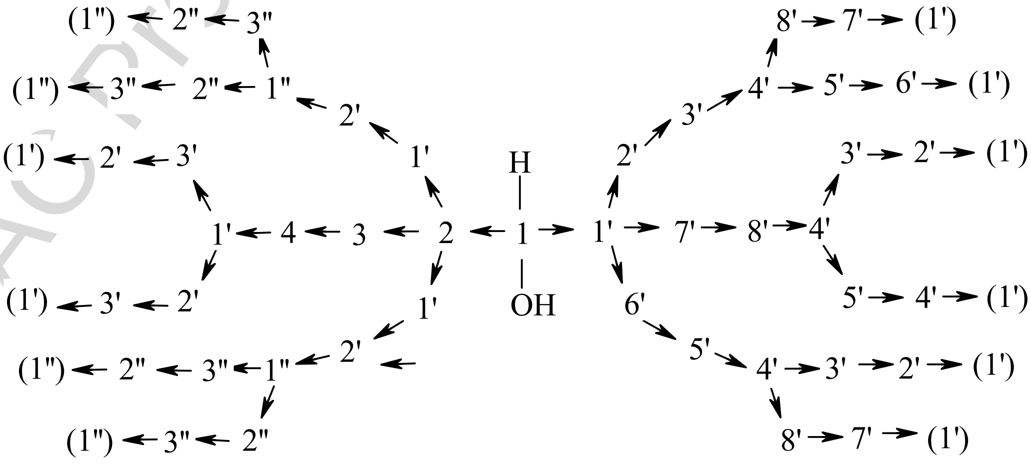
P-92.1.1.3 Sub-rule **1b**. Priority due to duplicate atoms

Custer (ref. 35) proposed an amendment to Sequence Rule **1a** to establish the priority between two cyclic substituents which give the same exploratory pathway. The sub-rule is expressed as 'a duplicate atom corresponding to an atom closer to the start of the exploration pathway precedes one further away'. The following example illustrates the sub-rule:



1-(bicyclo[2.2.2}octan-1-yl)-1-[1,5-dicyclopropyl-3-(2-cyclopropylethyl)]pentan-3-yl]methan-1-ol (PIN)

(numbering shown corresponds to the construction of digraph below)

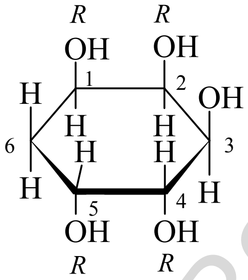


Explanation: The duplicate atoms on the right correspond to the carbon at the first level (C-1 of the bicycle[2.2.2]octan-1-yl) whereas those on the left correspond to atoms at the fourth level (C-1 of the cyclopropyl groups). As nearer duplicate atoms take precedence, the substituent on the right is assigned the priority 'b' and the other the priority 'c'. The first level of the exploration, sphere **I**, leads to the ranking O > H.

P-92.1.1.4 Nonstereogenic centers

In chiral compounds some centers may be nonstereogenic. No stereodescriptors are assigned to these centers.

Example:

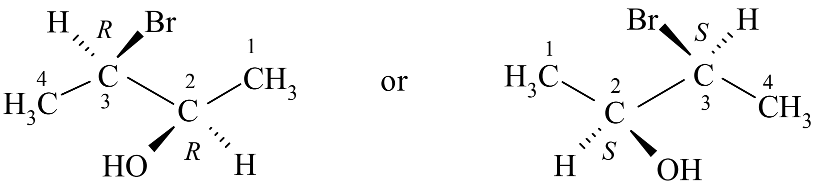


(1*R*,2*R*,4*R*,5*R*)-cyclohexane-1,2,3,4,5-pentol (PIN)
(the exchange of the hydrogen atom and the -OH group in position 3 generates the same enantiomer)
(not 6-deoxy-*allo*-inositol, see P-104.2.2)

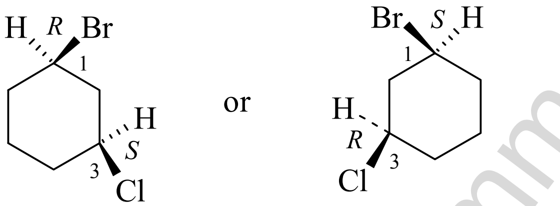
P-92.1.2 Relative configuration. The stereodescriptors '*rel'*, and '*R**' and '*S**'

Chirality centers, of which the relative but not the absolute configuration is known, may be labeled '*rel*' (for relative) (not to be confused with *r* for reference, see P-92.6.4) followed, in parentheses, by the stereodescriptors '*R*' and '*S*', each preceded by the appropriate locant (see E-4.10, ref. 1). The stereodescriptors may also be '*R**' and '*S**' (spoken R star, S star), preceded when necessary by appropriate locants (see E-4.10, ref. 1). These stereodescriptors '*R*', '*R**', '*S*', '*S**' are assigned by the sequence rule procedure, arbitrarily assuming that the stereogenic center first cited (which usually has the lowest locant) has the chirality descriptor '*R*' or '*R**'. The method using the stereodescriptor '*rel*' is preferred when preferred IUPAC names are to be specified. It is important to note that the descriptor '*rel*' applies to all stereogenic centers when more than one such center is present in a compound.

Examples:



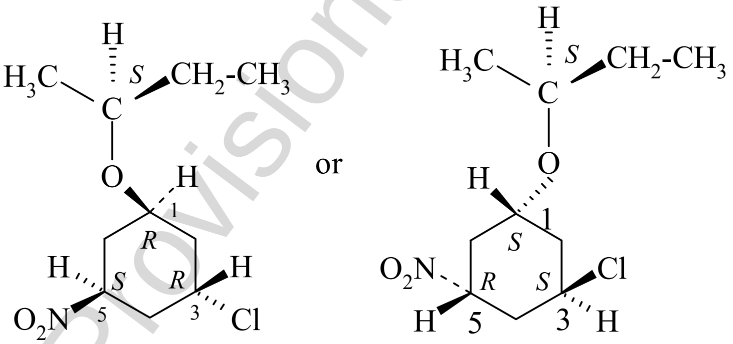
rel-(2*R*,3*R*)-3-bromobutan-2-ol (PIN)
(2*R**,3*R**)-3-bromobutan-2-ol



rel-(1*R*,3*S*)-1-bromo-3-chlorocyclohexane (PIN)
(1*R**,3*S**)-1-bromo-3-chlorocyclohexane

P-92.4.2 In compounds containing chirality centers with known absolute configurations and a sterically unrelated set of chiral centers with known relative configuration, the '*R**' and '*S**' descriptors must be used to designate the latter (see E-4.10, ref. 1). The prefix '*rel*-' cannot be used as it does apply to the entire molecule.

Example:



absolute configuration known

relative configuration known

(1*R**,3*R**,5*S**)-1-[(2*S*)-butan-2-yloxy]-3-chloro-5-nitrocyclohexane (PIN)

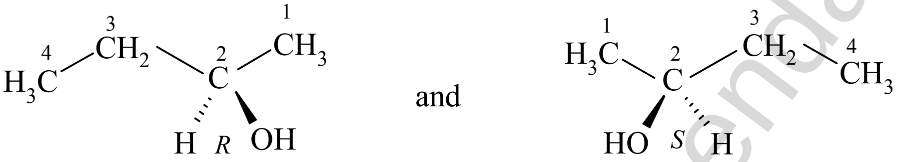
P-92.1.3 Racemates and meso compounds. The stereodescriptors '*rac*', '*RS'* and '*SR'*

A racemate is an equimolar mixture of a pair of enantiomers. It does not exhibit optical activity in solution.

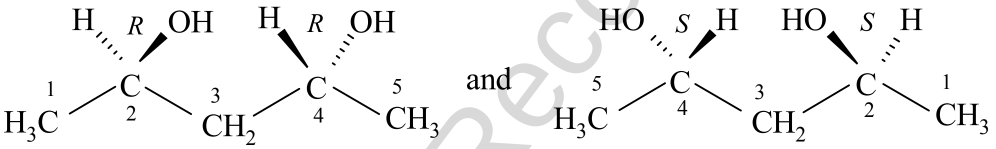
Different methods are used to characterize the name of a racemate or of a racemic compound. The prefixes '(±)' or '*rac*' (or '*racem*') or the stereodescriptors '*RS*' or '*SR*' may all be used in general nomenclature. The descriptor '*rac*' is used in preferred IUPAC names.

Racemates containing a single stereogenic center are labeled ‘*RS*’. If there is more than one center, the first (corresponding to the lowest locant assigned to stereodescriptors) is labeled ‘*RS*’ and the others are ‘*RS*‘ or ‘*SR*’ according to whether they are ‘*R*’ or ‘*S*’ when the first is ‘*R*’. The method used in preferred IUPAC names is to describe the descriptor having the lowest locant by ‘*R*’ and the others accordingly; the prefix ‘*rac*’ is placed in front of the set of descriptors and locants.

Examples:



rac-(2*R*)-butan-2-ol (PIN)
(±)-butan-2-ol
(*RS*)-butan-2-ol

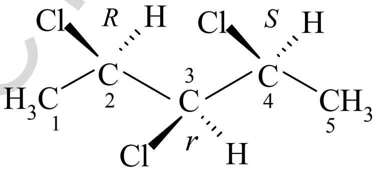


rac-(2*R*,4*R*)-pentane-2,4-diol (PIN)
(2*RS*,4*RS*)-pentane-2,4-diol

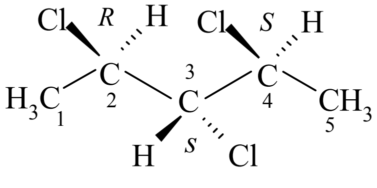
P-92.1.4 Pseudo-asymmetric centers. The stereodescriptors ‘*r*’ and ‘*s*’

P-92.1.4.1 An atom that is a tetrahedrally substituted atom and bonded to four different entities, two and only two of which have opposite configurations, is stereogenic. The descriptors ‘*r*’ and ‘*s*’ are used to denote such centers; they are assigned in accordance with Sequence Rule **5**, taking into consideration that ‘*R*’ has precedence over ‘*S*’ in the order of priority. The stereodescriptors ‘r’ and ‘*s*’ are reflexion invariant (see 2.5.3, ref. 30).

Example 1:



(2*R*,3*r*,4*S*)-2,3,4-trichloropentane (PIN)



(2*R*,3*s*,4*S*)-2,3,4-trichloropentane (PIN)

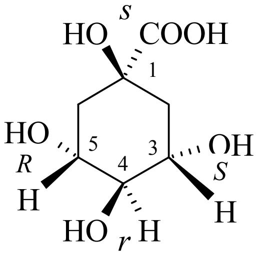
Guide to name construction:

Step 1: configuration ‘*R*’ or ‘*S*’ is assigned to stereogenic centers C-2 and C-4;

Step 2: configuration at C-3 is assigned by applying sequence rule 5, '*R*' precedes '*S*'.

In the above set of compounds, the exchange of the Cl and H atoms at C-3 of the compound described on the left generates the compound on the right, and '3*r*' becomes '3*s*'

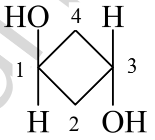
Example 2:

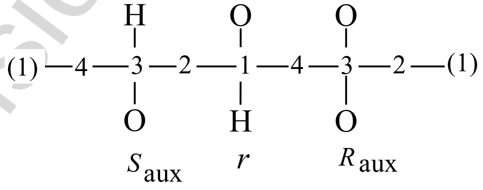


(1*s*,3*S*,4*r*,5*R*)-1,3,4,5-tetrahydroxycyclohexane-1-carboxylic acid (PIN)

P-92.1.4.2 The use of auxiliary stereodescriptors 'R_{aux}' and 'S_{aux}' leads to the specification of the configuration of pseudoasymetric centers. Achiral cyclic diols, for example, are named by this method.

Example 1:

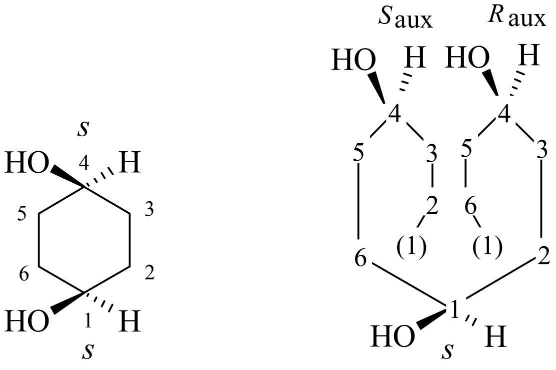




(1*r*,3r*)*-cyclobutane-1,3-diol (PIN)

Explanation: the digraph puts into evidence the opposite configuration at C-3 in the two branches. Sequence rule (5), '*R*' precedes '*S*', generates the stereodescriptor '*r*' for C-1 and, similarly, for C-3.

Example 2:



(1*s*,4*s*)-cyclohexane-1,4-diol (PIN)

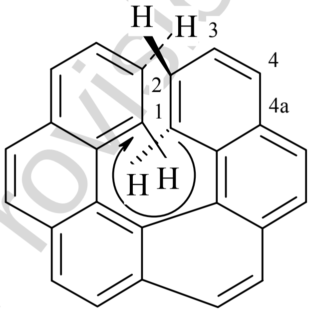
Explanation: the digraph permits to assign the ‘*s*’ configuration to C-1 (shown in the digraph) and C-4.

P-92.1.5 Helicity, axial and planar chirality. The stereodescriptors ‘*M*’, ‘*P*’, ‘R_a’, ‘S_a’, ‘R_p’ and ‘S_p’

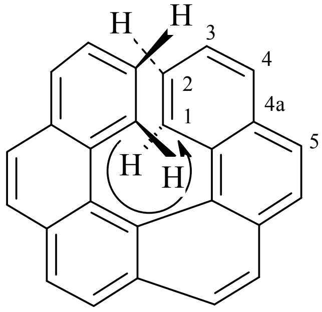
P-92.1.5.1 Helicity: The stereodescriptors ‘*M’* and ‘*P’*

Helicity is the chirality of a helical, propeller, or screw-shaped molecular entity (see subsection 2.6, ref. 31). A left-handed helix is described as ‘*M* ’ (or minus) and a right-handed helix as ‘*P* ’ (or plus), as expressed by the rotation angle θ (see torsion angle, P-94.2).

The chirality of hexahelicenes is denoted by the stereodescriptors ‘*P*’ and ‘*M* ’ . When the upper right ring is near the observer, and the upper left ring away from the observer, the path from front to rear along the periphery of the molecule gives a clockwise course denoted by ‘(+)’ or ‘*P*’. The anticlockwise course is denoted by ‘(−)’ or ‘*M* ’.



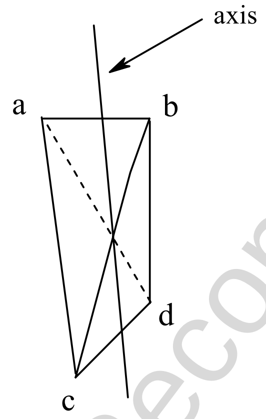
(*P*)-hexahelicene (PIN)



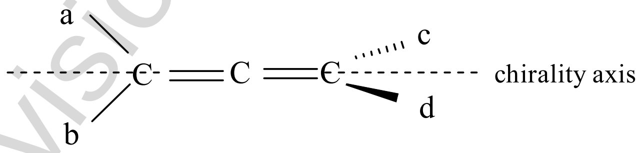
(*M*)-hexahelicene (PIN)

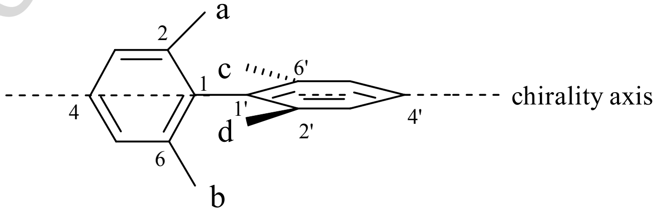
P-92.1.5.2 Axial chirality: The stereodescriptors ‘R_a’ or ‘*P*’ and ‘S_a’ or ‘*M* ’

Structures with axial chirality are regarded as elongated tetrahedra and viewed along the axis; it is immaterial from which side it is viewed (see subsection 2.6, ref. 31). Axial chirality is used to refer to stereoisomerism resulting from the nonplanar arrangement of four groups in pairs about a chirality axis. A chirality axis is the axis about which a set of atoms or groups is held so that it results in a spatial arrangement which is not superposable on its mirror image. For instance, in an allene ‘abC=C=Ccd’, the chiral axis is defined by the ‘C=C=C’ bonds, and in a 2,2′,6,6′-tetrasubstituted biphenyl the atoms 1,1′,4,4′ lie on the chiral axis.



In chiral compounds owing their chirality to a stereogenic center, it is necessary to have four different atoms or groups (‘a’, ‘b’, ‘c’, and ‘d’). With an elongated tetrahedron, this requirement is no longer necessary because of reduced symmetry. The only condition is that ‘a’ be different from ‘b’ and ‘c’ be different from ‘d’; thus compounds with two pairs of substituents ‘a’ and ‘b’ are chiral if ‘a’ is different than ‘b’.

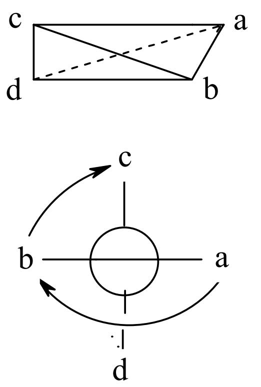




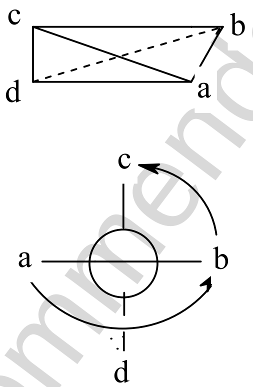
Descriptors ‘R_a’ and ‘S_a’ and ‘*M*’ and ‘*P*’ are assigned in accordance with two different methods.

P-92.1.5.3 The descriptors 'R_a / S_a'

Substituents (atoms or groups) are arranged in the elongated tetrahedral system. Two higher-ranking substituents are chosen, one in each pair, using the sequence rule. For the pairs 'a' > 'b' and 'c' > 'd', the chirality is described by 'R_a' if the path going from 'a' to 'b' to 'c' is clockwise, while looking toward 'd'. The symbol is 'S_a' if this path is anticlockwise.



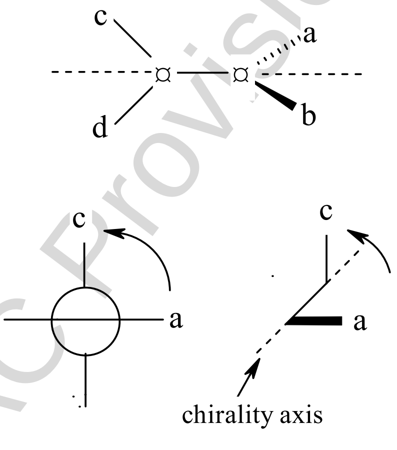
R_a



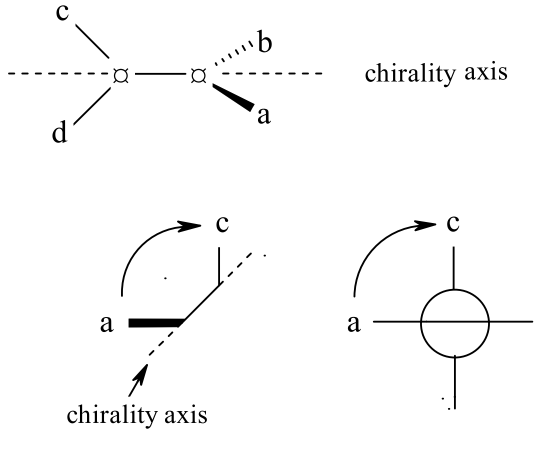
S_a

P-92.1.5.4 The descriptors '*M* ' and '*P*'

Looking along the chirality axis the atoms or groups are arranged in pairs. When proceeding from the nearer atom or group having priority in the pair to the further away atom or group having priority in the pair, the chirality is described by the symbols '*M*' if the path is anticlockwise; the symbol is '*P*' if the path is clockwise. Stereodescriptors 'R_a' and 'S_a' are used in preferred IUPAC names.

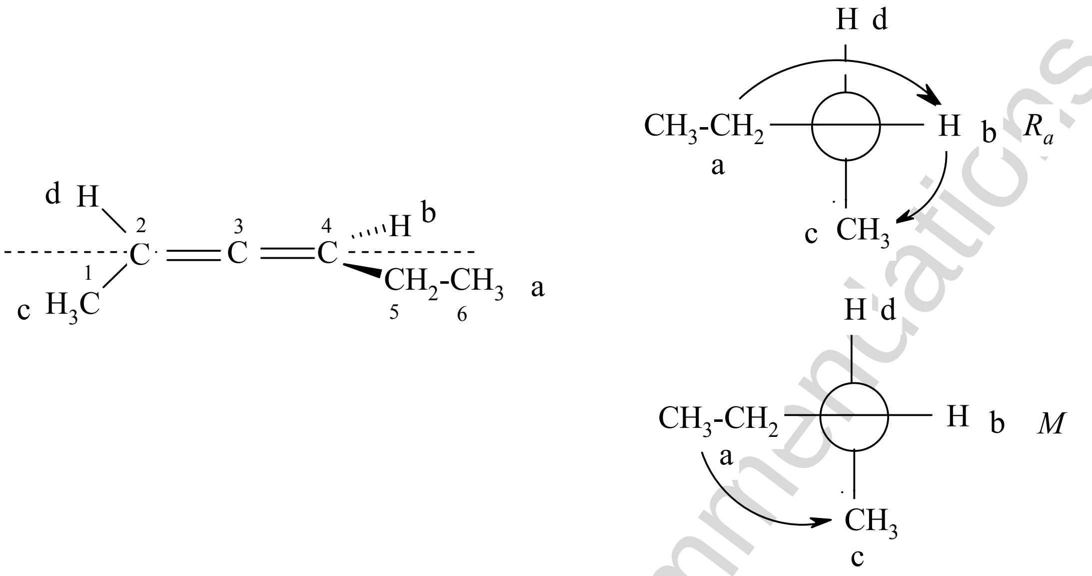


M



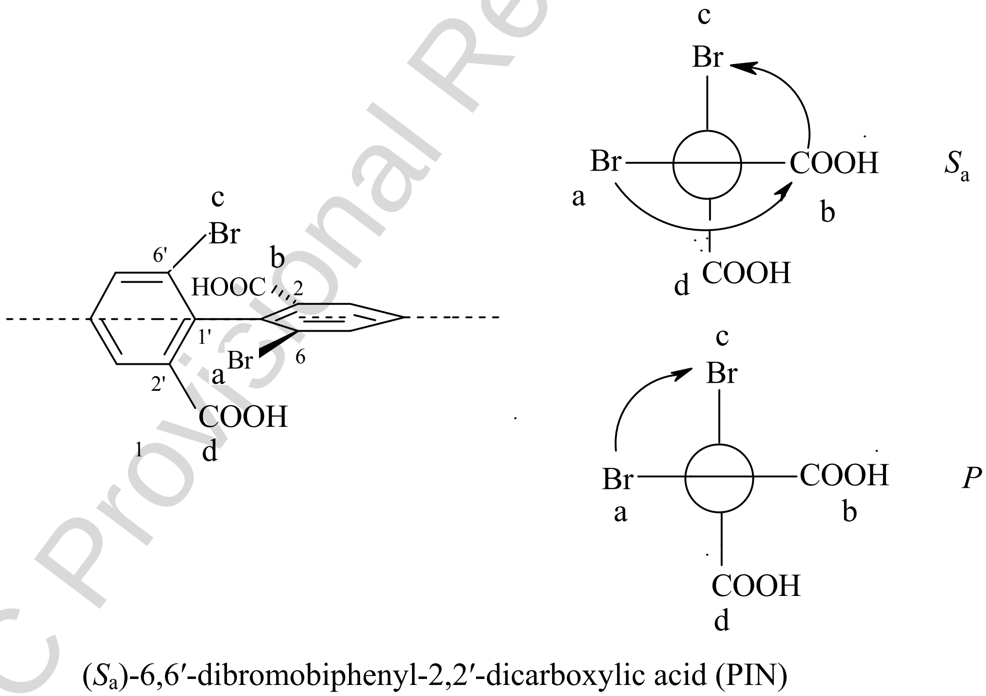
P

Example 1:



(*R*_a)-hexa-2,3-diene (PIN)
(*M*)-hexa-2,3-diene

Example 2:



(*S*_a)-6,6′-dibromobiphenyl-2,2′-dicarboxylic acid (PIN)
(*P*)-6,6′-dibromobiphenyl-2,2′-dicarboxylic acid

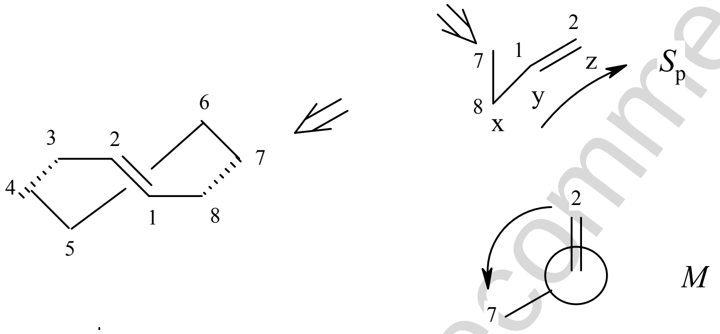
P-92.1.5.4 The stereodescriptors ‘*R*$_p$’ and ‘*S*$_p$’

Planar chirality is a term used to refer to stereoisomerism resulting from the arrangement of out of plane groups with respect to a plane (chirality plane) (see subsection 2.6, ref. 31). It is exemplified by the atropisomerism of (*E*)-cyclooctene (chiral plane = double bond and attached atoms) or a monosubstituted cyclophane (chiral plane = substituted ring). The configuration is specified by the stereodescriptors ‘R_p’ and ‘S_p’(or ‘*P*’ and ‘*M*’).

Three atoms are used to define the direction of rotation, clockwise or anticlockwise (‘x’, ‘y’, and ‘z’). A pilot atom, next to ‘x’, is chosen at an observation site (⇒) to determine the direction of rotation. A clockwise path is described by the stereodescriptors ‘*P*’ (helicity descriptor) or ‘R_p’ (CIP descriptor). The opposite path is described by ‘*M*’ (helicity descriptor) or ‘S_p’ (CIP descriptor).

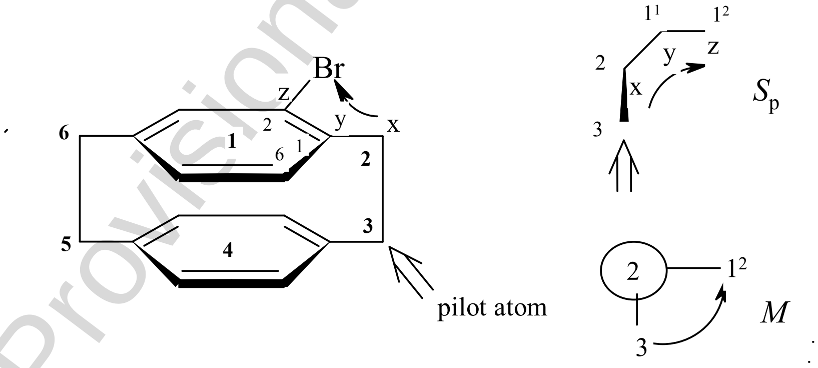
Stereodescriptors ‘R_p’ and ‘S_p’ are used in preferred IUPAC names.

Example 1:



(1*E*,S_p)-cyclooct-1-ene (PIN)
(1*E*,*M*)-cyclooct-1-ene

Example 2:

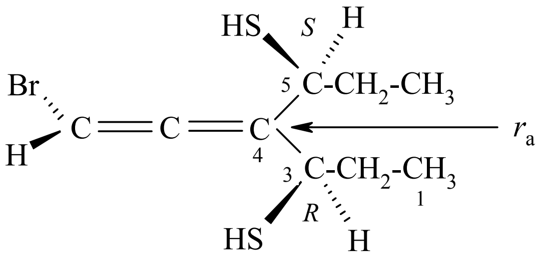


(S_p)-1^2-bromo-1,4(1,4)-dibenzenacyclohexaphane (PIN)
(*M*)-1^2-bromo-1,4(1,4)-dibenzenacyclohexaphane

P-92.1.6 Pseudoasymmetric axes. The stereodescriptors ‘r_a’ and ‘s_a’, ‘*m*’ and ‘*p*’

The descriptors ‘r_a’ or ‘*m*’, and ‘s_a’ or ‘*p’*, are used to denote a stereogenic unit that is exhibiting axial chirality due to the presence of two enantiomeric substituents groups; they are assigned in accordance with the sequence rule 5, taking into consideration that ‘*R*’ has precedence over ‘*S*’ in the order of priority. The stereodescriptors ‘r_a’, ‘s_a’, ‘*m*’ and ‘*p*’ are reflexion invariant (see 2.5.3, ref. 30).

Example:



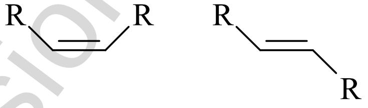
(*3R*,4r_a,*5S*)-4-(2-bromoethenylidene)heptane-3,5-dithiol (PIN)
(*3R*,4*m*,5*S*)-4-(2-bromoethenylidene)heptane-3,5-dithiol
(*3R*,*5S*)-*4*-[(*m*)-(2-bromoethenylidene)]heptane-3,5-dithiol
(*3R*,*5S*)-*4*-[(r_a)-(2-bromoethenylidene)]heptane-3,5-dithiol

P-92.1.7 Stereodescriptors '*E*', '*Z*', *cis/trans*-iomerism.

P-92.1.7.1 Definitions

The terms '*cis* and '*trans*' are used to show the relationship between two atoms or groups attached to separate atoms that are connected by a double bond or are contained in a ring. The two atoms or groups are said to be located 'cis' to each other if they lie on the same side of a plane. If they are on opposite sides, their relative position is described as 'trans'. The appropriate reference plane of a double bond is perpendicular to that of the relevant σ-bonds and passes through the double bond.

Examples:



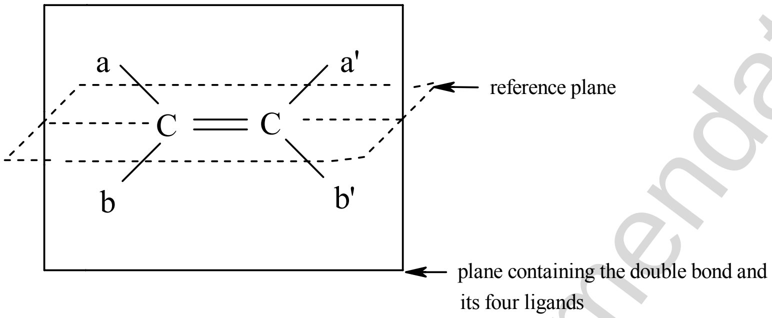
cis *trans*

The terms '*cis*' and '*trans*' are also used as stereodescriptors to describe the configuration of a compound (see P-92.2.1.1).

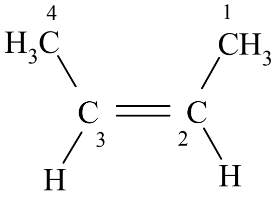
P-92.1.7.2 *cis*/*trans*- Isomerism. The stereodescriptors '*E*' and '*Z*'

The '*E*' and '*Z*' descriptors are assigned as follows to describe the configuration of a double bond. The sequence rule atom or group having precedence attached to one of a doubly bonded pair of atoms is compared with the sequence rule atom or group having precedence attached to the other atom; if the atoms or groups having precedence are on the same side of the reference plane, the italic capital letter '*Z*' is used as a stereodescriptor; if the atoms or groups having precedence are on opposite sides, the italic capital letter '*E*' is used. These setereodescriptors have been coined from the German language, '*Z*' is derived from 'zusammen' (together) and '*E*' from 'entgegen' (opposite). Placed in parentheses, they are cited at the front of a name. When the position of the double bond is denoted by a locant, this locant is also placed at the front of the stereodescriptor. When no locant is used to describe the double bond, no locant is placed at the front of the stereodescriptor.

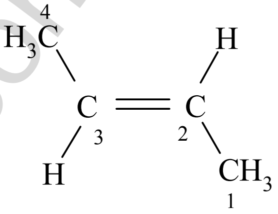
The '*E*' and '*Z*' descriptors are preferred to '*cis*' and '*trans*' in IUPAC names (see P-92.2.1.1)



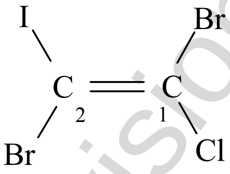
Examples:



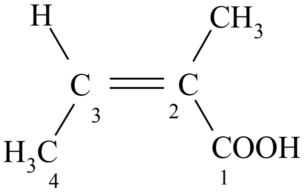
(2*Z*)-but-2-ene (PIN)



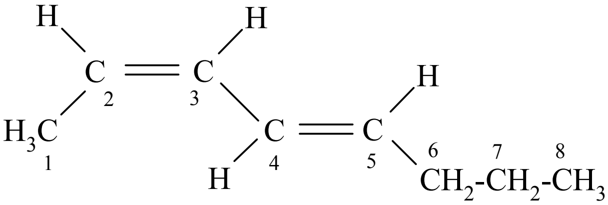
(2*E*)-but-2-ene (PIN)



(*Z*)-1,2-dibromo-1-chloro-2-iodoethene (PIN)



(*Z*)-2-methylbut-2-enoic acid (PIN)

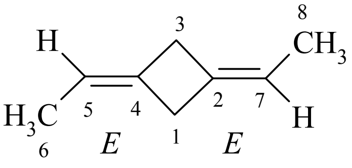


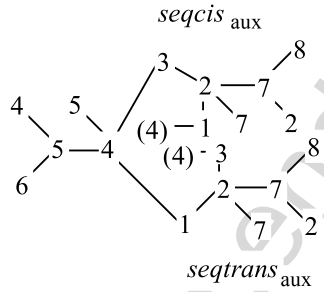
(2*Z*,4*E*)-octa-2,4-diene (PIN)

P-92.1.7.2.1 Use of auxiliary stereodescriptors

The use of auxiliary stereodescriptors leads to the assignment of '*Z*' and '*E*' stereodescriptors to sets of double bonds undistinguishable by direct application of sequence rule (1).

Example:





2,4-di[(*E*)-ethylidene]cyclobutane (PIN)
(*E*)-2,4-diethylidenecyclobutane

Explanation: In the digraph, when considering the two branches at C-4, one contains a *seqcis*$_{\text{aux}}$ double bond (path 3-2-7-8), the other branch contains a *seqtrans*$_{\text{aux}}$ double bond (path 1-2-7-8). As *seqcis*$_{\text{aux}}$ precedes *seqtrans*$_{\text{aux}}$, C-3 precedes C-1, the double bond at C-4 is *seqtrans*, or *E* that is the stereodescriptor used in the name of the compound. Similarly, the double bond at C-2 is *E*.

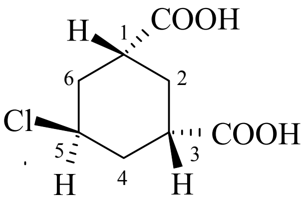
In names, the stereodescriptor *E* is used to describe each double bond; it is placed before the name of the substituent group having this configuration. This method is preferred to the use of the stereodescriptor *E*, to describe the whole molecule, considered as an extended double bond.

P-92.1.8 *cis/trans*-Isomerism. The stereodescriptors '*r*', '*c*', and '*t*'

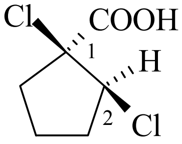
When one substituent and one hydrogen atom are attached to each of more than two positions of a monocycle, or when two different substituents are attached at the same position of a monocycle, then the lowest-numbered substituent named as a suffix is selected as a reference group. If none of the substituents is named as a suffix, then that substituent of the pair of substituents having the lowest locant, and which has precedence in the sequence rule, is chosen as the reference group; it is denoted as '*r*'. The relationship of substituents, relative to the reference group, is cited as '*c*' (for *cis*) or '*t*' (for *trans*), as appropriate. When alternative numberings of a ring are possible, that numbering is chosen which gives a '*cis*' attachment at the first point of difference.

The notation consisting of adding '*r*' (for reference substituent) followed by a hyphen and the locant of the lowest numbered of these substituents and '*c*' (for *cis*) and '*t*' (for *trans*) (as appropriate) followed by a hyphen and the locant for another substituent, as used in Section E of the 1979 edition of Nomenclature of Organic Chemistry (ref. 1) and in the Guide to IUPAC Nomenclature of Organic Compounds (ref. 2), is no longer recommended.

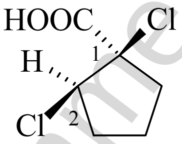
Examples:



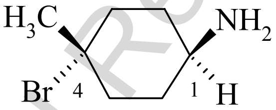
5*t*-chlorocyclohexane-1*r*,3*c*-dicarboxylic acid
(1*R*,3*S*,5*r*)-5-chlorocyclohexane-1,3-dicarboxylic acid (PIN)
(not *t*-5-chlorocyclohexane-*r*-1,*c*-3-dicarboxylic acid)



or



1,2*t*-dichlorocyclopentane-1*r*-carboxylic acid
rel-(1*S*,2S)- 1,2-dichlorocyclopentane-1-carboxylic acid (PIN)
(not 1,*t*-2-dichlorocyclopentane-*r*-1-carboxylic acid)



4*t*-bromo-4-methylcyclohexan-1*r*-amine
(1*s*,4*s*)-4-bromo-4-methylcyclohexan-1-amine (PIN)

P-92.1.9 P-92.1.7 Nontetrahedral configurations. Stereodescriptors ‘*TPY*-3’, ‘*TS*-3’, ‘*SS*-4’, ‘*TBPY*-3’, ‘*TBPY*-4’, ‘*TBPY*-5’, ‘*TPY*-5’, ‘*OC*-6, *A*,*C*’

P-92.1.9.1 When an atom is attached to 3, 4, 5, or 6 atoms or groups a number of geometrical configurations are possible. In general there will be some distortion from the idealized geometry of the regular solid due to differences between the atoms involved. Thus with five attached ligands they may be arranged as a trigonal bipyramid or square pyramid and with six as an octahedron. The notation described below for these systems is based on inorganic coordination nomenclature (ref. 14, Red Book I). Details of the geometry of systems with a coordination greater than six will be found in reference 14.

The stereodescriptors are composed of three parts.

(1) A symbol indicating overall geometry called a ‘polyhedral symbol’;
(2) A symbol called a ‘configuration index’;
(3) A symbol indicating the chirality associated with the central atom called a ‘chirality symbol’.

The three parts are enclosed in parentheses and separated from each other by hyphens to form the descriptor, which is cited in front of the name separated by a hyphen.

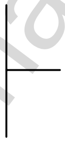
P-92.1.9.2 Polyhedral symbol

The polyhedral symbol takes the form of an abbreviation of the name of the closest idealized geometry (italic upper case letters) and a number indicating how may atoms or groups (ligands in coordination nomenclature) are attached (see Rule I-10.5.2, ref. 14). Table 8.1 describes the most frequently encountered polyhedrons related to structures of organic compounds. The configuration of molecules containing a tetrahedral center has been discussed in Sections P-91 and P-92.1 to P-92.6

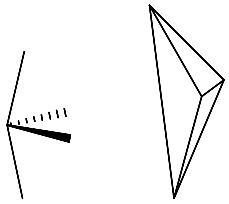
Table 8.1 List of polyhedral symbols

Idealized geometry	Attached atoms or groups	Polyhedral symbol
trigonal pyramid	3	*TPY*-3
T-shape	3	*TS*-3 (ref. 37)
see-saw	4	*SS*-4 (ref. 37)
trigonal bipyramid	5	*TBPY*-5
square pyramid	5	*SPY*-5
octahedron	6	*OC*-6

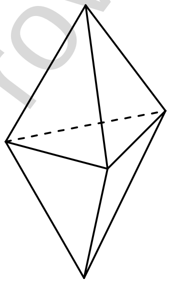
TPY-3



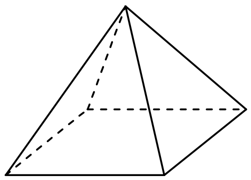
TS-3



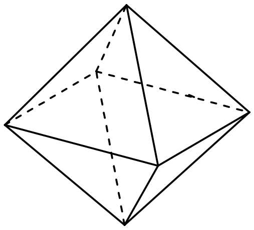
SS-4



TBPY-5



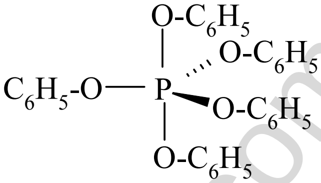
SPY-5



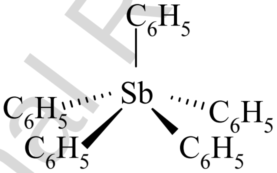
OC-6

The abbreviation and number are separated by a hyphen and enclosed in parentheses in front of the name of the compound, if no further information is required.

Examples:



(*TBPY*-5)-pentaphenoxy-λ^5-phosphane

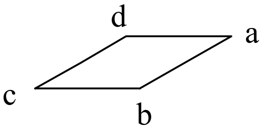


(*SPY*-5)-pentaphenyl-λ^5-stibane

P-92.1.9.3 Configuration index and priority rules

The configuration index is a series of numbers to identify where each atom or group is located (see Rule I-10-5.3, ref. 14). It is based on the CIP priority order of the atoms attached. The atom or atoms with highest priority are given priority number one (**1**); the next priority number two (**2**), and so on. In addition to the standard CIP sequence rules 1 and 2, two additional rules are needed:

(a) *trans*-maximum difference of priority (see I-10.5.3.3, ref. 14). Between atoms with the same priority number, high priority is assigned to the atom which is trans (opposite) to the atom having the lowest priority number; in the following planar structure, 'a' and 'c' (and 'b' and 'd') are '*trans*':

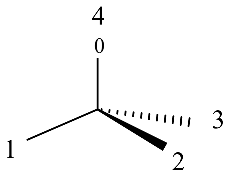


(b) Priming convention (see I-10-6.3.2, ref. 14). When there are two (or three) identical rings present, the priority numbers of one of them is primed (and the third double primed).
(c) Unprimed priority numbers are preferred to primed. In coordination nomenclature rings are di- and polydentates ligands.

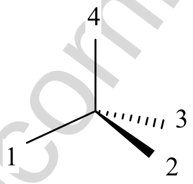
Each idealized geometry has its own rules for assignment of the configuration index.

P-92.1.9.3.1 Trigonal pyramid

The configuration of molecules containing a trigonal pyramidal center (*TPY*-3) is described in a similar way to that of tetrahedral centers (*T*-4) described above in P-91 and P-92.1 through P-92.6. The tetrahedral configuration is achieved by adding a phantom atom (0) to the central atom perpendicular to the base of the pyramid. No configuration index is used with the ‘*TPY*-3’ symbol. Priority numbers are ‘1’ > ‘2’ > ‘3’ > ’4’.



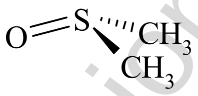
TPY-3 (a phantom atom is shown)



T-4 (for comparison)

Sulfoxides, when the central atom and substituents only are considered, constitutes a trigonal system. The polyhedral symbol is placed at the front of the name.

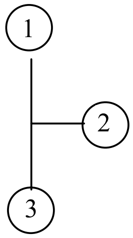
Example:



(*T*-4)-methylsulfinylmethane (PIN)
(*TPY*-3)-methylsulfinylmethane

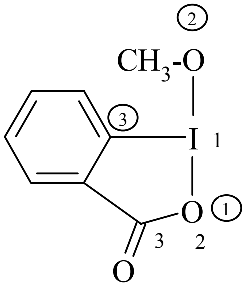
P-92.1.9.3.2 T-shape systems

The configuration index of the T-shape configuration follows the polyhedral symbol and consist of a single digit, the priority number of the atom or substituent group on the stem of the ‘T’ (as opposed to the cross piece of the ‘T’).



(*TPY*-3-2)

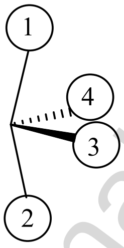
Example:



(*TPY*-3-3)-1-methoxy-1λ^3,2-benziodoxol-3(1*H*)-one
(*TBPY*-3)- 1-methoxy-1λ^3,2-benziodoxol-3(1*H*)-one (PIN, see P-92.1.7.3.4.2)

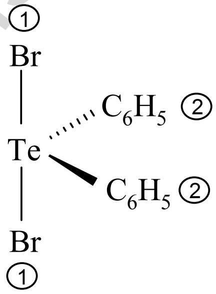
P-92.1.9.3.3 See-saw systems

The configurational index of a see-saw system is composed of the priority number indicating the two atoms or groups separated by the largest angle.



SS-4-12

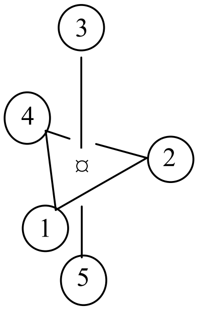
Example:



(*SS*-4-11)-dibromodiphenyl-λ^5-tellurane
(*TBPY*-4-dibromodiphenyl-λ^5-tellurane (PIN, see P-92.1.7.3.4.2)

P-92.1.9.3.4 Trigonal bipyramid

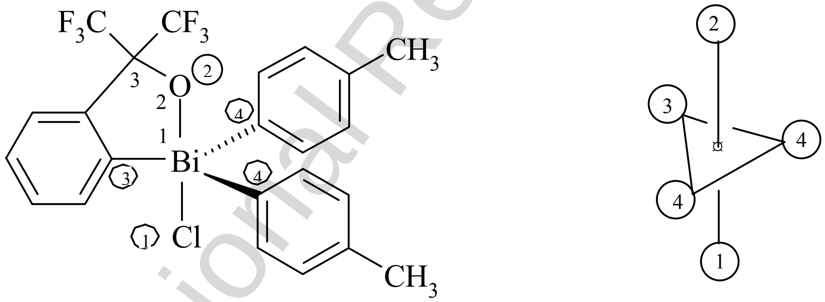
P-92.1.9.3.4.1 The configuration index of a trigonal bipyramid (see Rule I-5.4.4) is composed of the priority number of the two apical atoms (lower number first if different). They represent the reference axis of the system. Priority numbers are: ‘1’ > ‘2’ > ‘3’ > ‘4’ > ‘5’.



TBPY-5-35

The polyhedral symbol and configuration index, separated by a hyphen, are enclosed in parentheses in front of the name of the compound, if no further information is required.

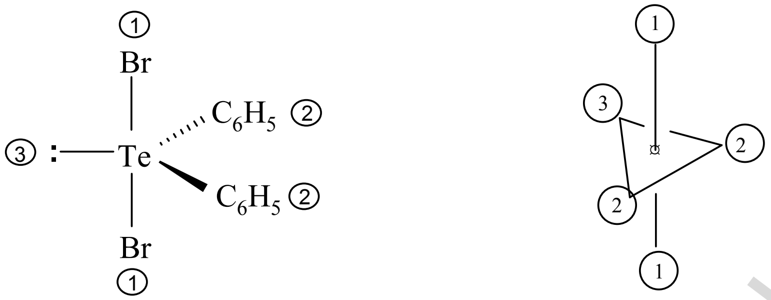
Example:



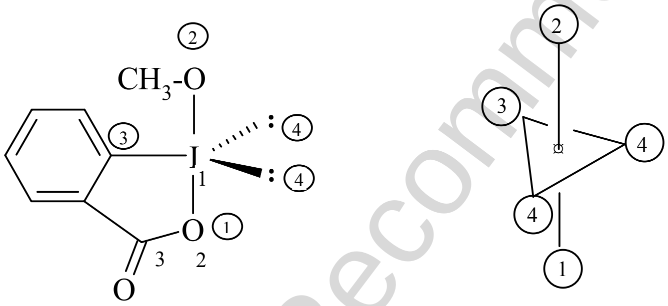
(*TBPY*-5-12)-1-chloro-1,1-bis(4-methylphenyl)-3,3-bis(trifluoromethyl)-1,3-dihydro-2,1λ^5-benzoxabismole (PIN)

P-92.1.9.3.4.2 The trigonal bipyramid system can be extended to central atoms substituted by four atoms or groups and one lone pair of electrons, and by three atoms or groups and two lone pairs of electrons; the use of a lone pair of electrons as a component in tetrahedral configuration is discussed in P-91.4.2.4 and illustrated in P-93.1.1.4.5. When one lone pair is present, the polyhedral symbol is (*TBPY*-4); the symbol is (*TBPY*-3) when two lone pairs of electrons are present. The configuration index is determined in the usual way, taking into account that a lone pair of electrons has the atomic number zero, as indicated in P-91.4.2.4. In preferred IUPAC names, the symbol (*TBPY*-4) is preferred to the see-saw system; similarly the symbol (*TBPY*-3) is preferred to the T-shape system.

Examples:



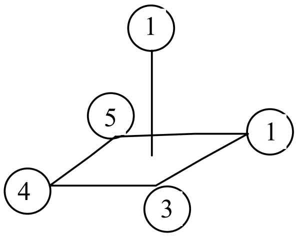
($TBPY$-4-11)-dibromodiphenyl-λ^5-tellurane (PIN)
(SS-4-11)-dibromodiphenyl-λ^5-tellurane (see P-92.1.7.3.3)



($TBPY$-3-12)-1-methoxy-1λ^3,2-benziodoxol-3(1H)-one (PIN)
(TPY-3-3)-1-methoxy-1λ^3,2-benziodoxol-3(1H)-one (see P-92.1.7.3.2)

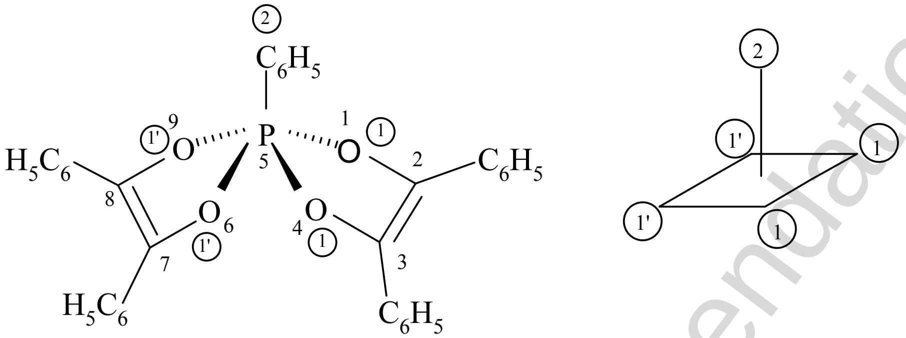
P-92.1.9.3.5 Square pyramid

The configuration index of a square pyramid (see Rule I-10.5.4.3, ref. 14) is given by two numbers. The first is the priority number of the apical atom and the second is the priority number of the atom trans (opposite) with reference to the atom having the highest priority (lowest priority number) in the base of the pyramid. If necessary, the rule of the '*trans*-maximum difference of priority numbers' is applied (see Rule I-10.5.3.2, ref. 14). The reference axis corresponds to the bond to the apical ligand. The polyhedral symbol and configuration index, separated by a hyphen, are enclosed in parentheses and cited in front of the name of the compound, if no further information is required. For the ranking order '1' > '2' > '3' > '4' > '5', the following configuration is denoted by the configuration index '24'.

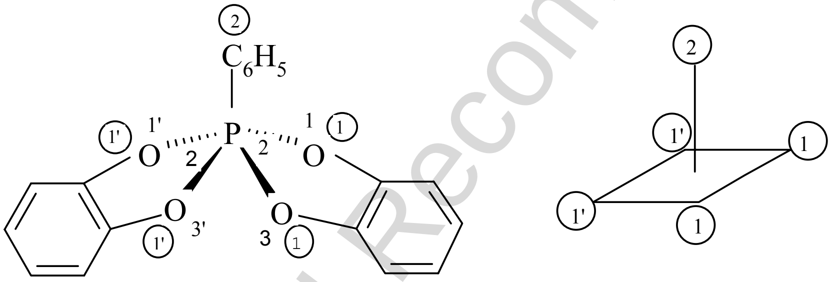


SPY-5-24

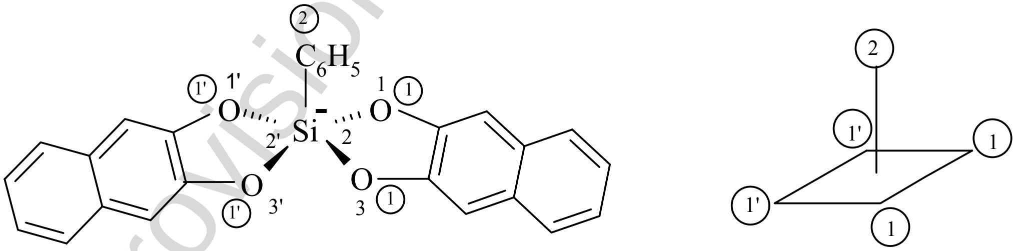
Examples:



(*SPY*-5-21′)-2,3,5,7,8-pentaphenyl-1,4,6,9-tetraoxa-5λ^5-phosphaspiro[4.4]nona-2,7-diene (PIN)



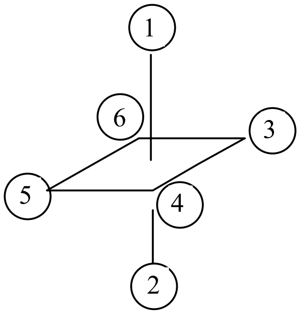
(*SPY*-5-21′)-2-phenyl-2λ^5,2′-spirobi[1,3,2-benzodioxaphosphole] (PIN)



(*SPY*-5-21′)-2-phenyl-2,2’-spirobi[naphtho[2,3-*d*][1,3,2]dioxasilol]-2-uide (PIN)

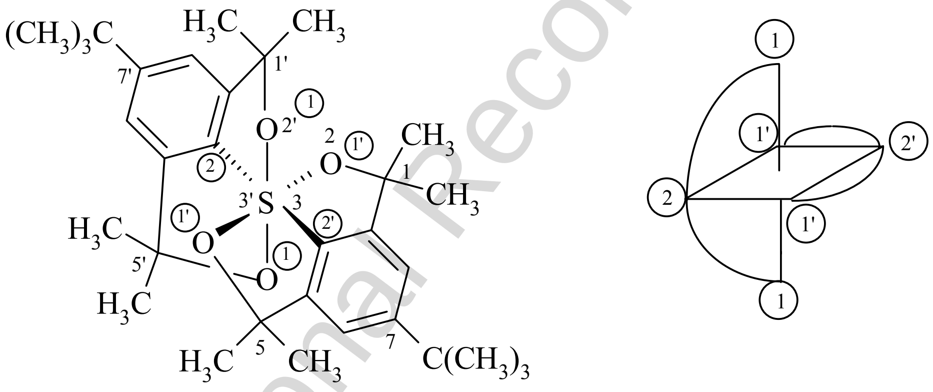
P-92.1.9.3.6 Octahedron

The configuration index of a octahedron (see Rule I-10.5.4.2, ref. 14) is given by two numbers. The first is the priority number of the atom ‘*trans’* (opposite) the atom of highest priority (lowest priority number). This defines the reference axis. The second number is the priority number of the atom ‘trans’ (opposite) the atom of highest priority (lowest priority number) in the plane perpendicular to the reference axis. If necessary, the principle of the ‘trans maximum difference’ of priority numbers’ is applied (see Rule I-10.5.3.2, ref. 14). The polyhedral symbol and configuration index, separated by a hyphen, are enclosed in parentheses and cited in front of the name of the compound, if no further information is needed. For the order of priority ‘1’ > ‘2’ > ‘3’ > ‘4’ > ‘5’ > ‘6’, the configuration index is ‘25’, as illustrated below.



(*OC*-6-25)

Examples:



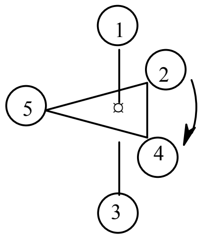
(*OC*-6-11′)-7,7′-di-*tert*-butyl-1,1,1′,1′,5,5,5′,5′-octamethyl-1*H*,1′*H*,5*H*,5′*H*-$3\lambda^6$,3′-spirobi[[1,2]oxathiolo[4,3,2-*hi*][2,1]benzoxathiole] (PIN)

P-92.1.9.4 Chirality

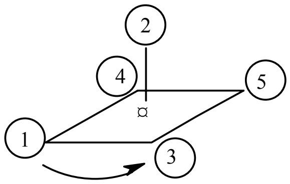
The chirality symbols ‘*A*/*C*’ are used to indicate the absolute configuration of compounds described by a polyhedral symbol and a configuration index, with the exception of the trigonal pyramidal configuration that is described by ‘*R*/*S*’ stereodescriptors.

P-92.1.9.4.1 The chirality symbols ‘*A*’ and ‘*C*’

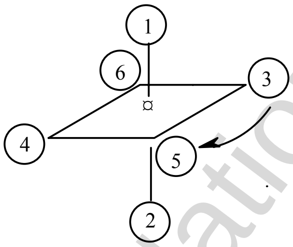
P-92.1.9.4.1.1 The atoms in the plane perpendicular to the reference axis are viewed from the side with the atom or group of highest priority (lowest priority number) on the reference axis. If the direction from the atom in this plane with highest priority (lowest priority number) to the atom with the next higher priority is clockwise the chirality symbol is ‘*C*’, if anticlockwise ‘*A*’. The term ‘anticlockwise’ is also called ‘counterclockwise’. The polyhedral symbol, configuration index and chirality symbol, each separated by a hyphen, are enclosed in parentheses and cited in front of the name of the compound (see Rule I-10.7.3. ref. 14). For the order of priority ‘1’ > ‘2’ > ‘3’ > ‘4’ > ‘5’ >’ 6’, the symbols are illustrated below:



TBPY-5-13-*C*

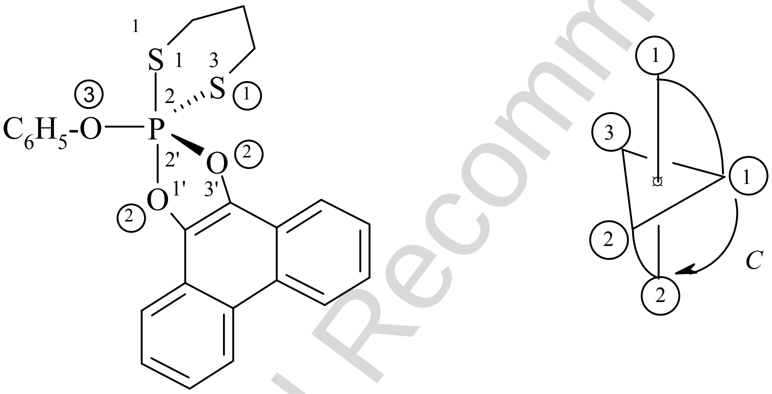


SPY-5-25-*A*

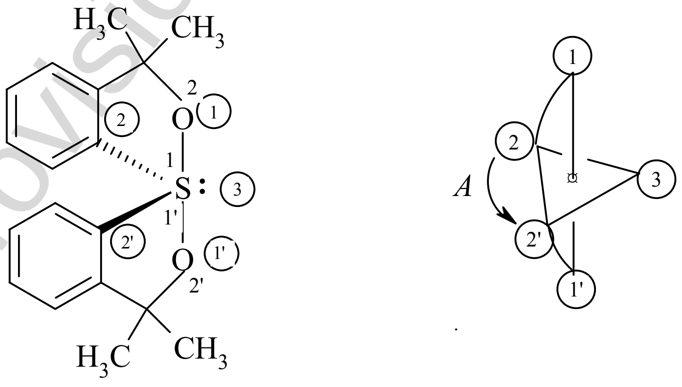


OC-6-24-*C*

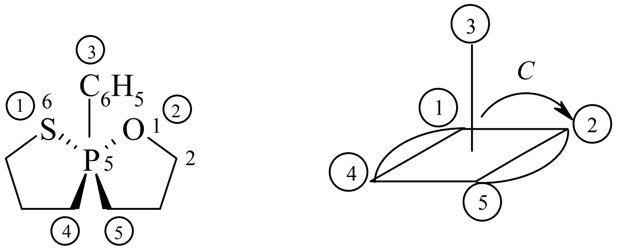
Examples:



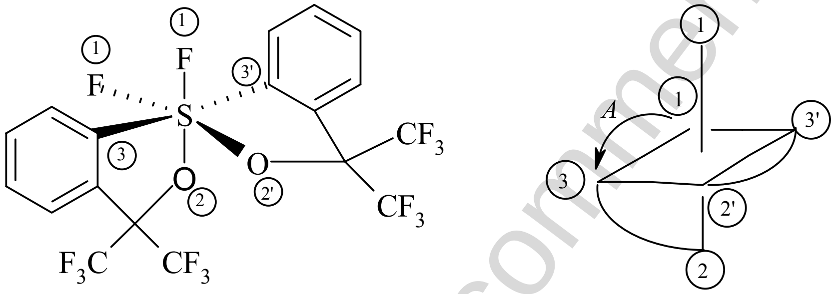
(*TBPY*-5-12-*C*)-2-phenoxy-2λ^5-spiro[1,3,2-dithiaphosphinane-2,2′-phenanthro[9,10-*d*][1,3,2]dithiaphosphole] (PIN)



(*TBPY*-4-11′-*A*)-3,3,3’,3’-tetramethyl-3*H*,3’*H*-1λ^4-spirobi[2,1-benzoxathiole] (PIN)



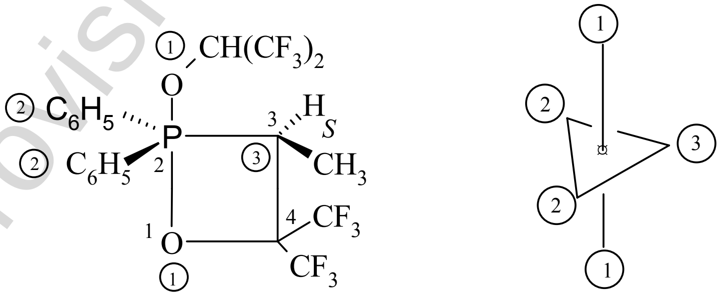
(*SPY*-5-34-*C*)-5-phenyl-1-oxa-6-thia-5λ^{5}-phosphaspiro[4.4]nonane (PIN)



(*OC*-6-22′-*A*)-1,1-difluoro-3,3,3′,3′-tetrakis(trifluoromethyl)-3*H*,3’*H*-1λ^{6}-spiro-bi[2,1-benzoxathiole] (PIN)

P-92.1.9.4.1.2 When necessary, the locant of the chiral center is included in front of the polyhedral descriptor, and other chiral centers are specified in accordance with the increasing value of locants as indicated in P-92.3.2.2; parentheses are put around the complete descriptor denoting the overall geometry of the molecule.

Examples:

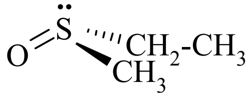


[2(*TBPY*-5-12),3*S*]-2-[(1,1,1,3,3,3-hexafluoropropan-2-yl)oxy]-3-methyl-2,2-diphenyl-4,4-bis(trifluoromethyl)-1,2λ^{5}-oxaphosphetane (PIN)

P-92.1.9.4.2 The chirality symbols ‘*R*/*S*’.

The stereodescriptors ‘*R*/*S*’ (as defined in P.92.3) are used to indicate the absolute configuration of a trigonal pyramidal system discussed in P-92.7.3.1. They are added after the ‘*TPY*-3’ symbol. A phantom atom of low priority, and not a pair of electrons, is used to create the tetrahedral configuration permitting the use of ‘*R*/*S*’ stereodescriptors in the manner described for tetrahedral configurations. Names associated with the tetrahedral configuration including a lone pair of electrons ion in place of an atom or substituent group are preferred to those expressing a trigonal pyramidal configuration including a phantom atom.

Example:



(*S*)-(methylsulfinyl)ethane (PIN)
(*TPY*-3-*S*)-(methylsulfinyl)ethane

P-92.2 Non-CIP stereodescriptors

P-92.2.0 Introduction

CIP stereodescriptors are preferred stereodescriptors in association with preferred IUPAC names constructed in accordance with the principles, rules and conventions described in Chapters 1 to 8 of this book. Stereodescriptors used before the CIP system was established are still recommended for general nomenclature and are mandatory in the field of Natural Products as indicated in Chapter 10.

P-92.2.1 Stereodescriptors used in preferred IUPAC nanes: '*cis*', '*trans*'; '*r*', '*c*', '*t*'; '*endo*',,'*exo*', '*syn*', '*anti*'.
P-92.2.2 Stereodescriptors no longer recommended in systematic IUPAC nomenclature but used in the nomenclature of natural products (see Chapter 10): 'D' and 'L'; '*erythro*', '*threo*'. '*meso*'; 'α', 'β', and 'ξ'; '*cis*', '*trans*', '*all-trans*'. '*ambo*'.

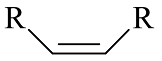
P-92.2.1 Stereodescriptors used in preferred IUPAC names: '*cis*', '*trans*', '*endo*', '*exo*', '*syn*', '*anti*'

P-92.2.1.1 The stereodescriptors '*cis*', '*trans*' , and '*r*', '*c*', '*t*'
P-92.2.1.2 The stereodescriptors '*endo*', '*exo*', '*syn*' and '*anti*'

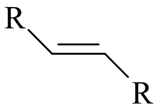
P-92.2.1.1 Stereodescriptors '*cis*' and '*trans*'

The stereodescriptors '*cis*' and '*trans*' are used to show the relationship between two atoms or groups attached to separate atoms that are connected by a double bond or are contained in a ring. The two atoms or groups are said to be located 'cis' to each other if they lie on the same side of a plane. If they are on opposite sides, their relative position is described as 'trans'. The appropriate reference plane of a double bond is perpendicular to that of the relevant σ-bonds and passes through the double bond. For a ring (the ring being in a conformation, real or assumed, without reentrant angles at the two substituted atoms) it is the mean plane of the ring(s).

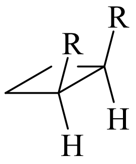
Examples:



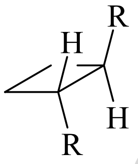
cis



trans

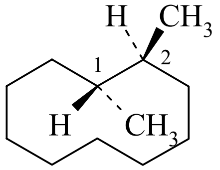


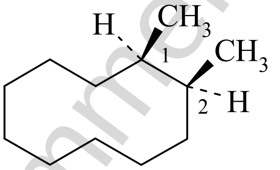
cis



trans

The structures below look like *cis/trans*-isomers, but are actually different conformations of the same *cis* stereoisomer. In the conformation on the left hand side, the stereogenic center at C-1 is located on a reentrant angle.



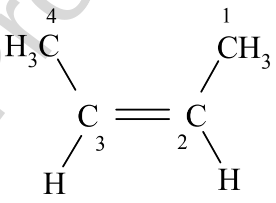


The stereodescriptors '*cis/trans*' are placed in front of the names, followed by a hyphen. Locants are placed in front of these descriptors when more than one double bond are present; locants and stereodescriptors are cited in parentheses. When alternative numberings are possible, that numbering is chosen which gives a '*cis*' attachment at the first point of difference.

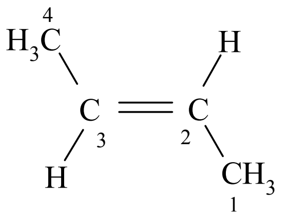
P-92.2.1.1.1 Application to double bonds

The '*cis*' and '*trans*' descriptors are recommended only in general nomenclature to describe the configuration of a double bond that are substituted once on each carbon atom. The '*cis*' and '*trans*' descriptors are placed at the front of the name when one double bond is present; when double bonds have to be identified by locants, these locants are reproduced at the front of the stereodescriptor, followed by a hyphen; parentheses are used to nest the entire stereodescriptor. Double bonds that are more substituted must be named by using the stereodescriptors '*E*' *and* '*Z*' described in P-92.1.6.2. For all double bonds, stereodescriptors '*E*' and '*Z*' are preferred to '*cis*' and '*trans*'.

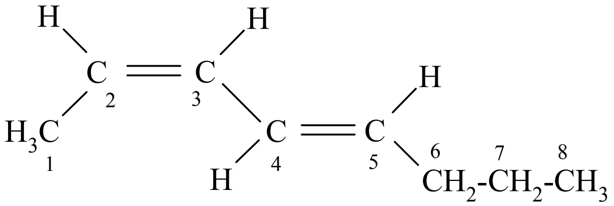
Examples:



cis-but-1-ene
(*Z*)-but-1-ene (PIN)



trans-but-2-ene
(*E*)-but-2-ene (PIN)

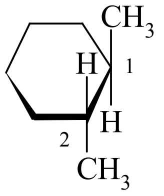


(2-*cis*,4-*trans*)-octa-2,4-diene
(2*Z*,4*E*)-octa-2,4-diene (PIN)

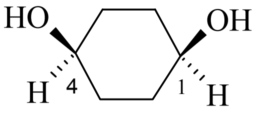
P-92.2.1.1.2 Application to substituted cyclic compounds.

P-92.2.1.1.2.1 When one substituent and one hydrogen atom are attached at each of two positions of a monocycle, the steric relations (the relative configuration) of the two substituents is expressed as ‘*cis*’ or ‘*trans*’, followed by a hyphen and placed before the name of the compound. No locants are required before the stereodescriptors. In names, ‘*cis*’ isomers are cited before ‘*trans*’ isomers, when a choice is possible. CIP stereodescriptors must be used to describe relative configuration in preferred IUPAC names, as shown in P-91.3 and P-92.1.2..

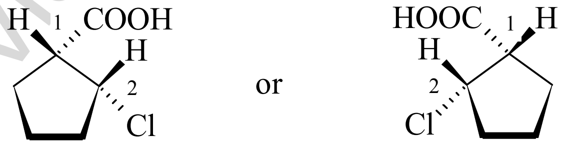
Examples:



trans-1,2-dimethylcyclohexane
rel-(1*R*,2*R*)-1,2-dimethylcyclohexane (PIN, see P-92.1.2)



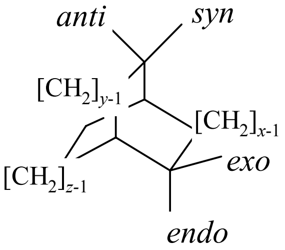
cis-cyclohexane-1,4-diol
(1*s*,4*s*)-cyclohexane-1,4-diol (PIN, see P-91.3)



cis-2-chlorocyclopentane-1-carboxylic acid
rel-(1*R*,2*R*)-2-chlorocyclopentane-1-carboxylic acid (PIN)

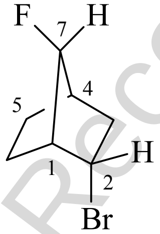
P-92.2.1.2 The stereodescriptors ‘*endo*’, ‘*exo*’, ‘*syn*’, ‘*anti*’ (relative configuration)

The stereodescriptors ‘*endo*’, ‘*exo*’, ‘*syn*’, ‘*anti*’ are used to indicate the relative orientation of groups attached to nonbridgehead atoms in bicyclo[x.y.z]alkanes, where ‘x’ ≥ ‘y’ > ‘z’ > 0, and with the additional provision that ‘x + y’ must be smaller than 7.

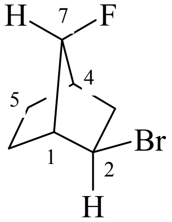


If the group is orientated toward the highest numbered bridge (‘’*z* bridge, e.g. C-7 in example below) it is given the description ‘*exo*’; if it is orientated away from the highest numbered bridge it is given the description ‘*endo*’. If the group is attached to the highest numbered bridge and is orientated toward the lowest numbered bridge (‘’*x* bridge, e.g. C-2 in example below) it is given the description ‘*syn*’; if the group is orientated away from the lowest numbered bridge it is given the description ‘*anti*’. The descriptors are always preceded by an appropriate locant.

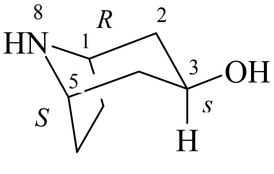
Examples:



(2-*endo*,7-*anti*)-2-bromo-7-fluorobicyclo[2.2.1]heptane
(2*S*,7*R*)-2-bromo-7-fluorobicyclo[2.2.1]heptane (PIN)



(2-*exo*,7-*syn*)-2-bromo-7-fluorobicyclo[2.2.1]heptane
(2*R*,7*S*)-2-bromo-7-fluorobicyclo[2.2.1]heptane (PIN)



(3-*exo*)-8-azabicyclo[3.2.1]octan-3-ol
(1*R*,3*s*,5*S*)-8-azabicyclo[3.2.1]octan-3-ol (PIN)

P-92.2.2 Descriptors no longer recommended in systematic IUPAC nomenclature but still used in the nomenclature of natural products described in Chapter 10: ‘D and L’; ‘*erythro*’, ‘*threo*’, ‘*meso*’; ‘α’, ‘β’, and ‘ξ’; ‘*cis*’, ‘*trans*’, ‘*all-trans*’; *ambo*.

P-92.2.2.1 The descriptors ‘D’ and ‘L’

The descriptors ‘D’ and ‘L’ are used to describe the configuration of amino acids and peptides (ref. 23 and P-103), carbohydrates (ref. 22 and P-102), and cyclitols (ref. 42 and P-104).

P-92.2.2.2 The descriptors ‘*erythro*’ and ‘*threo*’

The descriptors ‘*erythro*’ and ‘*threo*’ are used in the nomenclature of carbohydrates, along with descriptors such as ‘*arabino*’ and ‘*gluco*’ (see ref . 22 and P-102).

P-92.2.2.3 The stereodescriptors ‘α’, ‘β’, and ‘ξ’

The stereodescriptors ‘α’, ‘β’, and ‘ξ’ are used in the nomenclature of natural products described to describe the absolute configuration of alkaloids, terpenes and terpenoids, steroids, and other compounds as described in P-101.

P-92.2.2.4 The stereodescriptors ‘*cis*’, ‘*trans*’ and ‘*all-E*’ and ‘*all-trans*’ are used in the nomenclature of carotenoids and similar compounds (see ref. 40 and 48)

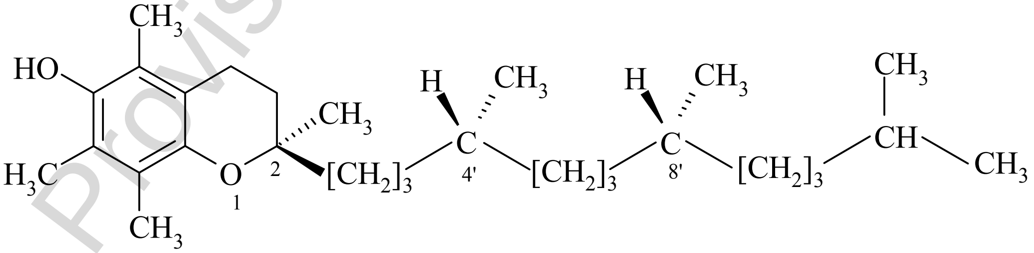
P-92.2.2.5 The descriptor ‘*meso*’

The descriptor ‘*meso*’ is used in the nomenclature of carbohydrates to designate compounds such as alditols and aldaric acids that are symmetrical and thus optically inactive (ref. 22 and P-102).

P-92.2.2.6 The stereodescriptor ‘*ambo*’

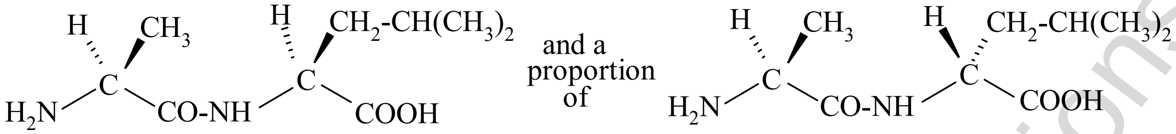
Formation of diastereoisomers by reaction at a nonstereogenic center of a chiral molecule or the reaction of a chiral compound with a racemic compound will not normally give a 50-50 mixture. To indicate this, the prefix ‘*ambo*’ is used.

Examples:



plus a proportion of the epimer at C-2

2-*ambo*-(2*R*,4′*R*,8′*R*)-α-tocopherol.



L-alanyl-*ambo*-leucine
(formed from L-alanine and DL-leucine)

P-93 Applications to specific parent structures

P-93.0 Introduction

Different systems are used to describe the configuration of acyclic and cyclic compounds. This Section describes these various systems and the selection of preferred descriptors to denote the tridimensional structure in preferred names. In Sections P-91 and P-92, the various stereodescriptors were described in accordance with different types of configuration. In this Section, they are applied on the basis of the parent structures, i.e., acyclic or cyclic. It is important to remember that stereodescriptors represent the entire molecule.

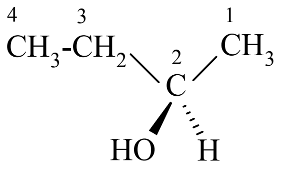
P-93.1 Specification of configuration of acyclic compounds

P-93.1.1 Specification of configuration due to chirality centers

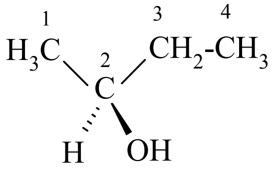
P-93.1.1.1 The presence of one center of chirality is denoted by the stereodescriptors '*R*' and '*S*', as described in P-92.1. These stereodescriptors, preceded by '*rel*' are preferred to '*R**' and '*S**' to indicate the relative configuration. The stereodescriptor '*rac*', is preferred to '*RS*' and '*SR*' to describe racemates.

Stereodescriptors are preceded by a locant when the chirality center needs to be described by a locant. When no locant is required in the name of the chiral compound, no locant is necessary before the stereodescriptor.

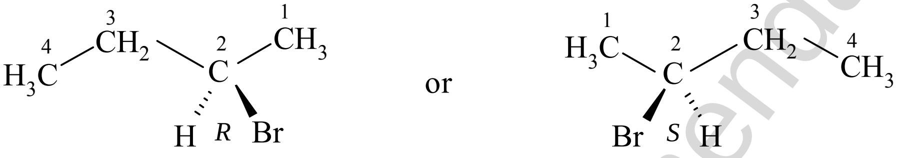
Examples:



(2*R*)-butan-2-ol (PIN)



(2*S*)-butan-2-ol (PIN)

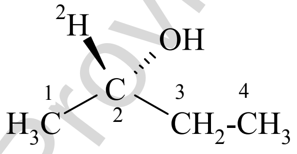


rel-(2*R*)-butan-2-ol (PIN)
(2*R**)-butane-2-ol

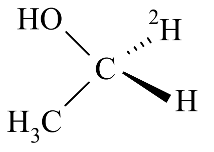
rac-(2*R*)-2-bromobutane (PIN)
(*RS*)-2-bromobutane
(±)-2-bromobutane

Sequences rules (1) and (2) are successively applied to specify the configuration of isotopically modified compounds. When inserted into the name at the same place as isotopic descriptors, the stereochemical affixes are cited first.

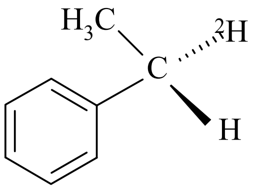
Examples:



(2*S*)-(2-^{2}H)-butan-2-ol (PIN)



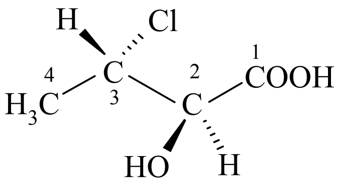
(1*S*)-(1-^{2}H$_{1}$)ethan-1-ol (PIN)



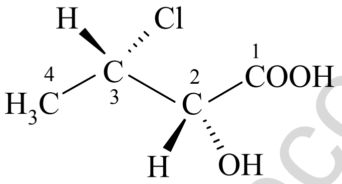
[(1*S*)-(1-^{2}H$_{1}$)ethyl]benzene (PIN)

P-93.1.1.1.2 When, in a parent structure, two or more stereodescriptors, '*R* and/or '*S*' are required to describe a single tridimensional (3D) structure, they are placed in front of the name and cited according to the ascending order of their corresponding locants, regardless of the kind of descriptor.

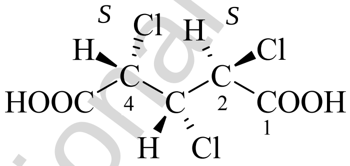
Examples:



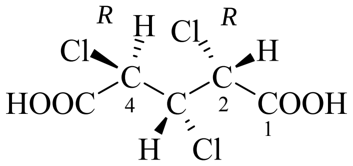
(2*R*,3*S*)-3-chloro-2-hydroxybutanoic acid (PIN)



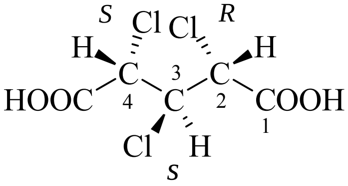
(2*S*,3*S*)-3-chloro-2-hydroxybutanoic acid (PIN)



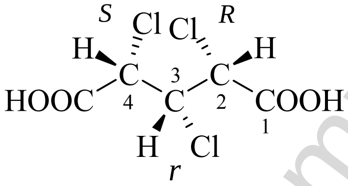
(2*S*,4*S*)-2,3,4-trichloropentanedioic acid (PIN)



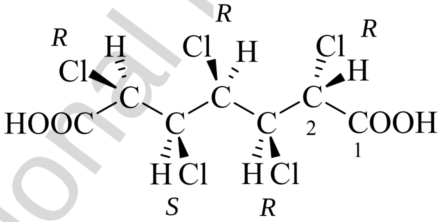
(2*R*,4*R*)-2,3,4-trichloropentanedioic acid (PIN)



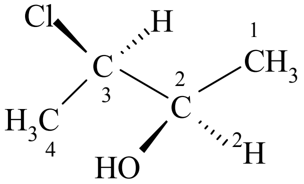
(2*R*,3*s*,4*S*)-2,3,4-triropentanedioic acid (PIN)
(Chirality center '*R*' receives the lowest locant [see P-14.4(k)]; application of sequence rule 5generates the stereodescriptor '*s*' at C-3)



(2*R*,3*r*,4*S*)-2,3,4-trichloropentanedioic acid (PIN)
(Chirality center '*R*' receives the lowest locant [see P-14.4(k)]; application of sequence rule 5 generates stereodescriptor '*r*' at C-3)



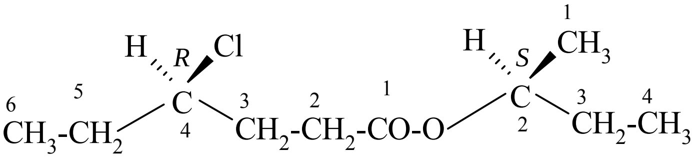
(2*R*,3*R*,4*R*,5*S*,6*R*)-2,3,4,5,6-pentachloroheptanedioic acid (PIN)
(application of Sequence rule 4 generates stereodescriptor '*R*' at C-4)



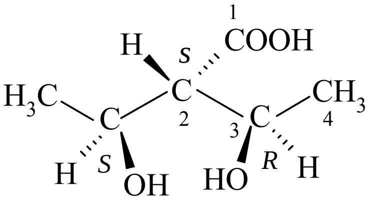
(2*R*,3*R*)-2-chloro-(3-$^2H_1$)-butan-2-ol (PIN)

P-93.1.1.1.3 Stereodescriptors, if any, denoting the absolute configuration of a component cited as a prefix or in functional class names, are cited immediately before each respective component.

Examples:



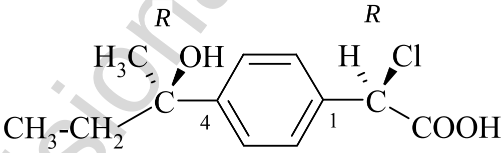
(2*S*)-butan-2-yl (4*R*)-4-chlorohexanoate (PIN)



(2*s*,3*R*)-3-hydroxy-2-[(1*S*)-1-hydroxyethyl]butanoic acid (PIN)

Guide to name construction:

Step 1: configurations '*R*' and '*S*' are assigned to the hydroxylated stereogenic centers;
Step 2: configuration '*s*' is assigned to the pseudo-asymetric carbon atom;
Step 3: the principal chain has the maximum of stereogenic centers having the '*R*' configuration [see P-44.4.5.3(a)];
Step 4: the name is constructed by citing the stereodescriptors at the front of the principal chain and of the substituent.



(2R)-2-chloro-2-{4-[(2*R*)-2-hydroxybutan-2-yl]phenyl}acetic acid (PIN)

P-93.1.1.1.4 Tetrahedral configuration of elements other than carbon

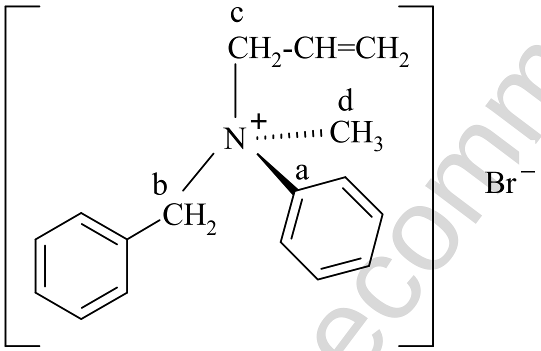
P-93.1.1.1.4.0 Introduction

The absolute configuration of any atom with four atoms or groups tetrahedrally arranged is described by '*R*' and '*S*' stereodescriptors. The assignment of these descriptors is the same as for carbon centered compounds.

P-93.1.1.1.4.1 Azanium (ammonium) and phosphanium (phosphonium) compounds

The four different atoms or groups are considered in priority order 'a' > 'b' > 'c' > 'd' in the manner described in P-91.4. Stereodescriptors are cited as indicated in P-92.3.2.

Examples:

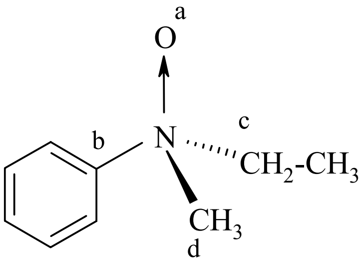


(*R*)-*N*-benzyl-*N*-methyl-*N*-(prop-2-en-1-yl)anilinium bromide (PIN)
(*R*)-benzyl(methyl)phenyl(prop-2-en-1-yl)azanium bromide
(*R*)-benzyl(methyl)phenyl(prop-2-en-1-yl)ammonium bromide

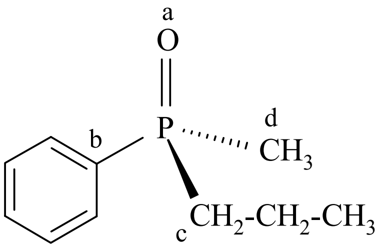
P-93.1.1.1.4.2 Amine oxides and phosphane oxides

With chiral amine oxides and phosphane oxides the oxygen atom is treated as the fourth atom. The nature of the bonding to this oxygen atom is not relevant.

Examples:



(*R*)-*N*-ethyl-*N*-methylaniline oxide (PIN)
[(*R*)-*N*-ethyl-*N*-methylaniliniumyl]oxidanide
(see P-74.2.1.2)

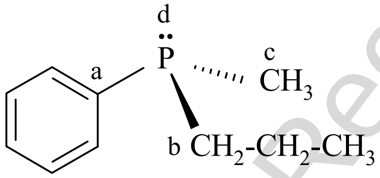


(S)-methyl(phenyl)propyl-λ^5-phosphanone
(S)-methyl(phenyl)propylphosphane oxide (PIN)

P-93.1.1.1.3 Phosphanes

A tetrahedral configuration is assumed for chiral λ^3-phosphanes. The lone pair of electrons is considered as the group of lowest precedence in the order 'a' > 'b' > 'c' > 'd' (see P-91.4.2.4).

Examples:

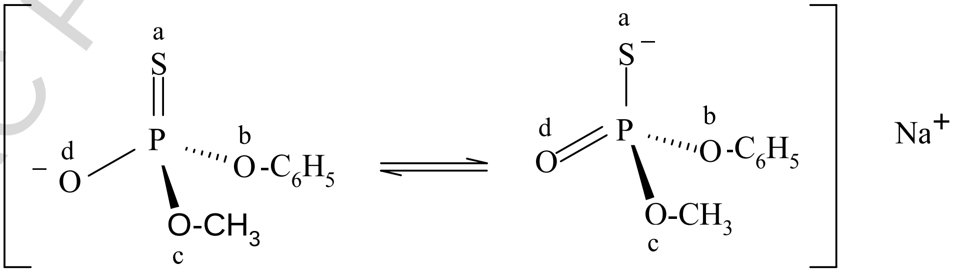


(R)-methyl(phenyl)propylphosphane (PIN)

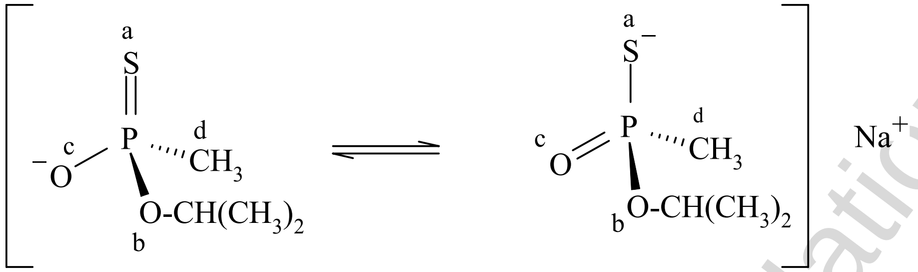
P-93.1.1.1.4.4 Phosphates, phosphonates and related compounds

The P=O bond, as conventionally written in phosphates, phosphonates and related compounds, is considered as a single bond, as there are already four atoms or groups in the tetrahedral configuration. Similarly, the formal arrangement of charges is not considered when determining the configuration of a chiral molecule. As the stereodescriptors 'R' and 'S' describe the entire structure, either a salt or an ester, the full name is placed in parentheses to denote the global configuration.

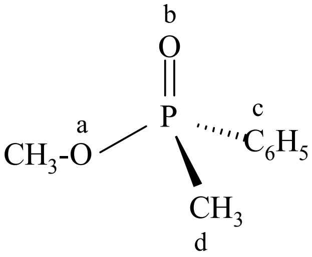
Examples:



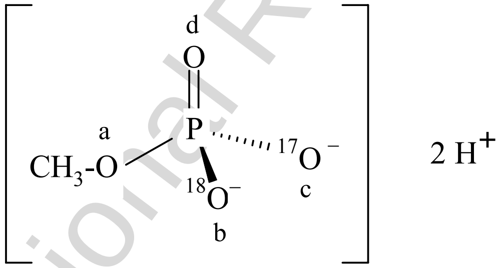
sodium (R)-(O-methyl O-phenyl phosphorothioate) (PIN)



sodium (*R*)-(*O*-propan-2-yl methylphosphonothioate) (PIN)
sodium (*R*)-[*O*-(1-methylethyl) methylphosphonothioate] (PIN)



(*S*)-[methyl methyl(phenyl)phosphinate] (PIN)

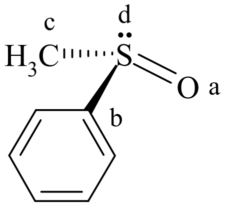


dihydrogen (*R*)-(*O*-methyl [^{17}O,^{18}O]phosphate) (PIN)

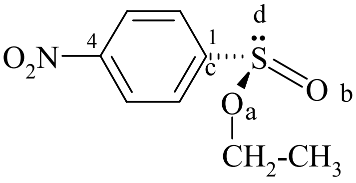
P-93.1.1.1.4.5 Sulfoxides and related compounds

The geometry of the sulfoxide group is tetrahedral when the lone pair of electrons is treated as if it were an atom. This lone pair of electrons has lowest priority. Chiral examples of other related sulfur compounds with three atoms attached to the sulfur atom are treated in the same way.

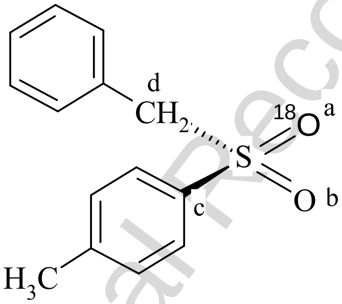
Examples:



(S)-methanesulfinylbenzene (PIN)



(R)-(ethyl 4-nitrobenzene-1-sulfinate) (PIN)

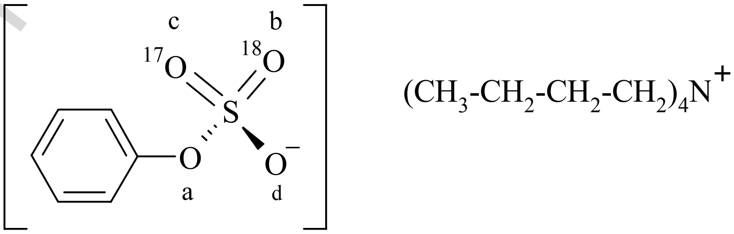


1-methyl-4-[(R)-phenyl($^{18}O_1$)methanesulfonyl]benzene (PIN)

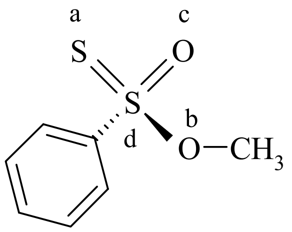
P-93.1.1.1.4.6 Sulfates, sulfonates and related compounds

Sulfates, sulfonates and related anions are treated in the same way as phosphate anions (see P-93.1.1.1.4.4).

Examples:



N,*N*,*N*-tributylbutanaminium (S)-[*O*-phenyl (^{17}O,^{18}O)sulfate] (PIN)
tetrabutylammonium (S)-[*O*-phenyl (^{17}O,^{18}O)sulfate]
tetrabutylazanium (S)-[*O*-phenyl (^{17}O,^{18}O)sulfate]

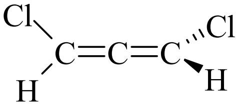


(*S*)-(*O*-methyl benzenesulfonothioate) (PIN)

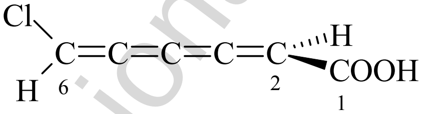
P-93.1.2 Allenes and cumulenes having an even number of double bonds

When appropriately substituted, allenes are chiral compounds having an axis of chirality. Chirality is thus described by the stereodescriptors ‘R_a’ and ‘S_a’ or ‘*M*’ and ‘*P*’, as described in P-92.1.5.1). Stereodescriptors ‘R_a’ and ‘S_a’ are preferred to ‘*M*’ and ‘*P*’.

Examples:



(R_a)-1,3-dichloropropa-1,2-diene (PIN)
(*M*)-1,3-dichloropropa-1,2-diene
(R_a)-1,3-dichloroallene
(*M*)-1,3-dichloroallene



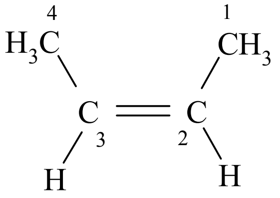
(S_a)-6-chlorohexa-2,3,4,5-tetraenoic acid (PIN)
(*P*)-6-chlorohexa-2,3,4,5-tetraenoic acid

P-93.1.3 Specification of configuration due to double bonds

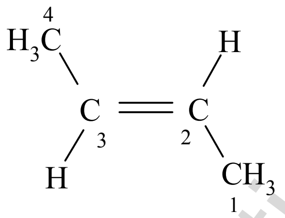
P-93.1.3.1 Description of the configuration of one double bond

The stereodescriptors ‘*E*’ and ‘*Z*’ are preferred to ‘*cis*’ and ‘*trans*’ to describe one or more C=C double bonds. Stereodescriptors ‘*cis*’ and ‘*trans*’ are used in general nomenclature only to describe double bonds having two hydrogen atoms, one on each carbon atom. Locants corresponding to those needed to describe a double bond are repeated before the stereodescriptors ‘*E*’ and ‘*Z*’, but not before ‘*cis*’ and ‘*trans*’

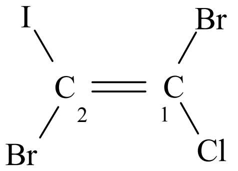
Examples:



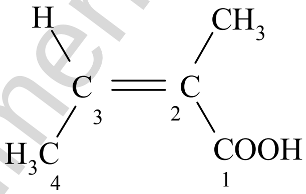
(2*Z*)-but-2-ene (PIN)
cis-but-2-ene



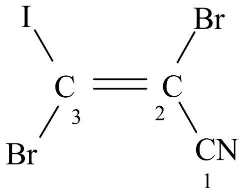
(2*E*)-but-2-ene (PIN)
trans-but-2-ene



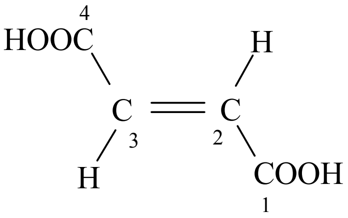
(1*Z*)-1,2-dibromo-1-chloro-2-iodoethene (PIN)



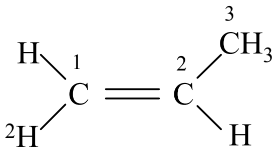
(2*Z*)-2-methylbut-2-enoic acid (PIN)



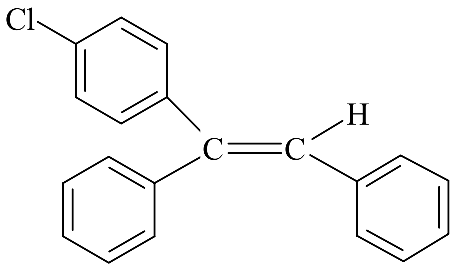
(2*E*)-2,3-dibromoprop-2-enenitrile (PIN.)
(2*E*)-2,3-dibromoacrylonitrile



(2*E*)-but-2-enedioic acid (PIN)
fumaric acid (the stereochemistry
is implied in the retained name)



(1*E*)-(1-$^{2}H_{1}$)prop-1-ene (PIN)
cis-(1-$^{2}H_{1}$)prop-1-ene



(*E*)-1,1′-[1-(4-chlorophenyl)ethene-1,2-diyl]dibenzene (PIN)

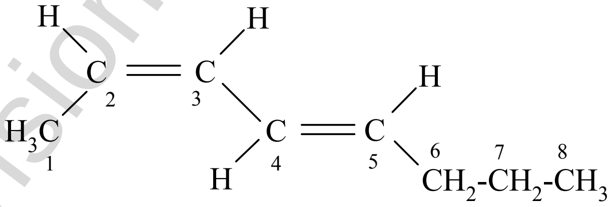
P-93.1.3.2 Compounds containing more than one double bond

The stereodescriptors ‘*E*/*Z*’ related to the parent are cited, preceded by the appropriate locant if more than one double bond is present, before the complete name of the compound, or before the name of the appropriate component. Chain locants are used when double bonds are ‘exo’ to the chain (see fourth example below). If more than one descriptor is used, the descriptors are cited in ascending order of their respective locants.

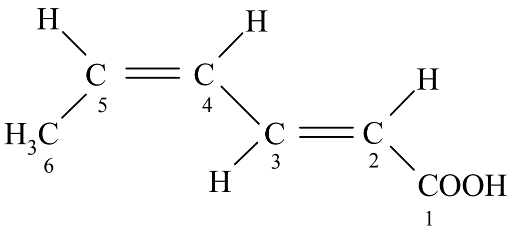
When alternative numberings of a chain or rings or ring systems are possible, that numbering is chosen which gives a ‘*cis*’ attachment at the first point of difference. Attention must be given to the fact that a ‘*cis*’ attachment is denoted by the stereodescriptor ‘*Z*’.

Stereodescriptors ‘*cis*’ and ‘*trans*’ may be used to describe double bonds having two hydrogen atoms, one on each carbon atom, but stereodescriptors ‘*E*’ and ‘*Z*’ are used in preferred IUPAC names. The stereodescriptors ‘*cis*’ and ‘*trans*’, placed in parentheses, are cited at the front of the name, preceded by the appropriate locant followed by a hyphen.

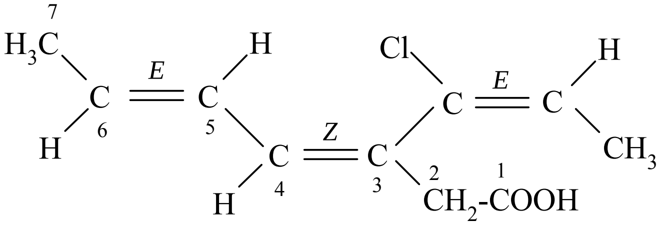
Examples:



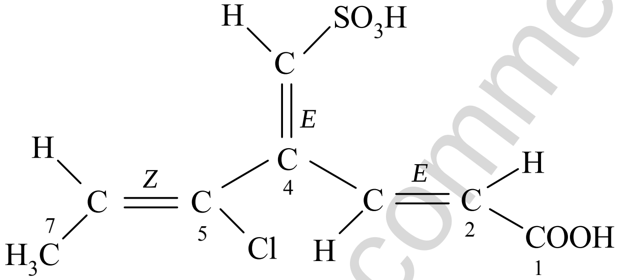
(2Z,4*E*)-octa-2,4-diene (PIN)
(2-*cis*,4-*trans*)-octa-2,4-diene



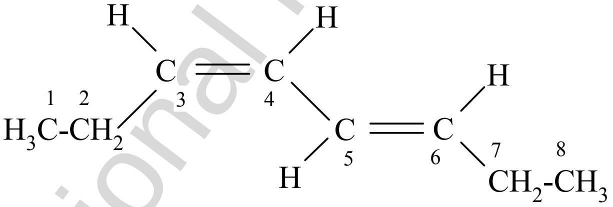
(2*E*,4*Z*)-hexa-2,4-dienoic acid (PIN)
(2-*trans*,4-*cis*)-hexa-2,4-dienoic acid



(3*Z*,5*E*)-3-[(1*E*)-1-chloroprop-1-en-1-yl]hepta-3,5-dienoic acid (PIN)
(3-*cis*,5-*trans*)-3-[(1*E*)-1-chloroprop-1-en-1-yl]hepta-3,5-dienoic acid



(2*E*,4*E*,5*Z*)-5-chloro-4-(sulfomethylidene)hepta-2,5-dienoic acid (PIN)

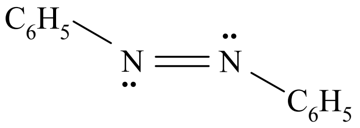


(3*Z*,5*E*)-octa-3,5-diene (PIN)
(3-*cis*,5-*trans*)-octa-3,5-diene
[the double bond with the *cis* configuration
receives the lowest locants (see P-44.4.5.1)]

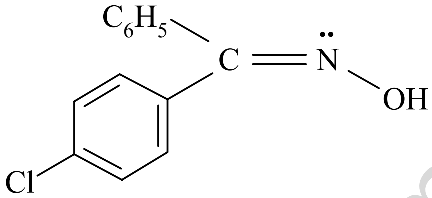
P-93.1.3.3 Descriptors '*E*' and '*Z*' to denote double bonds linked to heteroatoms

The stereodescriptors '*E*' and '*Z*' are also used to indicate the configuration of double bonds involving atoms other than carbon. A lone pair of electrons, when present, is considered to have the atomic number '0' (zero). The descriptors '*syn*' and '*anti*', and '*cis*' and '*trans*', are no longer recommended for these situations. No locant is required before the stereodescriptor when none is present in a name.

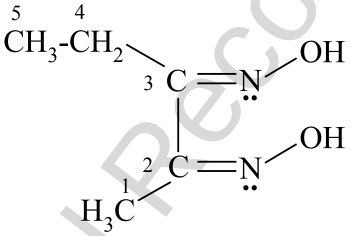
Examples:



(*E*)-diphenyldiazene
(not *trans*-diphenyldiazene)



(*Z*)-(4-chloro-α-phenylbenzylydene)hydroxylamine (PIN)
(*Z*)-(4-chlorophenyl)phenylmethanone oxime



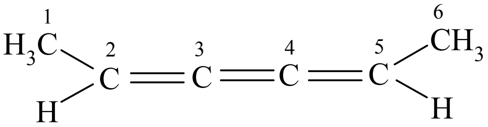
(2*Z*,3*E*)-pentane-2,3-diylidenebis(hydroxylamine) (PIN)
(2*Z*,3*E*)-pentane-2,3-dione dioxime

P-93.1.3.4 Cumulenes having odd number of double bonds

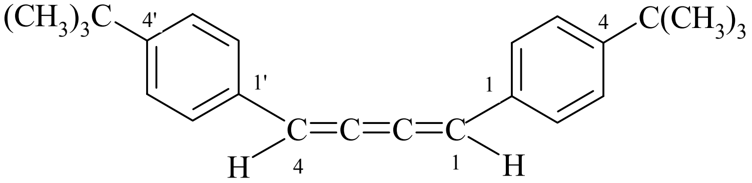
Cumulenes having an odd number of double bonds are planar molecules, like double bonds. The preferred stereodescriptors are '*E*' and '*Z*'. Stereodescriptors '*cis*' and '*trans*' may be used in general nomenclature.

The stereodescriptor '*E*' or '*Z*', describing the cumulene system, is preceded by composite locants indicating the starting point and the end point of the cumulated double bond system

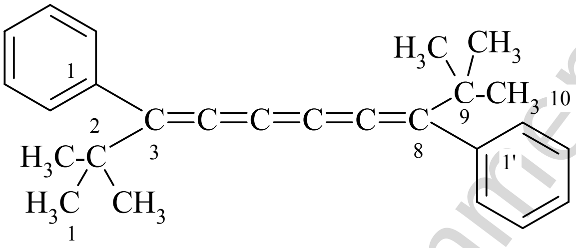
Examples:



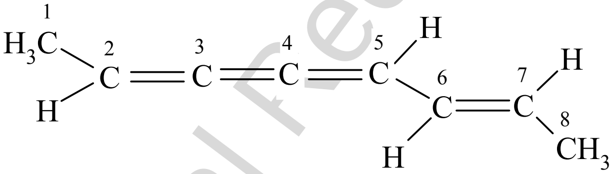
[2(5)*Z*]-hexa-2,3,4-triene
cis-hexa-2,3,4-triene



[1(4)*Z*]-1,1´-buta-1,2,3-triene-1,4-diylbis(4-*tert*-butylbenzene) (PIN)
(*cis*)-1,1´-buta-1,2,3-triene-1,4-diylbis(4-*tert*-butylbenzene)



[3(8)*E*]-1,1´-(2,2,9,9-tetramethyldeca-3,4,5,6,7-pentaene-3,8-diyl)dibenzene (PIN)
[3(8)*E*]-2,2,9,9-tetramethyl-3,8-diphenyl-deca-3,4,5,6,7-pentaene

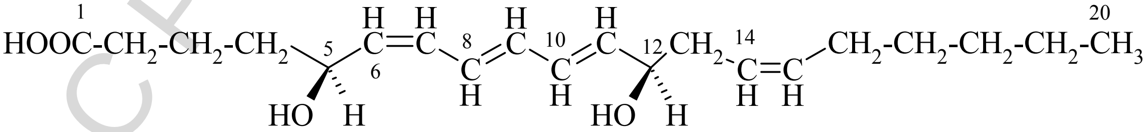


[2(5)*E*,6*E*]-octa-2,3,4,6-tetraene (PIN)
[2[5]-*trans*,6-*trans*]-octa-2,3,4,6-tetraene

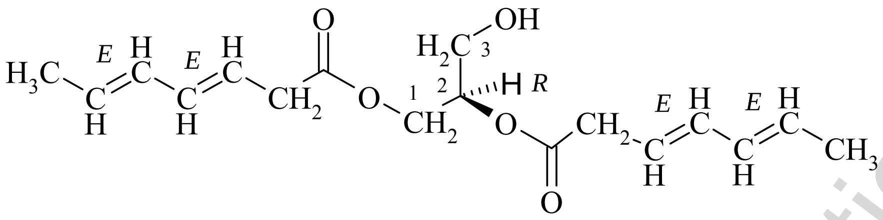
P-93.1.3.5 Specification of configuration in chiral unsaturated compounds

When chiral compounds contain C=C double bond(s), stereodescriptors are assigned as describe above. Stereodescriptors are cited at the front of the name or of any substituent group or appropriate portion of the name, in ascending order of the locants.

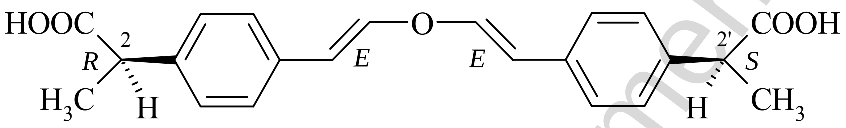
Examples:



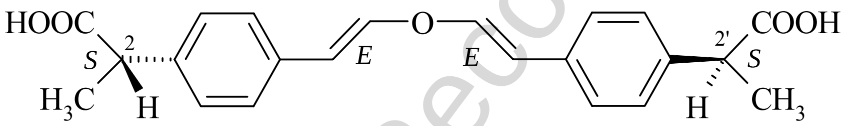
(5*S*,6*Z*,8*E*,10*E*,12*R*,14*Z*)-5,12-dihydroxyicosa-6,8,10,14-tetraenoic acid (PIN)
(5*S*,6-*cis*,8-*trans*,10-*trans*,12*R*,14-*cis*)-5,12-dihydroxyicosa-6,8,10,14-tetraenoic acid



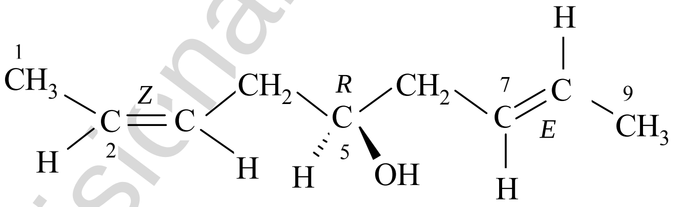
(2*R*)-3-hydroxypropane-1,2-diyl di(3*E*,5*E*)-hepta-3,5-dienoate (PIN)
(2*R*)-3-hydroxypropane-1,2-diyl di(3-*trans*,5-*trans*)-hepta-3,5-dienoate



(2*R*,2′*S*)-2,2′-{oxybis[(1*E*)-ethene-2,1-diyl-4,1-phenylene]}dipropanoic acid

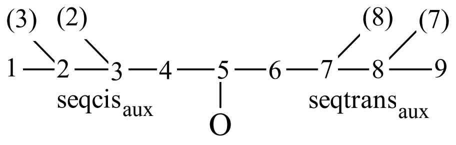


(2*S*,2′*S*)-2,2′-{oxybis[(1*E*)-ethene-2,1-diyl-4,1-phenylene]}dipropanoic acid



(2*Z*,5*R*,7*E*)-nona-2,7-dien-5-ol

Guide to name construction in accordance with the digraph:



Step 1: configurations ‘*seqcis*$_{aux}$’ and ‘*seqtrans*$_{aux}$’ are assigned to the double bonds, respectively ‘*Z*’ and ‘*E*’;
Step 2: the configuration ‘*R*’ at C-5 is determined in accordance with Sequence Rule **3**, *seqcis* precedes *seqtrans*;
Step 3: the chain is numbered to allocate low locant to the ‘Z’ double bond;

Step 4: the name is constructed by citing stereodescriptors and their locants at the front of the name, in the ascending order of locants.

P-93.2 Cyclic compounds

P-93.2.1 Monocyclic compounds
P-93.2.2 von Baeyer compounds
P-93.2.3 Spiro compounds
P-93.2.4 Fused and bridged fused compounds
P-93.2.5 Cyclophanes
P-93.2.6 Fullerenes
P-93.2.7 Ring assemblies

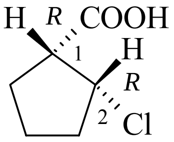
P-93.2.1 Monocyclic compounds

P-93.2.1.1 Chiral compounds

For chiral compounds, absolute configuration is described by using the stereodescriptors '*R*' and '*S*'. To describe the relative configuration the stereodescriptors '*R*' and '*S*' preceded by the term '*rel*' are preferred to '*R**'and '*S**', and also to '*cis*' and '*trans*' and '*r*', '*c*', and '*t*'. To describe the configuration of racemates, the stereodescriptors *R* and *S* preceded by the term *rac* are preferred to '*RS*' and '*SR*'. When relative configuration or racemates are described, the stereodescriptor '*R*' or '*R**' is cited for the chirality center having the lowest locant. It is to be noted that the prefixes '*rel*' or '*rac*' indicate the configuration of the entire molecule.

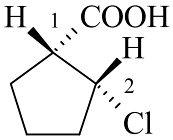
Example 1:

Absolute configuration:

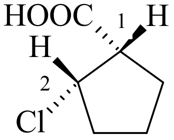


(1*R*,2*R*)-2-chlorocyclopentane-1-carboxylic acid (PIN)

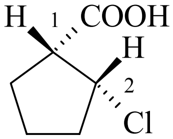
Relative configuration:



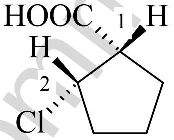
or



rel-(1*R*,2*R*)-2-chlorocyclopentane-1-carboxylic acid (PIN)
(1*R**,2*R**)-2-chlorocyclopentane-1-carboxylic acid
cis-2-chlorocyclopentane-1-carboxylic acid
[not *rel*-(1*S*,2*S*)-2-chlorocyclopentane-1-carboxylic acid]
[not (1*S**,2*S**)-2-chlorocyclopentane-1-carboxylic acid]



+

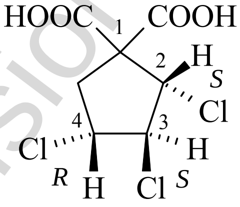


50% + 50%

rac-(1*R*,2*R*)-2-chlorocyclopentane-1-carboxylic acid (PIN)
(1*RS*,2*RS*)-2-chlorocyclopentane-1-carboxylic acid

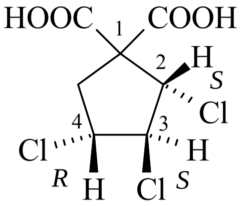
Example 2:

Absolute configuration:

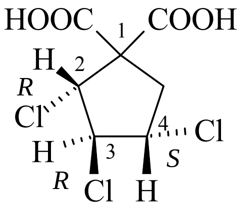


(2*S*,3*S*,4*R*)-2,3,4-trichlorocyclopentane-1,1-dicarboxylic acid (PIN)

Relative configuration:

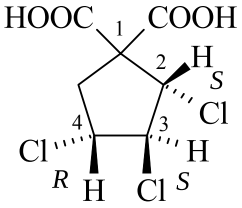


or

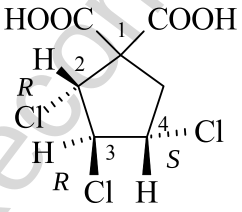


*rel-(*2*R*,3*R*,4*S*)-2,3,4-trichlorocyclopentane-1,1-dicarboxylic acid (PIN)
(2*R**,3*R**,4*S**)-2,3,4-trichlorocyclopentane-1,1-dicarboxylic acid
  [not *rel-(*2*S*,3*S*,4*R*)-2,3,4-trichlorocyclopentane-1,1-dicarboxylic acid]
  [not *(*2*S**,3*S**,4*R**)-2,3,4-trichlorocyclopentane-1,1-dicarboxylic acid]
2-*r*,3-*c*,4-*t*-trichlorocyclopentane-1,1-dicarboxylic acid

Racemate:

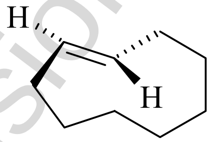


+

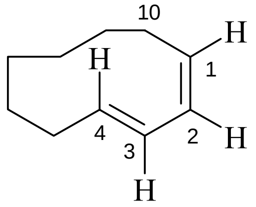


50% + 50%

rac-(2*R*,3*R*,4*S*)-2,3,4-trichlorocyclopentane-1,1-dicarboxylic acid (PIN)
(2*RS*,3*RS*,4*SR*)-2,3,4-trichlorocyclopentane-1,1-dicarboxylic acid



(1*E*)-cyclononene (PIN)



(1*Z*,3*E*)-cyclodeca-1,3-diene (PIN)
(1-*cis*,3-*trans*)-cyclodeca-1,3-diene
  [lowest locants are assigned to *Z* double
  bond (see P-44.4.5.1)]

P-92.2.1.2 Achiral compounds

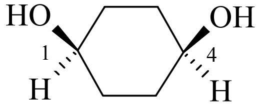
The configuration of achiral compounds is expressed in two ways:

(a) by using CIP stereodescriptors;

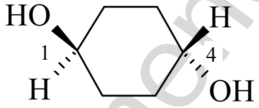
(b) by using ‘*cis*’, ‘*trans*’ or ‘*r*’, ‘*c*’, ‘*t*’ stereodescriptors.

Preferred IUPAC names are those using CIP stereodescriptors.

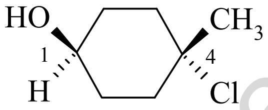
Examples:



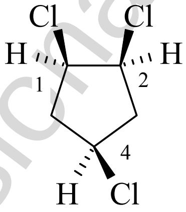
(1*s*,4*s*)-cyclohexane-1,4-diol (PIN)
cis-cyclohexane-1,4-diol



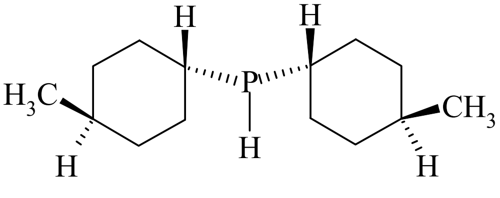
(1*r*,4*r*)-cyclohexane-1,4-diol (PIN)
trans-cyclohexane-1,4-diol



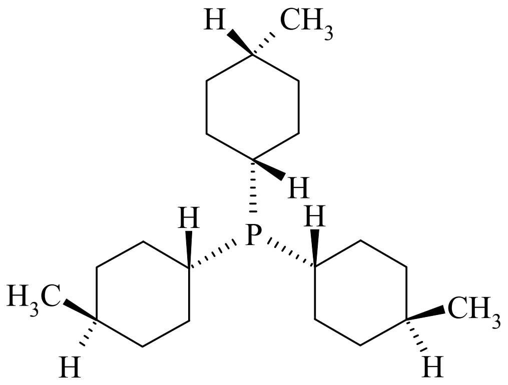
(1*r*,4*r*)-4-chloro-4-methylcyclohexan-1-ol (PIN)
4-*t*-chloro-4-methylcyclohexan-1*r*-ol



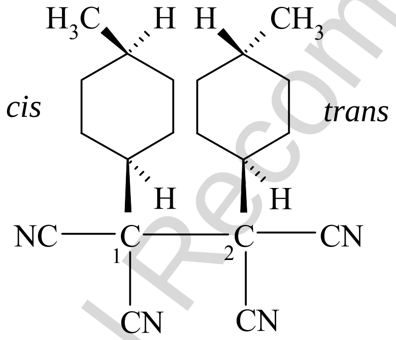
(1*R*,2*S*,4*r*)-1,2,4-trichlorocyclopentane (PIN)
1*r*,2*c*,4*c*-trichlorocyclopentane



bis[(1*r*,4*r*)-4-methylcyclohexyl]phosphane (PIN)
bis(*trans*-4-methylcyclohexyl)phosphane



[(1*s*,4*s*)-4-methylcyclohexyl]bis[(1*r*,4*r*)-4-methylcyclohexyl]phosphane (PIN)
(*cis*-4-methylcyclohexyl)bis(*trans*-4-methylcyclohexyl)phosphane

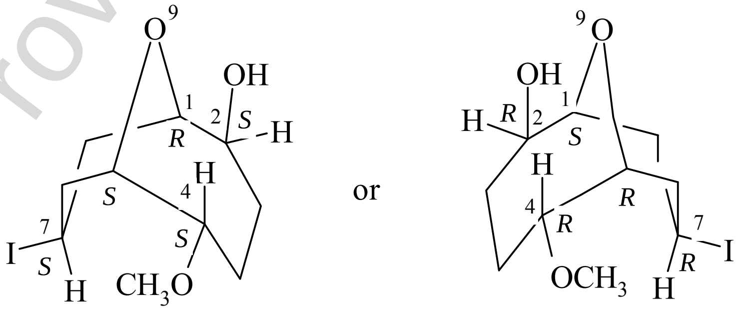


1-[(1*s*,4*s*)-4-methylcyclohexyl]-2-[(1*r*,4*r*)-4-methylcyclohexyl]ethane-1,1,2,2-tetracarbonitrile

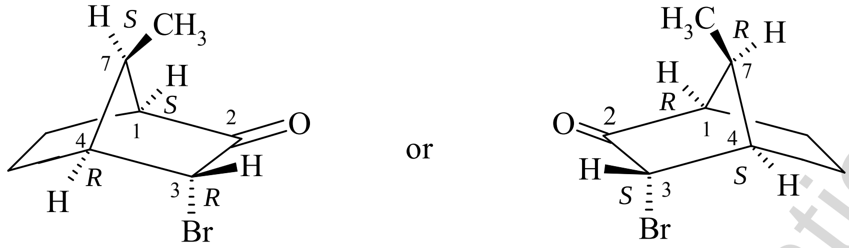
P-93.2.2 von Baeyer compounds

P-93.2.2.1 Chiral compounds

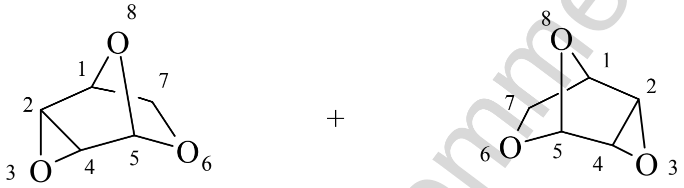
Examples:



rel-(1R,2*S*,4*S*,5*S*,7*S*)-7-iodo-4-methoxy-9-oxabicyclo[4.3.1]decan-2-ol (PIN)
(1*R**,2*S**,4*S**,5*S**,7*S**)-7-iodo-4-methoxy-9-oxabicyclo[4.3.1]decan-2-ol
(2-*exo*,4-*endo*,7-*exo*)-7-iodo-4-methoxy-9-oxabicyclo[4.3.1]decan-2-ol



rel-(1*R*,3*S*,4*S*,7*R*)-3-bromo-7-methylbicyclo[2.2.1]octan-2-one (PIN)
(1*R**,3*S**,4*S**,7*R**)-3-bromo-7-methylbicyclo[2.2.1]octan-2-one
(3-*endo*,7-*syn*)-3-bromo-7-methylbicyclo[2.2.1]octan-2-one



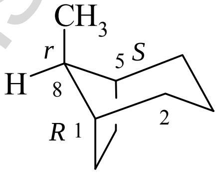
50% 50%

rac-(1*R*,2*S*,4*S*,5*R*)-3,6,8-trioxatricyclo[3.2.1.$0^{2,4}$]octane (PIN)
(1*RS*,2*SR*,4*SR*,5*RS*)-3,6,8-trioxatricyclo[3.2.1.$0^{2,4}$]octane

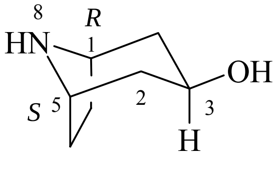
P-93.2.2.2 Achiral compounds

Pseudoasymmetric centers in achiral von Baeyer compounds are described by *r* and *s* sterodescriptors. The descriptors '*endo*', '*exo*', '*anti*' and '*syn*' may be used in general nomenclature to describe the relative configuration (see P-(2.2.1.2). CIP stereodescriptors are used in preferred IUPAC names.

Examples:



(1*R*,5*R*,8*r*)- 8-methylbicyclo[3.2.1]octane (PIN)
syn-8-methylbicyclo[3.2.1]octane



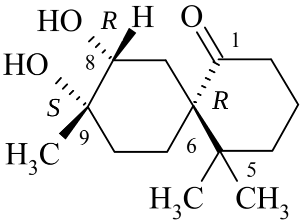
(1*R*,3*s*,5*S*)- 8-azabicyclo[3.2.1]octan-3-ol (PIN)
(3-*exo*)-8-azabicyclo[3.2.1]octan-3-ol

P-93.2.3 Spiro compounds

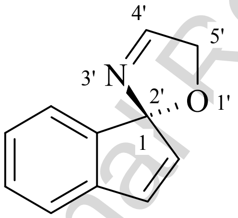
P-93.2.3.1 Chiral spiro atoms of the type Cabcd, where ‘a’ > ‘b’ > ‘c’ > ‘d’

The stereodescriptors *R* and *S* are used when the spiro atom is surrounded by four atoms arranged as ‘a’ > ‘b’ > ‘c’ > ‘d’. These stereodescriptors are preferred to ‘*cis*’ and ‘*trans*’ that can be used to describe the relative configuration of rings in dispiro compounds. The configuration of any chirality centers located on the spiro skeleton is described by stereodescriptors ‘*R*’ and ‘*S*’ by using the usual method.

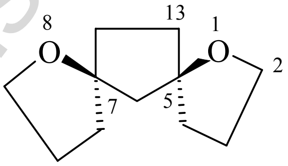
Examples:



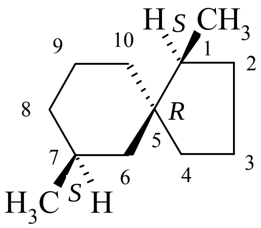
(6*R*,8*R*,9*S*)-8,9-dihydroxy-5,5,9-trimethylspiro[5.5]undecan-1-one (PIN)



(*R*)-5*H*-spiro[indene-1,2-(1,3)oxazole] (PIN)

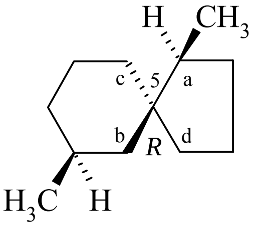


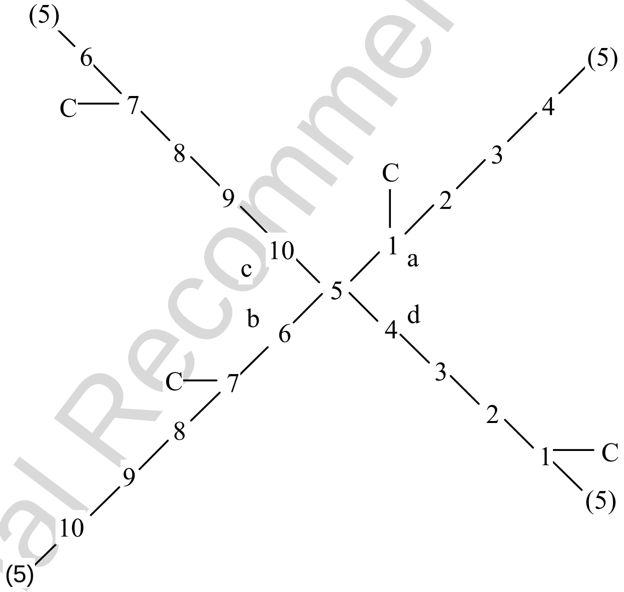
(5*R*,7*S*)-1,8-dioxadispiro[4.1.4.2]tridecane (PIN)
cis-1,8-dioxadispiro[4.1.4^7.2^5]tridecane (see P-92.1.5.2)



(1*S*,5*R*,7*S*)-1,7-dimethylspiro[4.5]decane

Construction of the digraph

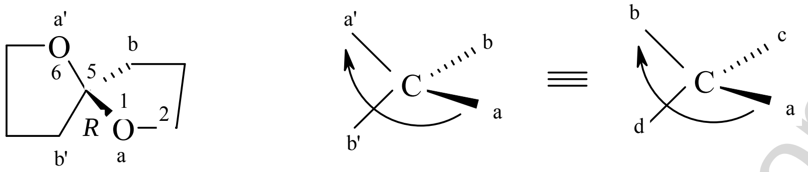




P-93.2.3.2 Chiral spiro atoms of the type Cab, where ‘a’ > ‘b’

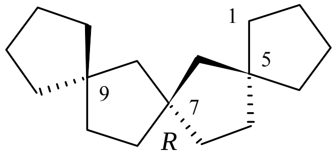
When a choice has to be made between two pairs of atoms or groups, as in the spiro compound below, an atom or group attached to the stereogenic center is chosen as reference, for example the oxygen atom in position 1 (see section 2.5, ref. 31). In the order of precedence ‘a ‘ > ‘a′’ > ‘b’ > ‘b′’, equivalent to ‘a’ > ‘b’ > ‘c’ > ‘d’, it is specified as ‘a’. The oxygen atom in position 6 is chosen as ‘a′’. Among the remaining atoms or groups, two $-CH_2-$ groups, precedence is given to the atom or group that is in the same ring as atom or group ‘a’; thus, the $-CH_2-$ group in position 4 is ‘b’ and the other $-CH_2-$ group is ‘b′’. Chirality is thus denoted by ‘*R*’.

Example 1:



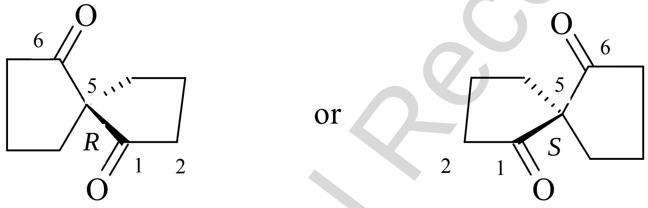
(5*R*)-1,6-dioxaspiro[4.4]nonane (PIN)

Example 2:



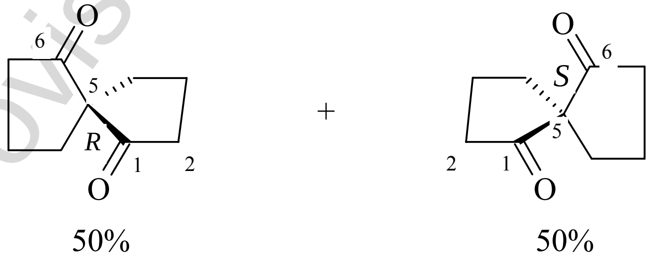
(7*R*)-trispiro[4.1.1.4^9.2^7.2^5]heptadecane (PIN)

Example 3:



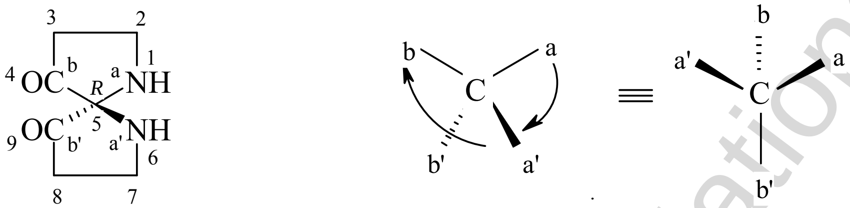
rel-(5*R*)-spiro[4.4]nonane-1,6-dione (PIN)
(5*R**)-spiro[4.4]nonane-1,6-dione

Example 4:



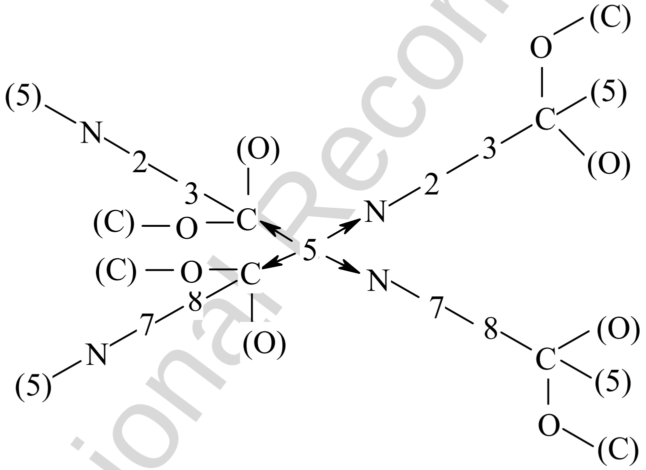
rac-(5*R*)-spiro[4.4]nonane-1,6-dione (PIN)
(5*RS*)-spiro[4.4]nonane-1,6-dione

Example 5:

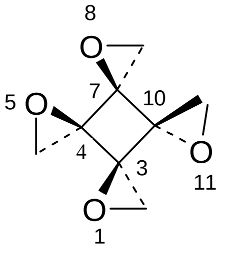


(5*R*)-1,6-diazaspiro[4.4]nonane-4,9-tetrone.(PIN)

In this (see section2.5, ref. 31), the analysis to determine the priority amongst pairs ‘a’ > ‘a′’ > ‘b’ > ‘b′’ starts at the nitrogen atom numbered 1, then to the nitrogen atom numbered 6; they are ranked a and b, respectively. The branch, as shown in the digraph below, leading to the group that has precedence, i.e., ‘a’ > ‘b’, is chosen as group ‘c’.



Example 6:



(3*R*,4*s*,7*S*,10*s*)-tetraoxatetraspiro[2.0.2^4.0.2^7.0.2^{10}.0^3]dodecane (PIN)
1*r*,5*c*,8*c*,11*t*-tetraoxatetraspiro[2.0.2^4.0.2^7.0.2^{10}.0^3]dodecane

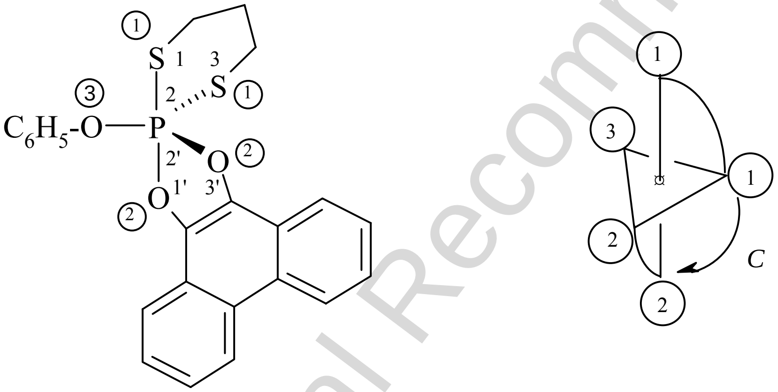
In this example, chiral and pseudoasymmetric centers are present. Application of sequence rules (3) and (4) are necessary.

Guide to name construction:

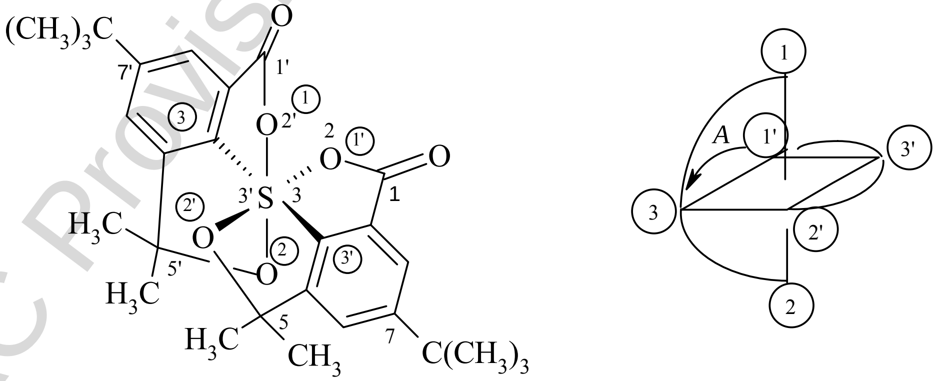
(a) the numbering is chosen that gives a ‘cis’ attachment at the first point of difference (see P-14.4 k); thus ‘1*r*,5*c*,8*c*,11*t*’, not ‘1*r*,5*t*,8*c*,11*c*’;
(b) configurations at C-3 and C-7 are determined by using sequence rule (4), *like* precedes *unlike*, in accordance with the methodology described in P-92.1.1.2;
(c) configurations at C-4 and C-10 are determined by using sequence rule (5), ‘*R*’ precedes ‘*S*’, in accordance with the methodology described in P-92.1.4.

P-93.2.3.3 Nontetrahedral stereogenic centers

As described in P-92.1.8, stereodescriptors used in coordination chemistry describe the relative and the absolute configuration of spiro compounds with λ^4, λ^5 and λ^6-hetero spiro atoms. Examples:



(*TBPY*-5-12-*C*)-2-phenoxy-2λ^5-spiro[1,3,2-dithiaphosphinane-2,2′-phenanthro[9,10-*d*][1,3,2]dithiaphosphole] (PIN)

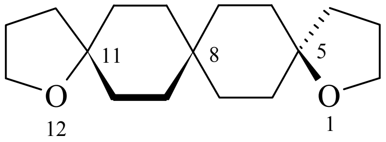


(*OC*-6-22′-*A*)-7,7′-di-*tert*-butyl-5,5,5′,5′-tetramethyl-1*H*,1′*H*,5*H*,5′*H*-3λ^6,3′-spirobi[[1,2]oxathiolo[4,3,2-*hi*][2,1]benzoxathiole]-1,1′-dione (PIN)

P-93 2.3.4 Axial chirality of spiro compounds

The stereodescriptors ‘*M*’ and ‘*P*’, or ‘R_a’ and ‘S_a’ are used to describe axial chirality of spiro compounds. The sterodescriptors ‘R_a’ and ‘S_a’ are used in preferred IUPAC names. Locants denoting the first and the last spiro atoms involved in the configuration are placed before the stereodescriptors.

Example:

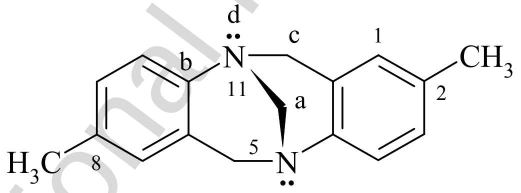


[(5(11)R_a]-1,12-dioxatrispiro[4.2.2.4^{11}.$2^{8.}$.2^{5}]nonadecane (PIN)
[(5(11)*M*]-1,12-dioxatrispiro[4.2.2.4^{11}.$2^{8.}$.2^{5}]nonadecane

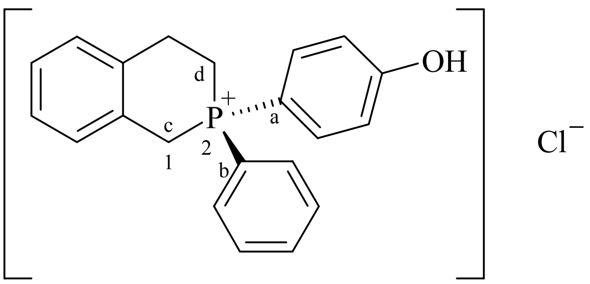
P-93.2.4 Fused and bridged fused compounds

P-93.2.4.1 A great variety of chiral and achiral carbocyclic and heterocyclic compounds are described by the appropriate symbols ‘*R*’, ‘*S*’, ‘*r*’, and ‘*s*’. A few examples illustrates the chirality associated with carbon and heteroatoms. The first example is the Tröger’s base showing the rare chirality associated with amines (see ref. 38).

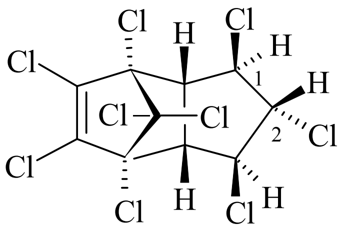
Examples:



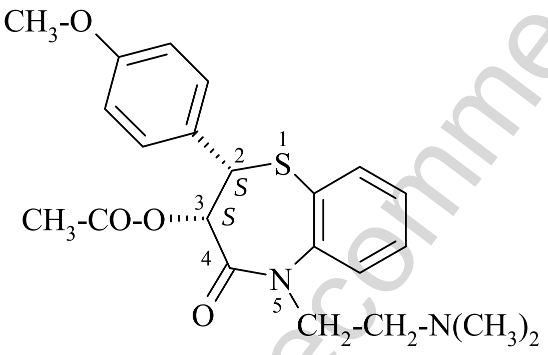
(5*S*,11*S*)-2,8-dimethyl-11-methanodibenzo[*b*,*f*][1,5]diazocine (PIN)
(the configuration of Tröger’s base at C-11 is shown)



(2*S*)-2-(4-hydroxyphenyl)-2-phenyl-1,2,3,4-tetrahydroisophosphinolinium chloride (PIN)



(1*R*,2*r*,3*S*,3a*R*,4*S*,7*R*,7a*S*)-1,2,3,4,5,6,7,8,8-nonachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1*H*- indene

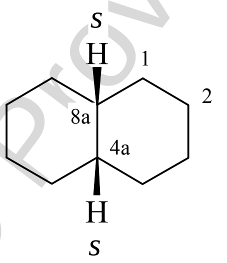


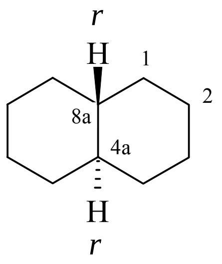
(2*S*,3*S*)-5-[2-(dimethylamino)ethyl]-2-(4-methoxyphenyl)-4-oxo-2,3,4,5-tetrahydro-1,5-benzothiazepin-3-yl acetate (PIN)

P-93.2.4.2 Configuration of saturated fused systems

Saturated fused systems exhibit '*cis-trans*' isomerism. The CIP '*r*' and '*s*' stereodescriptors are preferred to '*cis*' and '*trans*' to describe the pseudoasymmetric centers when appropriate. The '*cisoid*' and '*transoid*' non CIP stereodescriptors are, although they are not preferred in preferred IUPAC names.

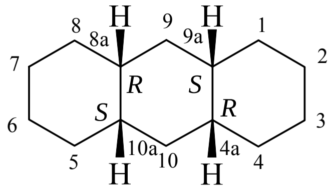
Examples:



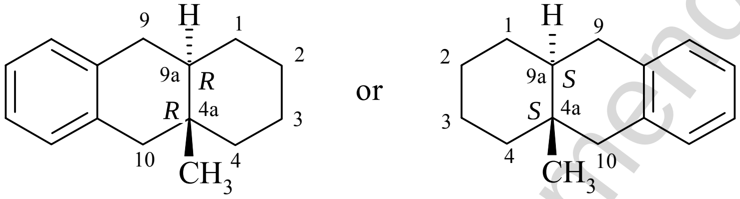


(4a*s*,8a*s*)-decahydronaphthalene (PIN)
cis-decahydronaphthalene

(4a*r*,8a*r*)-decahydronaphthalene (PIN)
trans-decahydronaphthalene



(4a*R*,8a*R*,9a*S*,10a*S*)-tetradecahydroanthracene (PIN)

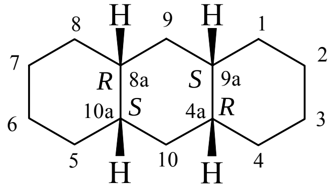


rel-(4a*R*,9a*R*)-4a-methyl-1,2,3,4,4a,9,9a,10-octahydroanthracene (PIN)
(4a*R**,9a*R**)-4a-methyl-1,2,3,4,4a,9,9a,10-octahydroanthracene

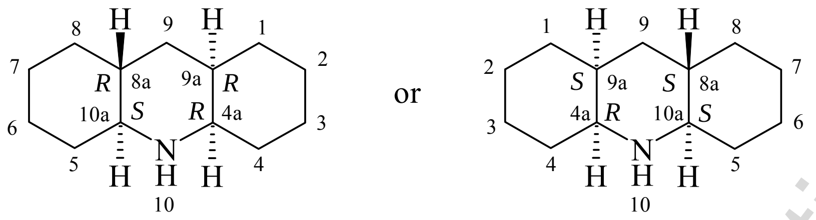
The descriptors '*cisoid*' and '*transoid*'

Steric relations at more than one pair of saturated fusion atoms in a fused system are denoted by '*cis*' and '*trans*', each followed by a hyphen, and, if necessary, the corresponding locant of the lower-numbered fusion atom and a second hyphen, all placed before the name of the ring system. Steric relations between the nearest atoms of *cis* or *trans* fusion pairs have been described by descriptors '*cisoid*' or '*transoid*' followed by a hyphen and when required, the corresponding locants and a second hyphen, the whole placed between the designations of the '*cis*' or '*trans*' junctions concerned. The term 'nearest atom' denotes those atoms linked together through the smallest number of atoms, irrespective of the numbering of the system. When a choice remains between nearest atoms, the pair containing the lower numbered atom is selected. The descriptors '*cisoid*' and '*transoid*' are not abbreviated. These descriptors are no longer recommended. The notation '*R*' and '*S*', with the descriptor '*rel*' is used instead for describing an enantiomer whose relative configuration only is known

Examples:



(4a*R*,8a*R*,9a*S*,10a*S*)-tetradecahydroanthracene (PIN)
cis-*cisoid*-*cis*-tetradecahydroanthracene (no longer recommended)
(this compound is achiral)

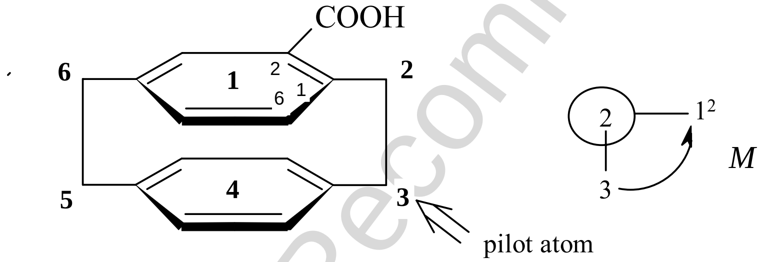


rel-(4a*R*,8a*R*,9a*R*,10a*S*)-tetradecahydroacridine (PIN)
cis-4a-*cisoid*-4a,10a-*trans*-10a-tetradecahydroacridine (no longer recommended)

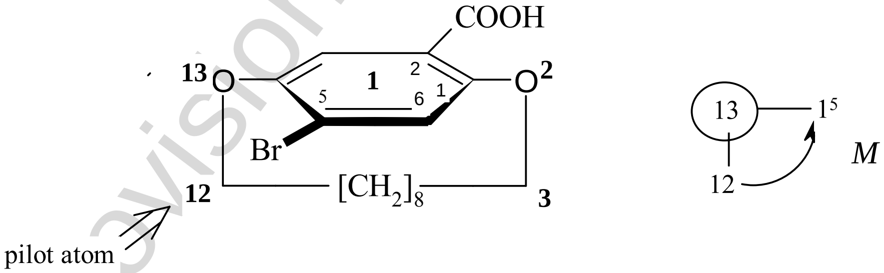
P-93.2.5 Cyclophanes

The descriptors 'R_p' and 'S_p' are preferred to '*P*' and '*M*' , respectively

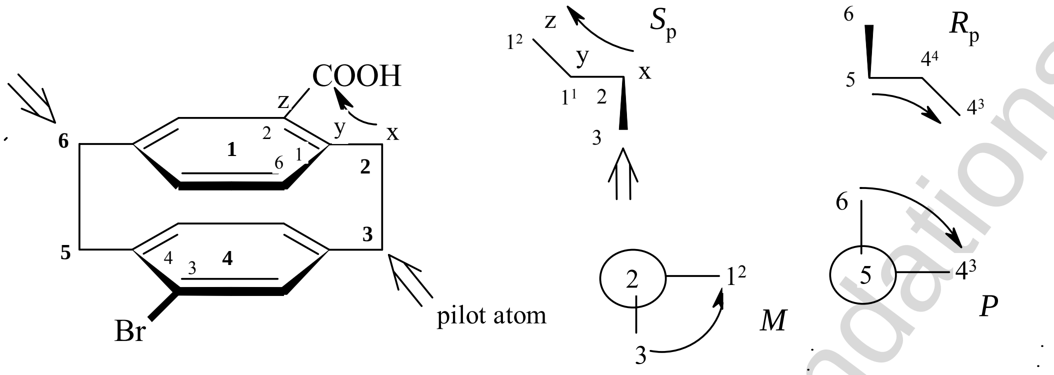
Example:



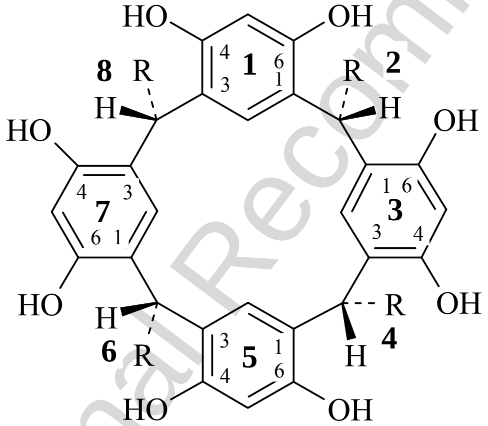
(S_p)-1,4(1,4)-dibenzenacyclohexaphane-1^2-carboxylic acid (PIN)
(*M*)-1,4(1,4)-dibenzenacyclohexaphane-1^2-carboxylic acid



(S_p)-1^5-bromo-1(1,4)-benzene-2,13-dioxacyclotridecaphane-1^2-carboxylic acid (PIN)
(*M*)-1^5-bromo-1(1,4)-benzene-2,13-dioxacyclotridecaphane-1^2-carboxylic acid



($1S_p$,$4R_p$)-4^3-bromo-1,4(1,4)-dibenzenacyclohexaphane-1^2-carboxylic acid (PIN)
(1*M*,4*P*)- 4^3-bromo-1,4(1,4)-dibenzenacyclohexaphane-1^2-carboxylic acid



R = $-CH_2-[CH_2]_7-CH_3$

(2*s*,4*s*,6*s*,8*s*)-2,4,6,8-tetranonyl-1,3,5,7(1,3)-tetrabenzenacyclooctaphane-1^4,1^6,3^4,3^6,5^4,5^6,7^4,7^6-octol (PIN)
2*r*,4*c*,6*c*,8*c*-tetranonyl-1,3,5,7(1,3)-tetrabenzenacyclooctaphane-1^4,1^6,3^4,3^6,5^4,5^6,7^4,7^6-octol

P-93.2.6 Fullerenes

P-93.2.6.1 Definitions and general methodology

Only general principles for describing stereochemical configuration of fullerenes are discussed briefly and exemplified in this section. Describing stereochemical configuration of fullerenes is extremely complex because of different factors such as the numbering of the fullerene molecule, systematic or trivial (in these recommendations, only the systematic numbering given in ref. 10 is used), the nature and disposition of substituent groups on the fullerene, and the plurality of stereodescriptors necessary to fully describe their stereochemical configuration. For a full discussion of the description of fullerene configuration, one must go to the original publication (Section 17 in ref. 10).

For the purpose of describing stereochemical configuration, fullerenes and their derivatives are classified into four types depending on the origin of their chirality.

P-93.2.6.1.1 Type 1. Inherently chiral parent fullerenes;
P-93.2.6.1.2 Type 2. Substituted fullerenes inherently chiral because of their substitution pattern;
P-93.2.6.1.3 Type 3. Substituted fullerenes noninherently chiral because of their substitution pattern;
P-93.2.6.1.4 Type 4. Chirality due to chiral substituents.
P-93.2.6.1.5 Superimposition of stereogenic elements in a fullerene molecule

The four types are classified by the 'substitution test' that consists of changing the substituents in a single fullerene unit into a 'achiral test substituent', 'T', and verifying the chirality of the fullerene so modified by the presence of 'T' substituents (see **Fig**. 9-1).

P-93..2.6.1.1 Type 1. Inherently chiral parent fullerenes.

The two fullerenes molecules described in Section P-27, (C_{60}-I_h)[5,6]fullerene and the (C_{70}-$D_{5h(6)}$)[5,6]fullerene, are achiral; they are not inherently chiral. To the contrary, the (C_{76}-D_2)[5,6}fullerene shown below is inherently chiral. The numbering of an inherently chiral fullerene applies to a specific enantiomer; the other enantiomer has a numbering that is the mirror-image of the first numbering. A description of the handedness of the numbering scheme is sufficient to unambiguously characterize the absolute configuration of the fullerene. The viewer looking at the polygon in which the numbering starts from outside the fullerene cage, traces a path from C-1 to C-2 to C-3, which is never aligned in a fullerene structure. If this path describe a clockwise direction, the configuration is indicated by the stereodescriptor '${}^{f,x}C$', where the superscript 'f' indicates that the descriptor refers to a fullerene, and the superscript 'x' is either 's' for the systematic numbering or 't' for the trivial numbering described in P-27.3. If the path from C-1 to C-2 to C-3 describes an anticlockwise direction, the descriptor is '${}^{f,x}A$'. Thus, the fullerene on the left hand side below is described by the stereodescriptor '${}^{f,x}C$'; its name is (${}^{f,s}C$)-(C_{76}-D_2)[5,6}fullerene. The fullerene on the right hand side is (${}^{f,s}A$)-(C_{76}-D_2)[5,6}fullerene. The systematic numbering is that used by Chemical Abstracts Service (ref. 16).

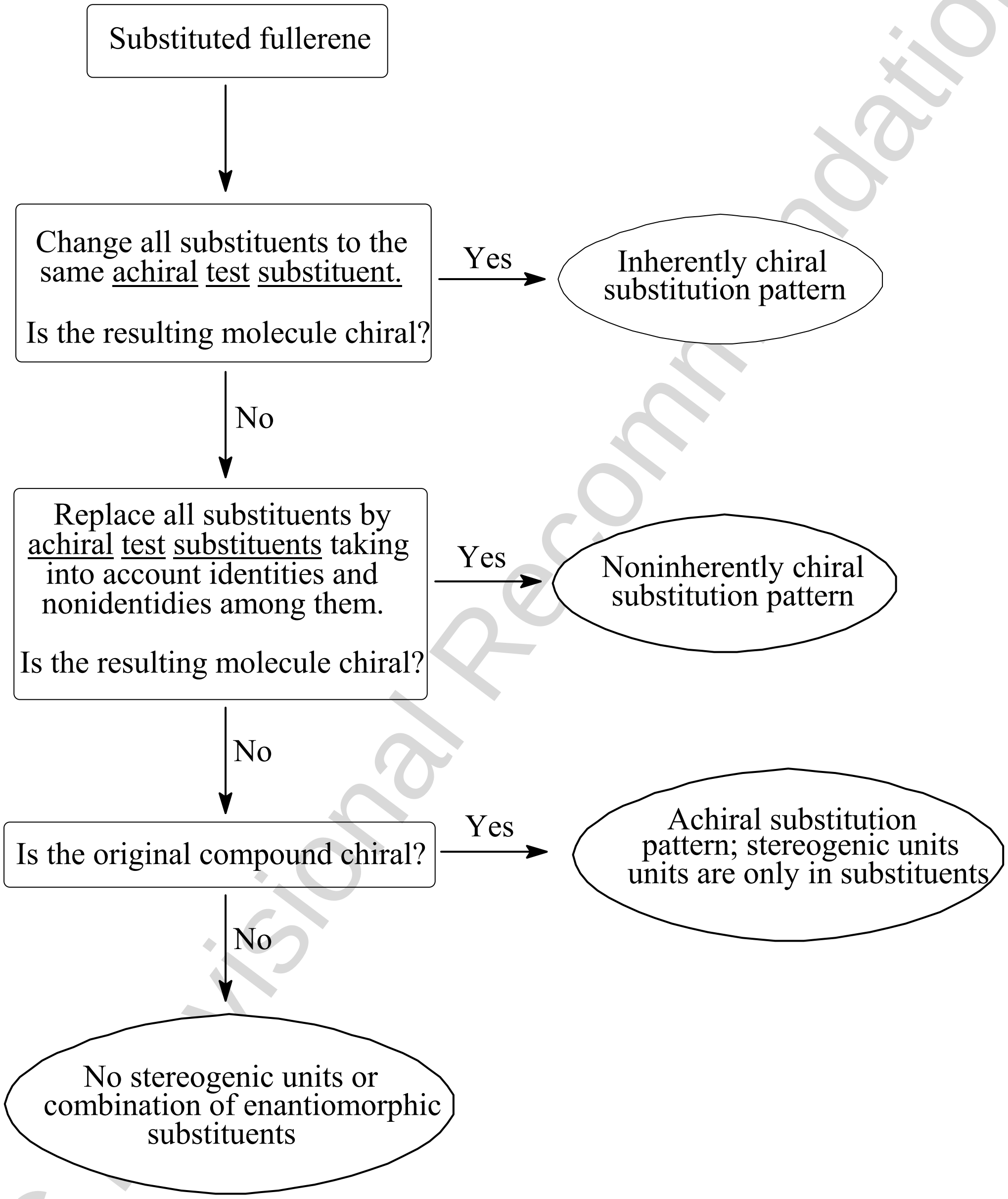
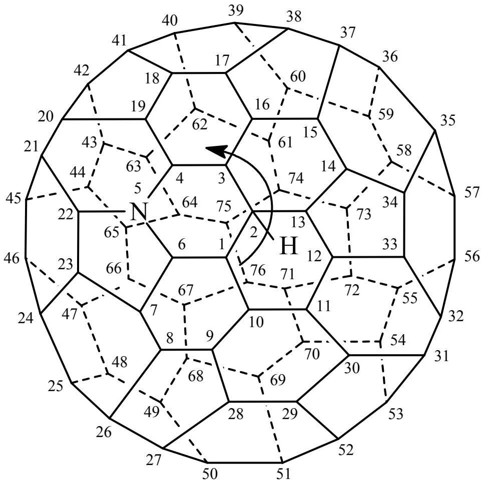
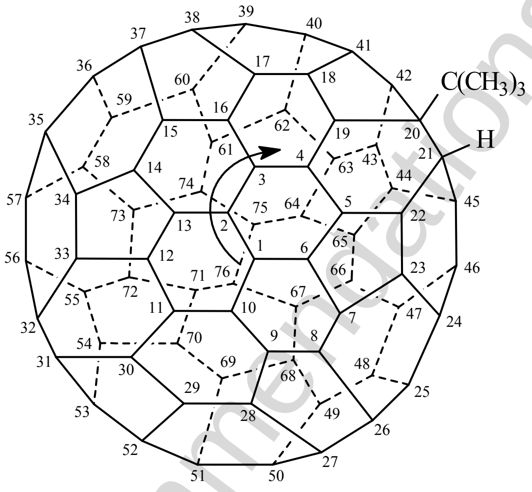


Fig. 9-1 Classification of fullerene chirality by a stepwise substitution pattern

Examples:



I



II

I (^{f,s}*A*)-2*H*-5-Aza -(C_{76}-D_2)[5,6]fullerene

II (^{f,s}*C*)-20-*tert*-Butyl-20,21-dihydro(C_{76}-D_2)[5,6]fullerene

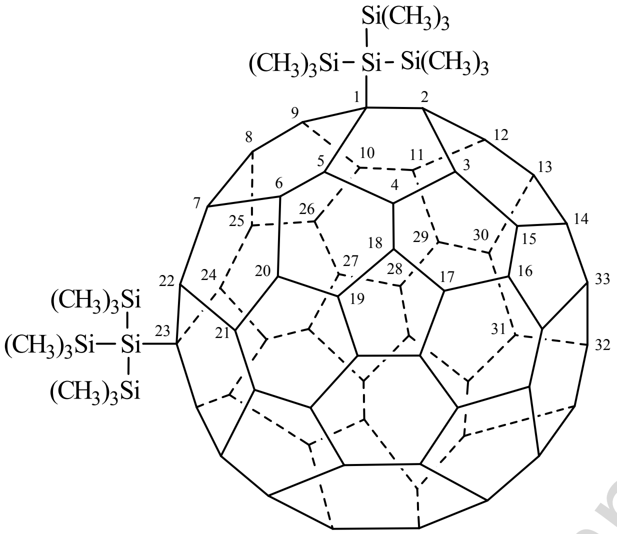
Note: The numbering used in these examples is that currently used in CAS index nomenclature (see ref 16).

P-93.2.6.1.2 Type 2. Substituted fullerenes inherently chiral because of their substitution pattern.

Derivatives of achiral (and chiral) parent fullerenes in which the presence of substituents, chiral or achiral, identical or different, on the fullerene skeleton, creates a chiral substitution pattern are said to have an inherently chiral substitution pattern.

Fullerene compounds of this type are all substituted achiral fullerenes. They have an inherently chiral substitution pattern if the existence of enantiomers is inherent to the geometrical arrangement of the substitution sites on the fullerene parent regardless of whether the substituents are identical or different. In these fullerene derivatives there is a unique numbering scheme that leads to the lowest set of locants for the substituents. As in P-63.2.6.1, the stereodescriptors are'^{f,x}*C*' and '^{f,x}*A*'.

Example:



(^{f,s}*C)*-1,23-Bis[1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl]-1,23-dihydro-(C_{60}-I_h)[5,6]-fullerene

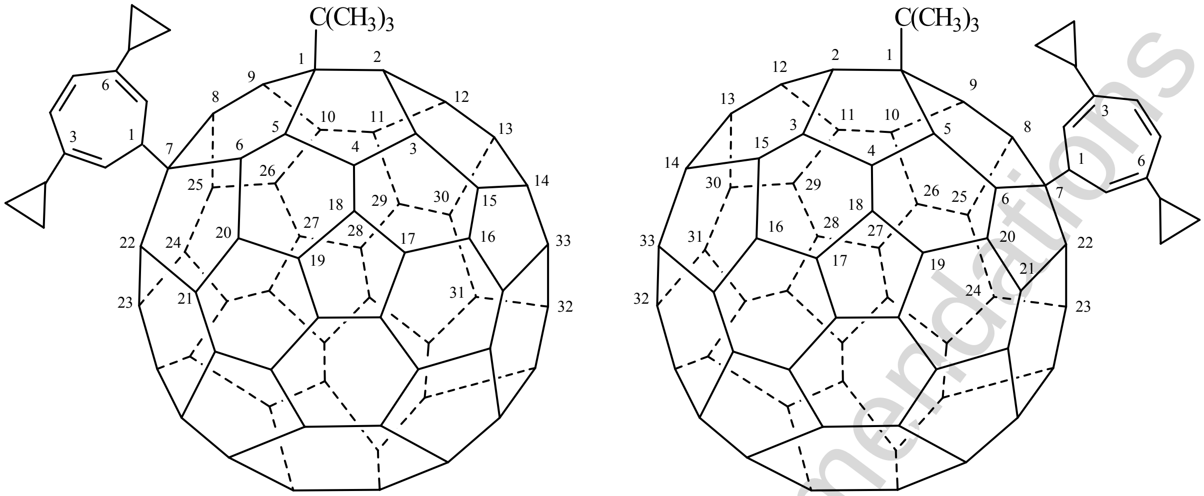
Explanation: Locants for the substituents are 1,23 for clockwise numbering. But for anticlockwise numbering they are 1,29 and since 1,23 is lower that 1,29 according to the principle of lowest locants (see P-14.) and therefore clockwise numbering is preferred. For the enantiomer, the lower locants 1,23 would be obtained on anticlockwise numbering and the descriptor would be (^{f,s}*A*)-.

P-93.2.6.1.3 Type 3. Substituted fullerenes noninherently chiral because of their substitution pattern.

Derivatives of achiral parent fullerenes in which a chiral substitution pattern on the fullerene is due to only to nonidentities among the substituents are have noninherently chiral substitution pattern.

The CIP system is used to rank substituents according to sequence rules (1) or (2) (see P-91.1.1). In the following enantiomeric disubstituted fullerenes, the *tert*-butyl group has precedence over the 3,6-dicyclopropylcyclohepta-2,4,6-trien-1-yl group. Stereodescriptors '^{f,x}*C*' and '^{f,x}*A*' are used to describe the absolute configuration, as indicated in P-93-2.6.1., in conformity with the path C-1 to C-2 to C-3 that is clockwise or anticlockwise.

Example:



(${}^{f,s}C$)- (${}^{f,s}A$)-

1-*tert*-Butyl-7-(3,6-dicyclopropylcyclohepta-2,4,6-trien-1-yl)-1,7-dihydro-(C_{60}-I_h)[5,6]fullerene

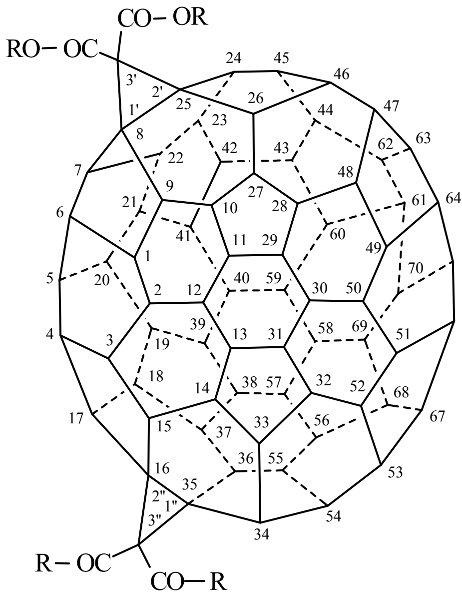
Explanation: This compound is chiral only because the substituents are constitutionally different. The parent fullerene is achiral and it does not have an inherently chiral substitution pattern because replacement of both substituents by the same achiral test substituent, 'T', results in an achiral compound. Therefore it has a noninherently chiral substitution pattern. The *tert*-butyl group is assigned the locant '1' because its CIP priority is higher than that of the 3,6-dicyclopropyl-cyclohepta-2,4,6-trien-1-yl group.

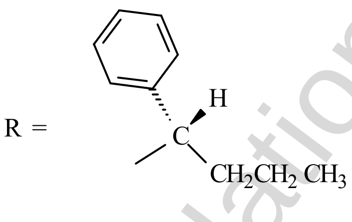
P-93.2.6.1.4 Type 4. Chirality due to chiral substituents.

Derivative of achiral parent fullerenes in which the presence of chiral substituents does not create a chiral substitution pattern have the stereogenic units located exclusively in the substituents.

In derivatives of this type, the chirality located in substituents is expressed by the usual CIP stereodescriptors. In the following example, the '*S*' configuration for the organyl group present in the –CO-O-R substituents is the only stereodescripto needed to express the configuration of the compound.

Example:





Configuration = *S*

tetrakis[(1*S*)-1-phenylbutyl] 3′*H*,3″*H*-dicyclopropa[8,25:16,35](C_{70}-$D_{5h(6)}$)-[5,6]fullerene-3′,3′,3″,3″-tetracarboxylate

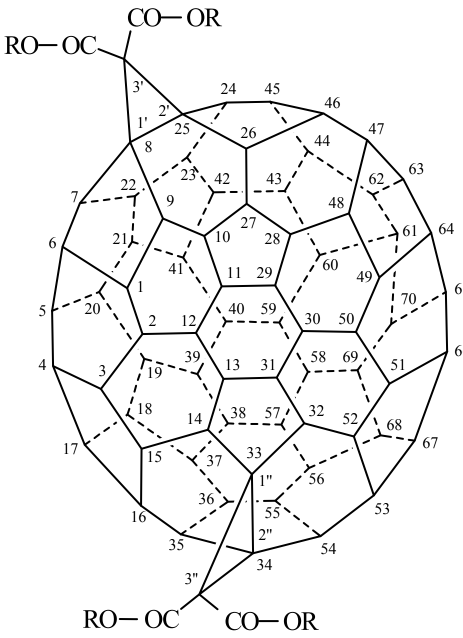
Explanations:

(a) This fullerene derivative is chiral. The parent fullerene is achiral and the derivative has an achiral substitution pattern. The configuration of the substituents are described by CIP stereodescriptors, as described in P-92. .

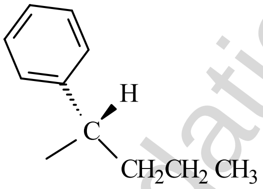
(b) If the esters of the acid in the above example were different, the parent fullerene and it substitution pattern would still be achiral and therefore any chirality of the original compound would be due to stereogenic centers located in the substituents.

P-93.2.6.2 Superimposition of stereogenic elements in a fullerene molecule. If a fullerene derivative with an inherently or noninherently chiral substitution pattern carries chiral substituents, the configuration of both types of stereogenic elements has to be indicated. The two types are independent of each other and the configuration of both must be specified for a full description of the compound.

Example:



R =



Configuration = *S*

Configuration = (${}^{f,s}C$)-

tetrakis[(1*S*)-1-phenylbutyl] (${}^{f,s}C$)-3′*H*,3′′*H*-dicyclopropa[8,25:33,34]-(C_{70}-$D_{5h(6)}$)[5,6]fullerene-3′,3′,3′′,3′′-tetracarboxylate

Explanation: The chiralities of the stereogenic centers in the esters are super-imposed on the descriptor for the fullerene with the inherently chiral substitution pattern. The enantiomer would be named:

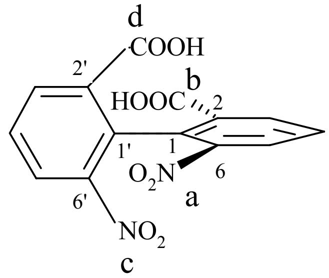
tetrakis[(1*R*)-1-phenyl-butyl] (${}^{f,s}A$)-3′*H*,3′′*H*-dicyclopropa[8,25:33,34]-(C_{70}-$D_{5h(6)}$)[5,6]fullerene-3′,3′,3′′, 3′′-tetracarboxylate

and the same for the various diastereoisomers.

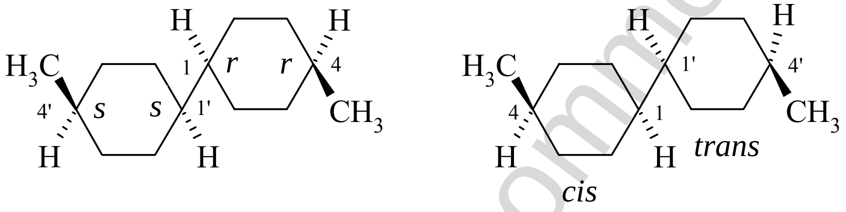
P-93.2.7 Ring assemblies

In preferred IUPAC names, appropriate CIP stereodescriptors are used to describe conformations in accordance with the nature of stereogenic centers. To describe axial chirality, the stereodescriptors ‘R_a’ and ‘S_a’ are preferred to P and M, respectively'.

Examples:

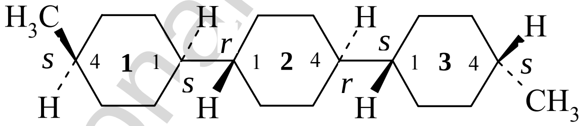


(*R*$_a$)-6,6′-dinitro-1,1′-biphenyl2,2′-dicarboxylic acid (PIN)
(*M*)-6,6′-dinitro-1,1′-biphenyl2,2′-dicarboxylic acid



(a) **(b)**

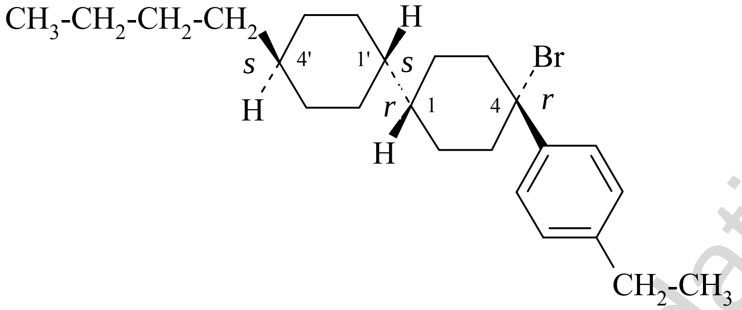
(a) [1*r*,1′*s*,4*r*,4′*s*]-4,4′-dimethyl-1,1′-bicyclohexane (PIN)
(b) [1(4)*cis*,1′(4′)*trans*]-4,4′-dimethyl-1,1′-bicyclohexane



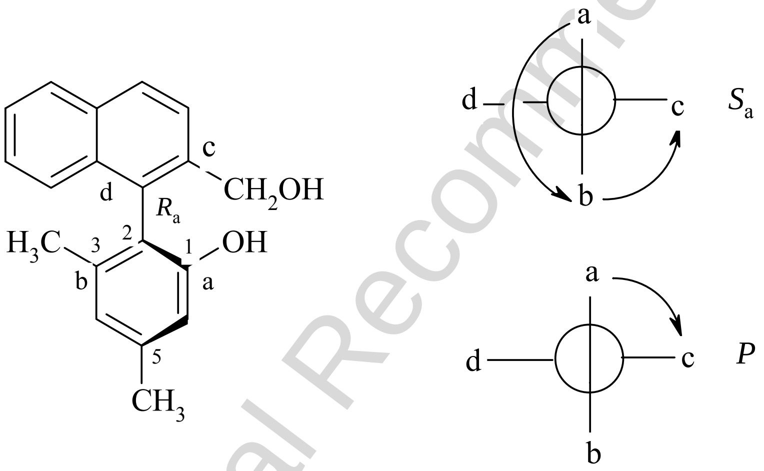
[1^1*s*,1^4*s*,2^1*r*,2^4*r*,3^1*s*,3^4*s*]-1^4,3^4-dimethyl-1^1,2^1:2^4,3^1-tercyclohexane (PIN)
[1^1(1^4)*cis*,2^1(2^4)*trans*,3^1(3^4)*cis*]-1^4,3^4-dimethyl-1^1,2^1:2^4,3^1-tercyclohexane

When more than two positions are substituted in an individual ring, achiral compounds are named by using the stereodescriptors ‘*r*’ and ‘*s*’. The normal numbering of ring assemblies is applied (see P-28.2 and P-28.3).

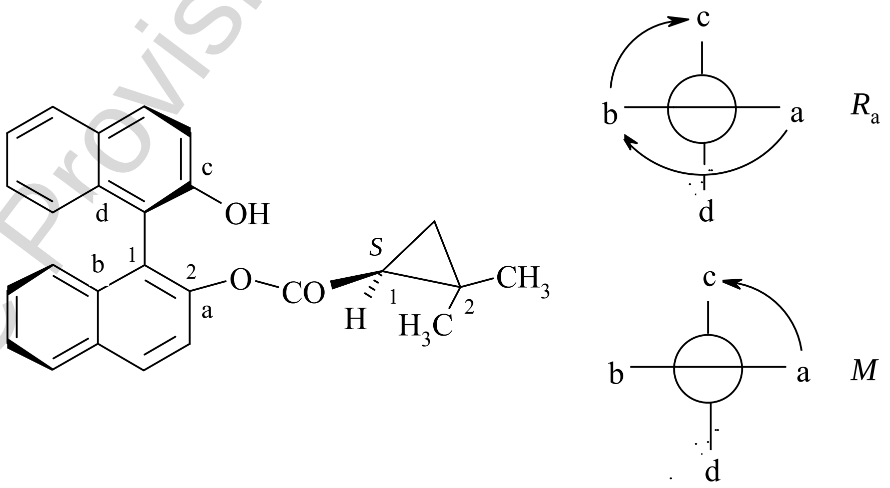
Example:



(1*r*,1′*s*,4*r*,4′*s*)-4-bromo-4′-butyl-4-(4-ethylphenyl)-1,1′-bicyclohexane (PIN)



(2S_a)-2-[2′-(hydroxymethyl)naphthalen-1-yl]-3,5-dimethylphenol (PIN)
(2*P*)-2-[2′-(hydroxymethyl)naphthalen-1-yl]-3,5-dimethylphenol



(1R_a)-2′-hydroxybinaphthalen-2-yl (1*S*)-2,2-dimethylcyclopropane-1-carboxylate (PIN)
(1*M*)-2′-hydroxybinaphthalen-2-yl (1*S*)-2,2-dimethylcyclopropane-1-carboxylate

P-93.3 Assemblies of chains and rings

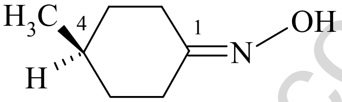
Preferred stereodescriptors, as described in Sections P-92 and P-93.1 and P-93.2, are used to describe assemblies of rings and chains.

P-93.3.1 Specification of chirality
P-93.3.2 Specification of *cis-trans* isomerism
P-93.3.3 Specification of chirality and *cis- trans* isomerism

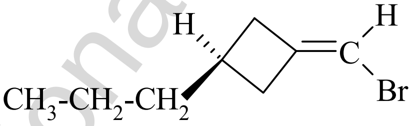
P-93.3.1 Specification of chirality

Compounds composed of a ring and a double bond arranged as an allene system exhibit axial chirality which is described by the chirality stereodescriptors R_a or S_a that are preferred to *M* and *P*, respectively.

Examples:



(R_a)-(4-methylcyclohexylidene)hydroxylamine (PIN)
(*M*)-(4-methylcyclohexylidene)hydroxylamine
(*M*)-4-methylcyclohexanone oxime



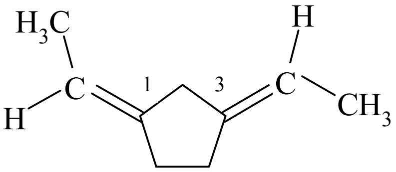
(S_a)-(3-(bromomethylidene)-1-propylcyclobutane (PIN)
(*P*)-(3-(bromomethylidene)-1-propylcyclobutane

P-93.3.2 Specification of '*cis-trans*' isomerism

Cumulenes having an odd number of double bonds in which a double bond has been replaced by a ring are considered here. Their configuration is described by the stereodescriptors associated with '*cis-trans*' isomerism, i.e., '*Z*' or '*E*'.

P-93.3.2.1 When the configuration of each double bond can be directly determined by applying the method recommended for double bonds described in P-92.1.6.2, stereodescriptors '*Z*' or '*E*' are used to describe the configuration of each double bond.

Example:



(1*Z*,3*E*)-1,3-diethylidenecyclopentane (PIN)

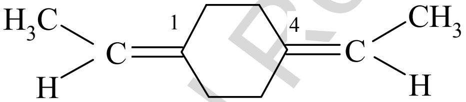
P-93.3.2.2 Two methods are used to describe the configuration of assemblies that cannot be named by the method described above in P-93.3.3.2.1:

(1) the entire molecule is described by using the stereodescriptors ‘*Z*’ and ‘*E*’, or ‘*cis*’ and ‘*trans*’, when the system is assimilated to an extended double bonds;

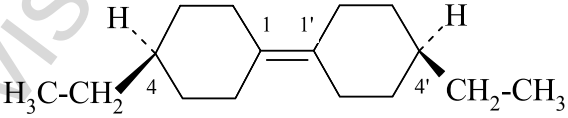
(2) auxiliary stereodescriptors are used as in P-921.6.2.1 to determine the configuration of each double bond;

Stereodescriptors describing the entire molecule are preferred to those determined by applying the method of auxiliairy descriptors; stereodescriptors ‘*Z*’ and ‘*E*’ are preferred to ‘*cis*’ and ‘*trans*’.

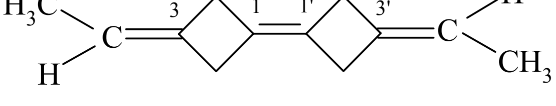
Examples:



[1(4)*Z*]-1,4-diethylidenecyclohexane (PIN) [method (1)]
[1(4)-*cis*]-1,4-diethylidenecyclohexane
1,4-di[(*Z*)-ethylidene]cyclohexane [method (2)]



[4(4′)-*Z*]-4,4′-diethyl-1,1′-bi(cyclohexylidene) (PIN) [method (1)]
[4(4′)-*cis*]-4,4′-diethyl-1,1′-bi(cyclohexylidene)

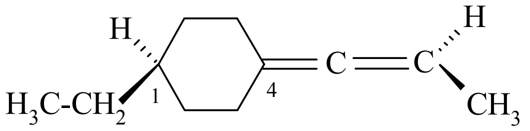


[3(3′)*E*]-3,3′-diethylidene-1,1′-bi(cyclobutylidene) (PIN)
[3(3′)-*trans*]-3,3′-diethylidene-1,1′-bi(cyclobutylidene)
3,3′-di[(*E*)-ethylidene-1,1′-bi(cyclobutylidene)

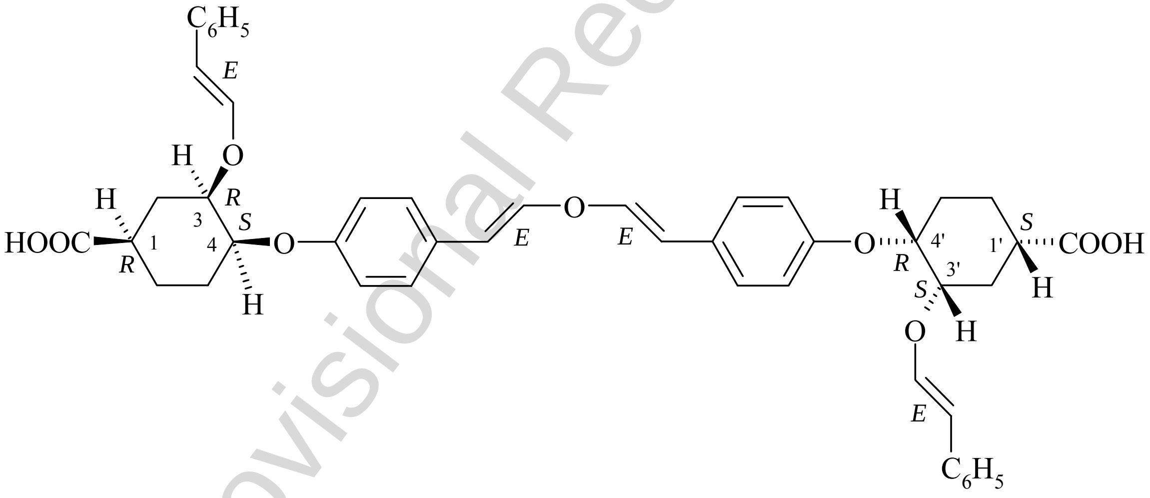
P-93.3.3 Specification of configuration in rings and chains

Stereodescriptors must be adapted to the many configurations that have to be described in compounds where rings and chains can be chiral. CIP stereodescriptors are preferred to non CIP stereodescriptors in preferred names.

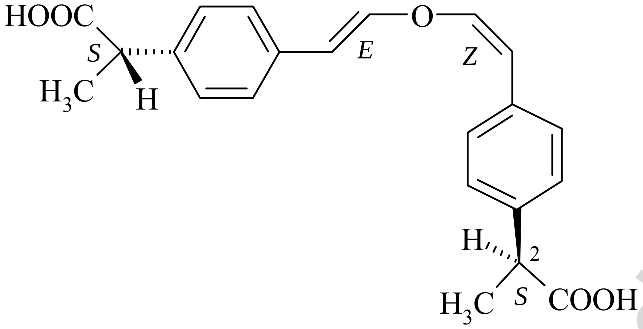
Examples:



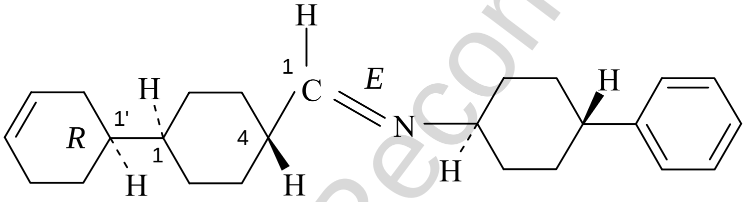
[1(4)-*Z*]-1-ethyl-4-(prop-2-en-1-ylidene)cyclohexane] (PIN)
[1(4)-*cis*]-1-ethyl-4-(prop-2-en-1-ylidene)cyclohexane
(1*S*,4S_{a})-1-ethyl-4-(prop-2-en-1-ylidene)cyclohexane
(the configuration of this compound can be described as *Z* for the entire molecule, or as a combination of a chiral center *S* at C-1 and axial chirality S_{a} for the allenic portion of the molecule)



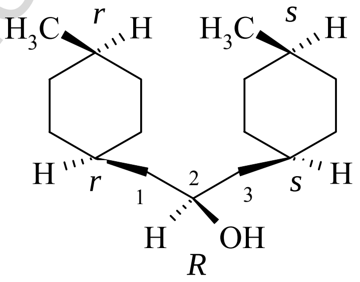
(1*R*,1′*S*,3*R*,3′*S*,4*S*,4′*R*)- 4,4′-{oxybis[(1*E*) -ethene-2,1-diyl-4,1-phenyleneoxy]}bis(3-{[(1*E*)-2-phenylethenyl]oxy}cyclohexane-1-carboxylic acid) (PIN)



(2*S*)-2-{4-[(1*E*)-{2-[(1*Z*)-2-{4-[(1*S*)-1-carboxyethyl]phenyl}ethenyl]oxy}ethenyl] phenyl}propanoic acid
(a multiplicative name is not allowed; lack of identical components in the linking substituent)



(1*E*)-1-[(1′*R*,1*r*,4*r*)-1,1′-bi(cyclohexan)-3′-en-4-yl]-*N*-[(1*r*,4*r*)-4-phenylcyclohexyl]methanimine (PIN)
(1*E*)-1-[(1′*R*,1(4)-*trans*)-1,1′-bi(cyclohexan)-3′-en-4-yl]-*N*-[(*trans*)-4-phenylcyclohexyl]methanimine



(2*R*)-1-[(1*r*,4*r*)-4-methylcyclohexyl]-3-[(1*s*,4*s*)-4-methylcyclohexyl]propan-2-ol (PIN)

Guide to name construction:

(a) in accordance with the corresponding digraph, stereodescriptors ‘r’ and ‘s’ are assigned to the two positions 1 and 4 of the cyclohexane rings as indicated in P-92.1.4.2;
(b) the cyclohexane ring having the stereodescriptors ‘1*r*’,’4*r*’ is attached to carbon C-1 of the chain;

(c) by using 'Sequence Rule **4** ('r' precedes 's'), the configuration '*R*' is assigned to carbon C-2 of the chain.

P-94 Conformation and conformational descriptors

P-95.1 Definition

A conformation is the spatial arrangement of the atoms affording distinction between stereoisomers which can be interconverted by rotations about formally single bonds, as exemplified for conformers A and B in Fig. 2.

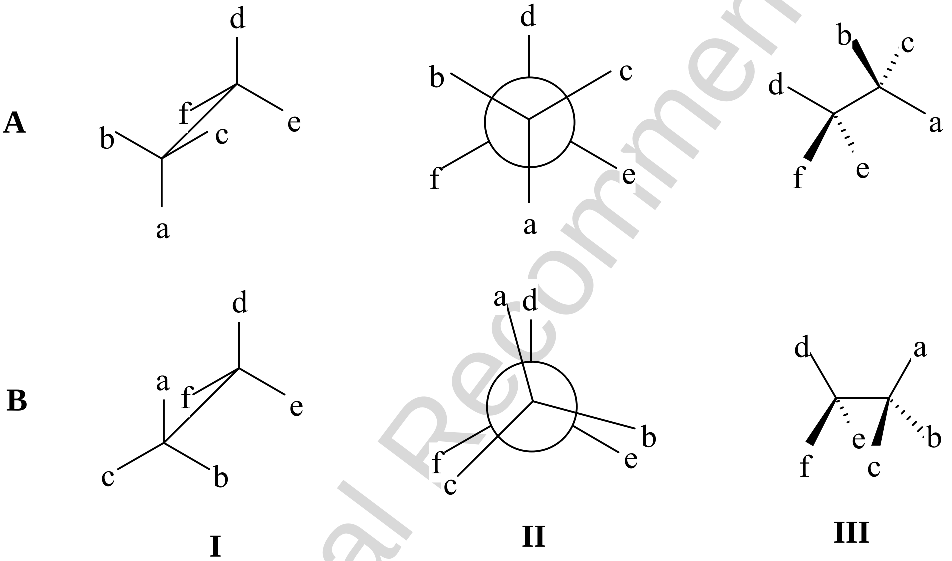


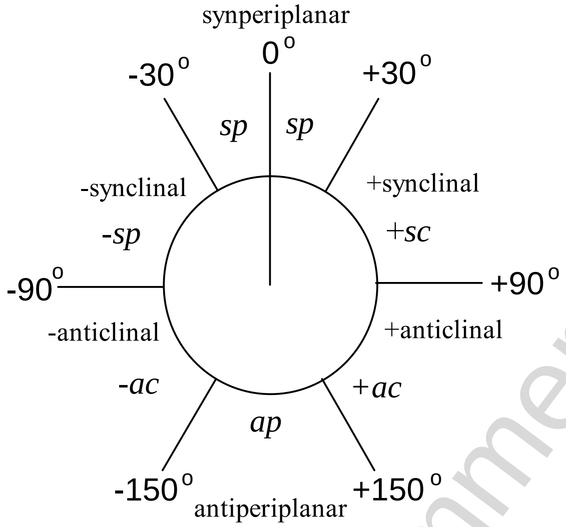
Fig. 9-2. Three different representations of two conformers A and B.

I Sawhorse projection
II Newman projection
III Zig-zag projection

P-94.2 Torsion angle

In an assembly of attached atoms X-A-B-Y, where neither X nor Y is collinear with A and B, the smaller angle subtended by the bonds X-A and Y-B in a plane projection obtained by viewing the assembly along the axis A-B is termed the 'torsion angle', denoted by the italicized Greek lower-case letter θ. The torsion angle is considered positive or negative according as the bond atom X or Y requires rotation to the right (clockwise) or left (anticlockwise), respectively, in order that its direction may coincide with that of the bond to the rear selected atom Y or X. The multiplicity of the bonding of the various atoms is irrelevant.. A torsion angle also exists if the axis for rotation is formed by a collinear set of more than two atoms directly attached to each other.

Conformations are described as synperiplanar (*sp*), synclinal (*sc*), anticlinal (*ac*), or antiperiplaner (*ap*), according as the torsion angle is within ±30° of 0°; ±60°, ±120°, or ±180°, respectively; the letters in parentheses are the corresponding abbreviations.



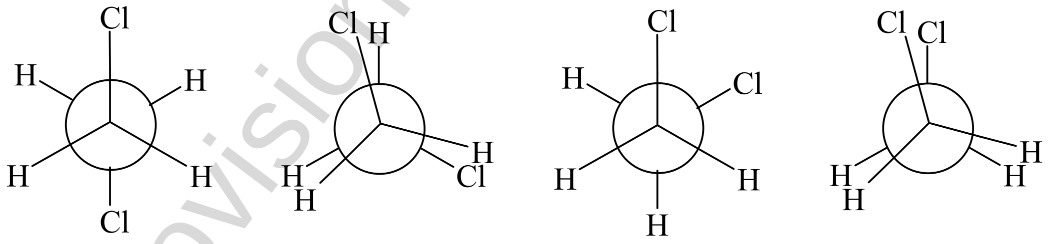
To choose the appropriate stereodescriptor, atoms or groups are selected from each set to define the torsion angle according to the following criteria:

(a) if all the atoms or groups of a set are different, that one of each set that has priority by the sequence rule;

(b) if one of a set is unique, that one;

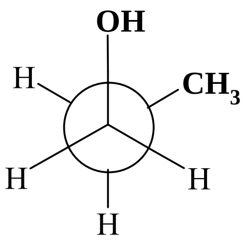
(c) if all of a set are identical, that one which provides the smallest torsion angle.

Examples:

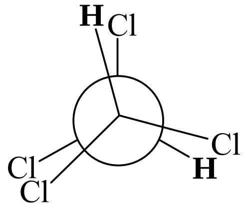


antiperiplanar anticlinal synclinal synperiplanar

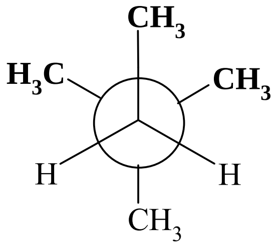
(The two chlorine atoms decide the conformation)



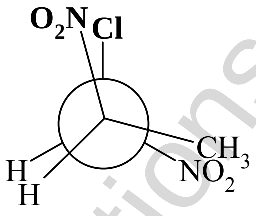
synclinal



anticlinal



synclinal



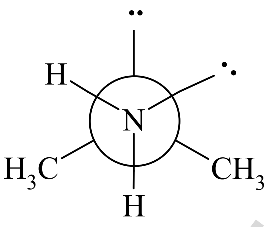
synperiplanar

Criteria for:

rear atom	2	2	3	1
front atom	2	2	2	1

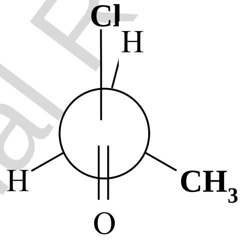
If A and B in X-A-B-Y are trigonal centers, a lone pair of electrons represented by two dots is taken into consideration to decide the description of the conformation, as illustrated by the example below describing the conformation of 1,1-dimethylhydrazine, $(CH_3)_2N\text{-}NH_2$; the lone pairs of electrons are the phantom atoms of the sequence rules symbolism. Similarly, trigonal centers involving double bonds are analyzed with the sequence rules by using duplicate atoms to determine the order of precedence.

Examples:



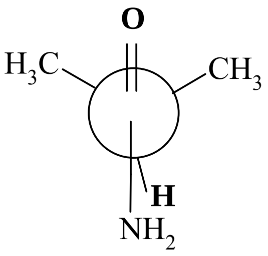
$(CH_3)_2N\text{-}NH_2$

synclinal



$CH_3\text{-}CH_2\text{-}CO\text{-}Cl$

anticlinal



$(CH_3)_2CH\text{-}CO\text{-}NH_2$

antiperiplanar

Criterion for:

rear atom	2	2	2
front atom	2	1	1

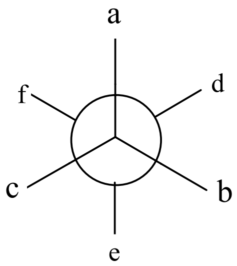
P-94.3 Specific stereodescriptors

Stereodescriptors are used to denote specific conformers, both aliphatic and alicyclic.

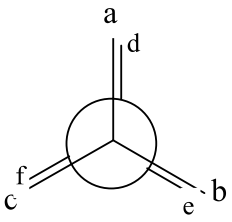
P-94.3.1 Eclipsed, staggered and gauche (or skew) conformations

P-94.3.1.1 Two atoms or groups attached to two adjacent stoms are said to be ‘eclipsed’ if the torsion angle between them is zero. They are said to be ‘staggered’ when they are as far apart as possible from an eclipsed conformation. ‘Gauche’ or ‘skew’ are synonymous with synclinal, which is preferred. The stereodescriptors ‘*trans*’ or ‘*anti*’ are not recommended in place of anticlinal, nor ‘*cis*’ or ‘*syn*’ in place of synclinal. Eclipsed and staggered are stereodescriptors used to denote the conformations when all ligands are identical.

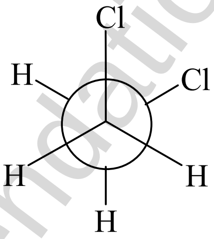
Examples:



staggered conformation
(all attached groups
are staggered)



eclipsed conformation
(the pairs ‘a-d’, ‘b-e’,
and ‘c-f’ are eclipsed)



synclinal (preferred)
gauche or skew

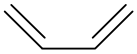
P-94.3.1.2 For a structure containing the grouping R_3C-C(Y)=X (with identical or different R groups) the conformation in which the torsion angle is such that X is antiperiplanar to one of the R group, and, in a Newman projection, the double bond bisects one of the R-C-R angle, is called a ‘bisecting conformation. The other conformation, in which X is synperiplanar to one of the R group, is called an eclipsing conformation.

Projections of CH_3-CH_2-CHO

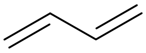
bisecting conformation eclipsing conformation

P-94.3.1.3 Stereodescriptors ‘s-*cis*’ and ‘s-*trans*’

The spatial arrangement of two conjugated double bonds about the intervening single bond is described as ‘s-*cis*’ if synperiplanar and ‘s-*trans*’ if antiperiplanar. This descriptor should not be applied to other systems such as *N*-alkyl amides (use ‘*E*/*Z*’ or ‘*sp*/*ap*’).



s-*cis*

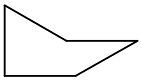


s-*trans*

P-94.3.2 Stereodescriptors for denoting the conformations of alicyclic rings

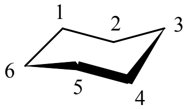
P-94.3.2.1 Envelope conformation

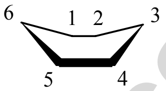
The envelope conformation is the conformation of a five-membered ring in which four atoms are coplanar and one atom projects out of the plane.

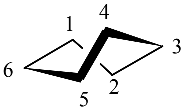


P-94.3.2.2 Chair, boat and twist conformations

When carbon atoms 1,2,4 and 5 of a six-membered ring occupy coplanar positions and when carbon atoms 3 and 6 are on opposite sides of the plane the conformation is called a chair form. It is a boat form when carbon atoms 3 and 6 are on the same side of the plane. The conformation passed through in the interconversion of two boat forms of six-membered ring is called the twist form; this term is preferred to skew boat, skew form or stretched form.



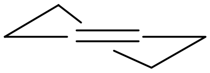




In carbohydrate stereochemistry, the term twist refers to a five-membered ring and the twist conformation is referred to as skew.

P-94.3.2.3 Half-chair

A molecule of a monounsaturated six-membered ring is described as being in a ‘half-chair’ conformation according as the atoms not directly linked to the double bond lie on oppoiste sides of the plane.



P-94.3.2.4 Crown conformation

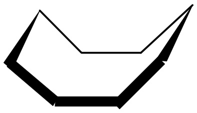
The conformation of a saturated cyclic molecular entity, containing an even number (≥ 8) of atoms in the ring, in which these atoms lie alternatively in each of two parallel planes and are symmetrically equivalent (D_{4d} for cyclooctane, D_{5d} for cyclodecane, etc), is called a ’crown conformation’.

cyclooctane

cyclodecane

P-94.3.2.5 Tub conformation

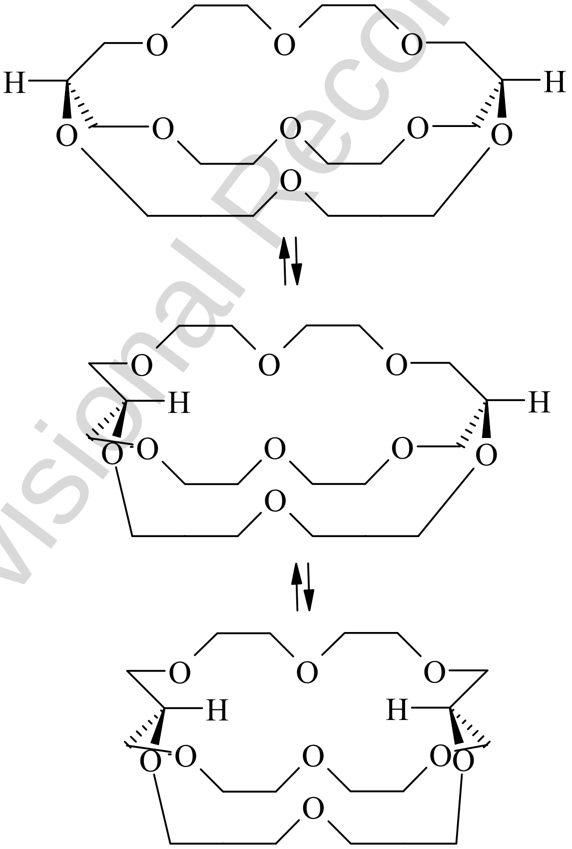
The conformation of an eight-membered ring in which the four atoms forming one pair on diametrically opposite bonds in the ring lie in one plane and all other ring atoms lie on one side of that plane is called a ‘tub conformation’.

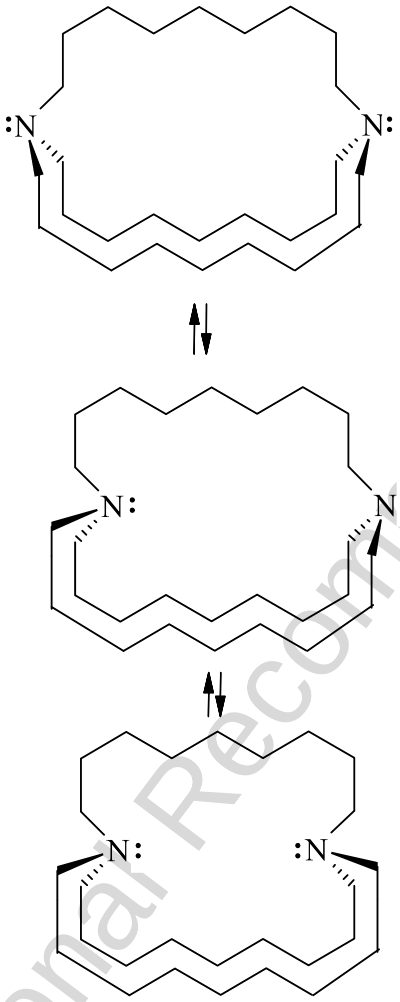


P-94.3.2.6 In-out isomerism

In-out isomerism is found in bicyclic systems having long enough bridges to allow the bridgehead exocyclic bond or lone pair of electrons to point either inside the structure or outside.

Examples:




:N
N:
N:
N:
N:
:N

CHAPTER 10 PARENT STRUCTURES FOR NATURAL PRODUCTS AND RELATED COMPOUNDS

P-100 Introduction

This Chapter is based on the recent publication ‘Revised Section F: Natural Products and Related Compounds, IUPAC Recommendations 1999’ (ref. 9).

In the field of natural products, three levels of nomenclature are recognized. A new compound, isolated from a natural source, is generally given a ‘trivial’ name. By common usage, these trivial names are commonly related to the biological origin of the material, but frequently not in a rational way, since the available structure is not known with great detail. These trivial names are considered to be ephemeral and replaced for chemical purposes by names describing the skeleton, the characteristic groups and the organyl substituent groups.

When the full structure is known, a ‘systematic name’ may be generated in accordance with Rules described in Chapters 1 through 8 of these recommendations. However, this name may be too cumbersome to be continually inserted into the text of a scientific paper. To overcome this difficulty and show the close similarity to related compounds, a ‘semisystematic name’ can be formed.

Semisystematic names are based on specific parents, generally including the stereochemistry, that can later on be used to fully describe a compound by using the rules of systematic nomenclature. There are two general types of semisystematic parent structures used for naming natural products and related compounds:

(a) parent hydrides, i.e., structures that do not have terminal heteroatoms or functional groups and therefore consist only of skeletal atoms and hydrogen, for example, in steroid (ref. 39), terpene, carotene (ref. 40), corrinoid (ref. 41), tetrapyrrole (ref. 42), alkaloid nomenclature. and lignans and neolignans (43). This type of semisystematic parent is analogous to the parents described in Chapter 2 and is treated in the same manner to generate complete names;

(b) functional parents, that are analogous to the functional parents described in Section P-35, and used in amino acid and peptide (ref. 23), carbohydrate (ref. 22), cyclitol (ref. 44) nucleoside (ref. 45), nucleotide, and lipid (ref. 45) nomenclature; they have characteristic groups implied in their name and can be modified by specific rules and by methods used in systematic nomenclature.

In this Chapter, Section P-101 describes the rules to form trivial names and semisystematic names used as parent hydrides, and those related to their skeletal transformation and functionalization for naming alkaloids, steroids, terpenes, and some related compounds. Section 102 describes the rules for naming carbohydrates, P-103 deals with the nomenclature of amino acids and peptides, P-104 describes the nomenclature for cyclitols, P-105 and P-106 deal with nucleosides and nucleotides, and finally P-107 discusses the nomenclature of lipids. If difficulties are encountered, consultation of the full publications may be necessary, as indicated in each Section. Preferred IUPAC names are indicated when a choice is possible.

P-101 Nomenclature for natural products based on parent hydrides (alkaloids, steroids, terpenes, carotenes, corrinoids, tetrapyrroles, and similar compounds)

P-101.1 Biologically based trivial names

P-101.1.1 When a compound is isolated from a natural source and a trivial name is required, the name should be based, whenever possible, on the family or genus or species name of the biological material from which it has been isolated. If appropriate, the class or order might also be used for the name of a compound that occurs in a number of related families.

P-101.1.2 The ending ‘une’ or, for euphonic reasons, ‘iune’ is used to indicate that the trivial name it terminates describes a compound of unknown structure.

P-101.2 Semisystematic nomenclature for natural products based on parent hydrides

As soon as the structure of a new natural product has been fully determined, the trivial name should be abandoned in favor of a systematic name formed by the Rules prescribed in Chapters 1 to 9 for systematic nomenclature of organic compounds. For a more complicated structure, an existing semisystematic name listed in P-101.2.7 is used to fully name the compound. If a previously known parent structure cannot be found, a new parent structure is formed and numbered as follows.

P-101.2.1 General guidelines for choosing a parent structure

P-101.2.1.1 A parent structure should reflect the basic skeleton (including nonterminal heteroatoms and hetero groups) that is common to most compounds of the class.

P-101.2.1.2 Parent structures should be chosen so that as many natural products as possible can be derived from each by well-defined operations and rules of the nomenclature of organic compounds.

P-101.2.1.3 A parent structure should include as much stereochemistry as possible that is common to the relevant class of natural products. Such parent structures are called ‘stereoparents’

P-101.2.2 Structural features allowed for parent structures

The following rules are applicable to new parent structures. Existing parent structure names are considered as retained names if they do not follow the new rules.

P-101.2.2.1 A parent structure should exceptionally include rings that are part of a characteristic group, such as a lactone or cyclic acetal.

P-101.2.2.2 A parent structure should not contain heteroatoms or groups.

P-101.2.2.3 A parent structure should contain acyclic hydrocarbon groups that occur in most of the compounds in the natural product class.

P-101.2.2.4 A parent structure should be as nearly fully saturated or fully unsaturated in terms of maximum number of noncumulative double bonds (mancude rings), while still representing the level of saturation (or unsaturation) of as many related compounds as possible.

P-101.2.2.5 A semisystematic name for a parent structure should be derived, as far as possible, from a trivial name formed in accordance with P-101. The endings to be used in place of ‘une’ or ‘iune’ must be assigned as follows:

(a) ‘ane’, if the entire stereoparent hydride is fully saturated;

(b) ‘ene’, if the cyclic or the main chain of the acyclic part contains the maximum number of noncumulative double bonds;

(c) ‘arane’, if, in an otherwise fully saturated parent structure, one or more individual mancude rings is present.

Existing names of parent structures in which endings are different from those indicated above, for example morphinan and ibogamine, are considered as retained names.

P-101.2.2.6 Indicated hydrogen, as defined in P-14.6, is used to describe isomers.

P-101.2.3 Numbering of parent structures

P-101.2.3.1 A numbering pattern established among a group of structurally related natural products is used for numbering the skeletal atoms of the stereoparent structure, providing that all skeletal atoms have been included in the numbering system.

P-101.2.3.2 If no numbering pattern has been become established among the members of a group of structurally related natural products, the stereoparent hydride is numbered according to the following guidelines:

(a) examine the skeleton to identify the senior ring or ring system system, according to P-44. The locant '1' is assigned to the atom of the preferred ring system whose locant would be '1' according to systematic numbering for that particular ring or ring system;

(b) assign all skeletal atoms of the senior ring system consecutive arabic numbers, including atoms of fusion positions in fused ring systems, beginning with the locant '1', and following the path prescribed for that particular type of ring or ring system;

(c) number acyclic substituents to skeletal atoms of ring components or connecting acyclic structures each in its entirety, including branches, in order of the increasing value of the locant of the skeletal atom to which it is attached;

(d) number skeletal atoms of acyclic connections to other ring or ring systems, if any, consecutively beginning with the atom next to the senior ring system, followed by the skeletal atoms of the other rings or ring systems as prescribed in (b) above; if two or more acyclic connections to other rings or ring systems are present, the one attached to the senior ring or ring system at the lowest numbered position is numbered first, then the ring attached to it, followed by the acyclic connector at the next lower position of the senior ring or ring system, etc.;

(e) number the larger group, in terms of the number of skeletal atoms, between two groups at a geminal disubstituted position, first; if there is still a choice, alphanumerical order is followed (Rule P-14.5) . If the two groups are then identical and attached to a stereoparent structure properly drawn (see Appendix in ref. 9), the group that is stereochemically α is numbered first; if the two groups are identical and attached to an acyclic terminal double bond, the group '*trans*' to the main chain is numbered first as described in the carotenoid recommendations (Rule 12.4 in ref. 40).

P-101.2.4 Identification of individual rings

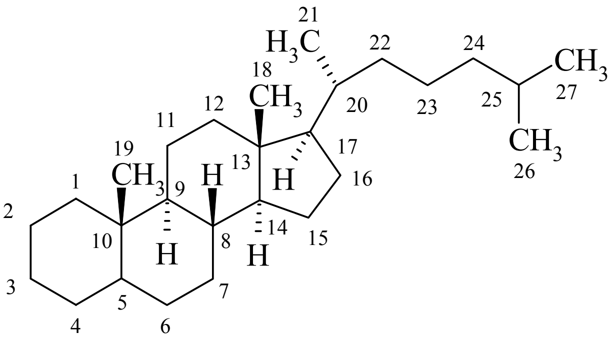
Since locants are used to describe skeletal modifications, as indicated in P-101.3, the identification of individual rings by letters A, B, C, etc., used in the past is no longer recommended, except for the rather special case of the removal of a terminal ring (see P-101.3.6). Nevertheless, to provide continuity with the use of this system, names using letters to identify rings are given where appropriate, but are no longer recommended.

P-101.2.5 Atomic connector, terminal segment and bond connector

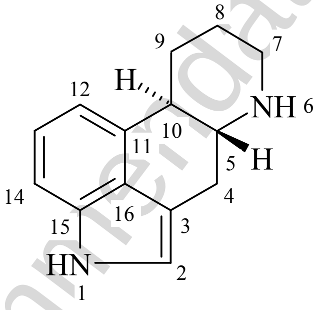
For nomenclature purposes, the fundamental structures are described by specific arrangements of atoms or groups of atoms called 'atomic connectors', 'terminal segments' and 'bond connectors', that must be taken into consideration in accordance with the additive or subtractive operations modifying a fundamental structure.

An 'atomic connector' is a chain of homogeneous skeletal atoms of the same element connecting any combination of bridgehead or ring junction atoms, rings, or ring systems (i.e. ring assemblies), substituted skeletal atoms in parent structure, or heteroatoms. A 'terminal segment' of a skeletal structure is an acyclic portion of homogeneous skeletal atoms connected at only one end by the features of structure that terminate atomic connectors. A 'bond connector' is a connection between any combination of bridgehead or ring junction atoms, rings or ring systems (i.e. ring assemblies), substituted skeletal atoms, or heteroatoms. The structures below illustrate atomic connectors, bond connectors and terminal segments. The use of these terms is further illustrated in P-101.3.1 in relation to the removal of skeletal atoms denoted by the prefix 'nor'.

Examples:



cholestane



ergoline

Atomic connectors:

In cholestane: 1-4, 6-7, 11-12, 15-16, and 22-24.
In ergoline: 2, 4, 7-9, and 12-14

Terminal portions:

In cholestane: 18, 19, 21, 26, and 27.
In ergoline: none

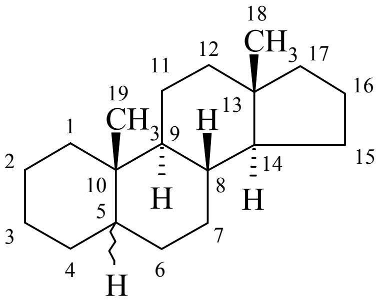
Bond connectors:

In cholestane: 5-10, 8-9, 8-14, 9-10, 13-14, 13-17, and 17-20
In ergoline: 1-15, 3-16, 5-6, 5-10, 10-11, 11-16, and 15-16

P-101.2.6 Stereochemical configuration of parent structures

The name of a parent structure usually implies (the 5α position in steroids is usually not defined), without further specification, the absolute configuration of all chiral centers and the configuration of double bonds when applicable. When a planar or quasi planar system of rings is denoted as a projection, as in this recommendation, an atom or group attached to the ring is called α if it lies below or β if it lies above the plane of the paper. Use of this system requires the orientations of structure as given in the examples used to exemplify the various rules. In the example below, the implied configurations shown define the attached hydrogen atoms and methyl groups at positions 8, 10, and 13, as β and at positions 9 and 14 as α; here, the configuration of the hydrogen atom at position 5 is not known and thus the orientation is ξ (xi), denoted by a wavy line in the formula. The stereodescriptors α, β and ξ used to describe implicit or indicated configuration are cited before the name of the fundamental parent structure without parentheses.

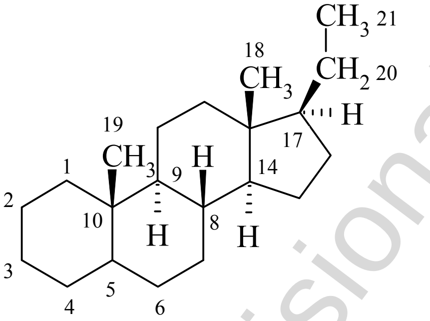
The α/β symbolism is used as defined above and extended in the following way to express different aspects of the configuration of modified fundamental parent structures.



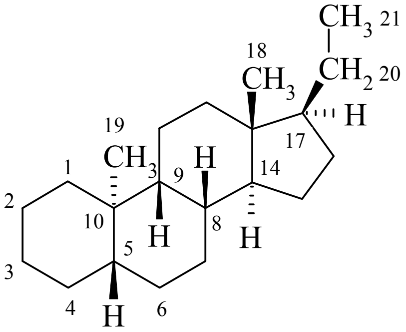
P-101.2.6.1 Configurations that are different from those in the parent structure

P-101.2.6.1.1 At chiral centers, the α/β system is used as described or in IUPAC-IUBMB recommendations for the nomenclature of steroids (ref. 39). Each chirality center is described by the stereodescriptor α, β, or ξ to indicate a configuration that must be specified and those that are inverted. The symbols α, β, or ξ, preceded by the appropriate locants, are placed immediately at the beginning of the name of the fundamental parent structure. In the following examples, configuration at C-5 must be specified; configurations at bridgeheads C-9 and C-10 are inverted when compared with those of the fundamental parent structure. This method is preferred to the alternative described in P-101.2.6.1.2 .

Examples:



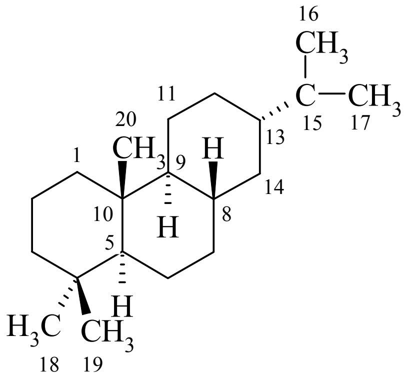
pregnane (PIN)
(fundamental parent structure)



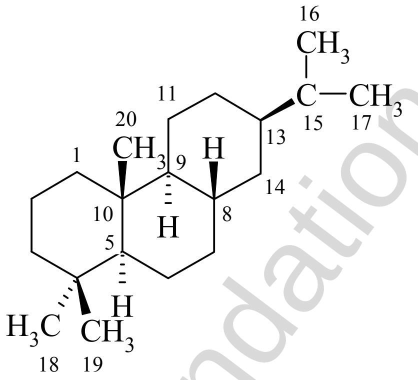
5β,9β,10α-pregnane (PIN)

A change in configuration of a nonbrigeheaded side chain that is part of the parent is denoted by the method specified for C-17 of steroids (see 3S-5.2, ref. 39), where α or β refers to the sidechain itself and not to the hydrogen atom in the same position.

Example:



abietane (PIN)
(fundamental parent structure)

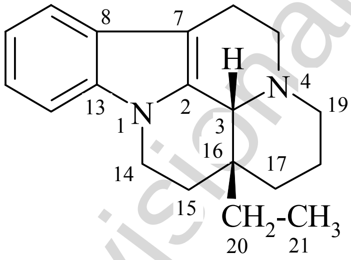


13β-abietane (PIN)

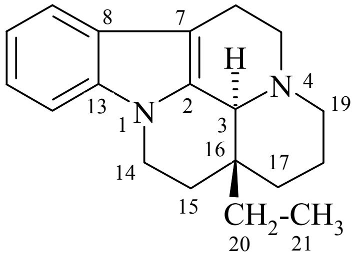
P-101.2.6.1.2 Configurational inversion at one of stereogenic centers whose configuration is implied or stated in the name of the fundamental parent structure can be indicated by the italicized prefix *epi* (derived from 'epimer') placed at the front of the name of the parent structure and prefixed by the locant of the affected atom. As method P-101.2.6.1.1 leads to preferred IUPAC names, this method may be used only in general nomenclature.

The preferred IUPAC name 13β-abietane, described above in P-101.2.6.1.1, can also be named 13-*epi*-abietane.

Example:



eburnamine (PIN)
(fundamental parent structure)



3-*epi*-eburnamine
3α-eburnamine (PIN)

P-101.2.6.1.4 The stereodescriptors *R* and *S*

The stereodescriptors '*R*' and '*S*' are used to describe the absolute configuration not specified by the α/β system described above, in accord with the CIP priority system and the rules and conventions described in Chapter 9 (see P-92.3). The stereodescriptors '*R*' and '*S*' are also used when a ring is opened and two chiral centers created, one of which may rotate, as described for vitamin D in P-101.8.4.

P-101.2.7 Semisystematic names of recommended fundamental stereoparent structures are listed in Table 10.1. All except retinal, cepham, and penam are parent hydrides.

Table 10.1 List of recommended names of stereoparent structures
(this list is nonlimiting; structures are shown in the Appendix in ref. 9)

1. Names recommended as preferred IUPAC names.

(a) alkaloids

aconitane
ajmalan
akuamilan
alstophyllan
aporphine
aspidofractidine
aspidospermidine
atidane
atisine
berbaman
berbine
cephalotaxine
cevane
chelidonine
cinchonan
conanine
corynan
corynoxan
crinan
curan
daphnane
dendrobane
eburnamine
emetan
ergoline
ergotaman
erythrinan
evonimine
evonine
formosanan
galanthamine
galanthan
hasubanan
hetisan
ibogamine
kopsan
lunarine
lycopodane
lycorenan
lythran
lythrancine
lythranidine
matridine
ormosanine
morphinan
nupharidine
oxayohimban
oxyacathan
pancracine
rheadan
rodiasine
samandarine
sarpagan
senecionan
solanidine
sparteine
spirosolane
strychinidine
tazettine
tropane
tubocuraran
tubulosan
veratraman
vincaleucoblastine
vincane
vobasan
vobtusine
yohimban

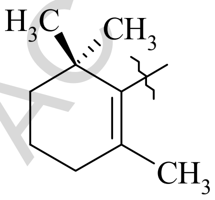
(b) steroids

androstane
bufanolide
campestane
cardanolide
cholane
cholestane
ergostane
estrane
furostan
gonane
gorgostane
poriferastane
pregnane
spirostan
stigmastane

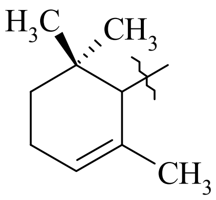
(c) terpenes (all are parent hydrides except retinal)

abietane
ambrosane
aristolane
atisane
beyerane
cadinane
β,φ-carotene[1]
β,ψ-carotene[1]
ε,κ-carotene[1]
ε,χ-carotene[1]
caryophyllane
cedrane
dammarane
drimane
eremophilane
eudesmane
gammacerane
germacrane
gibbane
grayanotoxane
guaiane
himalachane
hopane
kaurane
labdane
lanostane
lignan
lupane
neolignan
oleanane
ophiobolane
picrasane
pimarane
podocarpane
protostane
retinal
rosane
taxane
trichothecane
ursane

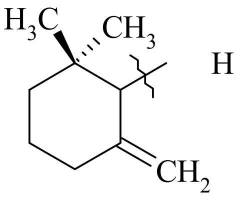
[1] Four different carotenes are exemplified; there are 28 carotene parent structures derived from all permutations of the seven following end groups:



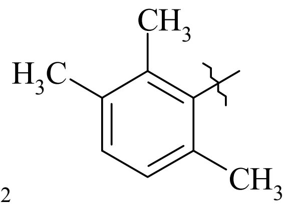
β



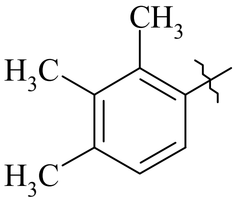
α (alpha)



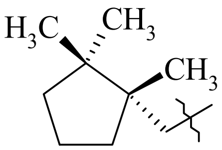
γ (gamma)



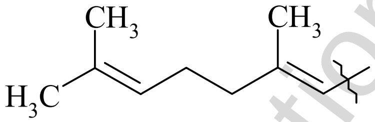
(theta)



χ (chi)



κ (kappa)



ψ (psi)

(d) Miscellaneous (all are parent hydrides except cepham and penam)

- biline
- cepham
- corrin
- penam
- prostane
- porphyrin
- thromboxane

(2) Names recommended for general nomenclature only

(a) Terpenes

- bisabolane
- bornane
- carane
- fenchane
- humulane
- menthane (*p*-isomer)
- pinane
- thujane

(b) Miscellaneous

- flavan
- isoflavan
- neoflavan

P-101.3. Skeletal modifications of parent structures

P-101.3.0 Introduction

The skeleton of parent structures can be modified in many ways, contracted, expanded, or rearranged by using operations described in P-13. These operations are denoted by specific nondetachable prefixes that are added to the name of the parent structure. Changes affecting the configuration must be shown as indicated in P-101.2.6 and P-102. Preferred IUPAC names result from a narrow interpretation of the number of operations that are allowed in order to preserve the integrity of the ring system and of the absolute configuration. In natural product nomenclature and general nomenclature, the number of operations is not subject to limitations.

This Section supersedes the provisional Section F Rules and Rules A-71 to related to terpene hydrocarbons as prescribed in the 1979 Recommendations (ref. 1).

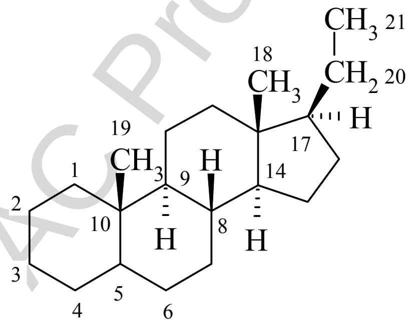
P-101.3.1 Removal of skeletal atoms without affecting the number of rings

P-101.3.1.1 The removal of an unsubstituted skeletal atom, saturated or unsaturated, from a ring or of an unsubstituted skeletal atom from an saturated acyclic portion of a parent structure with its attached hydrogen atom(s) is described by the nondetachable prefix ‘nor’; the loss of two or more such skeletal atoms are indicated by the usual numerical multiplicative prefixes ‘di’, ‘tri’ added before ‘nor’.

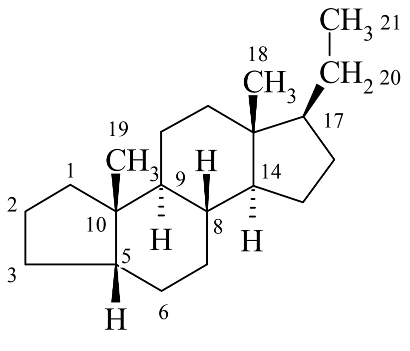
The position of the skeletal atom that is removed is denoted in all cases by its locants in the numbering of the fundamental parent structure. Although, because the locant of each skeletal atom removed is cited, an unambiguous name can be generated by the removal of any skeletal atom, carbon atom or heteroatom, it is traditional to remove skeletal atoms with the highest possible locant in an atomic connector in a cyclic portion of the skeletal structure. In carotenes, as an exception, the locant attached to ‘nor’ is the lowest possible (see Rule Carotenoid 5.1, ref, 27).

For preferred IUPAC names, modifications by the prefix ‘nor’ are limited to fundamental structures having two or more rings; ring contraction and chain shortening are limited to the removal of a maximum of two methylene groups. When the use of a fundamental structure is not allowed, preferred IUPAC names are substitutive names, systematically formed, with CIP stereodescriptors to describe configurations.

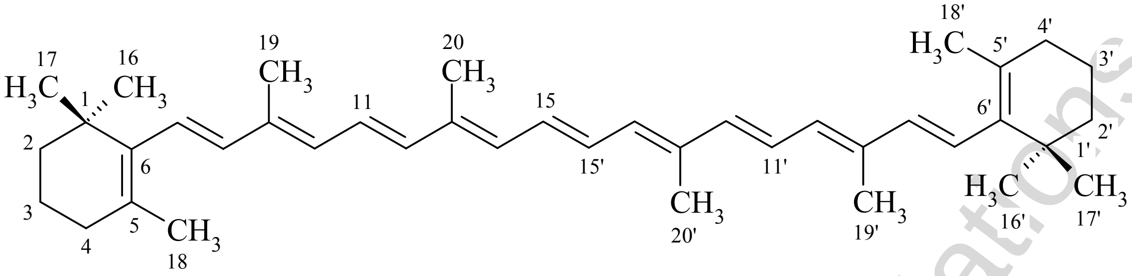
Examples:



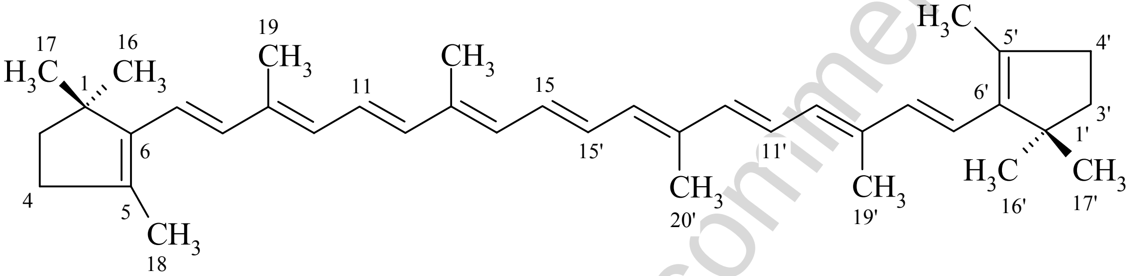
pregnane (PIN)
(fundamental parent structure)



4-nor-5β -pregnane (PIN)



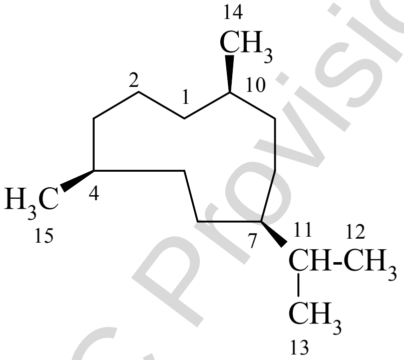
β,β-carotene (PIN)
(fundamental parent structure)



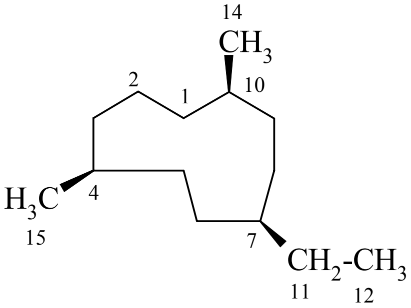
2,2′-dinor- β,β-carotene (PIN)

In an acyclic portion of a skeletal structure, the skeletal atom removed preferably is the one of an acyclic atomic connector or a terminal segment nearest to the free end of this acyclic portion. (This is done in order to maintain as far as possible the numbering of structural features of the compound and of compounds derived from it).

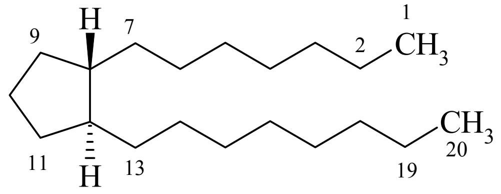
Examples:



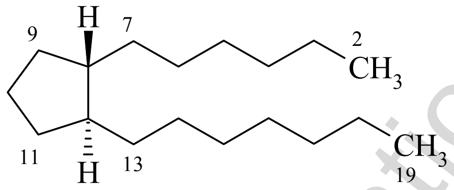
germacrane (PIN)
(fundamental parent structure)



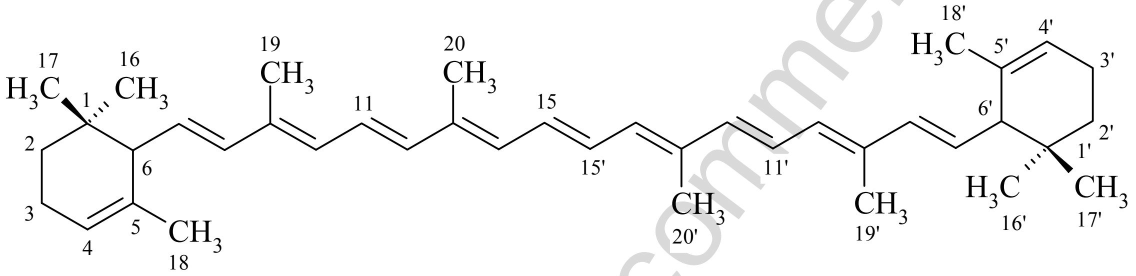
13-norgermacrane
(1*s*,4*R*,8*S*)-1-ethyl-4,8-dimethylcyclodecane (PIN)
(the prefix ‘nor’ is not permitted for
monocyclic stereoparents)



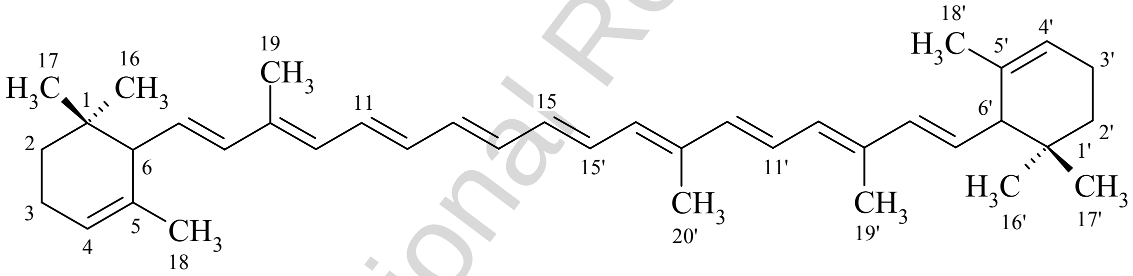
prostane (PIN)
(fundamental parent structure)



1,20-dinorprostane (PIN)



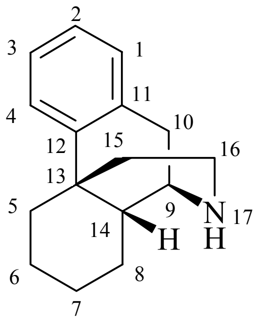
ε,ε-carotene (PIN)
(fundamental parent structure)



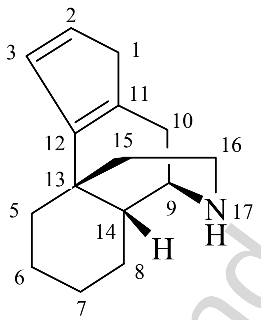
20-nor-ε,ε-carotene (PIN)

P-101.3.1.2 When the removal of an unsaturated skeletal atom from a mancude ring (containing the maximum number of noncumulative double bonds) in the parent structure results in the creation of a saturated ring position, this position is described by indicated hydrogen (see P-14.6). In names, the symbol *H*, denoted by the appropriate locant, is cited at the beginning of the name modified by the nondetachable prefix.

Example:



morphinane
(fundamental parent structure)



1*H*-4-normorphinane

P-101.3.2 Addition of skeletal atoms without affecting the number of rings

P-101.3.2.1 The addition of a methylene ($-CH_2-$) group between two skeletal atoms of a parent structure is described by the nondetachable prefix 'homo'; the addition of two or more methylene groups is indicated by the numerical multiplicative prefixes 'di', 'tri', etc. Positions of inserted methylene groups in the modified fundamental parent structure are indicated by the locants of the added methylene groups which are cited in front of the prefix 'homo', preceded by multiplicative prefixes when required.

The assignment of the locants to an added methylene group depends on whether it is considered to be inserted into an atomic connector or terminal acyclic portion or into a bond connector.

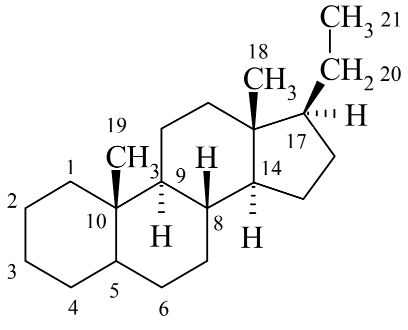
For preferred IUPAC names, modifications by the prefix 'nor' are limited to fundamental structures having two or more rings, and ring enlargement and chain lengthening are limited to the addition of a maximum of two methylene groups. When the use of a fundamental structure is not allowed, preferred IUPAC names are substitutive names systematically formed, with CIP stereodescriptors to describe configurations.

P-101.3.2.2 Numbering of additional skeletal atoms

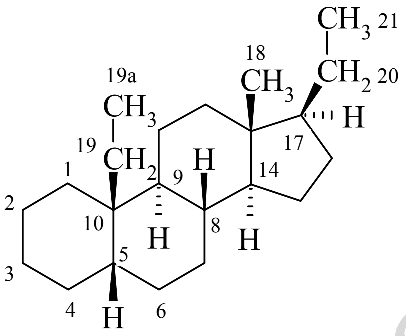
P-101.3.2.2.1 Methylene groups inserted into an atomic connector or into a terminal segment are identified by adding a letter 'a', 'b', etc., to the locant of the highest numbered skeletal atom of the atomic connector or terminal portion consistent with the location of double bonds remaining in the structure. If there are equivalent atomic connectors, the highest atomic connector is chosen, and the methylene group is inserted after the highest number skeletal atom in that connector.

Addition of acyclic side chains or extension of terminal portions of a side chain already attached to the stereoparent hydride may also be done by principles of substitutive nomenclature. The added substituent(s) are numbered as described above for 'homo' atoms.

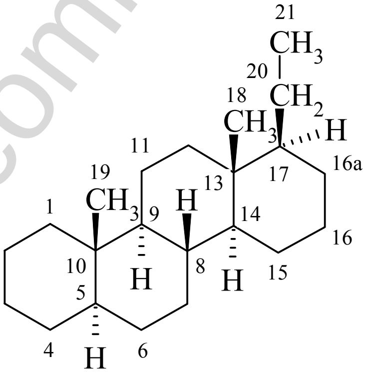
Examples:



pregnane (PIN)
(fundamental parent structure)



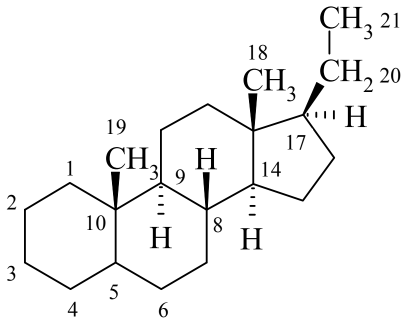
19a-homo-5β-pregnane (PIN)
(not 19-methyl-5α-pregnane;
extension of side chain not
allowed)



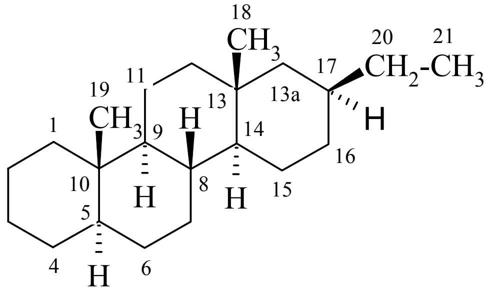
16a-homo-5α-pregnane (PIN)

P-101.3.2.2.2 Methylene groups inserted into a bond connector are identified by citing both locants of the skeletal atoms terminating the bond connector enclosing the second (higher) number in parentheses, followed by a letter ‘a’, ‘b’, etc. according to the number of methylene groups.

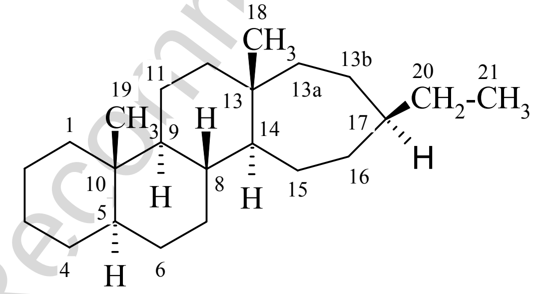
Examples:



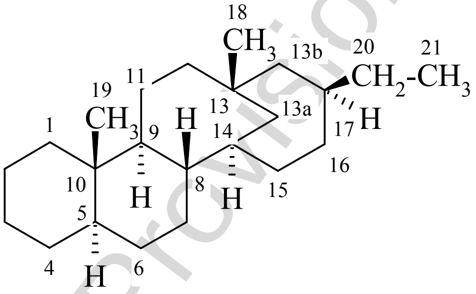
pregnane (PIN)
(fundamental parent structure)



13(17)a-homo-5α-pregnane (PIN)



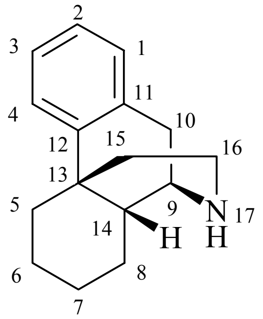
13(17)a,13(17)b-dihomo-5α-pregnane (PIN)
(has been called *D*(17a,17b)dihomo-
5α-pregnane)



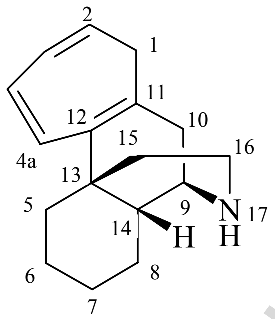
13(14)a,13(17)b-dihomo-5α-pregnane (PIN)

P-101.3.2.2.3 The insertion of a methylene group into a mancude ring or ring system (that contains the maximum number of noncumulative double bonds) or into a system of conjugated double bonds may create a saturated ring position that is described by ‘indicated hydrogen’ (see P-14.6). The position of the methylene group is prescribed by P-103.2.2.2, even though the saturated ring position may be elsewhere in the unsaturated ring system as denoted by the appropriate locant for the indicated hydrogen; this is a change for names of the homoporphyrins (see ref. 42, Rule TP-5.1). Two tautomeric forms, **A** and **B**, are represented below and specifically numbered and named.

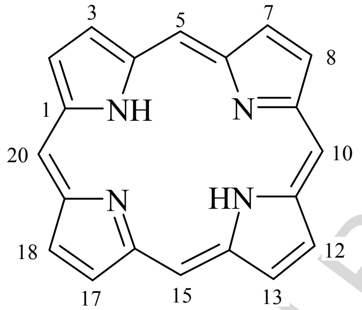
Examples:



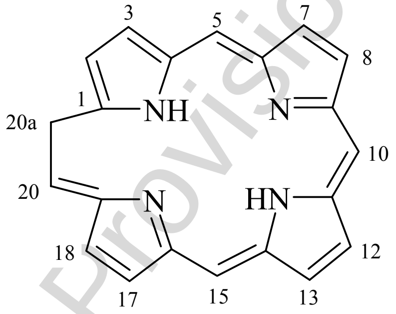
morphinan(PIN)
(fundamental parent structure)



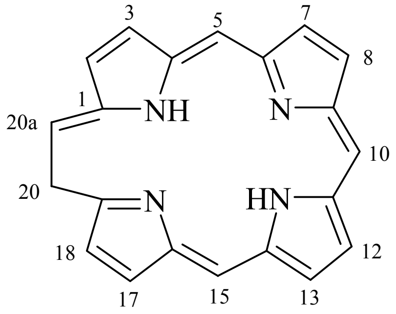
1*H*-4a-homomorphinan (PIN)



porphyrin (PIN)
(fundamental parent structure)



A 20a*H*-20a-homoporphyrin (PIN)



B 20*H*-20a-homoporphyrin (PIN)

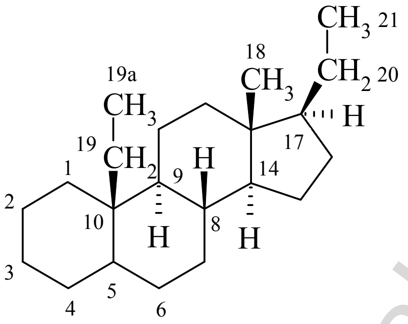
P-101.3.3 Bond formation

The creation of an additional ring by a conjunctive operation (see P-13.5.3) by means of a direct link between any two atoms of a parent structure is described by the nondetachable prefix 'cyclo' (not italicized) preceded by the locants of the skeletal atoms so connected. When necessary, the stereochemical configuration created by the new bond is denoted by α, β, or ξ descriptors in accord with P-101.2.5.1.1, or by describing the configuration of the hydrogen atom in accordance with P-101.2.5.1.2..

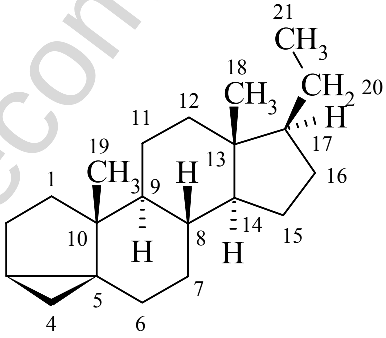
Stereochemical configurations of the parent structure are retained. New stereochemistry of the ring atoms having one hydrogen atom still present is indicated by the α/β stereodescriptors as described in P-105.5.1.2, or, if necessary, by the sequence rule method (*R*/*S*). The projection of the hydrogen atom below (α) or above (β) the reference plane of the ring system is indicated by the appropriate symbol and a capital italic letter *H* following the locant of the ring atom in the structure, all enclosed in parentheses, and cited before the appropriate prefix, in this case 'homo' (see P-103.5 for the prefix 'abeo'). This method of citation differs from that used in the Steroid Rules (ref. 39, Rule 3S-7.5).

For preferred IUPAC names, modifications by the prefix 'cyclo' are limited to fundamental structures having two or more rings, and ring formation is limited to the addition of a maximum of two more rings to a fundamental structure. When the use of a fundamental structure is not allowed, preferred IUPAC names are substitutive names systematically formed, with CIP stereodescriptors to describe configurations.

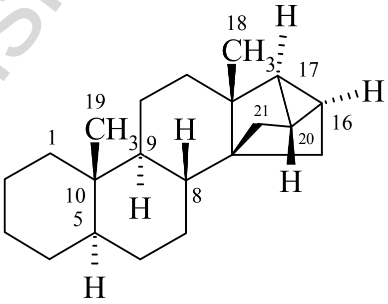
Example:



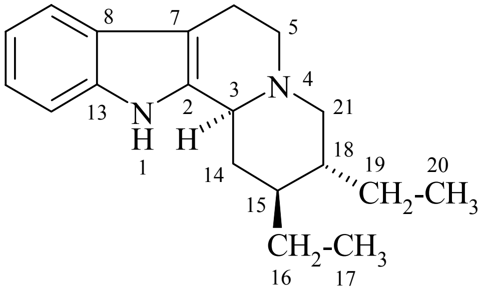
pregnane (PIN)
(fundamental parent structure)



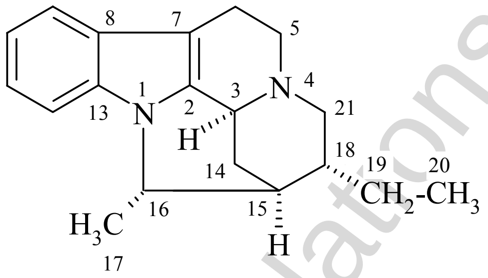
3α,5-cyclo-5α-pregnane (PIN)



(20*S*)-14,21:16β,20-dicyclo-5α,14β-pregnane (PIN)



corynan (PIN)
(fundamental parent structure)



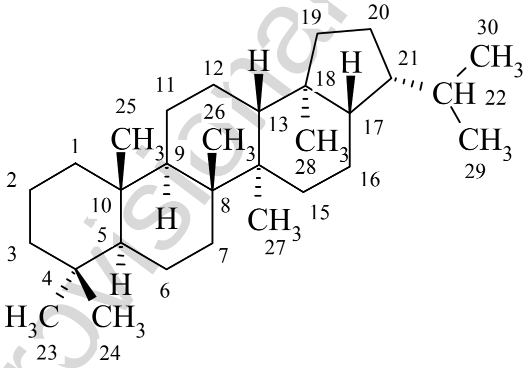
(16β*H*)-1,16-cyclocorynan (PIN)

P-101.3.4 Bond cleavage

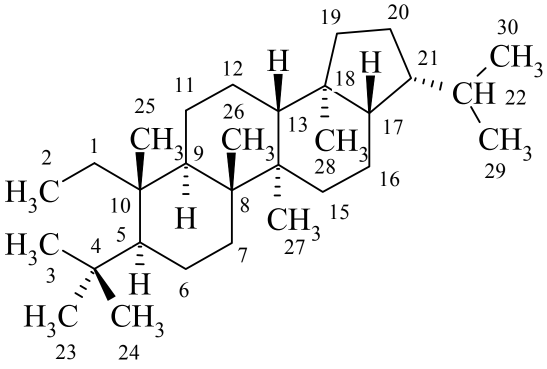
P-101.3.4.1 Cleavage of a ring bond (saturated or unsaturated) with the addition of appropriate number of hydrogen atoms at each new terminal group thus created is indicated by the prefix ‘seco’ (not italicized) and the locants of the cleaved bond. The original numbering is retained.

For preferred IUPAC names, modifications by the prefix ‘seco’ are limited to fundamental structures having three or more rings, and.ring opening is limited to one ‘seco’ operation. When the use of a fundamental structure is not allowed, preferred IUPAC names are substitutive names systematically formed, with CIP stereodescriptors to describe configurations.

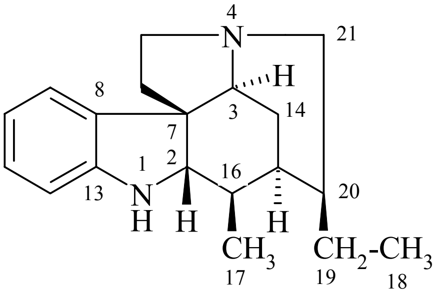
Example:



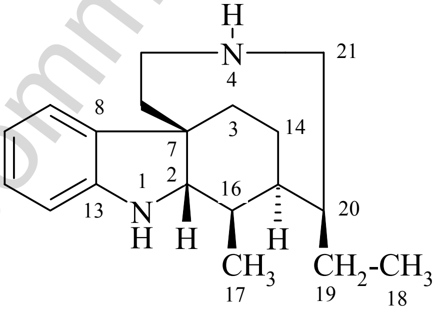
hopane (PIN)
(fundamental parent structure)



2,3-secohopane (PIN)



curan (PIN)
(fundamental parent structure)

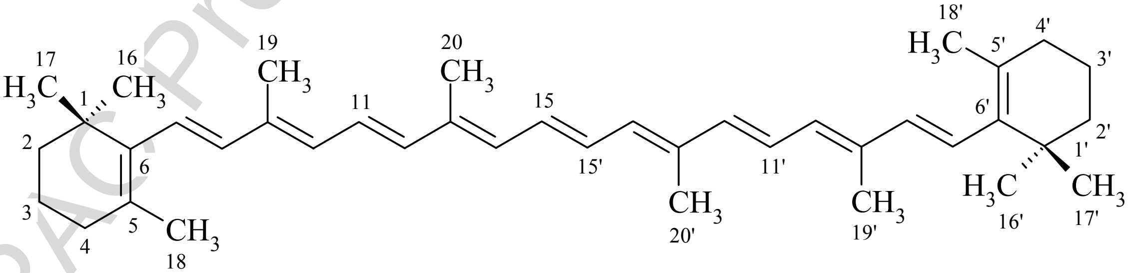


3,4-secocuran (PIN)

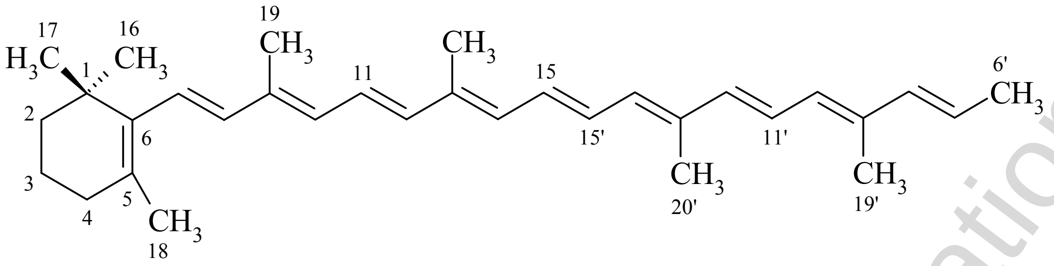
P-101.3.4.2 The unitalicized prefix ‘apo’ preceded by a locant is used to indicate removal of all of a side chain of a parent structure beyond the skeletal atom corresponding to that locant. Removal of more than one side chains is indicated by using the numerical multiplying prefixes ‘di’, ‘tri’, etc. preceded by the appropriate locants. Numbering of the skeletal atoms in the parent structure is retained in the resulting fragment.

This procedure is used only in carotenoid nomenclature (see ref. 40, Rule Carotenoid 10).

Example:



β-carotene (PIN)
(fundamental parent structure)



6′-apo-β-carotene (PIN)

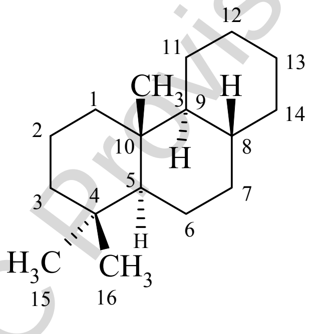
P-101.3.5 Bond migration

Parent structures that are not simple derivatives of accepted parents, but may be considered to arise from such parents by bond migration of one or more bonds, may be named by the following method. This method is described here, although it is not recommended to be used to generate preferred IUPAC names.

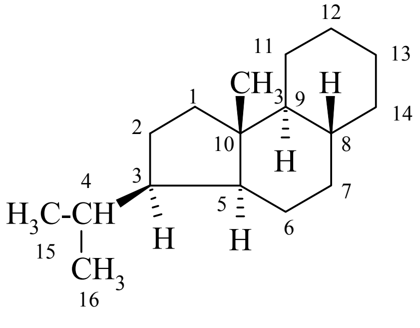
P-101.3.5.1 The nondetachable prefix ‘$x(y \rightarrow z)$-abeo-’, designates the migration from one end of a single bond from its original position in a parent structure to another position. In the prefix, ‘*x*’ is the locant of the stationary, i.e. unchanged, end of the migrating bond; ‘*y*’ is the locant of the position of the moving end of the migrating bond in the parent structure; and ‘*z*’ is the locant of the position of the moving end in the final structure. The numbering of the initial structure is retained.

Previously the prefix ‘abeo’ was italicized (ref 1, F-4.7; ref 2, R-1.2.7.1). For consistency with the other modifying prefixes it is now recommended that a roman font be used. The ‘abeo’ nomenclature described in this rule is permissive, not compulsory. It is most suitable for use in discussions on reaction mechanisms and biogenesis. In general systematic names, or names assigned by the ‘homo’, ‘nor’, ‘cyclo’, ‘seco’ method, are preferred.

Example:



podocarpane (PIN)
(fundamental parent structure)

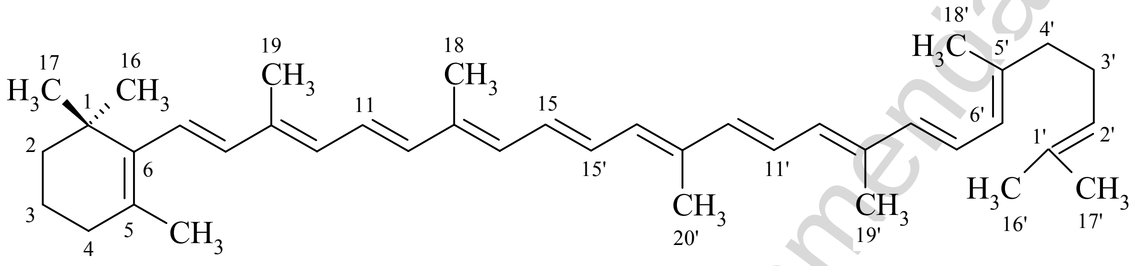


(3α*H*)-5(4→3)-abeo-podocarpane
3,5-cyclo-4,5-seco-3β-podocarpane (PIN)

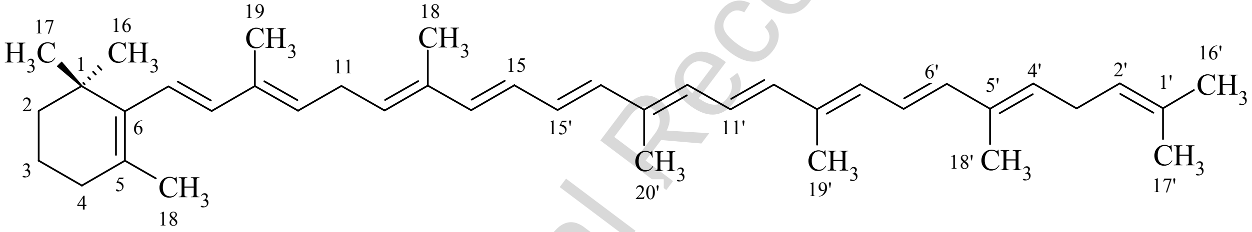
P-101.3.5.2 The italic prefix ‘*retro*’ preceded by a pair of locants is used to indicate a shift, by one position, of all single and double bonds of a conjugated polyene system delineated by the pair of locants; the conjugated polyene system cannot be part of a system of maximum number of noncumulative double bonds in a ring or ring system The first locant is the skeletal atom that has lost a hydrogen atom and the second locant the one that has gained a hydrogen atom.

The descriptor ‘*retro*’ is used in this manner only in carotenoid nomenclature (see ref 27, Carotenoid Rule 9)

Example:



β,ψ-carotene (PIN)
(fundamental parent structure)

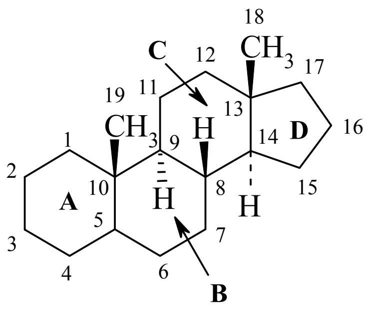


4′,11-*retro*-β,ψ-carotene (PIN)

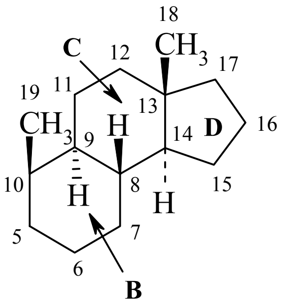
P-101.3.6 Removal of a terminal ring.

The removal of a terminal ring from a parent structure with the addition of an appropriate number of hydrogen atoms at each junction with the adjacent ring is indicated by the nondetachable prefix ‘des’ followed by the capital italic letter of the ring removed (see P-103.2). This is the only time that the capital letters are now used to identify rings in a parent structure. Stereochemistry implied by the name of the stereoparent structure remains the same, unless otherwise specified. Numbering of skeletal atoms of the parent structure is retained in the modified structure. This use of ‘des’ is restricted to steroids.

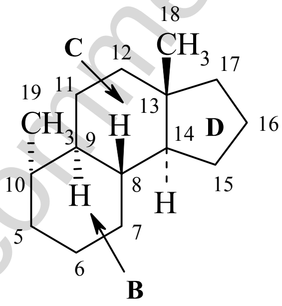
Example:



androstane (PIN)
(fundamental parent structure)



des-*A*-androstane (PIN)



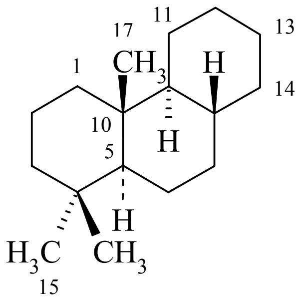
des-*A*-10α-androstane(PIN)

P-101.3.7 Combination of the prefixes ‘cyclo’, ‘seco’, ‘apo’, ‘homo’, and ‘nor’ for generating preferred IUPAC names

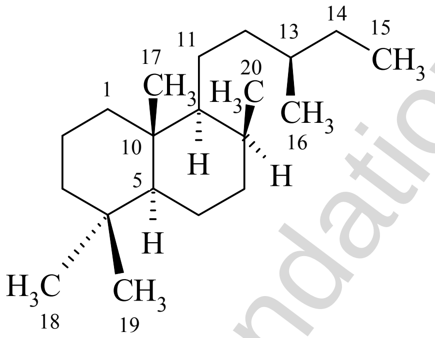
The modifications to a fundamental parent structure prescribed by the prefixes in the preceding recommendations (P-101.3.1 through P-101.3.4) may be combined to effect even more drastic changes in structure. The operation indicated by each prefix ‘cyclo’, ‘seco’, “apo’ ‘homo’, and ‘nor’ is applied to the fundamental parent structure sequentially as one ‘advances backward’, i.e. moves from right to left, from the name of the fundamental parent structure.

P-101.3.7.1 When different combinations of prefixes ‘cyclo’, ‘seco’, ‘apo’, ‘homo’, ‘nor’ can be used to effect the same transformation in structure, the combination of choice must express the fewest number of operations. Both detachable (e.g. alkyl) and nondetachable (e.g. homo or nor) prefixes are considered as modifications but detachable prefixes are preferred. Dihomo, dinor, etc. , are counted as two modifications each (see ref 26, 3S-6.3). When the number of operations is the same, the combination of homo/nor is preferred to cyclo/seco; choice between other combinations expressing the same number of operations is based on earlier alphabetical order of the prefixes.

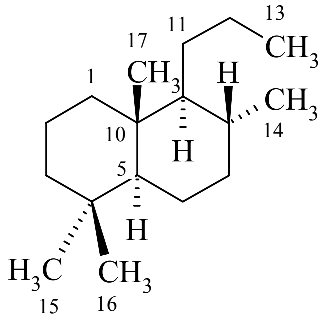
Examples:



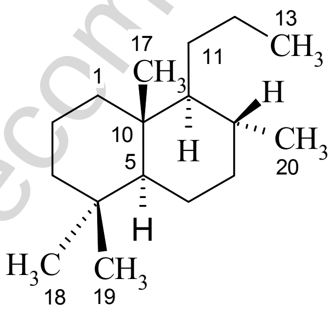
podocarpane (PIN)
(fundamental parent structure)



labdane (PIN)
(fundamental parent structure)



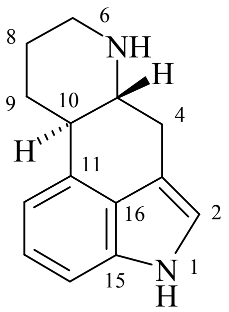
I



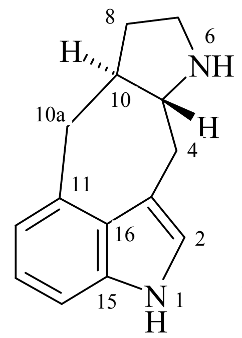
II

13,14-secopodocarpane **(I)** (PIN) not 8α-14,15,16-trinorlabdane **(II)**

Guide to name formation: Podocarpane may be used to generate the 'seco' compound by one operation; the same compound may be obtained from labdane in three operations. Thus, 13,14-secopodocarpane, the name resulting from the minimal use of structure modifying prefixes is the preferred IUPAC name. Compounds I and II are compared, irrespective of the fact that three operations are not allowed to generate preferred IUPAC names.



ergoline (PIN)
(fundamental parent structure)



10(11)a-homo-9-norergoline (PIN)
[not 5,9-cyclo-5,10-secoergoline, nor
(9*H*)-5(10→9)-abeoergoline]

P-101.3.7.2 The order of citation of combinations of structure modifying prefixes must avoid improper use of the prefixes as defined above or impossible situations when the corresponding operations are carried out in the manner prescribed above.

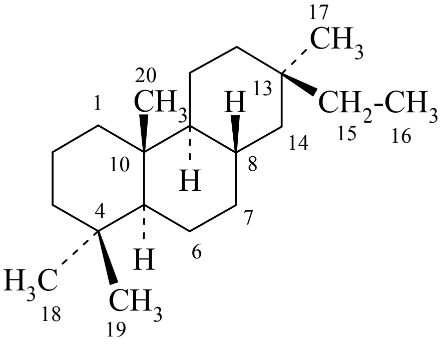
P-101.3.7.3 After satisfying P-101.3.7.1 and P-101.3.7.2, the nondetachable prefixes that indicate bond rearrangements (‘cyclo’ and ‘seco’) are cited, followed by those that indicate addition or removal of skeletal atoms (‘homo’ and ‘nor’). If more than one of any of these operations is needed, they are cited in alphabetical order before the name of the fundamental parent structure. Multiplying prefixes denoting multiple operations of the same kind do not affect the order.

Preferred IUPAC names result from modifications by two operations only involving the prefixes ‘cyclo’, ‘seco’, ‘homo’, and ‘nor’. In general nomenclature, more than two operations are allowed. Names are formed by citing the bond rearrangement prefixes ‘cyclo’ and ‘seco’, in that order from left to right, followed by removal/addition prefixes ‘homo’ and ‘nor, in that order from left to right, at the front of the name of the parent structure. Schematically this order may be shown as follows:

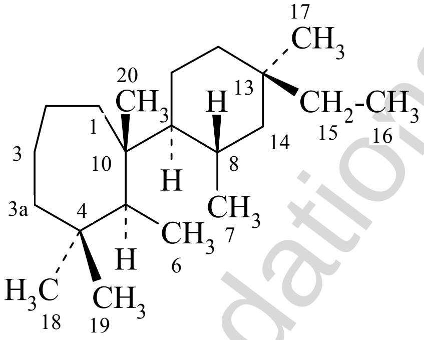
bond rearrangement	addition/removal of skeletal atoms	parent structure
cyclo, seco	apo, homo, nor	

Names in which the order of prefixes is cyclo/seco/homo/nor are preferred to those denoted by the alphabetical order apo/cyclo/homo/nor/seco for the four prefixes.

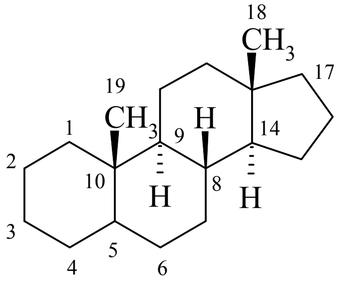
Examples:



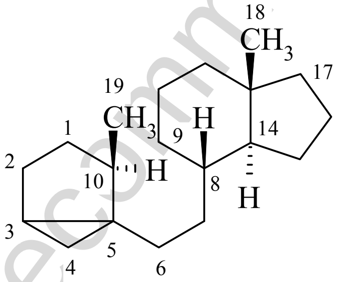
pimarane (PIN)
(fundamental parent structure)



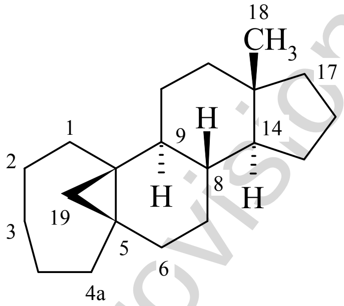
6,7-seco-3a-homopimarane (PIN)
3a-homo-6,7-secopimarane



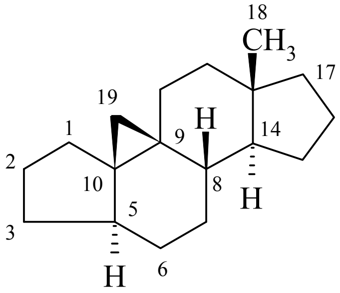
androstane (PIN)
(fundamental structure)



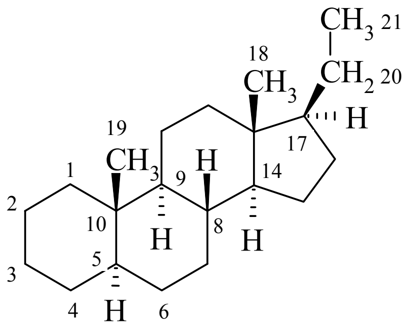
3α,5-cyclo-9,10-secoandrostane (PIN)



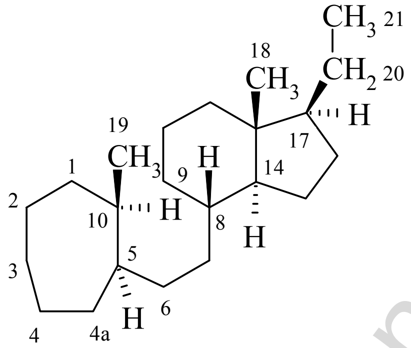
5β,19-cyclo-4a-homo-5β-androstane (PIN)



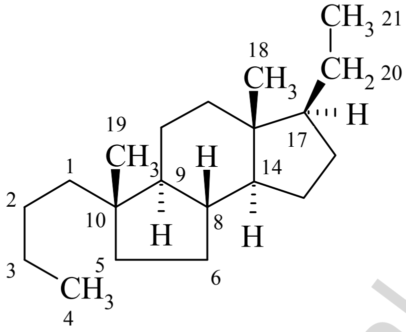
9β,19-cyclo-4-nor-5α,9β-androstane (PIN)



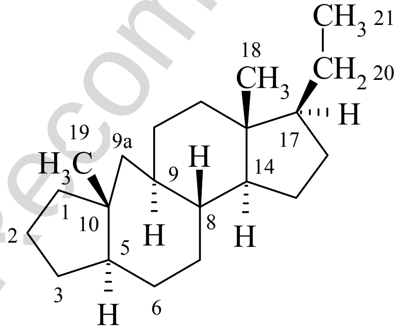
5-α-pregnane (PIN)
(fundamental structure)



9,10-seco-4a-homo-5α-pregnane (PIN)



4,5-seco-7-nor-5α-pregnane (PIN)



9a-homo-4-nor-5α-pregnane

P-101.4. Replacement of skeletal atoms

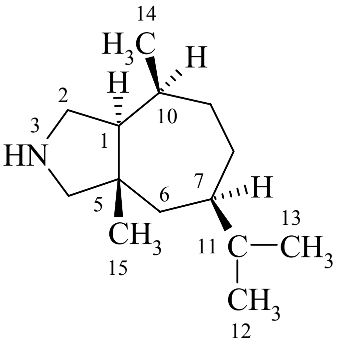
P-101.4.1 General methodology

The principles of skeletal replacement (‘a’) nomenclature, as described in P-15.4 to modify parent structures, are applied to replace carbon skeletal atoms by heteroatoms, such as O, S, N. Contrary to the recommended alphabetical order for citation in names in Revised Section F (ref. 9), the seniority order of the ‘a’ prefixes prescribed in P-15.4 is recommended for skeletal replacement. In addition to the methodology used to generate systematic names, skeletal replacement (‘a’) replacement is also used to replace heteroatoms in parent structures by carbon atoms and by other heteroatoms.

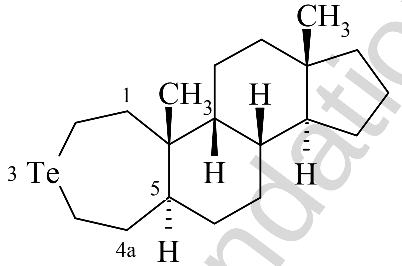
P-101.4.2 Skeletal replacement of carbon atoms by heteroatoms

Heteroatoms are denoted by ‘a’ prefixes that are cited before nondetachable prefixes expressing skeletal modifications in fundamental parent structures, each with a locant to indicate its position; the fixed numbering of the parent structure is maintained. Skeletal modifications, if any, must be completed before skeletal replacement (‘a’) nomenclature can be applied.

Examples:



3-azaambrosane (PIN)

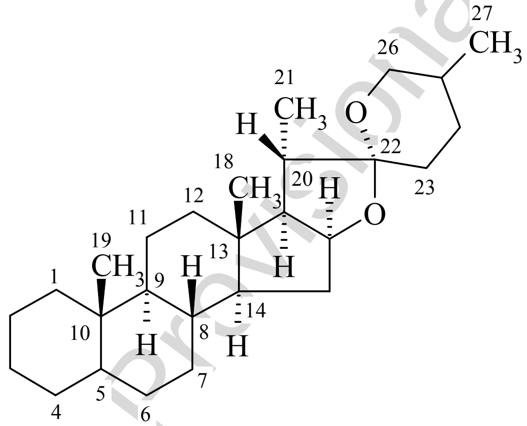


3-tellura-4a-homo-5α-androstane (PIN)

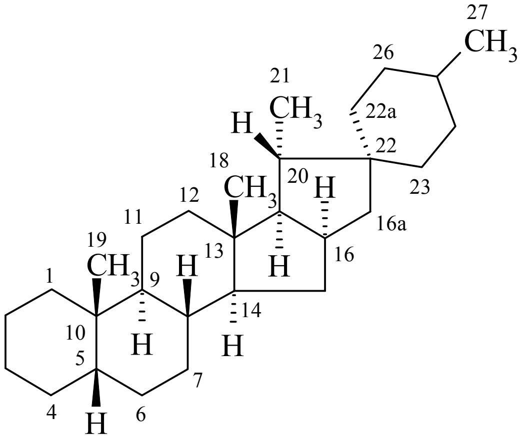
P-101.4.3 Replacement of skeletal heteroatoms by carbon atoms

Replacement of a heteroatom in a parent structure by a carbon atom is indicated by the 'a' prefix 'carba'. The original numbering is maintained. If the heteroatom is not numbered, the replacing carbon atom is numbered by affixing the letter 'a' to the locant of the immediately adjacent lower numbered skeletal atom. If the immediately adjacent lower numbered skeletal atom is a 'homo' atom, the letter 'b', 'c', etc., as appropriate, is used. Stereochemical configuration at the new carbon skeletal atom is described by methods for specifying additional stereochemistry (see P-101.2.6.1).

Examples:



spirostan (PIN)
(fundamental parent structure)

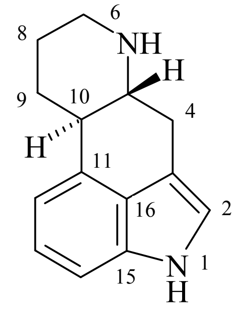


16a,22a-dicarba-5β-spirostan (PIN)

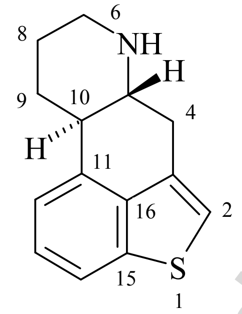
P-101.4.4 Replacement of heteroatoms by other heteroatoms

Replacement of a heteroatom in a stereoparent hydride by another heteroatom is denoted by the appropriate 'a' prefix and locant.

Example:



ergoline (PIN)
(fundamental parent structure)

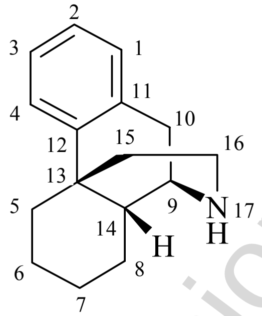


1-thiaergoline (PIN)

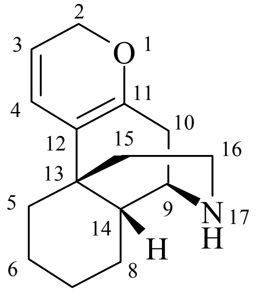
P-101.4.4 Indicated hydrogen

When the replacement of a skeletal atom in a portion of the structure of a parent structure that is mancude (contains the maximum number of noncumulative double bonds) or an extended conjugated system of double bonds results in the creation of a saturated skeletal position, that position is indicated by the symbolism of indicated hydrogen (see P-14.6).

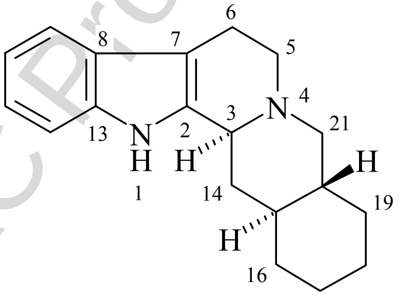
Examples:



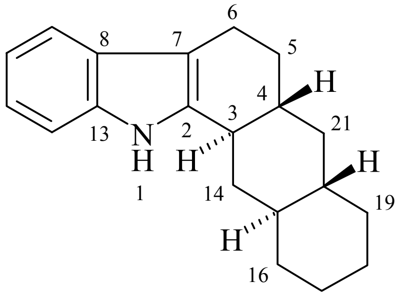
morphinan (PIN)
(fundamental parent structure)



2*H*-1-oxamorphinan (PIN)



yohimban (PIN)
(fundamental parent structure)



(4β*H*)-4-carbayohimban (PIN)

P-101.5. Additional rings and ring systems

Three types of rings and ring systems can be incorporated into parent structures:

P-101.5.1 Mancude rings and ring systems incorporated by fusion nomenclature
P-101.5.2 Rings and ring systems incorporated by bridged fused ring nomenclature
P-101.5.3 Rings and ring systems incorporated by spiro nomenclature

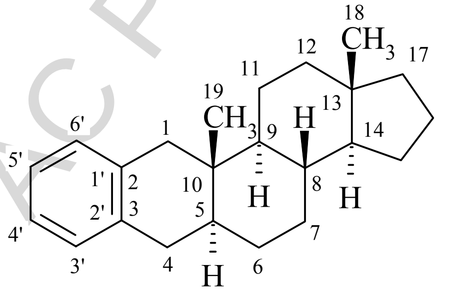
The methods, in certain cases adapted to parent structures, used for the construction of systematic names and described in Chapters 1 to 8 above, are applied.

P-101.5.1 Mancude rings and ring systems incorporated by fusion nomenclature

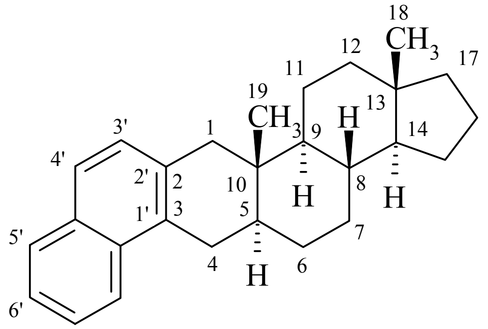
The parent structure as a component is used in fusion nomenclature in its normal state of hydrogenation. Accordingly, a double bond is not cited at the fusion site just because the other component contains the maximum of noncumulative double bonds. Furthermore, contrary to the rules prescribed in P-25, a fundamental parent structure is always chosen as the principal component and the attached component must be a mancude ring or ring system.

P-101.5.1.1 A ring or ring system considered as a mancude parent hydride in accordance with the rules prescribed in Chapter 2, carbocyclic or heterocyclic, fused to a parent structure is described by its fusion prefix name (see P-25) preceding the name of the parent structure. The skeletal atoms of the parent structure involved in the fusion are identified by plain (unprimed) locants and not by italicized letters '*a*', '*b*', etc.; the skeletal atoms of the mancude component, involved in the fusion, are identified by primed locant numbers. The position of the fusion is indicated by a fusion descriptor, including two sets of locants; the first cited set is that of the attached component, the second set relates to the principal component, the fundamental parent structure; the two sets are separated by a colon, enclosed in brackets, and cited between the two components. Where there is a choice, the locant for the mancude attached component are as low as possible and are cited in the same direction of numbering as for the parent structure. Terminal vowels, 'o' or 'a', in the name of the prefix are not elided when followed by a vowel, as prescribed for normal fusion nomenclature in P-25.3.1.2 (this is a change from previous recommendations).

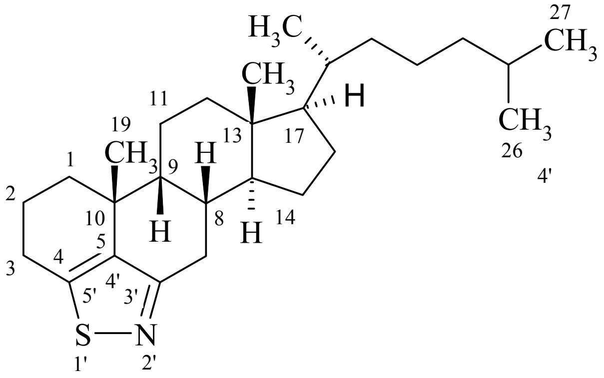
Examples:



benzo[2,3]-5α-androstane (PIN)
(locants 1′,2′ are omitted)



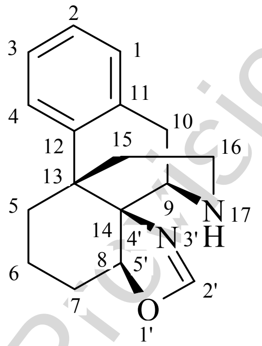
naphtho[2′,1′:2,3]-5α-androstane (PIN)



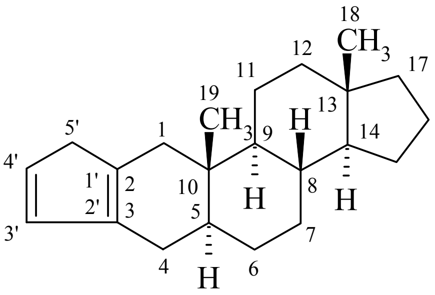
[1,2]thiazolo[5′,4′,3′:4,5,6]cholestane (PIN)
(not isothiazolo[5′,4′,3′:4,5,6]cholestane; the name isothiazole is no longer recommended as a fusion component, see P-25.3.2.1.3)

P-101.5.1.2 The attached component fused to a parent structure is a mancude compound (it contains the maximum number of noncumulative double bonds). Saturated positions on such components, including the fusion sites, that have at least one hydrogen atom are specified by an indicated hydrogen. They are also specified by a descriptor composed of the locant, followed by the configuration descriptor α or β and finally by the indicated hydrogen symbolism (see P-15.6), placed in parentheses at the front of the name as stereodescriptors are. Locants of the attached component are used to identify the position of the indicated hydrogen, but locants (unprimed) of the stereoparent hydride are used, if there is a choice between primed and unprimed locants.

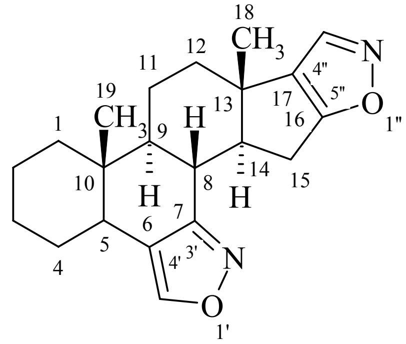
Examples:



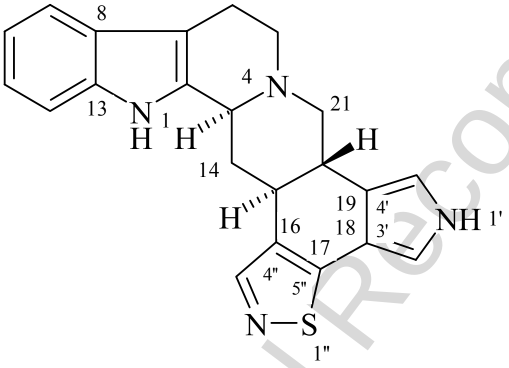
(8α*H*)-[1,3]oxazolo[5′,4′:8,14]morphinan (PIN)
(not 8α*H*-oxazolo[5′,4′:8,14]morphinan; the name oxazole without heteroatom locants is no longer recommended as a fusion component (see P-25.3.2.1.3); an indicated hydrogen atom denoted by the stereodescriptor (8α*H*) is necessary to complete the name)



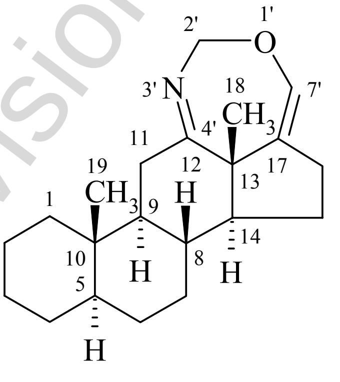
5′*H*-cyclopenta[2,3]-5α-androstane (PIN)



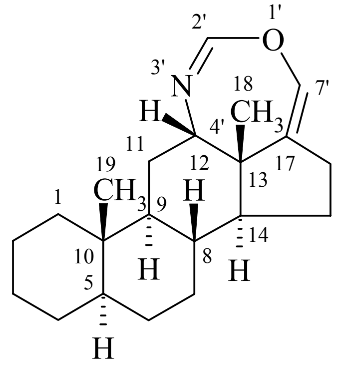
bis[1,2]oxazolo[4′,3′:6,7;5″,4″:16,17]-5α-androstane



1′*H*-pyrrolo[3′,4′:18,19][1,2]thiazolo[4″,5″:16,17]yohimban



2*H*′-[1,3]oxazepino[4′,5′,6′:12,13,17]-5α-androstane (PIN)



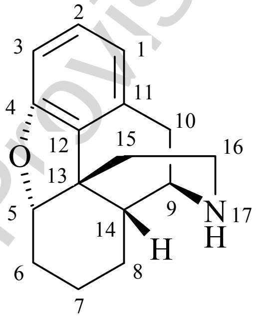
(12β*H*)-12*H*-[1,3]oxazepino[4′,5′,6′:12,13,17]-5α-androstane (PIN)

P-101.5.2 Rings and ring systems incorporated by bridges

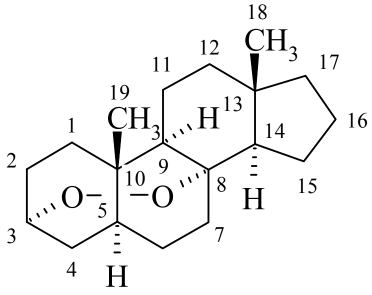
Atomic bridges added to parent structures may be described by the methods used in fusion nomenclature for bridged fused ring systems. The names of the bridges are those prescribed in P-25.4. This method is often used with heteroatom bridges. In fact, this method is often more useful than fusion procedures described in P-101.5.1 for describing certain types of heterocyclic rings fused to a parent structure, for instance 'epoxy' to denote a bridge rather than 'oxireno' to denote the ring fused as an attached component. The use of atomic bridges is preferred to fusion nomenclature to connect two nonadjacent atoms in a fundamental parent structure [epoxides and thioepoxides are exceptions as they can be named substitutively (see P-63.5)]. The prefixes used to denote bridges are nondetachable; they are cited in a name in front of the prefixes used to denote skeletal modifications, preceded by appropriate locants.

When a choice is possible, names formed by using fusion nomenclature are preferred IUPAC names.

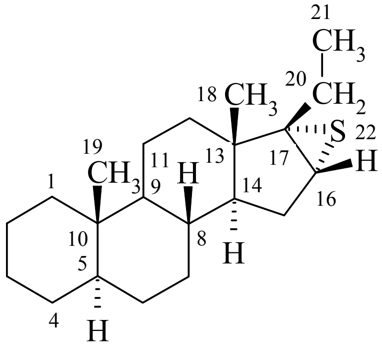
Examples:



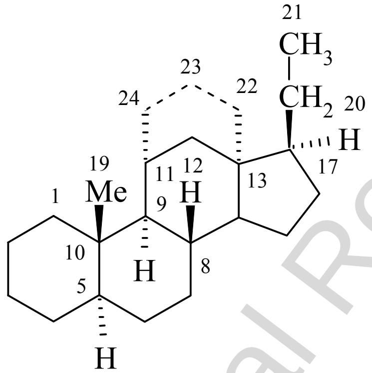
4,5α-epoxymorphinan(PIN)



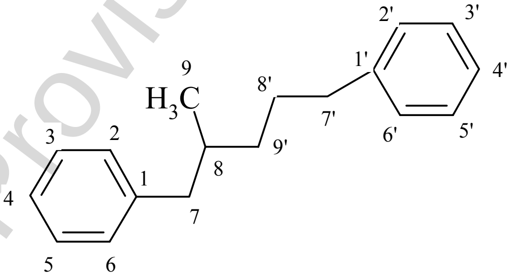
3α,8-epidioxy-5α,8α-androstane (PIN)



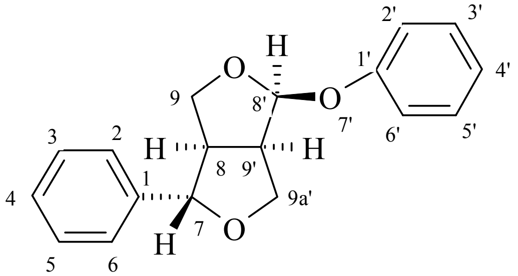
(16β*H*)-thiireno[16,17]-5α-pregnane (PIN, fusion name)
16α,17-epithio-5α-pregnane



11α,13-propano-18-nor-5α,13α-pregnane (PIN)
(not 11β,18-cyclo-12a,12b-dihomo-5α-pregnane;
nor 11α,18b-cyclo-18a,18b-dihomo-5α,13α-pregnane)



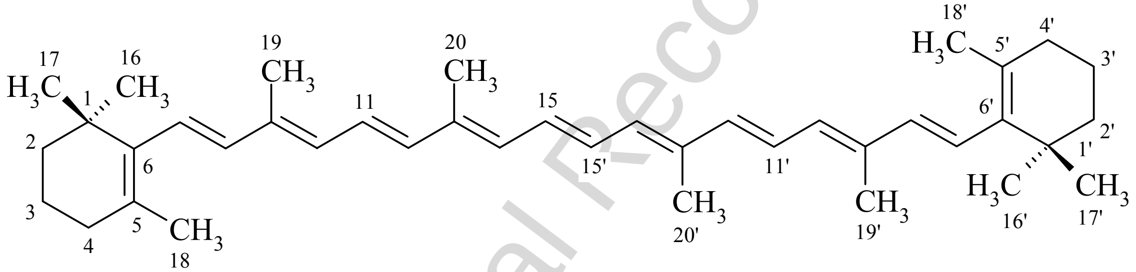
8,9′-neolignan
(fundamental parent structure)



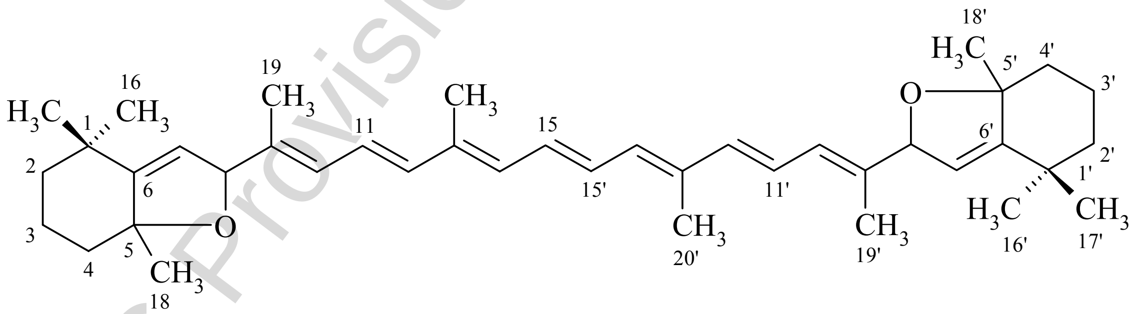
(7α,8α,8′β,9′α)-7,9a′:8′,9-diepoxy-7-oxa-9a′-homo-8,9′-neolignan

Contrary to the recommendations for systematic nomenclature of organic compounds, in carotenoid nomenclature, the bridge named ‘epoxy’ is considered detachable and the hydro/dehydro prefixes nondetachable. The name of the following bridged β,β-carotene is written in conformity with the rules of carotenoid nomenclature (ref. 40, Carotenoid rule 7.3).

Examples:



β,β-carotene (PIN)
(fundamental parent structure)

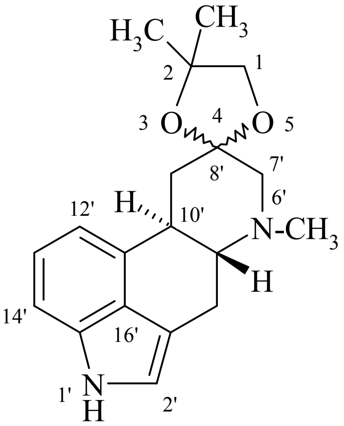


5,8:5′,8′-diepoxy-5,8,5′8′-tetrahydro-β,β-carotene (PIN)

P-101.5.3 Rings and ring systems incorporated by spiro nomenclature

Spiro compounds are named as prescribed in P-24.5 for monospiro compounds having at least one polycyclic component.

Example:



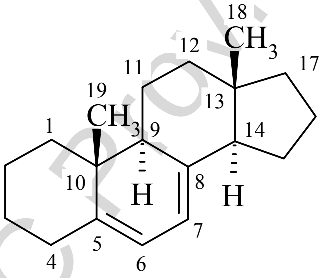
(4ξ)-2,2,6′-trimethylspiro[1,3-dioxolane-4,8′-ergoline] (PIN)

P-101.6 Modification of the degree of hydrogenation

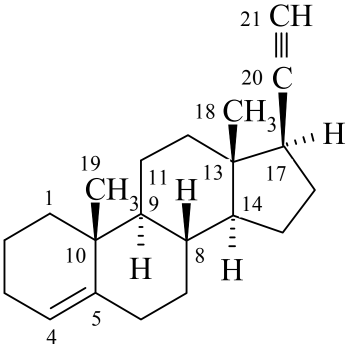
The general principles and rules for modifying the degree of hydrogenation of parent hydrides prescribed in Section P-31 are applied to parent structures. The endings ‘ene’ and ‘yne’ (see P-31.1) and the prefixes ‘hydro’ (see P-31.2) and ‘dehydro’ (see P-31.3) are used, depending on the subtractive or additive operation required.

P-101.6.1 Unsaturation in a compound whose parent structure is fully saturated or in the portion of a parent structure that is otherwise fully saturated and whose name ends in ‘an’, ‘ane’, or ‘anine’ is indicated by changing ‘an’ or ‘ane’ to ‘ene’ or ‘yne’ and by adding numerical mulytiplying prefixes as prescribed in P-31. Locants are placed immediately before the part of the name to which they relate.

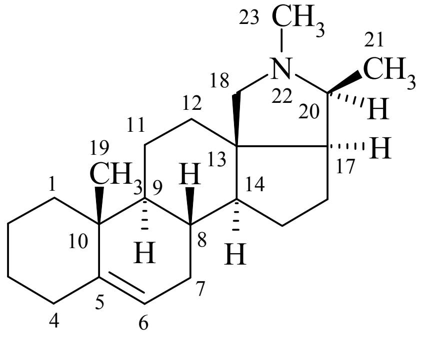
Examples



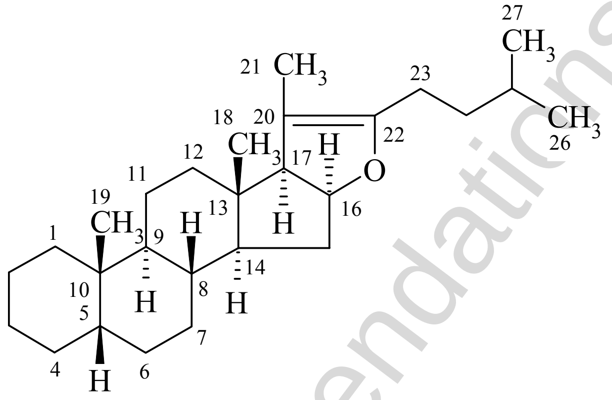
androsta-5,7-diene (PIN)



pregn-4-en-20-yne (PIN)



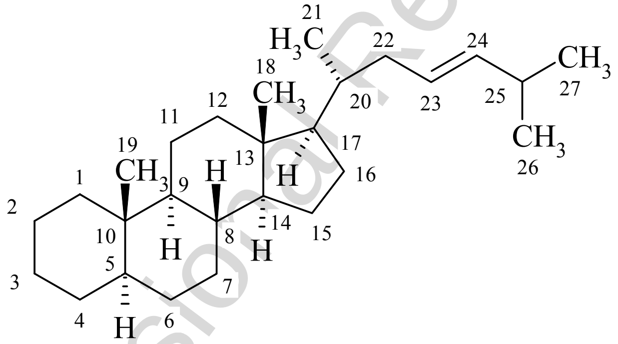
con-5-enine (PIN)



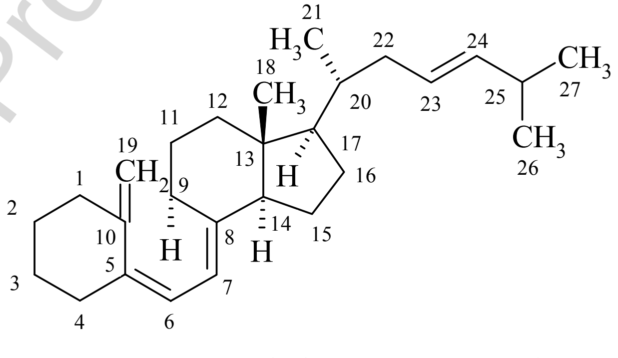
5β-furost-20(22)-ene (PIN)

P-101.6.2 The descriptors '*E*' and '*Z*', preceded by appropriate locants, are used to describe modified or additional stereochemical configurations for double bonds. The stereodescriptors '*cis*' and 'trans' are used in carotenoid nomenclature (ref. 40) and retinoid nomenclature (ref. 48).

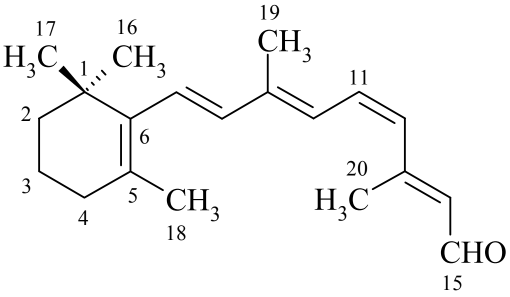
Example:



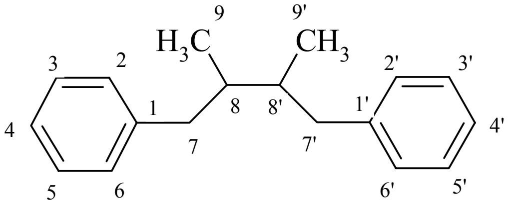
(23*E*)-5α-cholest-23-ene (PIN)



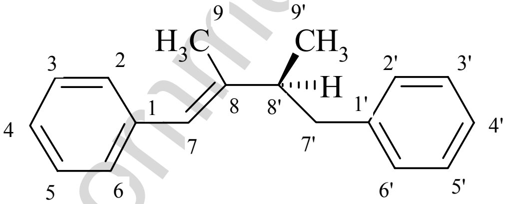
(5*Z*,7*E*)-9,10-secocholesta-5,7,10(19)-triene



11-*cis*-retinal (PIN)



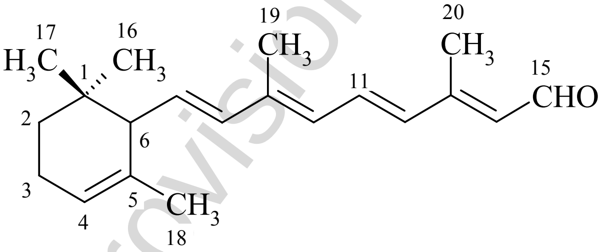
lignan (PIN)
(fundamental parent structure)



(7*E*,8′*S*)-lign-7-ene

P-101.6.3 The prefix *all* is used in front of stereodescriptors to indicate that all configurations are identical. This prefix is used only in the nomenclature of natural products, for example, *all-trans* to denote the fact that in retinal all double bonds are *trans*.

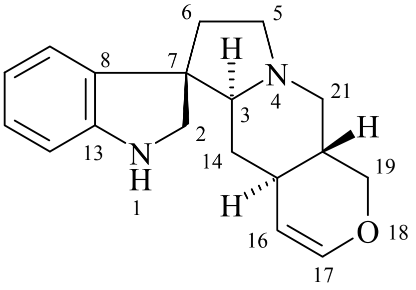
Example:



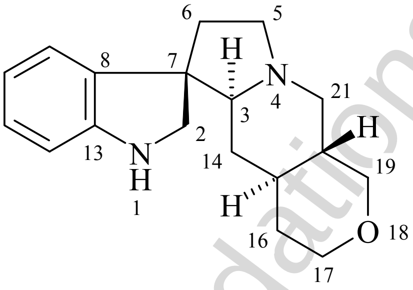
all-trans-retinal (PIN)

P-101.6.4 Saturation of double bonds in a parent structure whose name implies the presence of isolated double bonds and/or systems of conjugated double bonds is described by the prefix ‘hydro’, itself preceded by the locants of the saturated positions. The ‘hydro’ prefix is detachable and always cited immediately in front of the fundamental parent structure (see P-31.2).

Example:



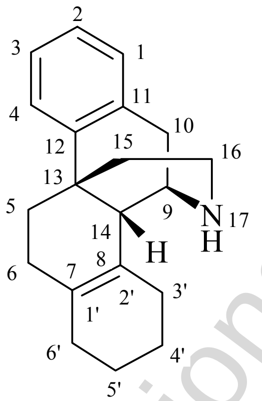
formosanan (PIN)
(fundamental parent structure)



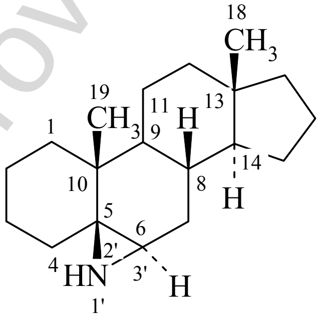
16,17-dihydroformosanan (PIN)

P-101.6.5 Saturated, or partially saturated, carbocyclic and heterocyclic ring components fused to a parent structure are named using ‘hydro’ prefixes. When there is a choice between primed and unprimed locants, the unprimed locants are used.

Examples:



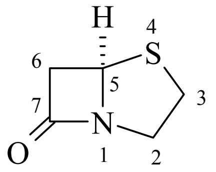
3′,4′,5′,6′-tetrahydrobenzo[7,8]morphinan (PIN)



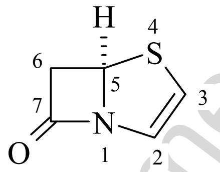
(6α*H*)-1′,6-dihydroazirino[2’,3’:5,6]-5β-androstane (PIN)
(for the symbol (6α*H*), see P-101.5.1.2)

P-101.6.6 The introduction of unsaturation additional to any unsaturation implied in a parent structure whose name does not end in ‘an’, ‘ane’, or ‘anine’, the conversion of an implied double bond into a triple bond, and the introduction of an additional double bond with rearrangement of an implied double bond, are denoted by the prefix ‘dehydro’, itself prefixed by a numerical multiplying term equal to the number of hydrogen atoms removed and the appropriate locants. The ‘dehydro’ prefix is detachable and always cited at the front of the fundamental parent structure, after any detachable alphabetized prefixes, when present.

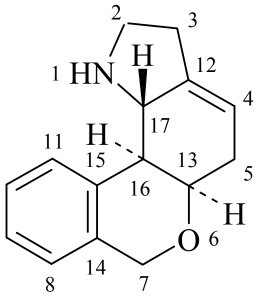
Examples:



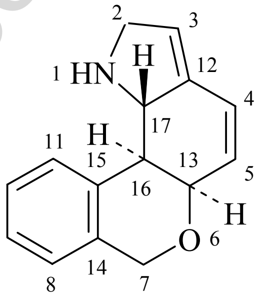
penam (PIN)
(fundamental parent structure)



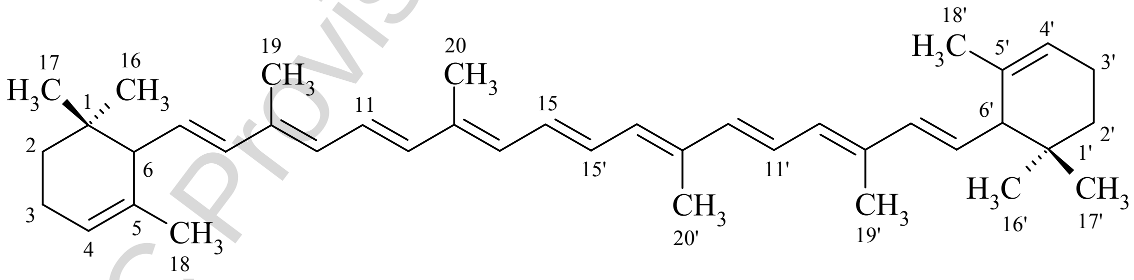
2,3-didehydropenam (PIN)



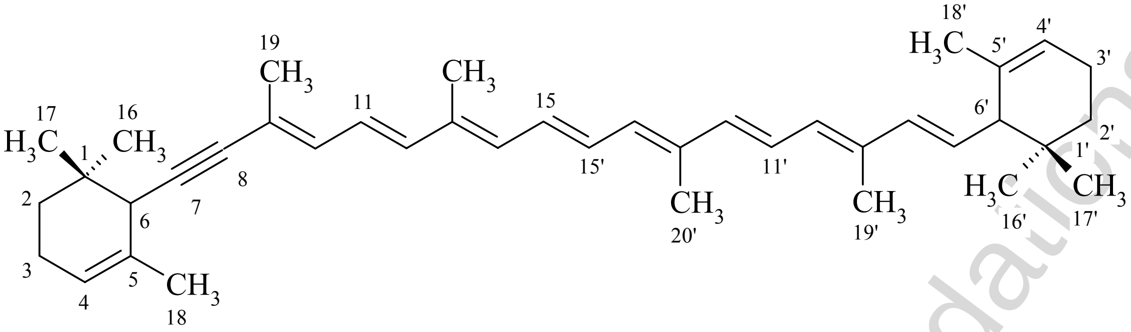
lycorenan (PIN)
(fundamental parent structure)



3,5-didehydrolycorenan (PIN)



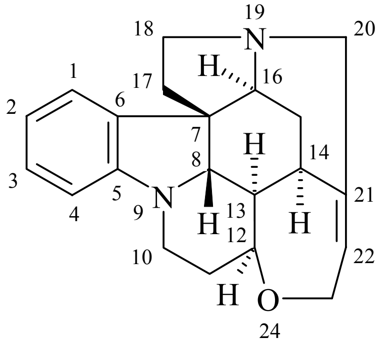
ε,ε-carotene (PIN)
(fundamental parent structure)



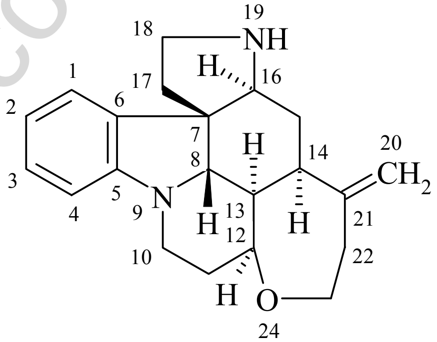
7,8-didehydro-ε,ε-carotene (PIN)

P-101.6.7 Rearrangement of double bonds may be indicated by a combination of 'hydro' and 'dehydro' prefixes. The 'dehydro' prefix is cited before the 'hydro' prefix, in accordance with the alphanumerical order.

Example:



strychnidine (PIN)
(fundamental parent structure)



20,21-didehydro-21,22-dihydro-19,20-secostrychnidine (PIN)

P-101.7 Derivatives of parent structures

Derivatives of parent structures are named according to principles, rules and conventions described in Chapters 1 to 8.

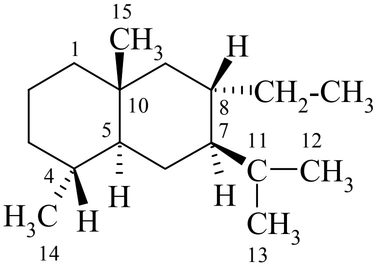
P-101.7.1 The suffixes and prefixes of the nomenclature of organic compounds are used in the prescribed manner to name atoms and groups that are considered to substitute for hydrogen atoms of parent structures. Preferred IUPAC names are based on the largest unmodified fundamental parent structures when a choice is possible. The stereodescriptors α, β and ξ are used to describe the configuration; they are cited in front of the prefix or suffix, preceded by the appropriate locant. Substitutive names so constructed are preferred to those that are formed by functional class nomenclature, except for some cyclic functional classes.

Substitution on rings and substitution on terminal segments are considered separately.

P-101.7.1.1 Substitution by alkyl groups

Organyl groups such as aryl groups and alkyl groups are introduced by substitutive nomenclature. This rule is implemented to introduce a methyl group in androstane in position 17β; the alternative method of subtracting a methylene group by using the nondetachable prefix ‘nor’ is not recommended.

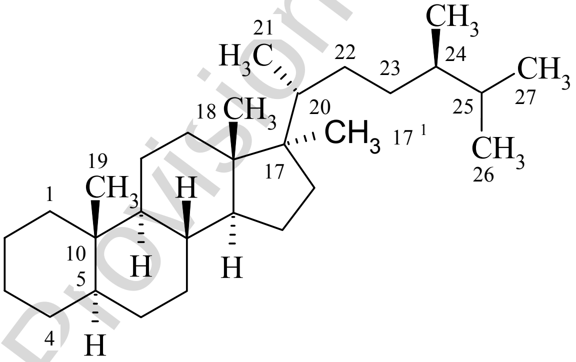
Example:



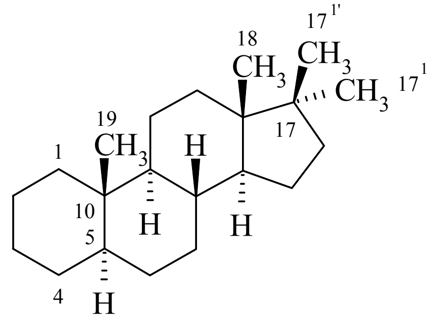
8α-ethyl-5α-eudesmane (PIN)

Rule 3S-2.7 in ref. 39 describes the methodology to name steroids with a side chain as part of the parent carbocycle and an alkyl substituent at C-17. Rule 3S-2.7 also describes the methodology to name steroids with two alkyl substituents at C-17. This methodology is applicable to any fundamental parent structure described in Section P-101.. Locants with superscript numbers are intended for the identification of the atoms, e.g. in ^{13}C-nmr assignments, not as locants for further substitution.

Examples:



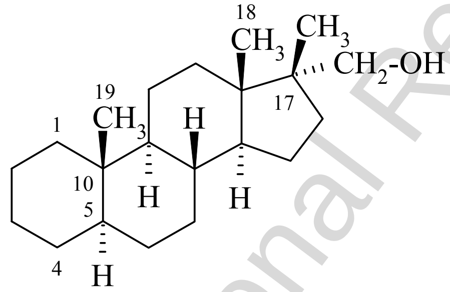
17-methyl-5α-campestane (PIN)
(the additional methyl group in position 17 is numbered 17^1;
other atoms are numbered as usual)



17,17-dimethyl-5α-androstane (PIN)
(both additional methyl groups are numbererd 17^1;
the β-methyl group is primed)

The principles, rules and conventions of substitutive nomenclature are used when a characteristic group cited as a suffix is present on an alkyl substituent group added to a fundamental parent structure.

Example:

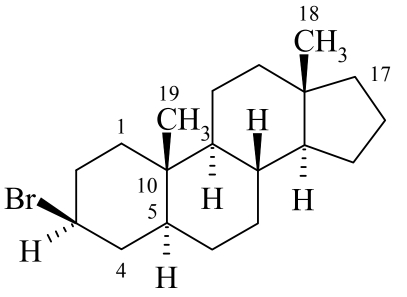


(17β-methyl-5α-androstan-17α-yl)methanol (PIN)
(not 21-nor-5α-pregnane)

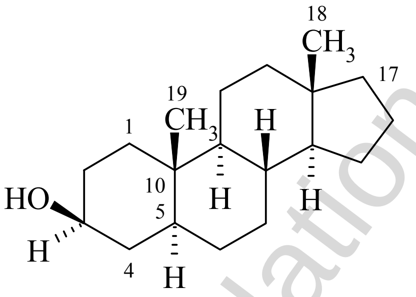
P-101.7.1.2 Substitution on rings

Suffixes are used in accordance with the seniority order of suffixes, considering the cyclic nature of the parent hydride. Detachable prefixes are cited in alphanumerical order. The endings ‘ene’ and ‘yne’ are cited in the normal way; the ‘hydro-dehydro’ prefixes are detachable but cited last among detachable prefixes.

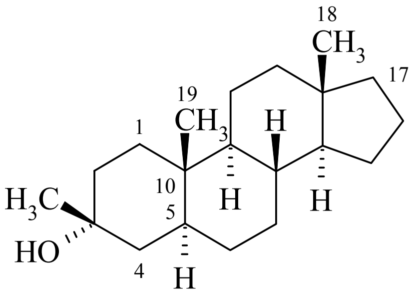
Examples:



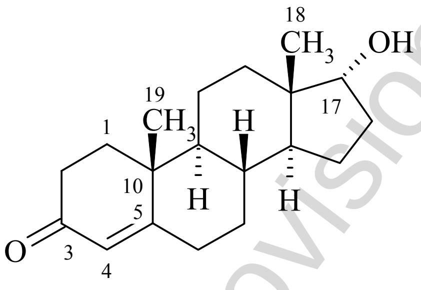
3β-bromo-5α-androstane (PIN)
5α-androstan-3β-yl bromide



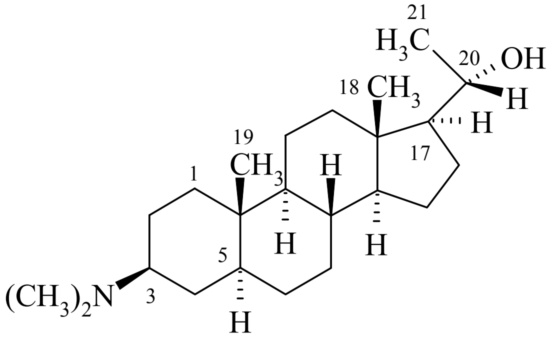
5β-androstan-3β-ol (PIN)



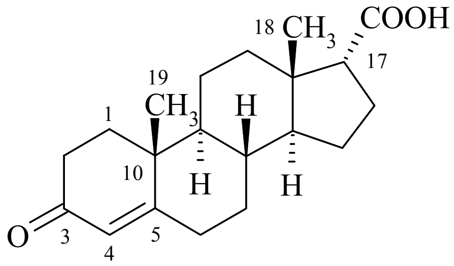
3β-methyl-5α-androstan-3α-ol (PIN)



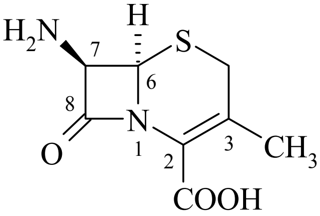
17α-hydroxyandrost-4-en-3-one (PIN)



(20*S*)-3β-(dimethylamino)-5α-pregnan-20-ol (PIN)



3-oxoandrost-4-ene-17α-carboxylic acid (PIN)
(not 21-nor-5α-pregnane-20-oic acid; the preferred name involves the fewest number of operations, see 101.3.7.1)

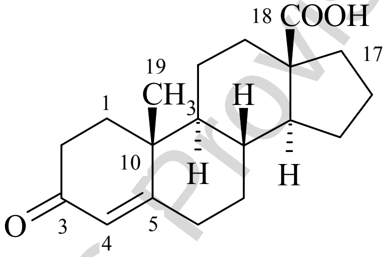


7β-amino-3-methyl-2,3-didehydrocepham-2-carboxylic acid (PIN)

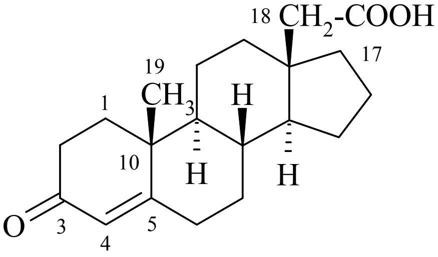
P-101.7.1.3 Substitution on terminal segments

Substitution on terminal segments by prefixes and suffixes expressing characteristic groups is recommended, even when a carbon atom included in a characteristic group is present. Lengthening a terminal segment by the addition of two methylene groups is allowed and denoted by the use of the prefix 'dihomo'. Further lengthening is possible, but alkyl groups must be used, as an exception to the rule related to seniority of the longest chain.

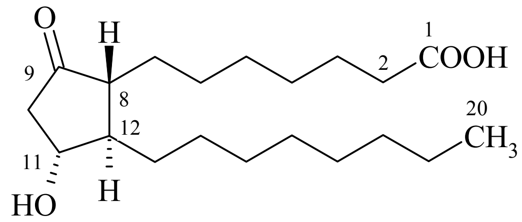
Examples:



3-oxoandrost-4-en-18-oic acid (PIN)



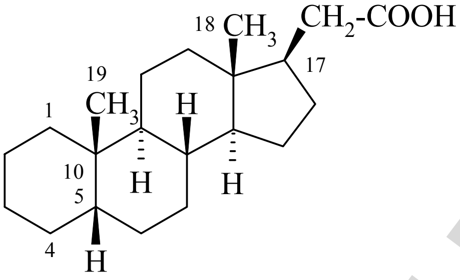
3-oxoandrost-4-ene-18-carboxylic acid (PIN)



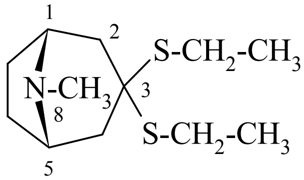
11α-hydroxy-9-oxoprostan-1-oic acid (PIN)

P-101.7.2 Modifications to principal characteristic groups such as esters (see P-65.4.3.2), acetals (see P-66.6.5), etc. are named by the usual methods described in Chapter 6. Cyclic modifications, such as lactones, cyclic acetals, etc. are named preferably as such rather than as fused or spiro ring systems, even if these names are functional class names (see also P-101.7.4).

Examples:



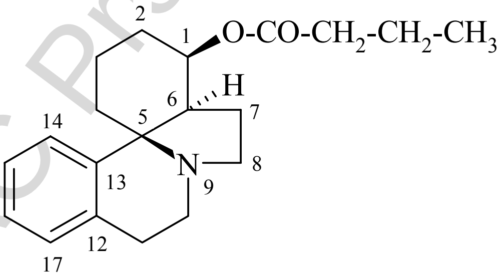
methyl 5β-androstane-17β-carboxylate (PIN)



3,3-bis(ethylsulfanyl)tropane (PIN)
tropan-3-one diethyl dithioketal

P-101.7.3 Names of substituent groups derived from parent stereoparent hydride structures are formed, by the general method described in P-29, by adding the suffixes ‘yl’, ‘ylidene’, or ‘ylidyne’, as appropriate, to the name of a parent, with elision of the final letter ‘e’, if present, before the letter ‘y’.

Example:

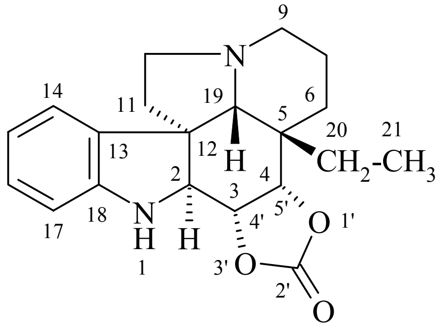


erythrinan-1β-yl butanoate (PIN)

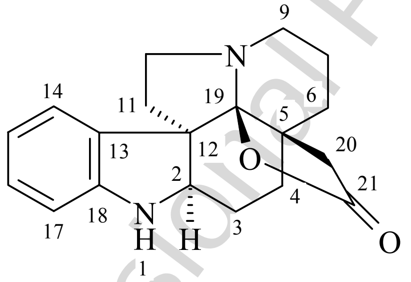
P-101.7.4 Addition of rings denoting functional groups

Rings denoting functional groups are preferably named by the usual methods described for constructing systematic names. Cyclic esters and lactones are named by the general method described for naming esters (see P-65.4.3.2). Names of acetals are formed by using the principles of functional class nomenclature (see P-66.6.5) rather than by fusion nomenclature described in P-101.5. When a choice is possible, a fusion name is preferred.

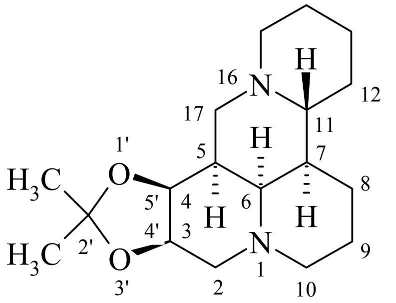
Examples:



(3β*H*,4β*H*)-3,4-dihydro[1,3]dioxolo[4′,5′-3,4]aspidospermidin-2′-one (PIN)
[not aspidospermidine-3α,4α-diyl carbonate(see P-65.4.3.2.6)]



21-noraspidospermidine-20,19-carbolactone (PIN, see P-65.4.3.4.1)
19-hydroxyaspidospermidine-21,19-lactone



(3α*H*,4α*H*)-2,2′-dimethyl-3,4-dihydro[1,3]dioxolo[4′,5′-3,4]matridine (PIN)
[not propan-2-one matridine-3β,4β-diyl acetal (see P-66.6.5)]
acetone matridine-3β,4β-diyl acetal

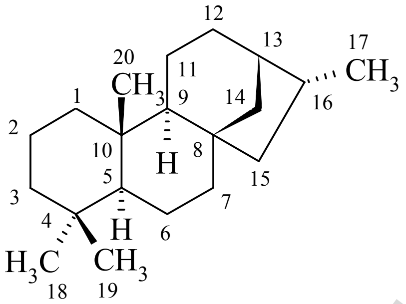
P-101.8. Further aspects of configuration specification

In addition to the specification of the absolute configuration of fundamental and modified parent structures using 'α', 'β', 'ξ', '*R*' and '*S*' stereodescriptors, many other stereochemical features have to be described. The principles, rules and conventions described in Chapter 9 are applied.

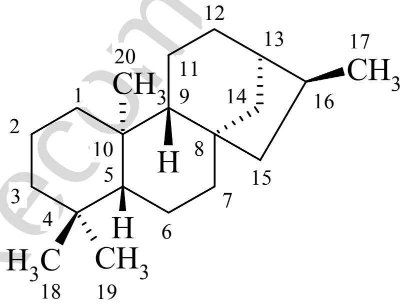
P-101.8.1 Inversion of configuration

Configurational inversion of all chirality centers is indicated by the italicized prefix '*ent*' (a contracted form for '*enantio*') placed at the front of the complete name of the compound. This prefix denotes inversion at all chirality centers (including those due to named substituents) whether these are cited separately or are implied in the name.

Example:



kaurane (PIN)



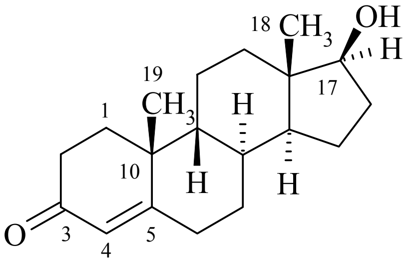
ent-kaurane (PIN)

P-101.8.2 Racemates

Racemates are named by citing the italicized stereodescriptor '*rac*' (an abbreviation for *racemo*) in front of the whole name of the compound including the prefix '*epi*', if present. In the case of a racemic compound, the enantiomeric structure drawn should be that one that shows the lowest numbered chirality center in the α-configuration. This may differ from the usual practice, which is to draw the enantiomeric structure having the same absolute configuration as the naturally occurring substance.

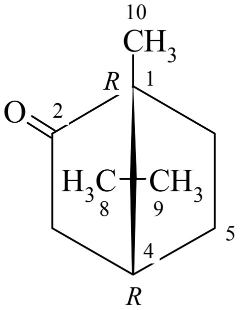
P-101.8.3 Relative configuration

When the relative, but not the absolute configurational relationships among chirality centers are known, the symbols '*R**' and/or '*S**' are used in accordance with Rule P-93.2. Alternatively, enantiomers of known relative, but unknown absolute configuration may be distinguished by the compound stereodescriptor (+)-*rel*- or (-)-*rel*-, where the plus and minus sign refer to the direction of rotation of polarized light at the sodium D line. Hence, the dextrorotatory form of the following structure would be named (+)-*rel*-17β-hydroxy-8α,9β-androst-4-en-3-one.

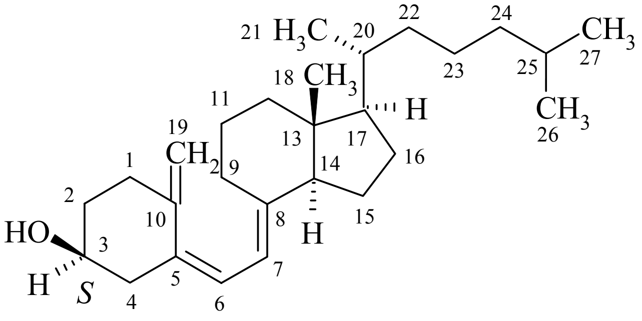


P-101.8.4 The stereodescriptors '*R*' and '*S*' are used to describe the absolute configuration of sterogenic centers for a compound whose parent structure is achiral, for example bornane. They are also used, in place of 'α', 'β', 'ξ', when a ring is opened creating two chiral portions one of which may rotate, as shown for vitamin D.

Example:

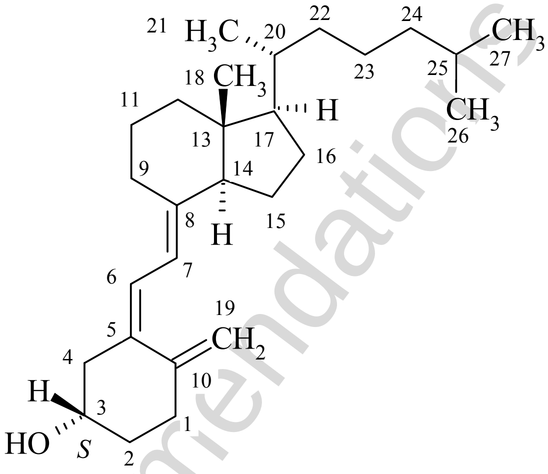


(1*R*,4*R*)-bornan-2-one
(+)-camphor
(1*R*,4*R*)-1,7,7-trimethylbicyclo[2.2.1]heptane-2-one (PIN)



(I)

≡



(II)

(3*S*,5*Z*,7*E*)-9,10-secocholesta-5,7,10(19)-trien-3-ol
(structures (I) and (II) are two conformations of the same
3-hydroxy derivative)

P-102 Nomenclature of carbohydrates

P-102.0 Introduction

Nomenclature of carbohydrates is based on the concept of parent monosaccharides having retained names that are preferred IUPAC names. These structures and names can be modified to indicate the nature of characteristic groups that are present, such as aldehydes, carboxylic acids, alcohols. They can also be combined to form di-, tri- and oligosaccharides.

The nomenclature has been recently revised (ref. 22). This Section describes the basic concepts of this specific type of nomenclature, in particular the extensive system of symbols and stereodescriptors to indicate the configuration of the many diastereoisomers and enantiomers.

P-102.1 Definitions
P-102.2 Parent monosaccharides
P-102.3 Configurational symbolism
P-102.4 Choice of a parent structure
P-102.5 Monosaccharides: aldoses and ketoses; deoxy and amino sugars
P-102.6 Monosaccharide derivatives
P-102.7 Disaccharides and oligosaccharides

P-102.1 Definitions

P-102.1.1 Carbohydrates

The generic term ‘carbohydrates’ includes monosaccharides, oligosaccharides and polysaccharides as well as substances derived from monosaccharides by reduction of the carbonyl group (alditols), by oxidation of one or more terminal groups to carboxylic acids, or by replacement of one or more hydroxy group(s) by a hydrogen atom, an amino group, a thiol group or similar heteroatomic groups. It also includes derivatives of these compounds. The term ‘sugar’ is frequently applied to monosaccharides and lower oligosaccharides.

Cyclitols are generally not regarded as carbohydrates. For the nomenclature of cyclitols, see P-104 and ref. 44.

P-102.1.2 Monosaccharides

Parent monosaccharides are polyhydroxy aldehydes H-[CHOH]$_n$-CHO or polyhydroxy ketones H-[CHOH]$_m$-CO[(CHOH]$_n$-H with three or more carbon atoms.

The generic term ‘monosaccharide’ (as opposed to oligosaccharide or polysaccharide) denotes a single unit without glycosidic connections to other such units. It includes aldoses, dialdoses, aldoketoses, ketoses, diketoses, as well as deoxy sugars and amino sugars, and their derivatives, provided that the parent compound has a (potential) carbonyl group.

P-102.1.2.1 Aldoses and ketoses

Monosaccharides with an aldehydic carbonyl or potential aldehydic carbonyl group are called aldoses; those with a ketonic carbonyl or potential carbonyl group are called ketoses.

The term ‘potential aldehydic group’ refers to the hemiacetal group arising from ring closure; the term ‘potential ketonic group’ refers to the hemiketal structure.

Cyclic hemiacetals or hemiketals of sugars with a five-membered ring (oxolane or tetrahydrofuran) ring are called ‘furanoses’, those with a six-membered ring (oxane or tetrahydropyran) ring ‘pyranoses’.

Dialdoses are monosaccharides containing two (potential) aldehydic groups.

Diketoses are monosaccharides containing two (potential) ketonic groups.

Ketoaldoses are monosaccharides containing one (potential) aldehydic group and one potential ketonic group; this term is preferred to the terms ‘aldoketoses’ and ‘aldosuloses’.

P-102.1.2.2 Deoxy sugars

Monosaccharides in which an alcoholic hydroxyl group has been replaced by a hydrogen atom are called ‘deoxy sugars’.

P-102.1.2.3 Amino sugars

Monosaccharides in which an alcoholic hydroxyl group has been replaced by an amino group are called ‘amino sugars’. When the hemiacetal group is replaced by an amino group, the compounds are called ‘glycosylamines’.

P-102.1.2.4 Glycosides

Glycosides are mixed acetals formally arising by elimination of water between the hemiacetal or hemiketal hydroxyl group of a sugar and a hydroxyl group of a second compound. The bond between the two components is called a ‘glycosidic bond’.

P-102.1.3 Oligosaccharides

Oligosaccharides are compounds in which monosaccharides units are joined by glycosidic linkages. According to the number of units, they are called disaccharides, trisaccharides, etc. The maximum number of units is not defined.

P-102.1.4 Polysaccharides

‘Polysaccharide’ (glycan) is the name given to a macromolecule consisting of a large number of monosaccharide (glycose) residues joined to each other by glycosidic linkages. The term ‘poly(glycose)’ is not a synonym for polysaccharide (glycan), because it includes monosaccharide residues joined to each other by nonglycoisidic linkages.

P-102.1.5 Preferred IUPAC names

Names of carbohydrates are either trivial or systematic. Many trivial names such as glucose, fructose, etc. are retained and used to describe the corresponding functional parents. This aspect of carbohydrate nomenclature is limited because it applies only to monosaccharides having four to six carbon atoms. A systematic carbohydrate nomenclature has been developed that is applicable to compounds with four or more carbon atoms, and is used extensively by carbohydrate chemists for compounds with more than six carbon atoms, and for unsaturated and branched sugars. Names generated by applying systematic nomenclature are called ‘systematic carbohydrate names’. Preferred IUPAC names are either retained names, unmodified or modified, or names generated in accordance with the principles, rules and conventions of substitutive nomenclature developed in Chapters 1 to 8. These systematically formed names are called ‘substitutive names’ or ‘systematic substitutive names’ to differentiate them from ‘systematic carbohydrate names. The system of preferred IUPAC names is based on the following criteria.

(1) retained names used in carbohydrate nomenclature and systematic substitutive names are selected as preferred IUPAC names. Systematic carbohydrate names may be used in general nomenclature.

(2) preferred IUPAC names for aldoses and ketoses with 4-6 carbon atoms are retained names; the following modifications also generate preferred IUPAC names:

(a) open-chain and ring forms

(b) alditols, aldonic acids, ketoaldonic acids, uronic acids, and aldaric acids

(c) *O*-substitution by alkyl, aryl, carboxylic acyl group prefixes

(d) glycosides and glycosyl substituent prefixes

(e) glycosyl halides and pseudohalides

(f) glycose phosphates and sulfates and other phosphorus or sulfur oxoacid esters

(g) deoxy compounds at the terminal CH_2OH position

(h) halo, halogenoid, and other permanent prefixes plus deoxy at the same position

(i) amino plus deoxy at the same position (*N*-substitution is allowed)

(j) replacement of oxygen atoms by other chalcogen atoms

(k) di- and oligosaccharides

(3) Preferred IUPAC names not generated according to (1) and (2) above are constructed as systematic substitutive names, for example:

(a) aldoses/ketoses having more than six carbon atoms

(b) deoxy at a chiral center (except as in (2)(i), above)

(c) *C*-substitution

(d) anhydro derivatives

(e) unsaturated derivatives

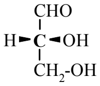
P-102.2 Parent structures and preferred IUPAC names

P-102.2.1 The bases for preferred IUPAC names are the structures of the parent monosaccharides in their acyclic form. Tables 10.2 and 10.3 give retained names for parent aldoses and ketoses with up to six carbon atoms. These retained names are used as preferred IUPAC names when the acyclic aldose or ketose has a carbon chain consisting of 4, 5 or 6 carbon atoms. Preferred IUPAC names of monosaccharides whose carbon skeleton is composed of more than 6 carbon atoms are systematic substitutive names.

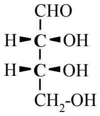
In Table 10.2 structures and retained names of the aldoses (in the aldehydic, acyclic form) with three to six carbon atoms are described. Only the D-forms are shown; the L-forms are the mirror images.

In Table 10.3 structures and retained names of the ketoses (in the ketonic, acyclic form) with three to six carbon atoms are described. Only the D-forms are shown; the L-forms are the mirror images.

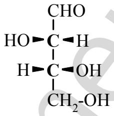
Table 10.2 Retained names (with recommended three-letter abbreviations in parentheses) and structures (in the aldehydic acyclic form) of the aldoses with three to six carbon atoms



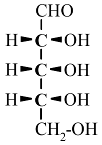
(*R*)-2,3-dihydroxypropanal (PIN)
D-glyceraldehyde
D-*glycero*



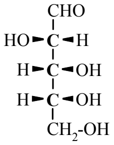
D-erythrose (PIN)
D-*erythro*



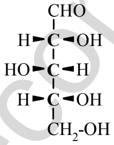
D-threose (PIN)
D-*threo*



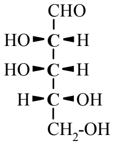
D-ribose (PIN)
D-*ribo*



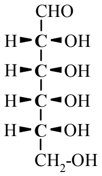
D-arabinose (PIN)
D-*arabino*



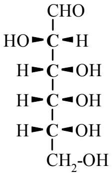
D-xylose (PIN)
D-*xylo*



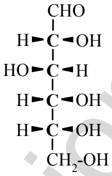
D-lyxose (PIN)
D-*lyxo*



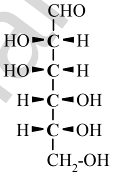
D-allose (PIN)
D-*allo*



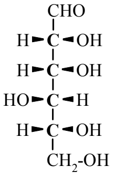
D-altrose (PIN)
D-*altro*



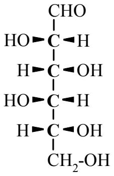
D-glucose (PIN)
D-*gluco*



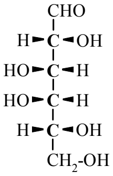
D-mannose (PIN)
D-*manno*



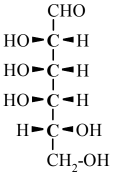
D-gulose (PIN)
D-*gulo*



D-idose (PIN)
D-*ido*

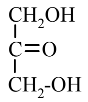


D-galactose (PIN)
D-*galacto*

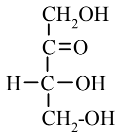


D-talose (PIN)
D-*talo*

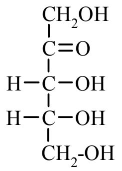
Table 10.3 Structures, with systematic and trivial names, of the 2-ketoses with three to six carbon atoms



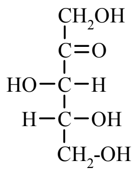
1,3-dihydroxypropan-2-one (PIN)
1,3-dihydroxyacetone
glycerone



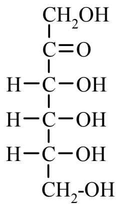
D-erythrulose (PIN)



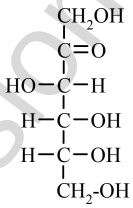
D-ribulose (PIN)



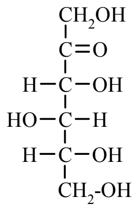
D-xylulose (PIN)



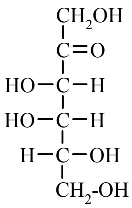
D-psicose (PIN)
D-*ribo*-hex-2-ulose



D-fructose (PIN)
D-*arabino*-hex-2-ulose



D-sorbose (PIN)
D-*xylo*-hex-2-ulose



D-tagatose (PIN)
D-*lyxo*-hex-2-ulose

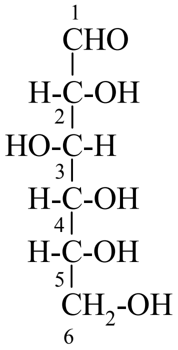
P-102.2.2 Numbering parent structures

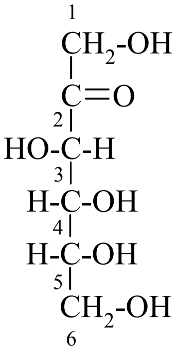
The carbon atoms of a monosaccharide are numbered consecutively in such a way that:

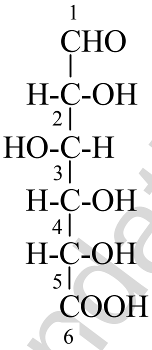
(1) a (potential) aldehyde group receives the locant 1 (even if a more senior function is present);

(2) the most senior of other functional groups expressed in the suffix receives the lowest possible locant, i.e carboxylic acid (derivatives) > (potential) ketonic carbonyl groups.

Examples:


D-glucose (PIN)

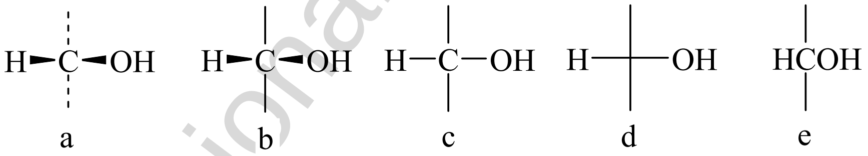

D-fructose (PIN)


D-glucuronic acid (PIN)

P-102.3 Configurational symbolism

P-102.3.1 The Fischer projection of the acyclic form

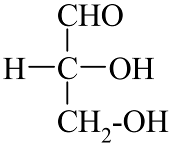
In this representation of a monosaccharide, the carbon chain is written vertically with the lowest numbered carbon at the top, as indicated in P-102.2.2. To define the configuration, each carbon atom is considered in turn and placed in the plane of the paper. Neighboring carbon atoms are below, and the H atoms and OH groups are above the plane of the paper. Various representations ‘b, c, d, e, and f’ of a carbon atom in a monosaccharide in the Fischer projection are as follows (structure ‘a’ is a tridimensional representation; the real Fischer projection is ‘d’); representation ‘e’ is commonly used in this Section:

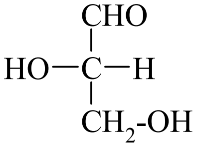


P-102.3.2 The stereodescriptors ‘D’ and ‘L’

The simplest aldose is glyceraldehyde. It contains one center of chirality and occurs therefore in two enantiomeric forms, called D-glyceraldehyde and L-glyceraldehyde; these are represented by the Fischer projection formulas given below. It is known that these projections correspond to the absolute configurations. The configurational stereodescriptors ‘D’ and ‘L’ must be written in small capital letters and linked by a hyphen to the name of the sugar.

Preferred IUPAC names are systematic substitutive names; the configuration is described by the preferred CIP stereodescriptors ‘*R*’ and ‘*S*’.

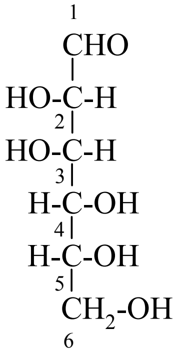

D-glyceraldehyde
(*R*)-2,3-dihydroxypropanal (PIN)


L-glyceraldehyde
(*S*)-2,3-dihydroxypropanal (PIN)

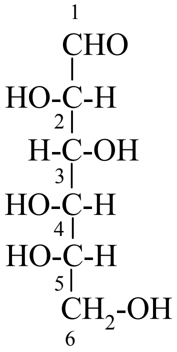
P-102.3.3 The configurational atom

A monosaccharide is assigned to the ‘D’ or ‘L’ series according to the configuration of the highest numbered center of chirality. This asymmetrically substituted carbon atom is called the ‘configurational atom’. Thus, if the hydroxy group projects to the right in the Fischer projection, the sugar belongs to the D-series, and receives the ‘D’ stereodescriptor.

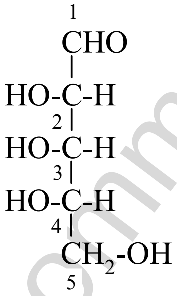
Examples:



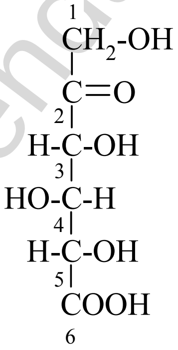
D-mannose (PIN)



L-glucose (PIN)



L-ribose (PIN)



D-sorbose (PIN)

P-102.3.4 Cyclic forms of monosaccharides

Most monosaccharides exist as cyclic hemiacetals or hemiketals. Two aspects of the internal cyclisation must be examined, first, the size of the ring, and secondly, the conformation of the newly created center of chirality.

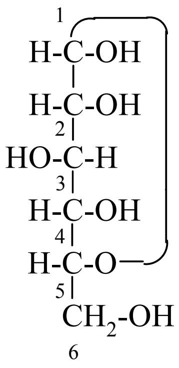
P-102.3.4.1 Ring size

Out of the various possible heterocyclic ring sizes resulting from hemiacetal or hemiketal formation, those with five and six members, including an oxygen atom, prevail and are discussed in this Section. Their names are based on those of the parent heterocycles furan and pyran, respectively. Names are formed by including the terms ‘furan’ and ‘pyran’ before the ending ‘ose’ in the name of a sugar. For example, D-mannose is changed to D-mannopyranose to indicate the cyclic form having a six-membered ring; furthermore, the generic term ‘pyranose’ includes all the sugars having a six-membered ring structure. Similarly, the sugars having a five-membered ring structure are ‘furanoses’; oxiroses, oxetoses and septanoses have a three-, four- or seven-membered cyclic structure, respectively.

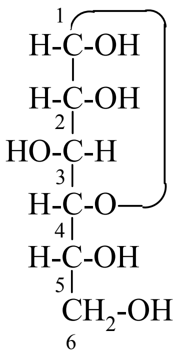
Different representations of cyclic forms are to be considered.

P-102.3.4.1.1 Hemiacetal or hemiketal formation is indicated in the Fischer projection of the cyclic form by a long bond joining the original aldehydic or ketonic group to the oxygen atom included in the ring.

Examples:



D-glucopyranose (PIN)



D-glucofuranose (PIN)

P-102.3.4.1.2 The Haworth representation

The Haworth representation is a perspective drawing. The ring is orientated almost perpendicular to the plane of the paper, but viewed from slightly above so that the edge closer to the viewer is drawn below the most distant edge, with the oxygen behind and C-1 at the right hand end. The cyclisation process is envisaged as proceeding stepwise, as exemplified for D-glucopyranose in Fig. 1, below. Two reorientations are necessary from the standard Fischer projection to prepare the acetalization or ketalization procedure; the first reorientation, step (a), consists in placing the nonterminal hydroxy groups vertically; the second one, step (c), is the reorientation of carbon C-5 to place the oxygen atom in the plane of the ring. The mode of cyclisation must be defined completely by expressing the configuration at carbon ‘1’.

P-102.3.4.2 Anomeric forms; use of stereodescriptors ‘α’ and ‘β’

P-102.3.4.2.1 In the cyclic form, the configuration of the newly created center of chirality C-1 must be expressed. This center is called the ‘anomeric center’. The two stereosiomers are called ‘anomers’; they are designated by the stereodescriptors ‘α’ and ‘β’ according to the configurational relationship between the anomeric center and the so called ‘reference center’.

P-102.3.4.2.2 Configurations ‘α’ and ‘β’ for monosaccharides

The anomeric reference center in a monosaccharide having a retained name is the configurational atom as defined in P-103.3.3. In the α-anomer, the exocyclic oxygen atom at the anomeric center is formally ‘*cis*’, in the Fischer projection, to the oxygen atom attached to the anomeric reference atom; in the β-anomer, the relationship is ‘*trans*’. The reference plane for determining the configurations ‘*cis*’ and ‘*trans*’ is perpendicular to the Fischer projection, including all carbon atoms of the monosaccharide.

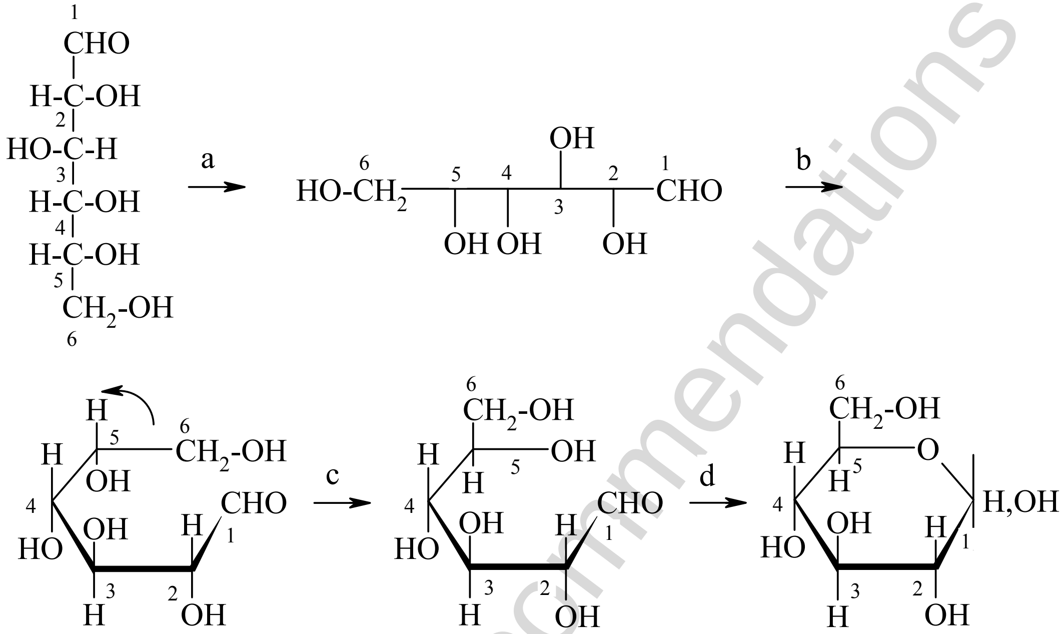
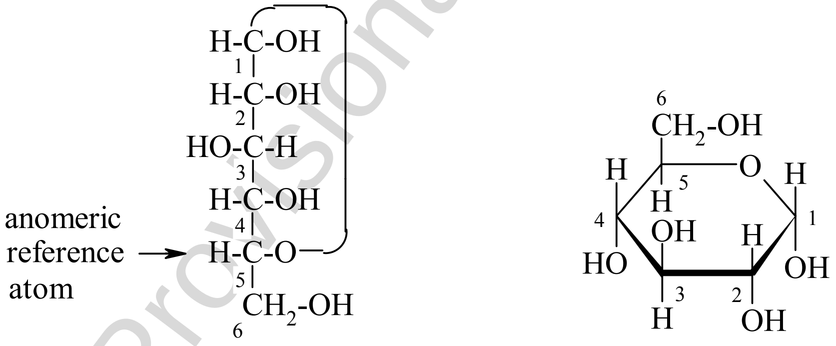


Fig. 1. Reorientation of Fischer projection to Haworth representation

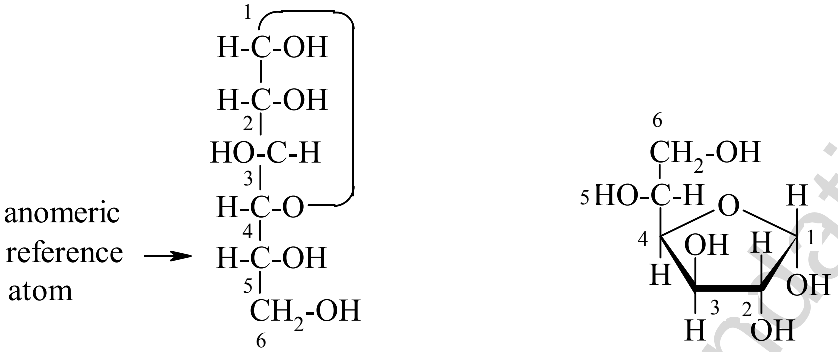
The anomeric stereodescriptor ‘α’ or ‘β’, followed by a hyphen, is placed immediately before the configurational stereodescriptor ‘D’ or ‘L’ of the retained name.

Examples:

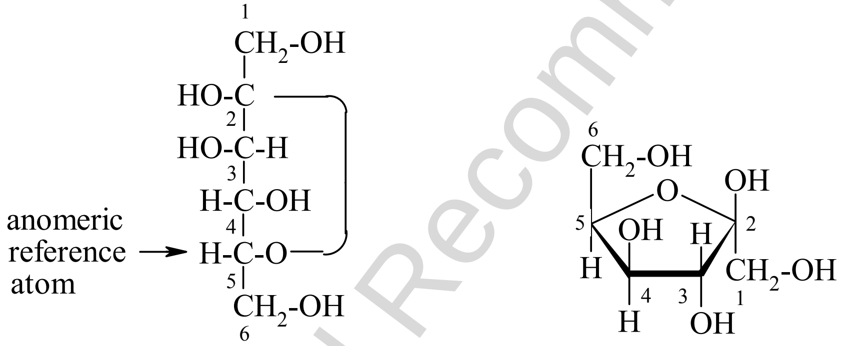


anomeric reference atom

α-D-glucopyranose (PIN)



α-D-glucofuranose (PIN)

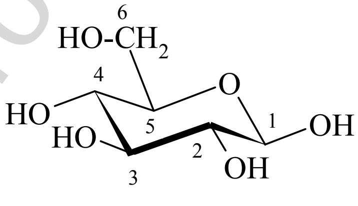


β-D-fructofuranose (PIN)

P-102.3.5 Conformation of monosaccharides

Pyranoses assume conformations that are not planar. For example β-D-glucopyranose assumes a chair conformation with characteristic substituent groups in equatorial conformation (hydrogen atoms are not shown):

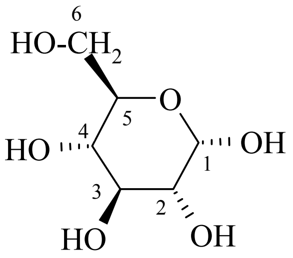
Example:



P-102.3.6 The Mills depiction

In this depiction, the main hemiacetal ring is drawn in the plane of the paper. Hashed wedges denote substituents below this plane, and solid wedges those above.

Example:



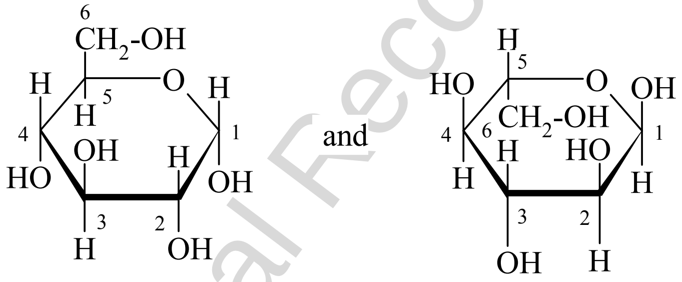
α-D-glucopyranose (PIN)

P-102.3.7 Stereodescriptors for denoting racemates and uncertain configurations

P-102.3.7.1 Stereodescriptors for denoting racemates

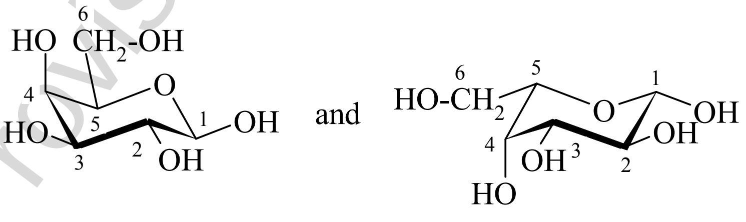
Racemates are indicated by the stereodescriptor ‘DL’.

Examples:



D-configuration L-configuration

α- DL-glucopyranose (PIN)



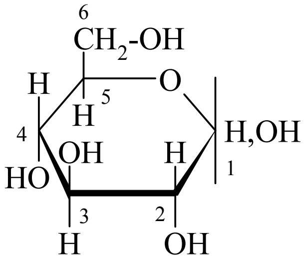
D-configuration L-configuration

β- DL-galactopyranose (PIN)

P-102.3.7.2 Mixtures of anomers

When a mixture of anomers has to be described, the stereodescriptors ‘α’ and ‘β’ are placed at the front of the name; in Haworth representations, the symbols H and OH replace the formal bonds at the anomeric carbon atom.

Examples:



α,β-D-glucopyranose (PIN)

P-102.4 Choice of parent structure

In cases where more than one monosaccharide structure is embedded in a large molecule, a parent structure is chosen on the basis of the following criteria, applied in the order given until a decision is reached:

(a) the parent that includes the functional group most senior in the order of classes (see P-42). If there is a choice, it is made on the basis of the greatest number of occurrences of the most senior functional group. Thus aldaric acid > uronic acid/ketoaldonic acid/aldonic acid > dialdose > ketoaldose/aldose > diketose > ketose;

(b) the parent with the greatest number of carbon atoms in the chain, e.g. heptose rather than hexose;

(c) the parent with the name that comes first in an alphabetical listing based on the following:

(i) the trivial name or the configurational prefix(es) of the systematic name, e.g., glucose (PIN) rather than gulose; a '*gluco*' rather than a '*gulo*' derivative;

Example: D-glucitol (PIN) rather than L-gulitol (see P-102.5.5.5.1);

(ii) the configurational symbol D rather than L;

Example: 5-*O*-methyl- D-galactitol (PIN) rather than 2-*O*-methyl- L-galactitol (see P-102.5.5.5.2);

(iii) the anomeric stereodescriptor α rather than β;

Example: α-D-fructofuranose β-D-fructofuranose 1,2′:1′,2-dianhydride (PIN) and not β-D-fructofuranose α-D-fructofuranose 1,2′:1′,2-dianhydride (see P-102.5.5.7.2).

(d) the parent with the most substituent groups cited as prefixes (bridging substitution, for example 2,3-*O*-methylene is regarded as multiple substitution for this purpose); the prefixes 'deoxy' and 'anhydro' are detachable and alphabetized, thus regarded as substituent groups;

(e) the parent with the lowest locants for substituent prefixes;

Example: 2,3,5-tri-*O*-methyl-D-mannitol (PIN) rather than 2,4,5-tri-*O*-methyl-D-mannitol [see P-102.5.5.5.3(a)]

(f) the parent with the lowest locant for the first cited substuent.

Example: 2-*O*-acetyl-5-*O*-methyl-D-mannitol (PIN) rather than 5-*O*-acetyl-2-*O*-methyl-D-mannitol [see P-102.5.5.5.3 (b)].

P-102.5 Monosaccharides

P-102.5.1 Aldoses

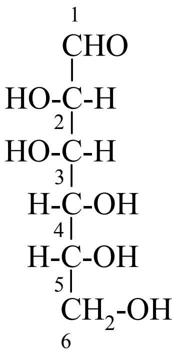
Names of aldoses are retained or substitutively formed. Retained names for aldoses with three to six carbon atoms are listed in Table 10.2. Except for glyceraldehyde, they are preferred IUPAC names. Names of aldoses having more than six carbon atoms are formed in two ways: by the procedures of systematic carbohydrate nomenclature, and by those of systematic substitutive nomenclature. Systematic substitutive names are preferred IUPAC names.

P-102.5.1.1 Systematic carbohydrate names

Systematic carbohydrate names of aldoses are formed from a stem name and a configurational prefix or prefixes. Stem names for the aldoses with three to ten carbon atoms are triose, tetrose, pentose, hexose, heptose, octose, nonose, and decose. The chain is numbered so that the carbonyl group receives the locant ‘1’.

P-102.5.1.1.1 The configuration of >CH-OH groups of the sugar is designated by the configurational prefix(es) listed in Table 10.2., such as ‘*glycero*’, ‘*gluco*’, ‘*manno*’, etc. Each name is qualified by a ‘D’ or ‘L’ stereodescriptor, as defined in P-102.3.2.

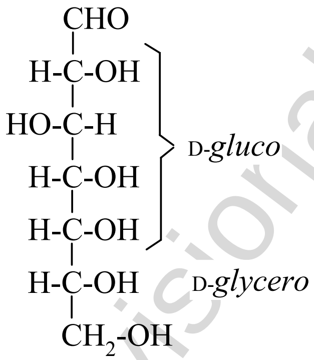
Example:



D-*manno*-hexose (systematic carbohydrate name)
D-mannose (PIN)

P-102.5.1.1.2 Aldoses composed of more than four chiral centers are named by adding two or more configurational prefixes (listed in Table 10.2) to the stem name. Prefixes are assigned in order to the chiral centers in groups of four, beginning with the group located next to the aldehydic group. The prefix relating to the group of carbon atoms farthest from the aldehydic group (which may contain fewer than four chiral centers) is cited first. These names are for use only in general nomenclature.

Examples:

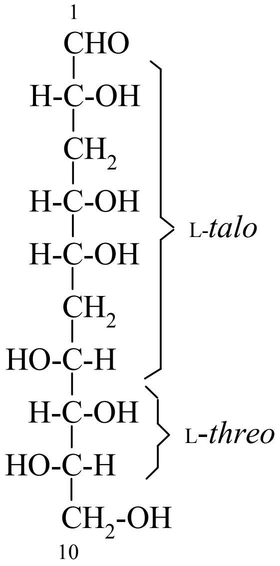


D-*glycero*- D-*gluco*-heptose
(not D-*gluco*- D-*glycero*-heptose)
(2*R*,3*S*,4*R*,5*R*,6*R*)-2,3,4,5,6-hexahydroxyheptanal (PIN)

P-102.5.1.1.3

When sequences of chiral centers are separated by nonchiral centers, the nonchiral centers are ignored, and the remaining set of chiral centers is assigned the appropriate configurational prefix (for four centers or less) or prefixes (for more than four centers).

Example:

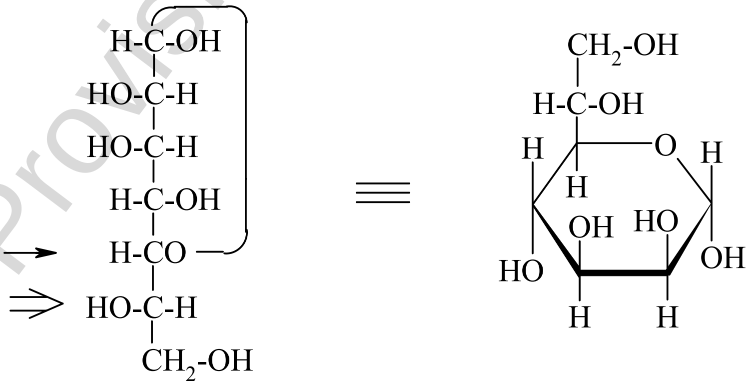


3,6-dideoxy-L-*threo*-L-*talo*-decose
(for deoxy sugars, see P-102.4.3)
(2*R*,4*S*,5*R*,7*R*,8*S*,9*S*)-2,4,5,7,8,9,10-heptahydroxydecanal (PIN)

P-102.5.1.1.4 Cyclic forms

For monosaccharides having more than six carbon atoms, the anomeric reference center is the highest numbered atom of the group of chiral centers next to the anomeric center that is involved in the heterocyclic ring and specified by a single configurational prefix. In the α-anomer, the exocyclic oxygen atom at the anomeric center is formally ‘*cis*’, in the Fischer projection, to the oxygen atom attached to the anomeric reference atom; in the β-anomer these oxygen atoms are formally ‘*trans*’.

Example:



→ denotes the anomeric reference atom; ⇒ denotes the configurational atom

L-*glycero*-α-D-*manno*-heptopyranose
(2*S*,3*S*,4*S*,5S,6*R*)-6-[(1*S*)-1,2-dihydroxyethyl]oxane-2,3,4,5-tetrol (PIN)

P-102.5.2 Ketoses

P-102.5.2.1 Classification

Ketoses are classified as 2-ketoses, 3-ketoses, etc. according to the lowest locant for the position of the (potential) carbonyl group.

P-102.5.2.2 Retained names

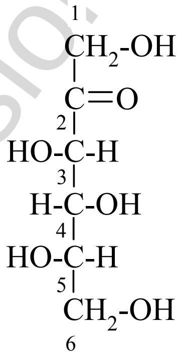
Retained names and structures are shown in Table 10.3. The retained names erythrulose, ribulose, xylulose, psicose, fructose, sorbose and tagatose are preferred IUPAC names for the 2-ketoses with four to six carbon atoms. Preferred IUPAC names for ketoses with more than six carbon atoms are formed by systematic substitutive nomenclature, the configuration being designated by the appropriate CIP stereodescriptors ‘*R*’, ‘*S*’, ‘*r*’*, etc.*

P-102.5.2.3 Systematic carbohydrate names

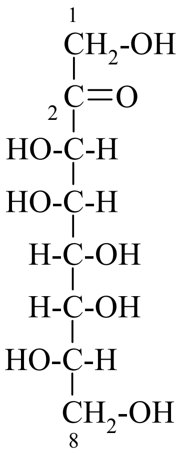
The systematic carbohydrate names of ketoses having four to six carbon atoms are formed from the stem name and the appropriate configurational prefix listed in Table 10.3. The stem names are formed from the corresponding aldoses stem names by replacing the ending ‘ose’ with ‘ulose’, preceded by the locant of the carbonyl group, e.g. ‘pent-2-ulose’ and ‘hex-3-ulose’. The chain is numbered so that the carbonyl group receives the lowest possible locant. When the carbonyl group is in the middle of a chain with an odd number of carbon atoms, a choice between alternative names is made according to alphanumerical order.

For 2-ketoses, configurational prefixes are given in the same way as for aldoses. Retained names are preferred IUPAC names. Systematic carbohydrate names for 3-ketoses and ketoses with more than six carbon atoms are used only in general nomenclature. Preferred IUPAC names are systematic substitutive names.

Examples:



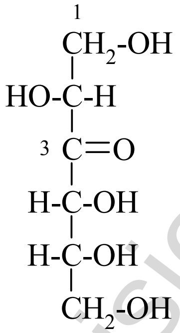
L-*xylo*-hex-2-ulose
L-sorbose (PIN)



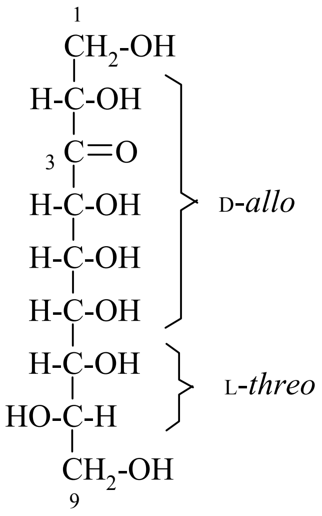
L-*glycero*-D-*manno*-oct-2-ulose
(3*S*,4*S*,5*R*,6*R*,7*S*)-1,3,4,5,6,7,8-heptahydroxyoctan-2-one (PIN)

For ketoses with the carbonyl group at C-3, or at a higher-numbered carbon atom, the carbonyl group is ignored and the set of chiral centers is given the appropriate prefix or prefixes according to Table 10.3.

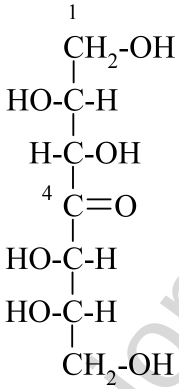
Examples:



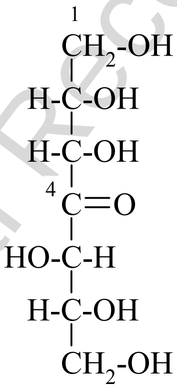
D-*arabino*-hex-3-ulose
(2*R*,4*R*,5*R*)-1,2,4,5,6-pentahydroxyhexan-3-one (PIN)



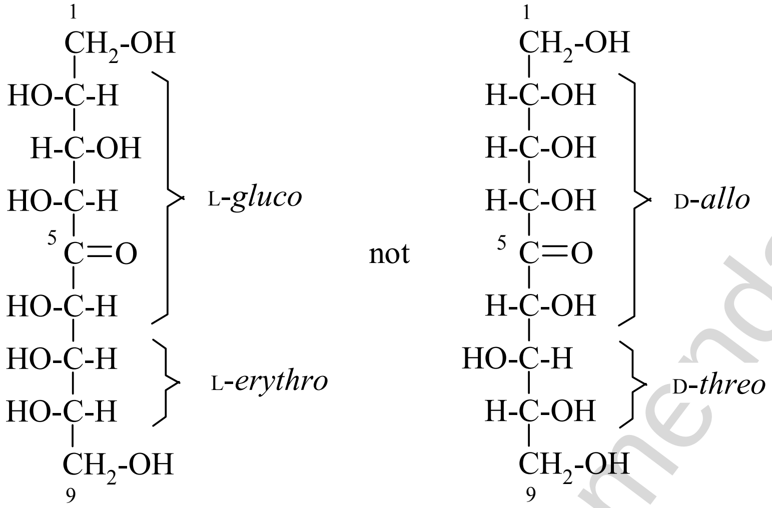
L-*threo*-D-*allo*-non-3-ulose
(2*S*,4*R*,5*R*,6*R*,7*R*,8*S*)-1,2,4,5,6,7,8-heptahydroxynonan-3-one



not



L-*gluco*-hept-4-ulose
(not D-*gulo*-hept-4-ulose; *gluco* is first in
alphanumerical order see P-102.)
(2*R*,3*S*,5*S*,6*S*)-1,2,3,5,6,7-hexahydroxyheptan-4-one (PIN)
(not (2*S*,3*S*,5*S*,6*R*)-1,2,3,5,6,7-hexahydroxyheptan-4-one)
(when there is a choice, the *R* configuration is assigned to the lowest locant)



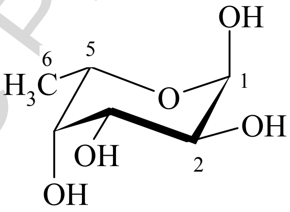
L-*erythro*-L-*gluco*-non-5-ulose
(not D-*threo*-D-*allo*-non-5-ulose; *erythro*-*gluco* is first in alphanumerical order)
(2*R*,3*S*,4*R*,6*S*,7*S*,8*S*)-1,2,3,4,6,7,8,9-octahydroxynonan-5-one (PIN)

P-102.5.3 Deoxy sugars

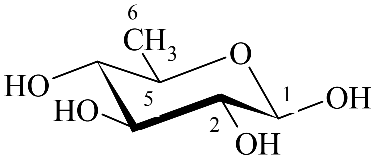
P-102.5.3.1 The prefix ‘deoxy’ means the removal of an ‘oxy’ group, –O–, with rejoining of the hydrogen atom. In these recommendations, the prefix ‘deoxy’ is classified as detachable; i.e., it is alphabetized among the substituents arising from substitutive nomenclature. This is a change from the previous status (see R-0.1.8.4, ref. 2) that classified the prefix ‘deoxy’ among nondetachable prefixes (see also the prefix ‘anhydro, that is now classified as detachable and alphabetized among all detachable prefixes).

P-102.5.3.2 Trivial names.

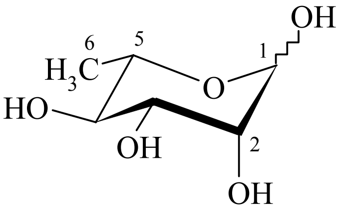
The following names are retained: fucose, quinovose and rhamnose. The corresponding structures are shown in the pyranose form. These names are used as preferred IUPAC names for the unmodified sugars. Systematic substitutive names are preferred IUPAC names for the formation of names of derivatives.



α-L-fucopyranose (PIN)
6-deoxy-α-L-galactopyranose



β-D-quinovopyranose (PIN)
6-deoxy-β-D-glucopyranose



L-rhamnopyranose (PIN)
6-deoxy-L-mannopyranose

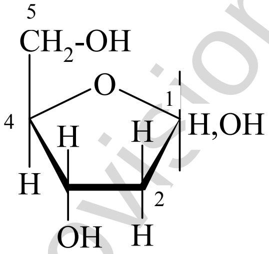
P-102.5.3.3 Carbohydrate names derived from retained names

Use of the prefix ‘deoxy’ in combination with a retained name other than glucose, mannose and galactose gives preferred IUPAC names when the deoxygenation does not involve the configuration at any chirality center, for example, 6-deoxy-D-allose. When the prefix ‘deoxy’ modifies a chirality center, a carbohydrate name is appropriate, but preferred IUPAC names are formed by substitutive nomenclature with CIP stereodescriptors (see P-102.5.3.4 for examples). As an exception, the combination of ‘amino’ and ‘dexoy at the same position is allowed in preferred IUPAC names.

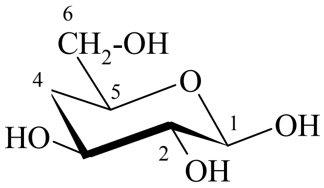
P-102.5.3.4 Systematic carbohydrate names

The systematic carbohydrate name consists of the prefix ‘deoxy’, preceded by the appropriate locant and followed by the stem name with such configurational prefixes as necessary to describe the chirality centers present in the deoxy compound. Configurational prefixes are cited in order commencing at the end furthest from C-1.

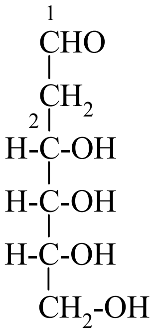
Examples:



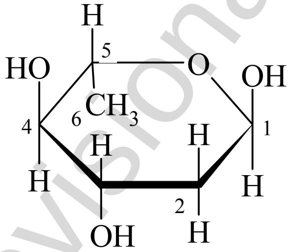
2-deoxy-D-*erythro*-pentofuranose
(often referred to as 2-deoxy-D-ribose)
(2*R*,3*S*,5ξ)-5-(hydroxymethyl)oxolane-3,5-diol (PIN)



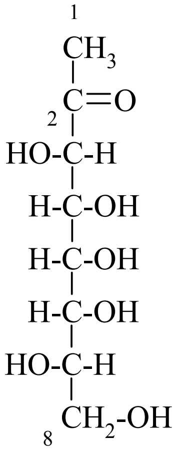
4-deoxy-β-D-*xylo*-hexopyranose
(not 4-deoxy-β-D-galactopyranose)
(2*R*,3*R*,4*S*,6*S*)-6-(hydroxymethyl)oxane-2,3,4-triol (PIN)



2-deoxy-D-*ribo*-hexose
(not 2-deoxy-D-allose)
(3*S*,4*S*,5*R*)-3,4,5,6-tetrahydroxyhexanal (PIN)



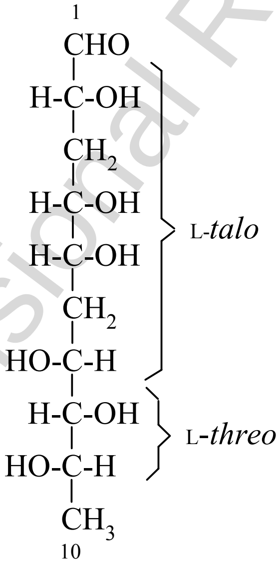
2,6-dideoxy-α-L-*arabino*-hexopyranose
(2*R*,4S,5*R*,6*S*)-6-methyloxane-2,4,5-triol (PIN)



1-deoxy-L-*glycero*-D-*altro*-oct-2-ulose
(3*S*,4*R*,5*R*,6*R*,7*S*)-3,4,5,6,7,8-hexahydroxyoctan-2-one (PIN)

When the –CH$_2$– group divides the chirality centers into two sets, it is ignored for the purpose of assigning the configurational prefix; the prefix(es) assigned should cover the entire sequence of chirality centers (see aldoses) (see P-102.5.1.1.3).

Example:



3,6,10-trideoxy-L-*threo*-L-*talo*-decose
(2*R*,4*S*,5*R*,7*R*,8*R*,9*S*)-2,4,5,7,8,9,10-heptahydroxydecanal (PIN)

P-102.5.4 Amino sugars and thiosugars and other chalcogen analogues

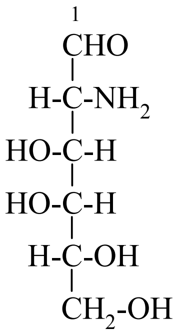
The replacement of a hydroxy group that is not an anomeric hydroxy group of a monosaccharide or a monosaccharide derivative by an amino group is envisaged as substitution of the appropriate hydrogen atom of the corresponding deoxy monosaccharide by an amino group. The configuration at the carbon atom carrying the amino group is expressed as that of an aldose, considering that the amino group has replaced a hydroxy group.

To the contrary, the replacement of a hydroxy group by a sulfanyl group is considered to be a functional replacement indicated by the prefix 'thio'.

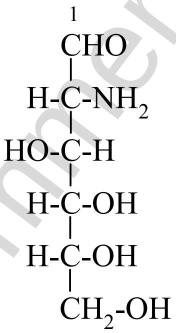
P-102.5.4.1 Amino sugars

P-102.5.4.1.1 Trivial names

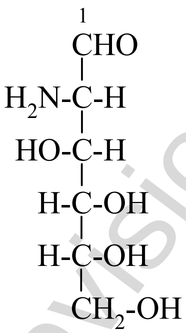
The following glycosamine names are retained but preferred IUPAC names are based on aldose names with amino and deoxy prefixes.



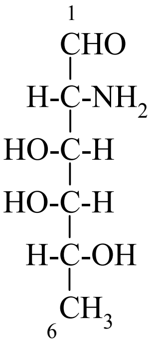
D-galactosamine
2-amino-2-deoxy-D-galactose (PIN)



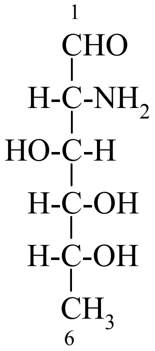
D-glucosamine
2-amino-2-deoxy-D-glucose (PIN)



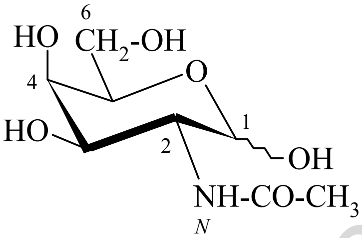
D-mannosamine
2-amino-2-deoxy-D-mannose (PIN)



D-fucosamine
2-amino-2,6-dideoxy-D-galactose (PIN)



D-quinovosamine
2-amino-2,6-dideoxy-D-glucose (PIN)

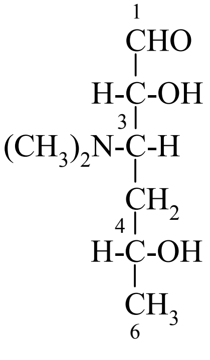


N-acetyl-D-galactosamine
N-acetamido-2-deoxy-D-galactopyranose (PIN)

P-102.5.4.1.2 Systematic carbohydrate names

Systematic carbohydrate names are formed, in two steps: in a first step a deoxy sugar is created by deoxygenation at the carbon atom where the amino group is to be introduced by substitution in a second step. Names of substituted amines are formed by using the name of the substituted amino group as a prefix.

Example:



3,4,6-trideoxy-3-(dimethylamino)-D-*xylo*-hexose
(2*R*,3*S*,5*R*)-3-(dimethylamino)-2,5-dihydroxyhexanal (PIN)

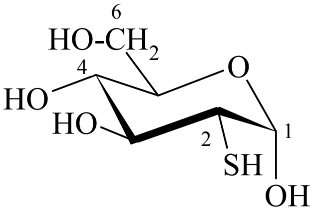
P-102.5.5 Thio sugars and other chalcogen analogues

The replacement of a hydroxy oxygen atom of an aldose or ketose, or of the oxygen atom of the carbonyl group of an acyclic aldose or ketose, by sulfur, selenium or tellurium is indicated by placing the prefix ‘thio’, ‘seleno’ or ‘telluro’, respectively, preceded by the appropriate locant, at the front of the systematic or trivial name of the aldose or ketose. In carbohydrate nomenclature, the prefixes ‘thio’, ‘seleno’ and ‘telluro’ are considered as detachable, alphabetized prefixes.

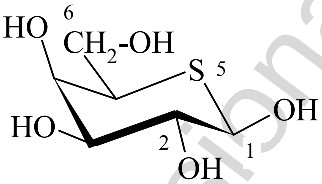
Replacement of the ring oxygen atom of the cyclic form of an aldose or ketose by sulfur, selenium, or tellurium is indicated in the same way, the number of the nonanomeric adjacent carbon atom of the ring being used as locant. In such a case, skeletal replacement expressed by ‘a’ replacement prefixes is not recommended.

Sulfoxides (and selenoxides or telluroxides) and sulfones (and selenones or tellurones) are named by functional class nomenclature (see P-63.6 for functional class names of sulfoxides and sulfones).

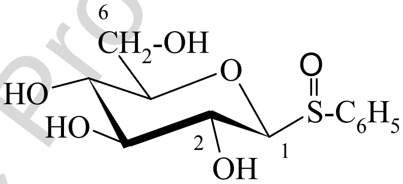
Examples:



2-thio-α-D-glucopyranose (PIN)



5-thio-β-D-galactopyranose (PIN)



β-D-glucopyranosyl phenyl sulfoxide
(for glycosyl groups, see P-102.6.1.1)
(2*S*,3*R*,4*S*,5*S*,6*R*)-2-(benzenesulfinyl)-6-(hydroxymethyl)oxane-3,4,5-triol (PIN)

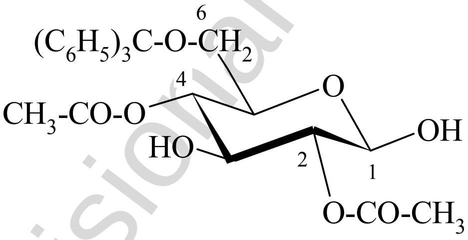
P-102.5.6 Derivatives of monosaccharides

P-102.5.6.1 *O*-Substitution

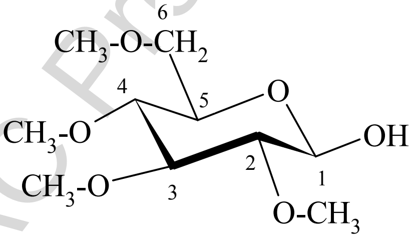
In order to maintain the integrity of structures and take advantage of retained names to imply the absolute configuration, *O*-substitution is allowed in carbohydrate nomenclature. Substituents replacing the hydrogen atom of an alcoholic hydroxy group of a monosaccharide or monosaccharide derivative are denoted as *O*-substituents. The substitution of an anomeric hydroxy group is discussed in P-102.5.5.2.2. The *O*-locant is not repeated for multiple substitutions by the same atom or group. Number locants are used as necessary to specify the positions of substituents; they are not required for compounds fully substituted by identical atoms or groups.

P-102.5.6.1.1 *O*-Acetyl and *O*-alkyl substitution. Names using acyl groups are preferred to names based on ester nomenclature ending in 'ate'.

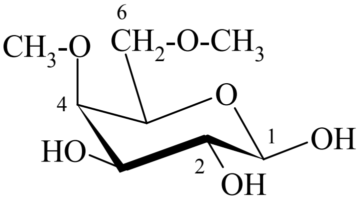
Examples:



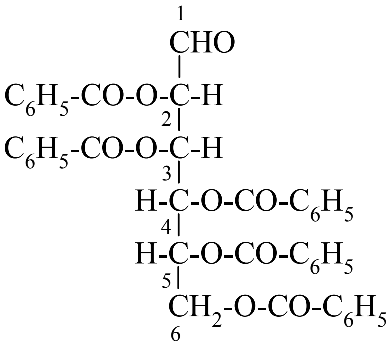
2,4-di-*O*-acetyl-6-*O*-trityl-β-D-glucopyranose (PIN)



2,3,4,6-tetra-*O*-methyl-β-D-glucopyranose (PIN)



4,6-di-*O*-methyl-β-D-galactoyranose (PIN)



2,3,4,5,6-penta-*O*-benzoyl-D-mannose (PIN)

P-102.5.6.1.2 Phosphoric acid esters

Esters of sugars with phosphoric acid are generally termed ‘phosphates’. In biochemical usage, the term ‘phosphate’ indicates the phosphate residue regardless of the state of ionization or the counter ions present. Preferred IUPAC names must differentiate between a true phosphate, $–O-PO(O^-)_2$, and an acid phosphate, i.e., $–O-PO(OH)_2$, called a (dihydrogen phosphate). The prefixes ‘phosphono’, for $–PO(OH)_2$, and ‘phosphonato’, for $PO(O^-)_2$, are also used, to denote *O*-phosphonic acid derivatives.

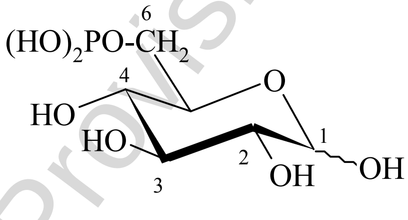
The term ‘phospho’ is used in place of ‘phosphono’ and ‘phosphonato’ in biochemical contexts.

When the sugar is esterified by two or more phosphate groups, the numerical terms ‘bis’, ‘tris’ are used, as ‘bis(phosphate)’, ‘tris(phosphate)’.

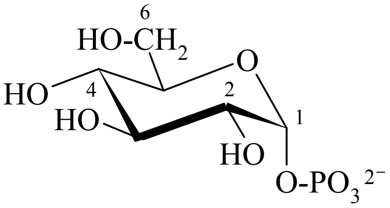
Phosphonates are treated in the same way as phosphates.

All phosphate esters names, including 1-phosphates, are preferred IUPAC names.

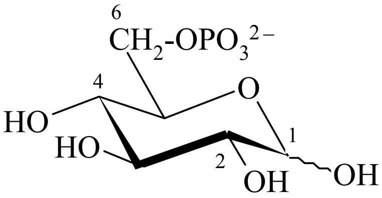
Examples:



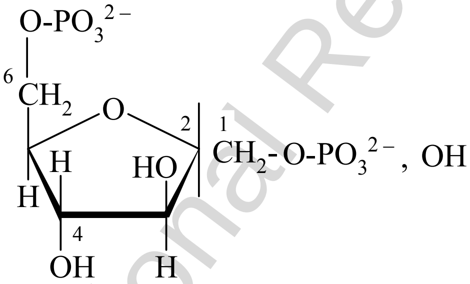
D-glucopyranose 6-(dihydrogen phosphate) (PIN)
6-*O*-phosphono-D-glucopyranose



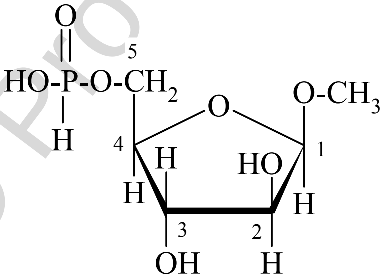
α-D-glucopyranosyl phosphate
α- D-glucopyranose 1-phosphate (PIN)



D-glucopyranose 6-phosphate (PIN)
6-*O*-phosphonato- D-glucopyranose



D-fructofuranose 1,6-bisphosphate (PIN)
1,6-di-*O*-phosphonato-D-fructofuranose

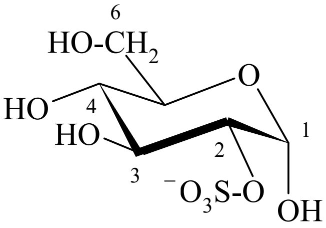


methyl β-D-ribofuranoside 5-(hydrogen phosphonate) (PIN)
methyl 5-deoxy- β-D-ribofuranosid-5-yl hydrogen phosphonate

P-102.5.6.1.2 Esters with sulfuric acid

Esters of sugars with sulfuric acid are named by adding the term ‘sulfate’ after the name of the sugar, with the appropriate locant. The prefixes ‘sulfo’ for $–SO_3H$, and ‘sulfonato’ for $SO_3^–$, can be used to denote *O*-derivatives.

Example:



α-D-glucopyranose 2-sulfate (PIN)
2-*O*-sulfonato-α-D-glucopyranose

P-102.5.6.2 Glycosides

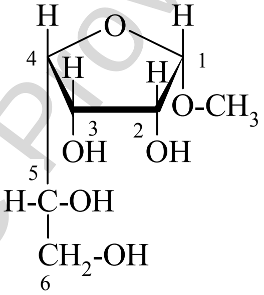
P-102.5.6.2.1 Definitions

Glycose is a less frequently used term for monosaccharide. Glycosides are mixed acetals (ketals) derived from cyclic forms of monosaccharides, having thus an *O*-substituted anomeric –OH group, such as –OR. See ref. 22 for a full discussion on the use of the term glycoside.

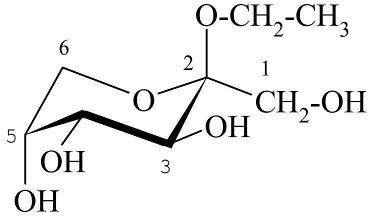
P-102.5.6.2.2 Names

Glycosides are named by using functional class nomenclature. The name of the class ‘glycoside’ is adapted to the name of each cyclic monosaccharide, by changing the letter ‘e’ at the end of the name to ‘ide’, for example glucopyranose becomes glucopyranoside, fructofuranose becomes fructofuranoside. The class name is preceded, as a separate word, by the name of the substituent group that is part of the acetal or ketal function.

Examples:



methyl α-D-gulopyranoside (PIN)



ethyl β-D-fructopyranoside (PIN)

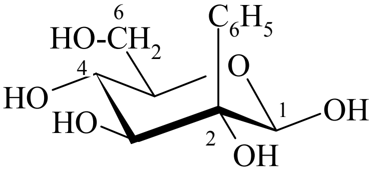
P-102.5.6.3 *C*-substitution

- P-102.5.6.3.1 Substitution at a nonterminal carbon atom
- P-102.5.6.3.2 Substitution replacing a hydroxy group
- P-102.5.6.3.3 Substitution at a terminal carbon atom

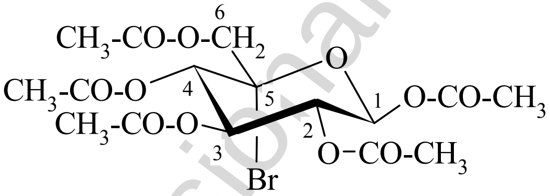
P-102.5.6.3.1 Substitution at a nonterminal carbon atom

The compound is named as a *C*-substituted monosaccharide. The group having priority in accordance with the CIP priority system is regarded as equivalent to –OH for assignment of configuration. Any ambiguity (e.g. at a carbon atom where ring formation occurs) is avoided by using the *R*,*S* system to specify the configuration at the modified chirality center. Preferred IUPAC names are substitutive names.

Example:



2-*C*-phenyl-β-D-glucopyranose
(2*R*,3*R*,4*S*,5*S*,6*R*)-6-(hydroxymethyl)-3-phenyloxane-2,3,4,5-tetrol (PIN)

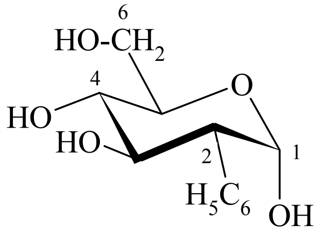


penta-*O*-acetyl-5-*C*-bromo-β-D-glucopyranose
(2*R*,3*R*,4*R*,5*S*,6*S*)-6-bromo-6-[(acetyloxy)methyl]oxane-2,3,4,5-tetrayl tetraacetate (PIN)

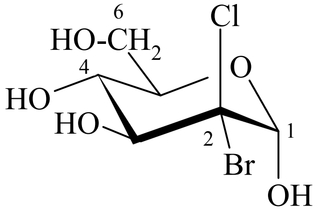
P-102.5.6.3.2 Substitution replacing a nonterminal hydroxy group

The compound is named as a substituted derivative of a deoxy sugar. The group replacing the –OH group determines the configuration. Any potential ambiguity must be dealt with by the use of the '*R*/*S*' system. The '*R*/*S*' system must be used to assign the preferred configuration of a chirality center twice substituted; this method is preferable to that establishing the configuration by making the substituent with high CIP priority equivalent to the –OH group.

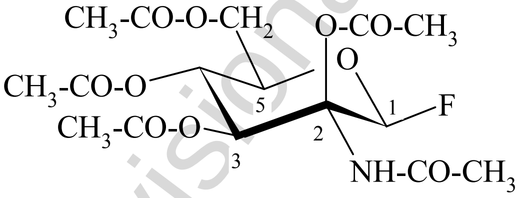
Example:



2-deoxy-2-phenyl-α-D-glucopyranose
2-deoxy-2-*C*-phenyl-α-D-glucopyranose
(2*R*)-2-deoxy-2-phenyl-α-D-*arabino*-hexopyranose
(1*S*,2*R*,3*R*,4*S*,5*R*)-6-(hydroxymethyl)-3-phenyloxane-1,3,4-triol (PIN)



(2*R*)-2-bromo-2-chloro-2-deoxy-α-D-*arabino*-hexopyranose
2-bromo-2-chloro-2-deoxy-α-D-glucopyranose
(2*S*,3*R*,4*S*,5*S*,6*R*)-3-bromo-3-chloro-6-(hydroxymethyl)oxane-2,3,4-triol (PIN)

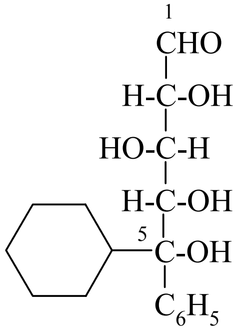


2-acetamido-2,3,4,6-tetra-*O*-acetyl-β-D-mannopyranosyl fluoride
(2*S*,3*S*,4*S*,5*S*,6*R*)-3-acetamido-6-[(acetyloxy)methyl]-2-fluorooxane-3,4,5-triyl triacetate (PIN)

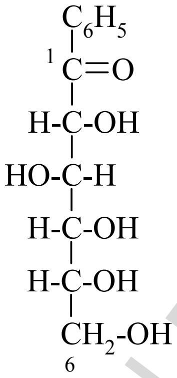
P-102.5.6.3.3 Substitution at a terminal carbon atom

Substitution at a terminal carbon atom of a carbohydrate chain creates a new chirality center; the configuration is indicated by the '*R*/*S*' system. Preferred IUPAC names are formed substitutively.

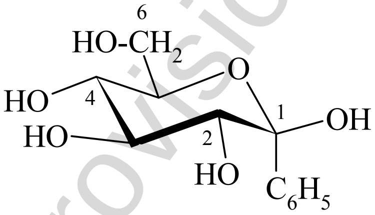
Examples:



(5*R*)-5-*C*-cyclohexyl-5-*C*-phenyl-D-xylose
(2*R*,3*S*,4*S*,5*R*)-5-cyclohexyl-2,3,4,5-tetrahydroxy-5-phenylpentanal (PIN)



1-phenyl-D-glucose
(2*R*,3*S*,4*R*,5*R*)-1-phenyl-2,3,4,5,6-pentahydroxyhexan-1-one (PIN)



1-*C*-phenyl-β-D-glucopyranose
(2*R*,3*R*,4*S*,5*S*,6*R*)-5-(hydroxymethyl)-2-phenyloxane-2,3,4,5-tetrol (PIN)

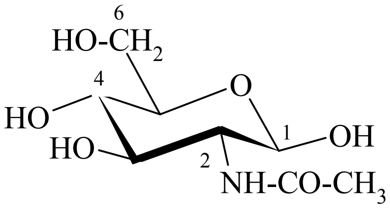
P-102.5.6.4 *N*-substitution

Substitution of the –NH_2 group of an amino sugar is dealt with in two different ways:

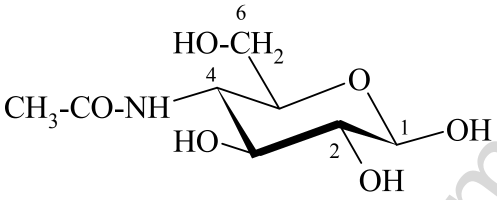
(1) The whole substituted amino group is designated as a prefix as in 2-acetamido (or 2-butylamino)-2-deoxy-D-glucose.

(2) If the amino sugar has a retained trivial name, the substitution is indicated by a prefix preceded by the capital italicized letter *N*.

Examples:



2-acetamido-2-deoxy-β-D-glucopyranose (PIN)
N-acetyl-β-D-glucosamine



4-acetamido-4-deoxy-β-D-glucopyranose (PIN)

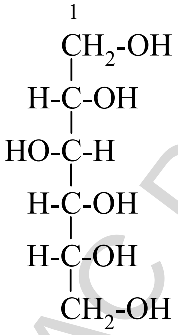
P-102.5.6.5 Alditols

Alditols are named by changing the ending ‘ose’ in the name of the corresponding aldose into ‘itol’.

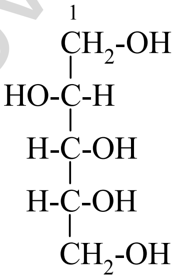
P-102.5.6.5.1 Choice of a parent structure

When the same alditol can be derived from either of two different aldoses, or from an aldose or a ketose, the recommended structure is derived from Rule P-102.3, with the exception of the retained names fucitol and rhamnitol.

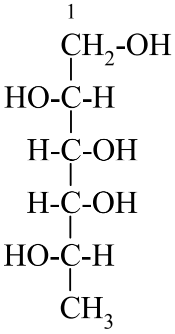
Examples:



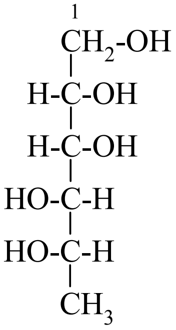
D-glucitol (PIN)
(not L-gulitol)



D-arabinitol (PIN)
(not D-lyxitol)



L-fucitol (PIN)
1-deoxy-D-galactitol

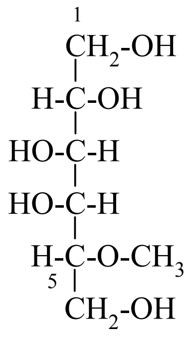


L-rhamnitol (PIN)
1-deoxy- L-mannitol

P-102.5.6.5.2 *meso*-Forms

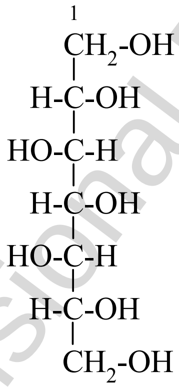
The prefix '*meso*' must be included in the preferred names of erythritol, ribitol and galactitol. The stereodescriptor 'D' or 'L' must be given when a derivative of a '*meso*' form has become asymmetric by substitution. It is also necessary to use the stereodescriptor 'D' or 'L' in the case where there are more than four contiguous chirality centers.

Example:



$$\begin{array}{r}
{}^{1}CH_2\text{-}OH\\
H\text{-}C\text{-}OH\\
HO\text{-}C\text{-}H\\
HO\text{-}C\text{-}H\\
H\text{-}C\text{-}O\text{-}CH_3\\
{}^{5}\ CH_2\text{-}OH
\end{array}$$

5-*O*-methyl-D-galactitol (PIN)
(a ' D' configuration is senior to 'L')



$$\begin{array}{r}
{}^{1}CH_2\text{-}OH\\
H\text{-}C\text{-}OH\\
HO\text{-}C\text{-}H\\
H\text{-}C\text{-}OH\\
HO\text{-}C\text{-}H\\
H\text{-}C\text{-}OH\\
CH_2\text{-}OH
\end{array}$$

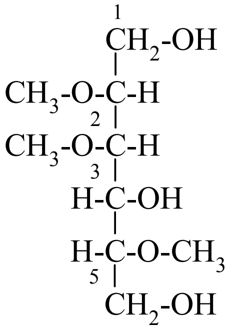
meso- D-*glycero*-L-*ido*-heptitol
(a ' D' configuration is senior to 'L')
(2S,3R,4r,5S,6R)-heptane-1,2,3,4,5,6,7-heptol (PIN)

P-102.5.6.5.3 Choice of parent structure for substituted alditols

The parent structure must have:

(a) the lowest locants for substituent prefixes in accordance with criterion (e) in Rule P-102.4.

Example:

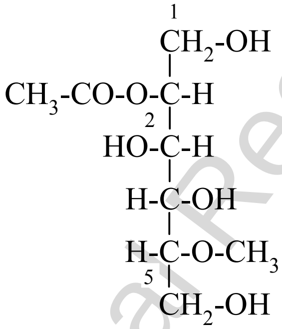


$$\begin{array}{rcl} & \overset{1}{\mathrm{C}} & \mathrm{H_2\text{-}OH} \\ & | & \\ \mathrm{CH_3\text{-}O\text{-}} & \mathrm{C} & \mathrm{\text{-}H} \\ & {}_{2}| & \\ \mathrm{CH_3\text{-}O\text{-}} & \mathrm{C} & \mathrm{\text{-}H} \\ & {}_{3}| & \\ \mathrm{H\text{-}} & \mathrm{C} & \mathrm{\text{-}OH} \\ & | & \\ \mathrm{H\text{-}} & \mathrm{C} & \mathrm{\text{-}O\text{-}CH_3} \\ & {}_{5}| & \\ & \mathrm{C} & \mathrm{H_2\text{-}OH} \end{array}$$

2,3,5-tri-*O*-methyl-D-mannitol (PIN)
(not 2,4,5-tri-*O*-methyl-D-mannitol)

(b) the lowest locant for the first cited substituent in alphanumerical order, in accordance with criterion (f) in Rule P-102.4.

Example:

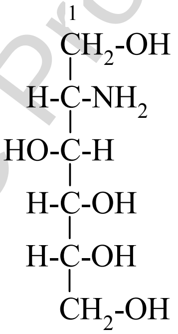


$$\begin{array}{rcl} & \overset{1}{\mathrm{C}} & \mathrm{H_2\text{-}OH} \\ & | & \\ \mathrm{CH_3\text{-}CO\text{-}O\text{-}} & \mathrm{C} & \mathrm{\text{-}H} \\ & {}_{2}| & \\ \mathrm{HO\text{-}} & \mathrm{C} & \mathrm{\text{-}H} \\ & | & \\ \mathrm{H\text{-}} & \mathrm{C} & \mathrm{\text{-}OH} \\ & | & \\ \mathrm{H\text{-}} & \mathrm{C} & \mathrm{\text{-}O\text{-}CH_3} \\ & {}_{5}| & \\ & \mathrm{C} & \mathrm{H_2\text{-}OH} \end{array}$$

2-*O*-acetyl-5-*O*-methyl-D-mannitol (PIN)
(not 5-*O*-acetyl-2-*O*-methyl-D-mannitol)

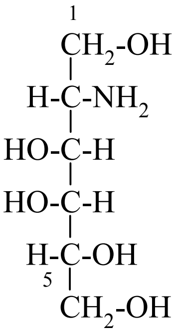
P-102-5.6.5.4 Aminoalditols

Alditols derived from galactosamine and glucosamine are aminoalditols. They have retained names, galactosaminitol and glucosaminitol, respectively.



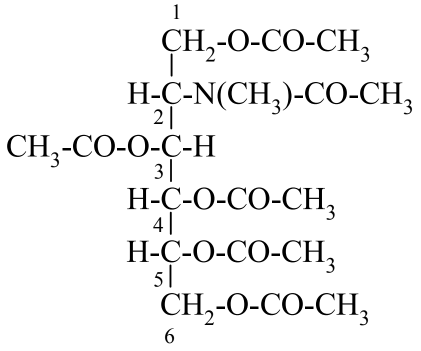
$$\begin{array}{rcl} & \overset{1}{\mathrm{C}} & \mathrm{H_2\text{-}OH} \\ & | & \\ \mathrm{H\text{-}} & \mathrm{C} & \mathrm{\text{-}NH_2} \\ & | & \\ \mathrm{HO\text{-}} & \mathrm{C} & \mathrm{\text{-}H} \\ & | & \\ \mathrm{H\text{-}} & \mathrm{C} & \mathrm{\text{-}OH} \\ & | & \\ \mathrm{H\text{-}} & \mathrm{C} & \mathrm{\text{-}OH} \\ & | & \\ & \mathrm{C} & \mathrm{H_2\text{-}OH} \end{array}$$

D-glucosaminitol
2-amino-2-deoxy-D-glucitol (PIN)



$$\begin{array}{rcl} & \overset{1}{\mathrm{C}} & \mathrm{H_2\text{-}OH} \\ & | & \\ \mathrm{H\text{-}} & \mathrm{C} & \mathrm{\text{-}NH_2} \\ & | & \\ \mathrm{HO\text{-}} & \mathrm{C} & \mathrm{\text{-}H} \\ & | & \\ \mathrm{HO\text{-}} & \mathrm{C} & \mathrm{\text{-}H} \\ & | & \\ \mathrm{H\text{-}} & \mathrm{C} & \mathrm{\text{-}OH} \\ & {}_{5}| & \\ & \mathrm{C} & \mathrm{H_2\text{-}OH} \end{array}$$

D-galactosaminitol
2-amino-2-deoxy-D-galactitol (PIN)



1,3,4,5,6-penta-*O*-acetyl-2-deoxy-2-(*N*-methylacetamido)-D-glucitol (PIN)

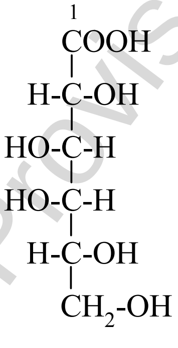
P-102.5.6.6 Monosaccharide carboxylic acids

P-102.5.6.6.1 Definitions

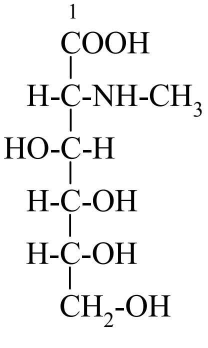
P-102.5.6.6.2 Aldonic acids.
P-102.5.6.6.3 Ketoaldonic acids.
P-102.5.6.6.4 Uronic acids.
P-102.5.6.6.5 Aldaric acids.

P-102.5.6.6.2 Aldonic acids

Aldonic acids are monocarboxylic acids formally derived from aldoses by oxidation of the aldehydic group to a carboxylic acid. Aldonic acids are divided into aldotrionic acids, aldotetronic acids, etc. according to the number of carbon atoms in the chain. The names of individual compounds are formed by changing the ending ‘ose’ of the retained or systematic name of the aldose to ‘onic acid’. The locant 1 is assigned to the carboxy group.
Examples:



D-galactonic acid (PIN)

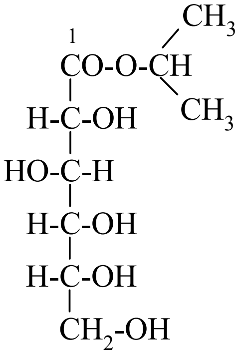


2-deoxy-2-(methylamino)-D-gluconic acid (PIN)

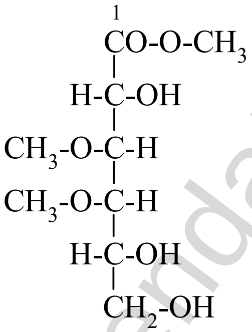
P-102.5.6.6.2.1 Derivatives of aldonic acids

Aldonic acids are treated as carboxylic acids having a retained name. They can form salts, esters, anhydrides, acyl groups and acid halides and pseudohalides, amides, hydrazides, nitriles and chalcogen analogues as described in Sections 65 and 66 for systematic nomenclature. Preferred IUPAC names are formed by using the described methodology for this type of name.

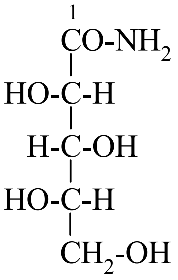
Examples:



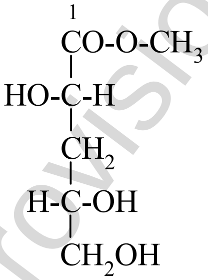
propan-2-yl D-gluconate (PIN)



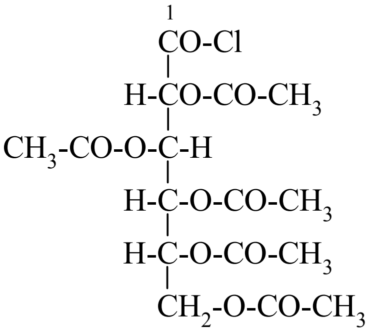
methyl 3,4-di-*O*-methyl-D-galactonate (PIN)



L-xylonamide (PIN)



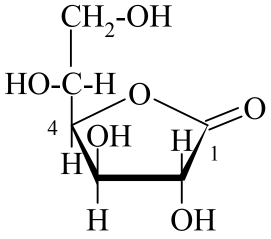
methyl 3-deoxy- D-*threo*-pentonate (PIN)



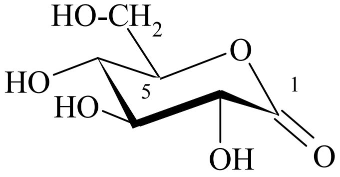
penta-*O*-acetyl- D-gluconoyl chloride (PIN)

Lactones and lactams are named by adapting Rules P-65.6.3.3.2 and P-66.1.4.1, respectively. Two locants are used before the lactone or lactam term: the first one is the locant 1 denoting the carboxy group position; the second locant denotes the position of attachment on the carbon chain. To name lactams, the amino group, $-NH_2$, must be generated and cited. The use of Greek letters to indicate the size of a lactone or lactam ring is not recommended. Preferred IUPAC names are formed substitutively on the basis of heterocyclic rings, with CIP stereodescriptors.

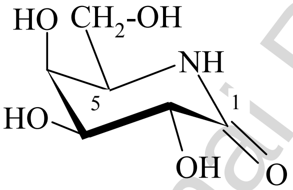
Examples:



D-glucono-1,4-lactone
(3R,4*R*,5*R*)- 4-[(1*R*)-1,2-dihydroxyethyl]-3,4-dihydroxyoxolan-2-one (PIN)



D-glucono-1,5-lactone
(2*R*,3*S*,4*S*,5*R*)-2,4-dihydroxy-5-(hydroxymethyl)oxolan-2-one (PIN)

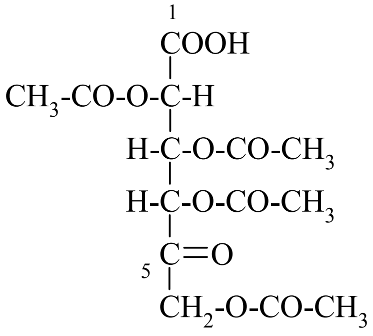


5-amino-5-deoxy- D-galactono-1,5-lactam
(3*R*,4*S*,5*S*,6*R*)-3,4,5-trihydroxy-6-(hydroxymethyl)piperidin-2-one (PIN)

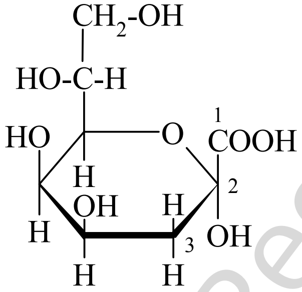
P-102.5.6.6.3 Ketoaldonic acids

Ketoaldonic acids are oxo carboxylic acids formally derived from aldonic acids by oxidation of a secondary –CHOH group to a carbonyl group. Names of individual ketoaldonic acids are formed by changing the ending ‘ulose’ in the name of the corresponding ketose to ‘ulonic acid’, preceded by the locant of the ketonic group. The numbering starts at the carboxy group.

Examples:



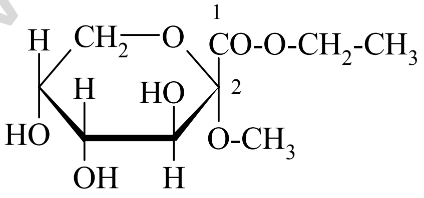
2,3,4,6-tetra-*O*-acetyl- D-*arabino*-hex-5-ulosonic acid
(1*S*,2*R*,3*S*)-2,3,4-tris(acetyloxy)-5-oxohexanoic acid (PIN)



3-deoxy-α-D-*manno*-oct-2-ulopyranosonic acid
(2*R*,4*R*,5*R*,6*R*)-6-[(1*R*)-1,2-dihydroxyethyl]-2,4,5-trihydroxyoxane-1-carboxylic acid (PIN)

Glycosides are named by changing the component ‘pyranose’ into ‘pyranoside’ in the name, to give ‘-ulopyranosidonic acid’. Names of derivatives of ketoaldonic acids are formed as described in P-102.5.6.6.2.1 for aldonic acids. When a glycoside is esterified, parentheses are used to isolate the glycosidic portion of the name.

Example:

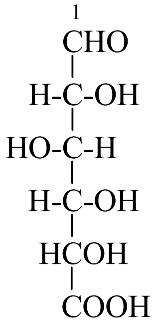


ethyl (methyl α-D-*arabino*-hex-2-ulopyranosid)onate
ethyl (2*R*,3*S*,4R,5*R*)-3,4,5-trihydroxy-2-methoxyoxane-2-carboxylate (PIN)

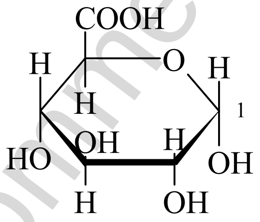
P-102.5.6.6.4 Uronic acids

P-102.5.6.6.4.1 Uronic acids are carboxylic acids formally derived from aldoses by oxidation of the terminal –CH_2OH group to a carboxy group. Names of individual uronic acids are formed by changing the ending 'ose' in the retained or systematic name of the corresponding aldose to 'uronic acid'. The numbering of the aldose is kept intact; the locant '1' is still assigned to the (potential) aldehydic group.

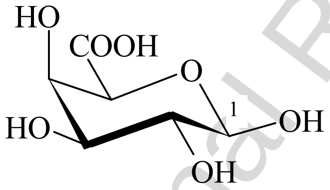
Examples:



D-glucuronic acid (PIN)



α-D-glucopyranuronic acid (PIN)

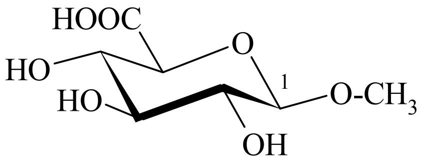


β-D-galactopyranuronic acid (PIN)

P-102.5.6.6.4.2 Glycosides of uronic acids

Names of glycosides of uronic acids are formed by changing the 'pyran' component in the name of the acid to 'pyranoside', with elision of the final letter 'e', to give 'pyranosiduronic acid'.

Example:

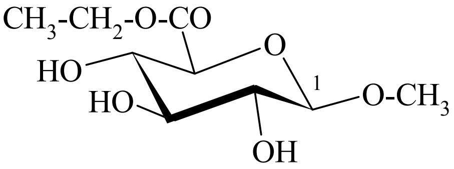


methyl β-D-glucopyranosiduronic acid (PIN)

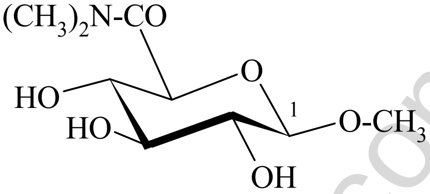
P-102.5.6.6.4.3 Derivatives of uronic acids

Names of derivatives are formed as indicated in P-102.5.6.6.2.1 and P-46.

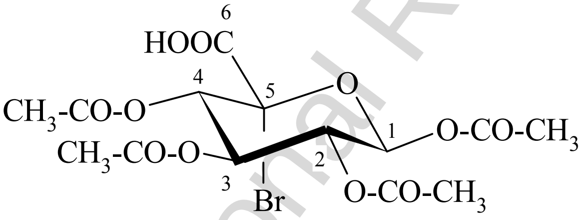
Examples:



ethyl (methyl β-D-glucopyranosid)uronate (PIN)



N,*N*-dimethyl(methyl β-D-glucopyranosid)uronamide (PIN)

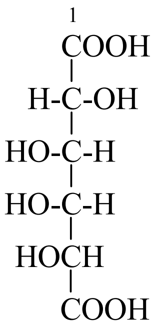


1,2,3,4-tetra-*O*-acetyl-5-bromo-β-L-idopyranuronic acid
(5*R*)-1,2,3,4-tetra-*O*-acetyl-5-bromo-α-D-*xylo*-hexopyranuronic acid
(2*R*,3*S*,4*R*,5*R*,6*R*)-2-bromo-3,4,5,6-tetra-(acetyloxy)oxane-2-carboxylic acid (PIN)

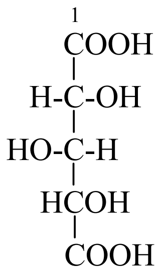
P-102.5.6.6.5 Aldaric acids

P-102.5.6.6.5.1 Aldaric acids are carboxylic acids formed by the oxidation of both terminal groups (–CHO and –CH_2OH) of aldoses to carboxy groups. Names of aldaric acids are formed by changing the 'ose' ending in retained or systematic names of parent aldoses to 'aric acid'. Choice of a parent structure is made in accordance with P-102.5.5.5.1. The stereodescriptor '*meso*' must be added for sake of clarity to the names of the appropriate aldaric acids.

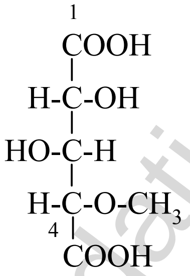
Examples:



L-altraric acid (PIN)
(not L-talaric acid)



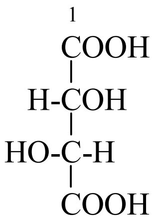
meso-xylaric acid (PIN)



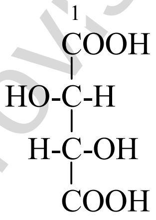
4-*O*-methyl-D-xylaric acid (PIN)
(not 2-*O*-methyl-L-xylaric acid)

P-102.5.6.6.5.2 Stereodescriptors for tartaric acids

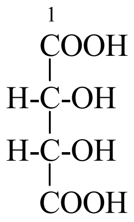
Tartaric acid is the retained name to describe the aldaric acids corresponding to the parent aldoses, erythrose and threose. '*R*' and '*S*' are preferred stereodescriptors for denoting the configuration of tartaric acid. Salts and esters are referred to as tartrates.



(2*R*,3*R*)-2,3-dihydroxybutanedioic acid (PIN)
(2*R*,3*R*)-tartaric acid
L-threaric acid
(+)-tartaric acid



(2*S*,3*S*)-2,3-dihydroxybutanedioic acid (PIN)
(2*S*,3*S*)-tartaric acid
D-threaric acid
(-)-tartaric acid



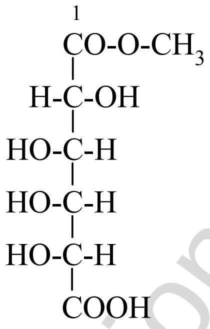
$$\begin{array}{c} {}^{1}\\ \text{COOH}\\ |\\ \text{H-C-OH}\\ |\\ \text{H-C-OH}\\ |\\ \text{COOH} \end{array}$$

(2*R*,3*S*)-2,3-dihydroxybutanedioic acid (PIN)
(2*R*,3*S*)-tartaric acid
erythraric acid
meso-tartaric acid

P-102.5.6.6.5.3 Derivatives of aldaric acids

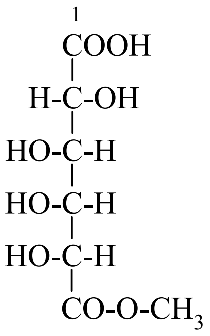
Derivatives of aldaric acids formed by modifying the carboxy group (into esters, amides, hydrazides, nitriles, amic acids, etc.) are named by the methods described in P-102.5.6.6.2.1 and P-65.

Examples:



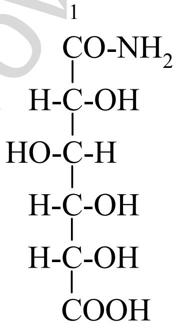
$$\begin{array}{c} {}^{1}\\ \text{CO-O-CH}_3\\ |\\ \text{H-C-OH}\\ |\\ \text{HO-C-H}\\ |\\ \text{HO-C-H}\\ |\\ \text{HO-C-H}\\ |\\ \text{COOH} \end{array}$$

1-methyl hydrogen L-altarate (PIN)



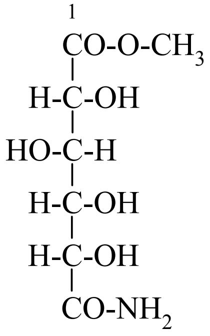
$$\begin{array}{c} {}^{1}\\ \text{COOH}\\ |\\ \text{H-C-OH}\\ |\\ \text{HO-C-H}\\ |\\ \text{HO-C-H}\\ |\\ \text{HO-C-H}\\ |\\ \text{CO-O-CH}_3 \end{array}$$

6-methyl hydrogen L-altarate (PIN)



$$\begin{array}{c} {}^{1}\\ \text{CO-NH}_2\\ |\\ \text{H-C-OH}\\ |\\ \text{HO-C-H}\\ |\\ \text{H-C-OH}\\ |\\ \text{H-C-OH}\\ |\\ \text{COOH} \end{array}$$

D-glucar-1-amic acid (PIN)



$$\begin{array}{c} {}^{1}\\ \text{CO-O-CH}_3\\ |\\ \text{H-C-OH}\\ |\\ \text{HO-C-H}\\ |\\ \text{H-C-OH}\\ |\\ \text{H-C-OH}\\ |\\ \text{CO-NH}_2 \end{array}$$

1-methyl D-glucar-6-amate (PIN)

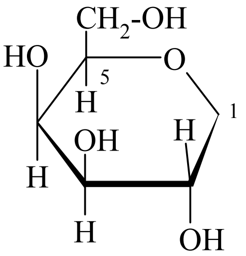
P-102.5.6.7 Anhydrides

Anhydrides are intramolecular or intermolecular derivatives of monosaccharides.

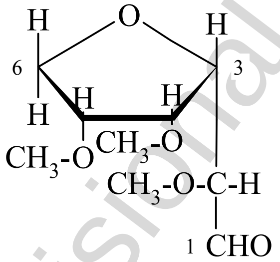
P-102.5.6.7.1 Intramolecular anhydrides

An intramolecular ether (commonly called intramolecular anhydride), formally arising by elimination of water from two hydroxyl groups of a single molecule of a monosaccharide (aldose, ketose) or monosaccharide derivative, is named by adding the detachable prefix 'anhydro', preceded by a pair of locants identifying the two hydroxy groups, to the name of the monosaccharide.

Examples:



1,5-anhydro-D-galactitol
(2*R*,3*R*,4*R*,5*S*)-6-(hydroxymethyl)oxane-3,4,5-triol (PIN)

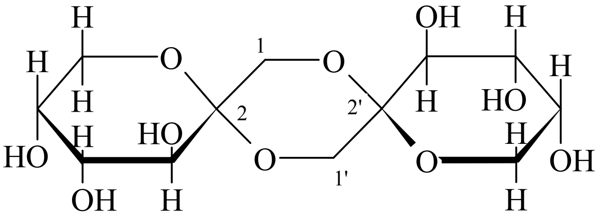


3,6-anhydro-2,4,5-tri-*O*-methyl- D-glucose
(2*R*)-2-[(2*S*,3*R*,4*R*)-dimethoxyoxolan-2-yl]-2-methoxyacetaldehyde (PIN)

P-102.5.6.7.2 Intermolecular anhydrides

The cyclic product of condensation of two monosaccharide molecules with elimination of two molecules of water (commonly called an intermolecular anhydride) is named by placing the term 'dianhydride' after the names of the two parent monosaccharides. When the two parents are different, the senior parent according to the selection criteria for selecting the parent structure (see P-102.4), is cited first. The position of each anhydride link is indicated by a pair of locants showing the position of the two hydroxy groups involved, the locants relating to one monosaccharide (in a mixed anhydride, the second monosaccharide named) are primed. The pair of locants immediately precedes the term 'dianhydride'.

Example:



α-D-fructopyranose β-D-fructopyranose 1,2′:1′,2-dianhydride
(α-D-fructopyranose is cited first; according to P-102.4 (c), α precedes β)
(3*R*,4*R*,5*S*,6*R*,9*S*,12*R*,13*S*,14*S*)-1,7,10,15-tetraoxadispiro[5.2.5^9.2^6]hexadecane-3,4,5,12,13,14-hexol (PIN)

P-102.6 Monosaccharides and derivatives as substituent groups

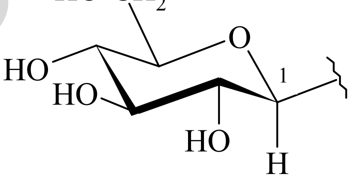
P-102.6.1 Glycosyl groups

P-102.6.1.1 Glycosyl groups

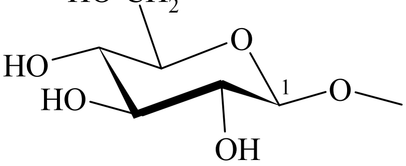
Substituent groups formed by removal of the anomeric hydroxy group from a cyclic monosaccharide are named by replacing the final letter ‘e’ of the monosaccharide name by ‘yl’. The term ‘glycosyl residue’ is used in the nomenclature of carbohydrates. Terms of this nature are widely used in naming glycosides, when they are not the parent structures, and oligosaccharides.

No locant is added to the name of the substituent to indicate the position of the free valence. A sinuous line denotes the free valence, as recommended for cyclic substituent groups in systematic nomenclature.

Examples:



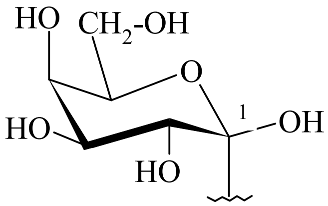
β-D-glucopyranosyl (PIN)
(the hydrogen atom at
position 1 is shown)



β-D-glucopyranosyloxy (PIN)

When the free valence is formed at carbon ‘1’ by subtraction of a hydrogen atom, the substituent group is named as a glycosyl group but the presence of the hydroxy group is denoted by substitution at carbon ‘1’. In this case, the stereodescriptor ‘α’ or ‘β’ refers to the free valence, not to the –OH group.

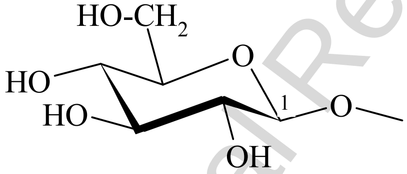
Example:



1-hydroxy-α-D-galactopyranosyl (PIN)

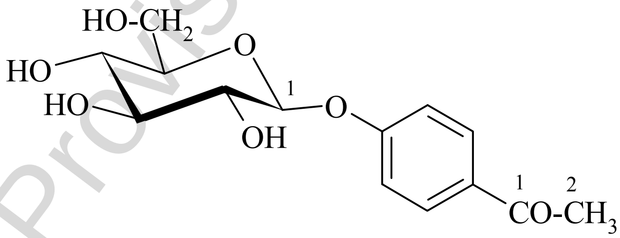
P-102.6.1.2 *O*-Glycosyl compounds

The substituent group formed by removal of a hydrogen atom from the anomeric –OH group is considered as a compound substituent group formed by the ‘glycosyl’ group and an ‘oxy’ group.

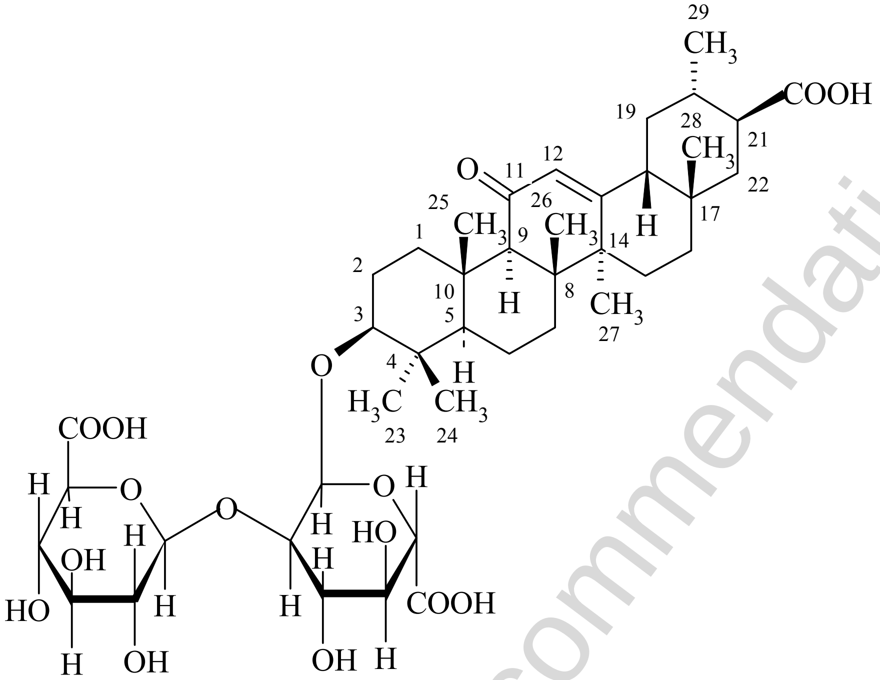


β-D-glucopyranosyloxy (PIN)

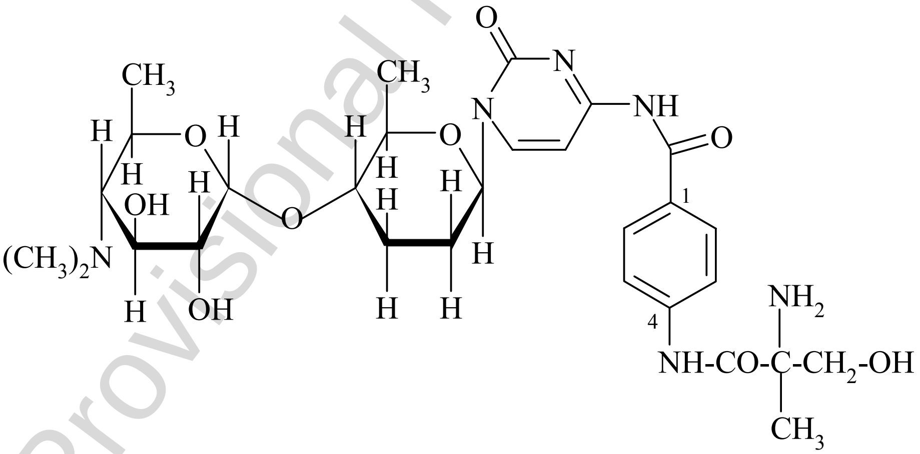
Examples:



1-[4-(β-D-glucopyranosyloxy)phenyl]ethan-1-one (PIN)
(not 4′-(β-D-glucopyranosyloxy)acetophenone; acetophenone is no longer recommended as a preferred IUPAC name)
(not 4-acetylphenyl β-D-glucopyranoside; a ketone is senior to a hydroxy compound)



21β-carboxy-11-oxo-30-norolean-12-en-3β-yl (2-*O*-β-D-glucopyranosyluronic acid)-α-D-glucopyranosiduronic acid (PIN)



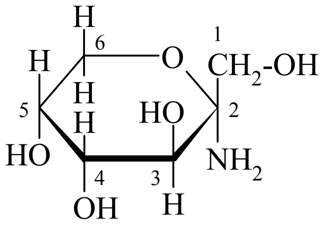
4-[(*RS*)-2-amino-3-hydroxy-2-methylpropanamido]-*N*-(1-{5-[(4,6-dideoxy-4-(dimethylamino)-α-D-glucopyranosyl)oxy]-1-[(2*R*,5*S*,6*R*)-6-methyloxan-2-yl]}-2-oxo-1,2-dihydropyrimidin-4-yl)benzamide (PIN)

Guide to name construction: the principal function is an amide; the cyclic amide, benzamide, is senior to the acyclic amide, propanamide)

P-102.6.1.3 *N*-Glycosyl compounds (glycosylamines)

N-Glycosyl derivatives are conveniently named as glycosylamines.

Example:

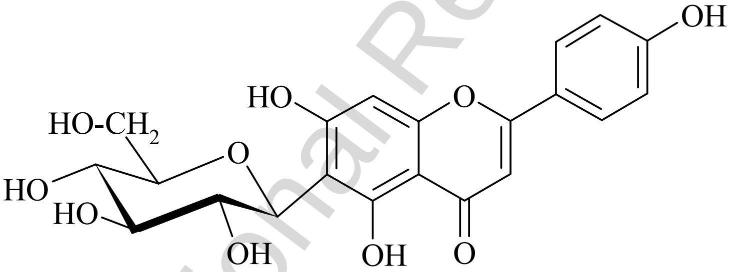


α-D-fructopyranosylamine (PIN)

P-102.6.1.4 *C*-glycosyl compounds

Compounds arising formally from the elimination of water from the glycosidic hydroxy group and a hydrogen atom bound to a carbon atom (thus creating a C-C bond) are named using the appropriate glycosyl group.

Examples:

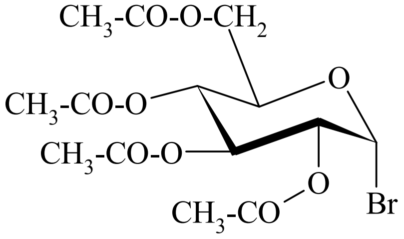


6-(β-D-glucopyranosyl)-5,7-dihydroxy-2-(4-hydroxyphenyl)-4*H*-chromen-4-one (PIN)
6-(β-D-glucopyranosyl)-4′,5,7-dihydroxyflavone

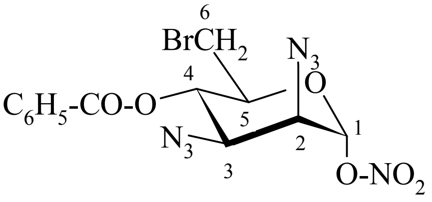
P-102.6.1.5 Glycosyl halides, pseudohalides and esters

Glycosyl halides and pseudohalides are named by using functional class nomenclature, by adding, as a separate word, the class name ‘chloride’, ‘isocyanate’, etc. to the name of the appropriate glycosyl group. Esters in position 1 of oxoacids other than *P* and *S* acids are treated like glycosyl halides and pseudohalides.

Example:



2,3,4,6-tetra-O-acetyl-α-D-glucopyranosyl bromide (PIN)

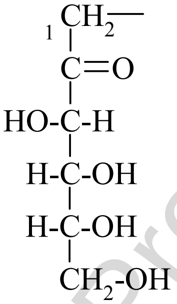


2,3-diazido-4-*O*-benzoyl-6-bromo-2,3,6-trideoxy-α-D-mannopyranosyl nitrate (PIN)

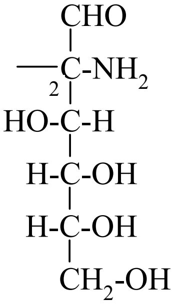
P-102.6.1.6 Substituent groups other than glycosyl groups

A hydrogen atom may be removed from any position of a monosaccharide other than C-1. This formation of a free valence is denoted by the suffix 'yl', but a locant is necessary to indicate the position of the free valence and to distinguish such a name from that of glycosyl substituents for which the locant 1 is omitted. These prefixes can be formed by replacing the final letter 'e' of the systematic or trivial name of a monosaccharide by *n*-*C*-yl, *n*-*O*-yl. The symbol '*C*' is omitted when the free valence is derived from a position at which hydrogen atoms only are attached.

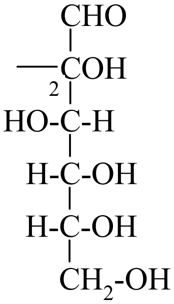
Examples:



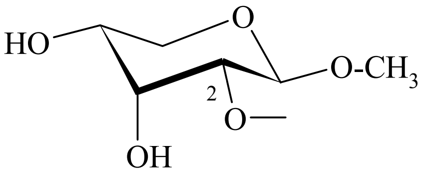
1-deoxy-D-fructos-1-yl (PIN)



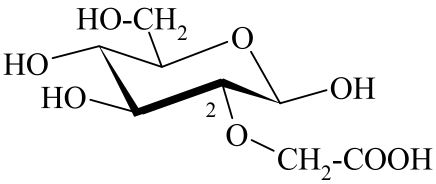
2-amino-2-deoxy-D-glucos-2-*C*-yl (PIN)



D-glucos-2-*C*-yl (PIN)



methyl β-D-ribopyranosid-2-*O*-yl (PIN)



2-(β-D-glucopyranos-2-*O*-yl)acetic acid (PIN)
(not 2-*O*-carboxymethyl β-D-glucopyranose; this name is not constructed in conformity with P-102.4.3(a) for selecting a parent structure; a carboxylic acid is senior to a hydroxy compound).

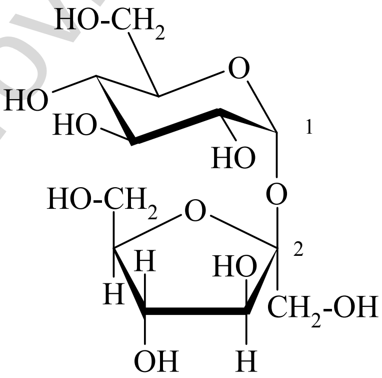
P-102.7 Disaccharides and oligosaccharides

Names of disaccharides and oligosaccharides are formed by the principles, rules and conventions described above for monosaccharides. As names may become very long and cumbersome, full systematic names have been replaced by a system based on symbols, such as Glc for glucose. A brief description of the extended form, the condensed and the short form is given in this Section.

P-102.7.1 Disaccharides

P-102.7.1.1 Disaccharides without a free hemiacetal group

Disaccharides which can be regarded as formed by elimination of one molecule of water from two glycosidic (anomeric) hydroxyl groups, are named as glycosyl glycosides. The parent (cited as the ‘glycoside’) is chosen in accordance with criteria described in P-102.4. Both anomeric descriptors must be cited in the name.
Example:



β-D-fructofuranosyl α-D-glucopyranoside (PIN)
(not α-D-glucopyranosyl β-D-fructofuranoside; gluco precedes fructo in the alphabetical order)
sucrose (trivial name)

P-102.7.1.2 Disaccharides with a free hemiacetal group

Disaccharides which can be regarded as formed by elimination of one molecule of water from one glycosidic (anomeric) hydroxyl group and one alcoholic hydroxyl group, are named as glycosylglycoses. Locants and anomeric descriptors must be cited in the full name.

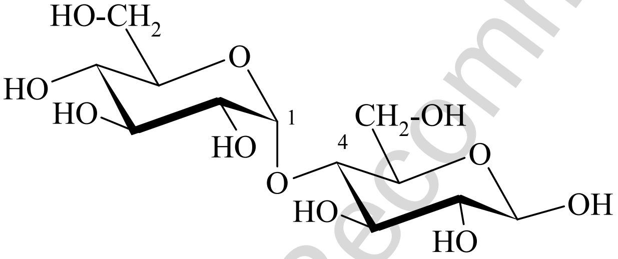
There are two established methods for citing locants:

(1) in parentheses between the components with an arrow going from the locant of the glycosyl component to that of the glycose component;

(2) at the front of the glycosyl component.

Method (1) leads to preferred IUPAC names.

Example:



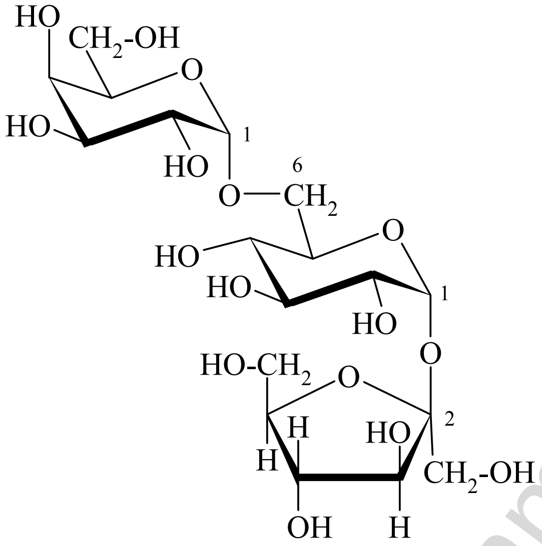
(1) α-D-glucopyranosyl-(1→4)-β-D-glucopyranose (PIN)
(2) 4-*O*-α-D-glucopyranosyl-β-D-glucopyranose
β-maltose (trivial name; not β-D-maltose)

P-102.7.2 Oligosaccharides

P-102.7.2.1 Oligosaccharides without a free hemiacetal group

A trisaccharide, for example, is named as a glycosylglycosyl glycoside or glycosyl glycosylglycoside as required. A choice between the two residues linked through their anomeric positions for citation as the 'glycoside' portion can be made on the basis of P-102.4. Alternatively, a sequential (end-to-end) naming approach may be used, regardless of P-102.4. The name is formed by the preferred method for naming disaccharides.

Example:

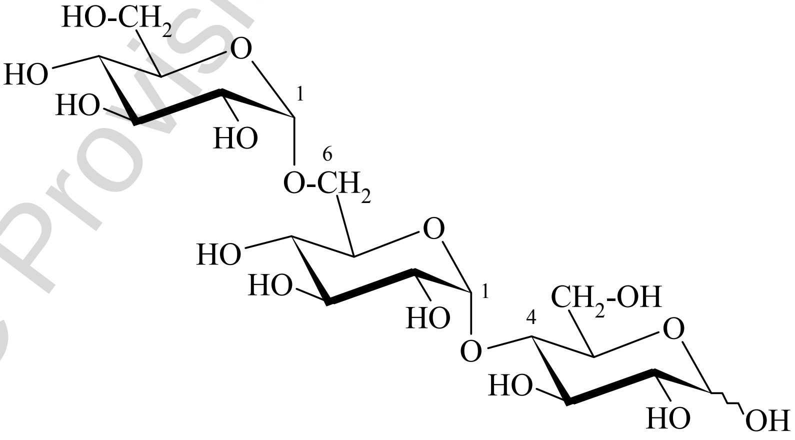


β-D-fructofuranosyl α-D-galactopyranosyl-(1→6)-α-D-glucopyranoside (PIN)
(glucose, not fructose, is selected as the ‘glycoside’)
α-D-galactopyranosyl-(1→6)-α-D-glucopyranoside β-D-fructofuranoside
(sequential method)
raffinose (trivial name)

P-102.7.2.2 Oligosaccharides with a free hemiacetal group

An oligosaccharide of this type is name as a glycosyl[glycosyl]*n*glycose, the ‘glycose’ portion being the parent. The conventional depiction has the ‘glycose’ portion on the right. Names are formed as described in P-102.7.2.1.

Example:



α-D-glucoyranosyl-(1→6)-α-D-glucopyranosyl-(1→4)-D-glucopyranose (PIN)
panose (trivial name)

P-103 Amino acids and peptides

P-103.0 Introduction

This Section describes the nomenclature of amino acids that constitute the building blocks of peptides and proteins. They are functional parents having retained names listed in Table 10.3. Less common amino acids also have retained names. The nomenclature of amino acids is composed of two types of names: names based on retained names for functional parents, with a limited capacity of functionalization and substitution, and systematic substitutive names for all other compounds.

The nomenclature of these amino acids is described in the document entitled 'Nomenclature and Symbolism for Amino Acids and Peptides' (ref. 23). In this Section, the nomenclature of these amino acids is restricted to their derivatives outside the field of peptides and proteins and their use in the construction of preferred IUPAC names.

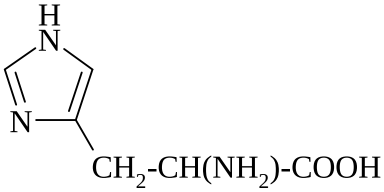
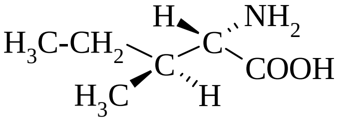
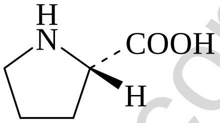
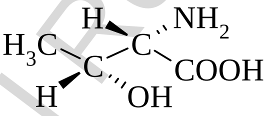
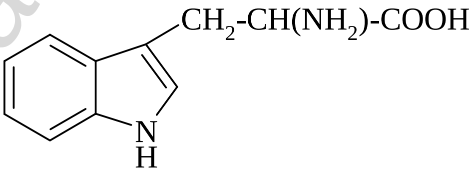
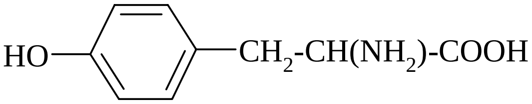
P-103.1 Nomenclature based on retained names
P-103.2 Substitutive names of amino acids
P-103.3 Nomenclature of peptides

P-103.1 Nomenclature based on retained names (see Tables 3 and 4)

P-103.1.1 Configuration of α-amino carboxylic acids
P-103.1.2 Functional modifications of α-amino carboxylic acids
P-103.3 Derivatives of α-amino carboxylic acids
P-103.4 α-Amino carboxylic acids as substituent groups

Table 10.3. Retained names of α-amino acids

Retained name	*Symbols*		*Formula*
alanine (PIN)	Ala	A	CH_3-CH(NH_2)-COOH
arginine (PIN)	Arg	R	H_2N-C(=NH)-NH-[CH_2]$_3$-CH(NH_2)-COOH
asparagine (PIN)	Asn	N	H_2N-CO-CH_2-CH(NH_2)-COOH
aspartic acid (PIN)	Asp	D	HOOC-CH_2-CH(NH_2)-COOH
cysteine (PIN)	Cys	C	HS-CH_2-CH(NH_2)-COOH
glutamine (PIN)	Gln	Q	H_2N-CO-[CH_2]$_2$-CH(NH_2)-COOH
glutamic acid(PIN)	Glu	E	HOOC-[CH_2]$_2$-CH(NH_2)-COOH
glycine (PIN)	Gly	G	H_2N-CH_2-COOH

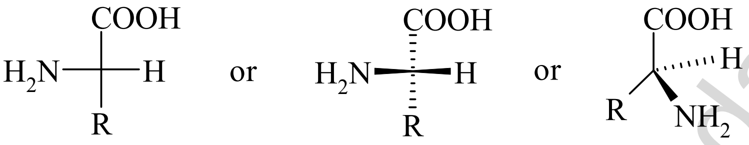
histidine (PIN)	His	H	
isoleucine* (PIN)	Ile	I	
leucine (PIN)	Leu	L	$(CH_3)_2CH-CH(NH_2)-COOH$
lysine (PIN)	Lys	K	$H_2N-[CH_2]_4-CH(NH_2)-COOH$
methionine (PIN)	Met	M	$CH_3-S-[CH_2]_2-CH(NH_2)-COOH$
phenylalanine (PIN)	Phe	F	$C_6H_5-CH_2-CH(NH_2)-COOH$
proline* (PIN)	Pro	P	
serine (PIN)	Ser	S	$HO-CH_2-CH(NH_2)-COOH$
threonine* (PIN)	Thr	T	
tryptophan (PIN)	Trp	W	
tyrosine (PIN)	Tyr	T	
valine (PIN)	Val	V	$(CH_3)_2CH-CH(NH_2)-COOH$
unspecified amino acid	Xaa	X	

---

* L-forms shown

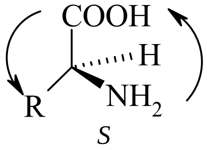
P-103.1.1 Configuration of α-amino carboxylic acids

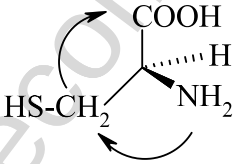
The absolute configuration at the α-carbon atom of the α-amino carboxylic acids is designated by the stereodescriptor ‘D’ or ‘L’ to indicate a formal relationship to ‘D’ or ‘L’ glyceraldehyde. The stereodescriptor ‘ξ’ (Greek letter xi) indicates unknown configuration.



Three tridimensional representations of the ‘L’ configuration
(The ‘L’ configuration of isoleucine, proline and threonine is shown in Table 10.3)

The ‘L’ configuration corresponds to the ‘*S*’ configuration in the CIP system, except for cysteine that has the ‘*R*’ configuration..





R for L-cysteine

P-103.1.2 Functional modifications of α-amino carboxylic acids

Retained names are use to form preferred IUPAC names of salts and esters, and those of alkyl, aryl and acyl derivatives substituted on *N*, *O*, and *S* atoms.

The carboxy group –COOH can be transformed into various characteristic groups such as a hydroxymethyl group, $-CH_2$-OH, or an aldehyde group, –CHO. Some names derived from retained amino acid names are recommended to be used for naming acyl groups, amides, alcohols, aldehydes, and even ketones, in the context of peptide and protein nomenclature. They can be used in general nomenclature, but not as preferred IUPAC names that must be systematically constructed as indicated in P-103.2.

P-103.1.2.1 Ionization of characteristic groups

Names of zwitterions, anions and cations are derived from the rules expressed in Chapter 7.

Examples:

NH_3^+-CH_2-COO^-	2-azaniumylacetate (PIN) glycine zwitterion
H_2N-CH_2-COO^-	glycinate (PIN) glycine anion

$\mathrm{NH_3^+{-}CH_2{-}COOH}$	glycinium (PIN) glycine cation

Specific names are recommended for the monoanion and the dianion of aspartic acid and glutamic acid:

$\mathrm{^{-}OOC{-}CH_2{-}CH_2{-}CH(NH_3^+){-}COO^{-}}$	hydrogen glutamate (PIN) glutamate(1-)
$\mathrm{^{-}OOC{-}CH_2{-}CH_2{-}CH(NH_3^+){-}COO^{-}\ \ Na^+}$	sodium hydrogen glutamate (PIN) sodium glutamate(1-)
$\mathrm{^{-}OOC{-}CH_2{-}CH_2{-}CH(NH_2){-}COO^{-}}$	glutamate (PIN) (by definition glutamate = 2−) glutamate(2-) (see 3AA-6, ref. 23) glutamic acid dianion
$\mathrm{^{-}OOC{-}CH_2{-}CH_2{-}CH(NH_3^+){-}COO^{-}\ \ 2Na^+}$	disodium glutamate (PIN)
$\mathrm{NH_3^+{-}[CH_2]_4{-}CH(NH_3^+){-}COO^{-}}$	lysinium (PIN) (by definition “-ium” = 1+) lysinium(1+) (see 3AA, ref. 23) lysine monocation
$\mathrm{NH_3^+{-}[CH_2]_4{-}CH(NH_3^+){-}COO^{-}\ \ Cl^{-}}$	lysinium chloride (PIN) (by definition “-ium” = 1+) lysinium(1+) chloride (see 3AA, ref. 23) lysine monohydrochloride)
$\mathrm{NH_3^+{-}[CH_2]_4{-}CH(NH_3^+){-}COOH}$	lysinediium (PIN) lysinium(2+) (see 3AA, ref. 23)

P-103.1.2.2 Acyl groups

Preferred IUPAC names of acyl groups , $\mathrm{H_2N{-}CHR{-}CO{-}}$, are formed by changing the ending ‘ine’ (or ‘an’ in tryptophan) into ‘yl’, for example alanyl, valyl, tryptophyl. ‘Cysteinyl’ is used instead of ‘cysteyl’; ‘cystyl’ is derived from ‘cystine’.

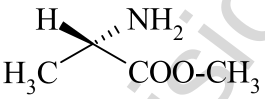
The following names are used to name the acyl groups derived from dicarboxylic amino acids and their corresponding amides.

HOOC-CH_2-CH(NH_2)-CO–	α-aspartyl (PIN) aspart-1-yl
–CO-CH_2-CH(NH_2)-COOH	β-aspartyl (PIN) aspart-4-yl
–CO-CH_2-CH(NH_2)-CO–	aspartoyl
HOOC-CH_2-CH_2-CH(NH_2)-CO–	α-glutamyl (PIN) glutam-1-yl
–CO-CH_2-CH_2-CH(NH_2)-COOH	γ-glutamyl glutam-5-yl (PIN)
–CO-CH_2-CH_2-CH(NH_2)-CO–	glutamoyl
H_2N-CO-CH_2-CH(NH_2)-CO–	asparaginyl
H_2N-CO-CH_2-CH_2-CH(NH_2)-CO–	glutaminyl

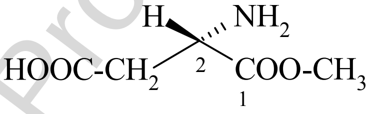
P-103.1.2.3 Esters

Preferred IUPAC names of esters, R-CO-OR′, are formed by the general method of using the ‘ate’ ending obtained by replacing the ‘ic acid’ ending or the final letter ‘e’ of the retained name (or adding the ending ‘ate’ to the name tryptophan) and the name of the substituent group R′.

Example:



methyl L-alaninate (PIN)
alanine methyl ester

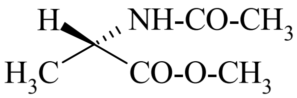


1-methyl L-aspartate (PIN)

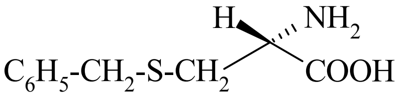
P-103.1.2.4 Nitrogen, oxygen and sulfur substituted amino acids

Retained names are used to indicate nitrogen, oxygen and sulfur substitution. Locants *N*, *O* and *S*, as appropriate, indicate the location of the substitution. For lysine, locants N^2 and N^6 are used to denote the two amino groups located at positions 2 and 6, respectively.

Examples:



methyl *N*-acetyl-L-alaninate (PIN)

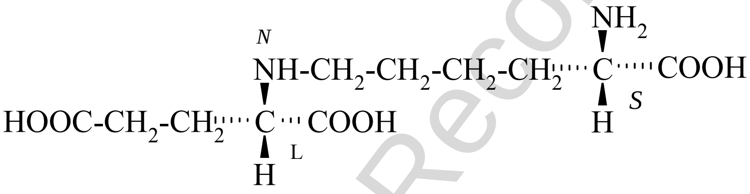


S-benzyl-L-cysteine (PIN)

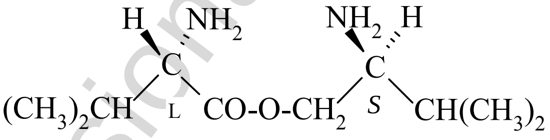
P-103.1.2.5 Addition of chirality centers

By substitution, added atoms or groups may add new chirality centers. Preferred IUPAC names are formed by using '*R*' and '*S*' stereodescriptors for all new chirality centers.

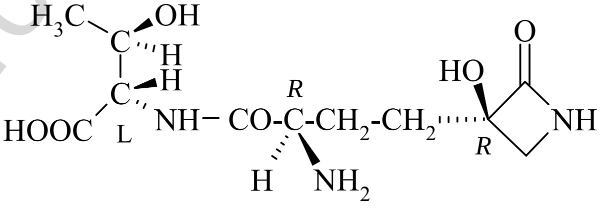
Examples:



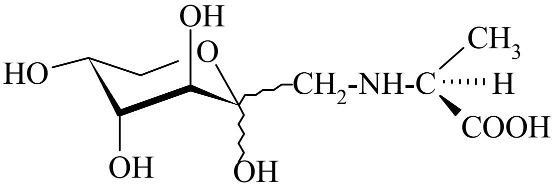
N-[(2*S*)-(5-amino-5-carboxypentyl)]-L-glutamic acid (PIN)



(2*S*)-2-amino-3-methylbutyl L-valinate (PIN)



N-{(2*R*)-2-amino-4-[(3*R*)-3-hydroxy-2-oxoazetidin-3-yl]butanoyl}-L-threonine (PIN)

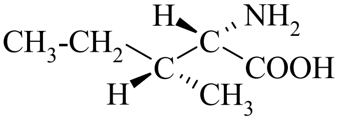
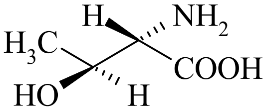


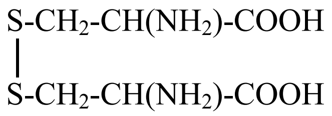
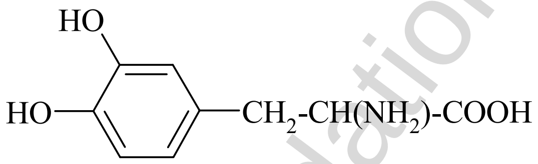
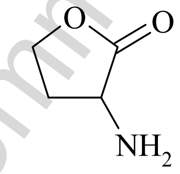
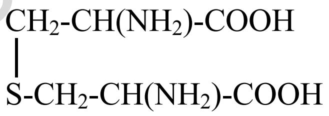
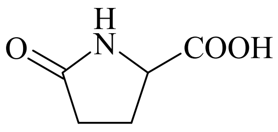
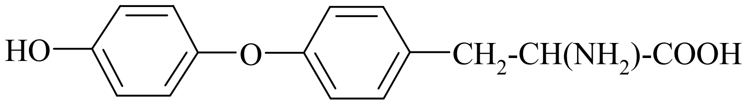
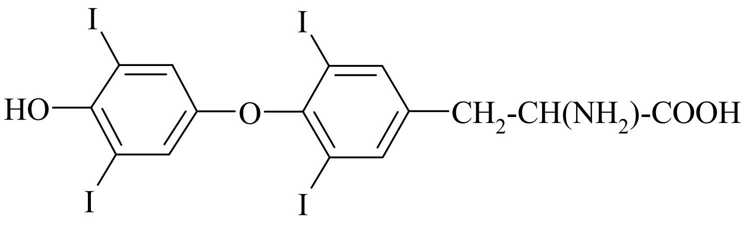
N-(1-deoxy-D-fructopyranos-1-yl)-L-alanine (PIN)

P-103.1.2.6 Other retained names

Several other trivial names are used in addition to those listed in Table 10.3. A few of them and their symbols are described in Table 10.4. They are used as preferred IUPAC names; they can be functionalized and substituted as shown in sections P-1.2. Stereodescriptors D, L and DL are used as required. The L configuration of alloisoleucine and allothreonine is shown. The publication 'Nomenclature and symbolism for amino acids and peptides' (ref. 23) must be consulted for the complete description of the use of less common amino acids.

Table 10.4 Amino acids with trivial names (other than those listed in Table 10.3)

Retained name	*Symbol*	*Structure*
β-alanine (PIN)	(βAla)	$H_2N-CH_2-CH_2-COOH$
alloisoleucine (PIN)	aIle	
allothreonine (PIN)	aThr	
allysine (PIN)	---	$HCO-[CH_2]_3-CH(NH_2)-COOH$
citrulline (PIN)	Cit	$NH_2-CO-NH-[CH_2]_3-CH(NH_2)-COOH$
cystathionine (PIN)	Al | HCy	$CH_2-CH(NH_2)-COOH$ | $S-[CH_2]_3-CH(NH_2)-COOH$
cysteic acid (PIN)	Cya	$^{-}O_3S-CH_2-CH(NH_2)-COOH$

cystine (PIN)	Cys | Cys	 $\begin{array}{l} S\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH \\ \vert \\ S\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH \end{array}$
dopa (PIN)	----	
homocysteine (PIN)	Hcy	$HS\text{-}CH_2\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$
homoserine (PIN)	Hse	$HO\text{-}CH_2\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH$
homoserine lactone (PIN)	Hsl	
lanthionine (PIN)	Ala | Cys	 $\begin{array}{l} CH_2\text{-}CH(NH_2)\text{-}COOH \\ \vert \\ S\text{-}CH_2\text{-}CH(NH_2)\text{-}COOH \end{array}$
ornithine (PIN)	Orn	$H_2N\text{-}[CH_2]_3\text{-}CH(NH_2)\text{-}COOH$
5-oxoproline (PIN)	Glp	
sarcosine(PIN)	Sar	$CH_3\text{-}NH\text{-}CH(NH_2)\text{-}COOH$
thyronine (PIN)	-----	
thyroxine (PIN)	Thx	

P-103.2 Substitutive names of amino acids and derivatives

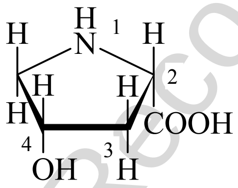
Names of derivatives of amino acids described in P-103.1 other than salts, esters and formed by *N*, *O* or *S* substitution are formed substitutively. Preferred names are constructed in accordance with principles, rules and conventions recommended for the formation of systematic substitutive names.

P-103.2.1 Carbon substitution
P-103.2.2 Substituent groups
P-103.2.3 Amides, anilides and hydrazides
P-103.2.4 Aldehydes, alcohols and ketones

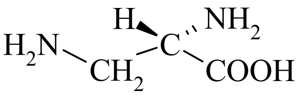
P-103.2.1 Carbon substitution

Preferred IUPAC names of amino acids substituted on carbon atoms are systematic substitutive names. CIP stereodescriptors are used.

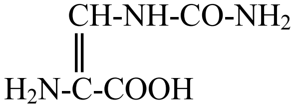
Examples:



pyrrolidine-2-carboxylic acid (PIN)
(2*S*,4*S*)-4-hydroxyproline (PIN)
(4*S*)-4-hydroxy-L-proline
cis-4-hydroxy-L-proline

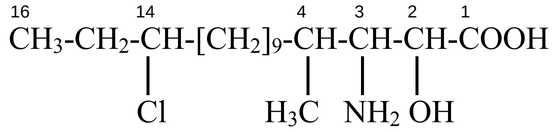


(2*S*)-2,3-diaminopropanoic acid (PIN)
L-2,3-diaminopropanoic acid
(2*S*)-2-amino-β-alanine (see ref. 49)
3-amino-L-alanine



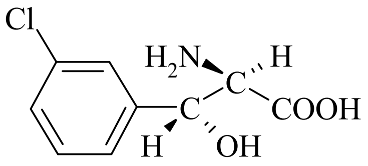
$$\begin{array}{ll} & \mathrm{CH\text{-}NH\text{-}CO\text{-}NH_2} \\ & \| \\ \mathrm{H_2N\text{-}} & \mathrm{C\text{-}COOH} \end{array}$$

(2*E*)-3-(carbamoylamino)-2-aminoprop-2-enoic acid (PIN)
(2*E*)-2,3-didehydro-3-ureido-L-alanine (see ref. 49)

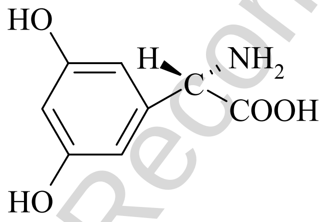


$$\overset{16}{\mathrm{CH_3}}\text{-}\mathrm{CH_2}\text{-}\underset{\substack{|\\ \mathrm{Cl}}}{\overset{14}{\mathrm{CH}}}\text{-}[\mathrm{CH_2}]_9\text{-}\underset{\substack{|\\ \mathrm{H_3C}}}{\overset{4}{\mathrm{CH}}}\text{-}\underset{\substack{|\\ \mathrm{NH_2}}}{\overset{3}{\mathrm{CH}}}\text{-}\underset{\substack{|\\ \mathrm{OH}}}{\overset{2}{\mathrm{CH}}}\text{-}\overset{1}{\mathrm{COOH}}$$

(2ξ,3ξ,4ξ,14ξ)-3-amino-14-chloro-2-hydroxy-4-methylhexadecanoic acid (PIN)
3-[(1ξ,14ξ)-11-chloro-1-methyltridecyl]-2-hydroxy-β-alanine



(2*R*,3*R*)-2-amino-3-(3-chlorophenyl)-3-hydroxypropanoic acid (PIN)
3-chloro-(*R*)-β-hydroxy-D-tyrosine



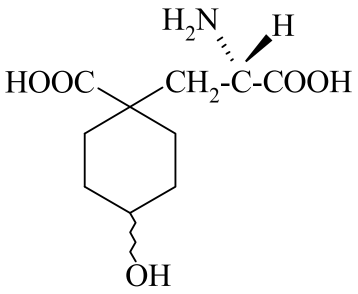
(2*S*)-2-amino-3-(3,5-dihydroxyphenyl)acetic acid (PIN)
L-(3,5-dihydroxyphenyl)glycine

P-103.2.2 Substituent groups

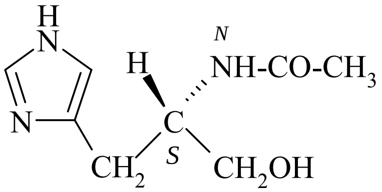
P-103.2.1.1 Substituent groups with the free valence on a carbon atom

Preferred IUPAC names are formed by the rules, principles and conventions of substitutive nomenclature when α-amino carboxylic acids must be cited as substituent groups in presence of characteristic groups having seniority for citation as suffix.

Examples:



1-[(2*S*)-2-amino-2-carboxyethyl]-4ξ-hydroxycyclohexane-1-carboxylic acid (PIN)



N-[(2*S*)-1-hydroxy-3-(1*H*-imidazol-4-yl)propan-2-yl]acetamide (PIN)

P-103.2.1.2 Substituent groups with the free valence on a nitrogen atom

Preferred IUPAC names are formed by the rules, principles and conventions of substitutive nomenclature when α-amino carboxylic acids must be cited as substituent groups in presence of characteristic groups having seniority for citation as suffix.

Substituent groups derived by subtracting a hydrogen atom from the amino group of an amino acid may also named by changing the ending ‘e’ into ‘o’ in names of appropriate amino acids, by adding the letter ‘o’ to tryptophan and by constructing the names asparto and glutamo, from aspartic acid and glutamic acid, respectively (see 3AA-7, ref. 23).

Examples:

–HN-CH_2-COOH	glycino (carboxymethyl)amino (PIN)

When there is more than one nitrogen atom in the amino acid, the use of a locant of the form N^x with a superscript is recommended.

Examples:

–HN-$[CH_2]_4$-CH(NH_2)-COOH

N^6-lysino
(4-amino-5-carboxypentyl)amino (PIN)

–HN-C(=NH)-NH-$[CH_2]_3$-CH(NH_2)-COOH

N^ω-arginino
N′-[(3-amino-4-carboxybutyl)amino]carbamimidamido (PIN) (see P-66.1.5.4.2)

–HN-CO-$[CH_2]_2$-CH(NH_2)-COOH

N^5-glutamino
(4-amino-4-carboxy)butanamido (PIN)

P-103.2.1.3 Substituent groups with the free valence on an oxygen or sulfur atom

Preferred IUPAC names are formed by the rules, principles and conventions of substitutive nomenclature when α-amino carboxylic acids must be cited as substituent groups in presence of characteristic groups having seniority for citation as suffix.

Substituent groups formed by subtraction of a hydrogen atom from an oxygen or sulfur atom may also be named by changing the final letter ‘e’, when appropriate, into ‘*x*-yl’, *x* being the locant of the atom from which the hydrogen atom has been subtracted, for example cystein-*S*-yl, threonin-O^3-yl, alanin-3-yl, or by adding ‘*x*-yl’ to aspartic, glutamic and tryptophan, for example aspartic-2-yl, tryptophan-2-yl.

Example:

$–S-CH_2-CH(NH_2)-COOH$

cystein-*S*-yl
(2-amino-2-carboxyethyl)sulfanyl (PIN)

P-103.2.3 Amides, anilides, hydrazides and analogous derivatives

Preferred IUPAC names of amides, anilides, hydrazides and analogous derivatives derived from amino acids are systematic substitutive names.

Names of amides derived from amino acids are formed by changing the final letter ‘e’ in the names of amino acids, when appropriate, into ‘amide’ or adding the term ‘amide’ to the name tryptophan.

Examples:

$H_2N-CH_2-CO-NH_2$	2-aminoacetamide (PIN) glycinamide

Note that the 4-amide of aspartic acid has its own name, asparagine, and the 5-amide of glutamic acid is glutamine. Their 1-amides are named aspartic 1-amide and glutamic 1-amide, respectively.

Preferred IUPAC names of anilides are formed by *N* substitution of the amide group by a phenyl group or substituted phenyl group. The ending ‘anilide’, in place of ‘amide’, may be used in general nomenclature.

Example:

$H_2N-CH_2-CO-NH-C_6H_5$	2-amino-1-*N*-phenylacetamide (PIN) glycinanilide

Substitution on nitrogen atoms in amides of amino acids is expressed by the methods described for amides (P-66.1.1.3) and amines (P-62.2.1.1.2).

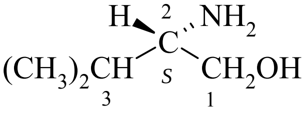
Examples:

$CH_3-NH-CH_2-CO-NH-CH_2-CH_3$	1-*N*-ethyl-2-(methylamino)acetamide (PIN)
$CH_3-CO-NH-CH_2-CO-NH_2$	2-(acetylamino)acetamide (PIN)

P-103.2.4 Alcohols, aldehydes, and ketones

Preferred IUPAC names of alcohols, aldehydes and ketones corresponding to amino acids with retained trivial names are formed systematically by using the principles, rules and conventions of substitutive nomenclature. The endings ‘ol’ and ‘al’ added to the retained names, with elision of the final letter ‘e’, may be used in general nomenclature. Stereoisomers are denoted by ‘*R*’ and ‘*S*’ stereodescriptors.

Examples:



(*S*)-2-amino-3-methylbutan-1-ol (PIN)
valinol

$(CH_3)_2CH\text{-}CH_2\text{-}CH(NH_2)\text{-}CHO$

2-amino-4-methylpentanal (PIN)
leucinal

$H_2N\text{-}CH_2\text{-}CO\text{-}CH_2Cl$

1-amino-3-chloropropan-2-one (PIN)

P-103.3 Nomenclature of peptides

Nomenclature of peptides is highly specialized and well documented in reference 19.

P-103.3.1 Names of peptides

To name peptides, the names of acyl groups ending in ‘yl’ (see P-103.2.6) are used. Thus if the amino acids glycine, $H_2N\text{-}CH_2\text{-}COOH$, and alanine, $H_2N\text{-}CH(CH_3)\text{-}COOH$, condense so that glycine acylates alanine, the dipeptide formed, $H_2N\text{-}CH_2\text{-}CO\text{-}NH\text{-}CH(CH_3)\text{-}COOH$, is named glycylalanine. If they condense in the reverse order, the product $H_2N\text{-}CH(CH_3)\text{-}CO\text{-}NH\text{-}CH_2\text{-}COOH$ is named alanylglycine. Higher peptides ane named similarly, e.g. alanylleucyltryptophan.

P-103.3.2 Symbols of peptides

The peptide glycylglycylclycine is symbolized Gly-Gly-Gly. This involves modifying the symbols Gly for glycine, $H_2N\text{-}CH_2\text{-}COOH$, by adding hyphens to it, in three ways:

(a) Gly- = $H_2N\text{-}CH_2\text{-}CO–$
(b) -Gly = $–HN\text{-}CH_2\text{-}COOH$
(c) -Gly- = $–HN\text{-}CH_2\text{-}CO–$

Thus the hyphen, which represents the peptide bond, removes a –OH group from the –COOH group of the amino acid when written on the right of the symbol, and a hydrogen atom, when written on the left of the symbol.

P-103.3.3 Indication of configuration in peptides

The stereodescriptor ‘L’ is not indicated in the symbols of peptides. To the contrary, stereodescriptor ‘D’ is indicated at the front of the acyl group or name of each component having that configuration. When present, symbols for less common amino acids are always preceded by the stereodescriptor ‘D’ or ‘L’.

Example:

Leu-D-Glu-L-aThr-D-Val-Leu (the symbol aThr is for allothreonine)

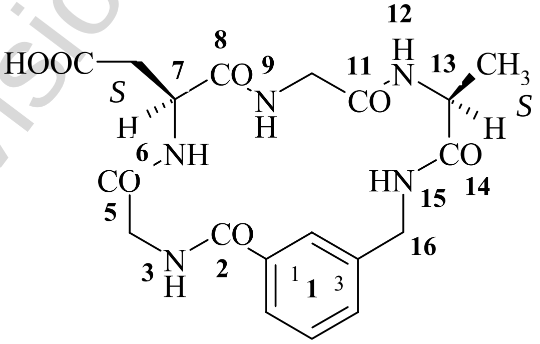
P-103.3.4 Cyclic peptides

Names of cyclic peptides are composed of the name of the peptide preceded by the prefix ‘cyclo’. The symbolic representation, placed in parentheses, is also preceded by the prefix ‘cyclo’. Stereodescriptors ‘D’ are cited in peptides composed entirely of amino acid residues with regular peptide bonds (eupeptide linkage) (see ref. 49). Synthetic cyclopeptides require stereodescriptors ‘*R*’ and ‘*S*’ when symbols of amino acid residues are not used.

Preferred IUPAC names are systematic substitutive names.

Examples:

cyclo-(leucyl-D-phenylalanyl-prolyl-valyl-ornithyl-leucyl-D-phenylalanyl-prolyl-valyl-ornithyl-)
cyclo-(Leu-D-Phe-Pro-Val-Orn-Leu-D-Phe-Pro-Val-Orn-)



2-[(7*S*,13*S*)-2,5,8,11,14-pentoxo-3,6,9,12,15-pentaaza-1(1,3)-benzenacyclohexadecaphan-7-yl]acetic acid (PIN)

The prefixes ‘endo’ and ‘des’ used in peptide nomenclature deserve a special mention, as ‘endo’ is used in a different context and ‘des’ with a different meaning than in the nomenclature of organic compounds.

P-103.3.5 The prefix 'endo'.

In peptide nomenclature, the prefix 'endo' (nonitalic) is used to denote the insertion of an amino acid residue in a well identified position in the peptide. For example, the name endo-4a-tyrosine-angiotensin II means that the the amino acid residue 'tyrosyl' has been inserted between the positions 4 and 5 in the structure of tyrosine. The prefix 'endo' is not to be confused with the recommended stereodescriptor '*endo*' (written in italics) described in P-92.2.1.2.

P-103.3.6 The prefix 'des'

The subtractive prefix 'des', in peptide nomenclature, is used to denote the removal of an amino acid residue from any position in a peptide structure. For example, the name des-7-proline-oxytocin means that the amino-acid residue 'prolyl', located in position 7 of the peptide oxytocin, has been removed. In the modification of parent structures described in Section P-101, the prefix 'des' is used to indicate the removal of a terminal ring in steroids with the addition of the appropriate number of hydrogen atoms at each junction with the adjacent ring (see P-101.3.6).

P-104 Cyclitols

P-104.1 Definitions

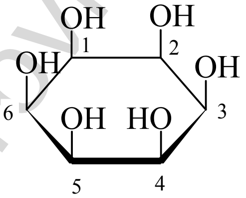
Cyclitols are cycloalkanes in which three or more ring atoms are each substituted with one hydroxyl group. Inositols, cyclohexane-1,2,3,4,5,6-hexols, are a specific group of cyclitols.

Preferred IUPAC names are retained names of inositols and *O*-alkyl, aryl and acyl derivatives.

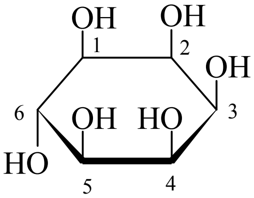
P-104.2 Name construction

Various methods are recommended for naming cyclitols.

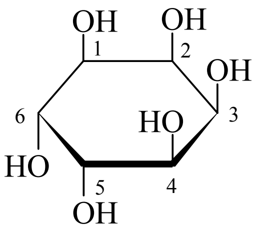
P-104.2.1 Stereoisomeric inositols are described by adding italicized prefixes at the front of the name 'inositol'. Positional numbers described in P-104.2.3 are shown in parentheses. Names denoted by the prefixes are preferred IUPAC names.



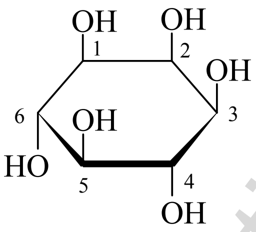
cis-inositol (PIN)
(1,2,3,4,5,6/0-)



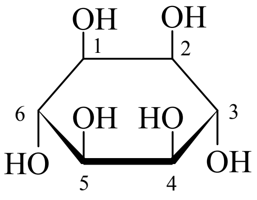
epi-inositol (PIN)
(1,2,3,4,5/6-)



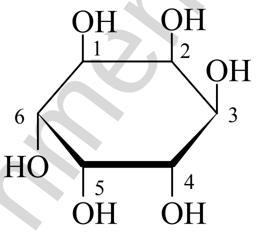
allo-inositol (PIN)
(1,2,3,4/5,6-)



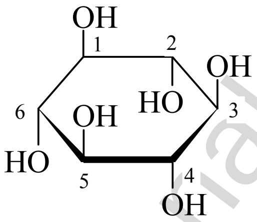
myo-inositol (PIN)
(1,2,3,5/4,6-)



muco-inositol (PIN)
(1,2,4,5/3,6-)

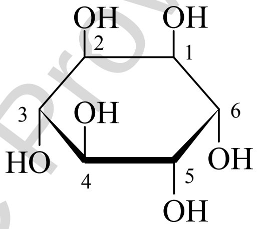


neo-inositol (PIN)
(1,2,3/4,5,6-)

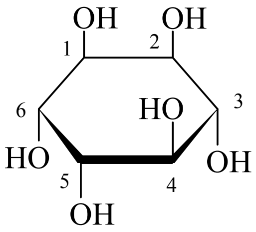


scyllo-inositol (PIN)

(1,3,5/2,4,6-)



1D-*chiro*-inositol (PIN)
(1,2,4/3,5,6-)
(formerly D-*chiro*-inositol
or (+)-inositol)

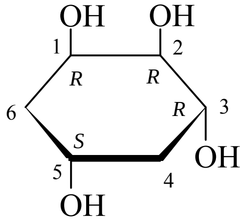


1L-*chiro*-inositol (PIN)
(1,2,4/3,5,6-)
(formerly L-*chiro*-inositol
or (−)-inositol)

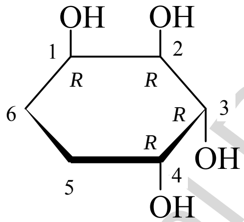
The absolute configuration is denoted by 'D' and 'L' are determined in the following way. For the planar ring representation where the hydroxy group numbered 1 is above the plane of the ring, the configuration 'L' corresponds to a clockwise numbering, and the configuration 'D' corresponds to an anticlockwise numbering, as illustrated by the two enantiomeric *chiro*-inositols.

P-104.2.2 Cyclitols, with the exception of inositols, are named systematically based on the parent hydride cyclohexane by using the CIP method and its sequence rules for describing stereoisomers. This method is preferred to the method of positional numbers described in P-104.2.3.

Examples:



(1*R*,2*R*,3*R*,5*S*)-cyclohexane-1,2,3,5-tetrol (PIN)



(1*R*,2*R*,3*R*,4*R*)-cyclohexane-1,2,3,4-tetrol (PIN)

P-104.2.3 Locants are assigned to hydroxy groups in cyclitols, and thus the direction of numbering is described, with reference to the steric relations and nature of the substituents attached to the ring. The substituents lying above the plane of the ring constitute a set, and those lying below another set. Lowest locants are related to one set of the substituents according to the following criteria, which are applied successively until a decision is reached.

(a) to the substituents considered as a numerical series, without regard to configuration;

(b) if one set of the substituents is more numerous than the other, to the more numerous;

(c) if the set are equally numerous and one of them can be denoted by lower numbers, to that set;

(d) to substituents other than unmodified hydroxyl groups;

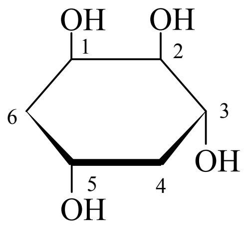
(e) to the substituent first cited in the alphanumerical order;

(f) to those designations that lead to an L rather than a D configuration, as determined by method (1) above (applies to meso compounds only)

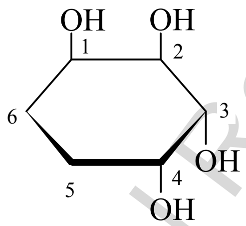
(g) the positional numbers are described by means of the numerator consisting of the set of substituents with the lowest locants, arranged in ascending order. The denominator is the other set. The fraction is denoted by the solidus (/) symbol.

Preferred IUPAC names are formed by the method in P-104.4.2.

Examples:



1L-1,2/3,5-cyclohexanetetrol
(1*R*,2*R*,3*R*,5*S*)-cyclohexane-1,2,3,5-tetrol (PIN)



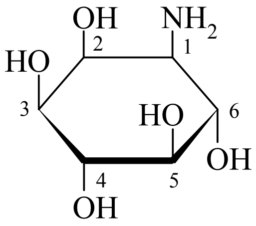
1L-1,2/3,4-cyclohexanetetrol
(1*R*,2*R*,3*R*,4*R*)-cyclohexane-1,2,3,4-tetrol (PIN)

P-104.3 Derivatives of cyclitols

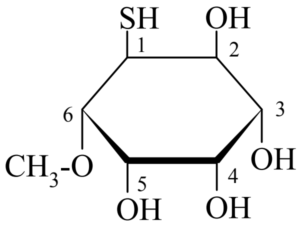
P-104.3.1 Derivatives of inositols

Inositols are modified in the same way as carbohydrates to generate preferred IUPAC names for their derivatives. There is no limit to *O*-substitution by alkyl (aryl) and acyl groups (see P-102.5.6.1). Hydroxy groups can be exchanged for amino groups using the 'deoxy' operation (see P-102.5.6.4). When characteristic groups that are senior to hydroxyl groups are put in the place of a hydroxyl group, fully substitutive names must be constructed. The numbering of the inositol remains unchanged and the configuration is expressed by an 'L' or 'D' stereodescriptor.

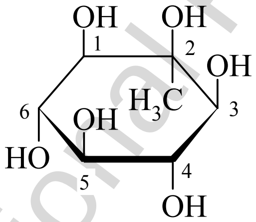
Examples:



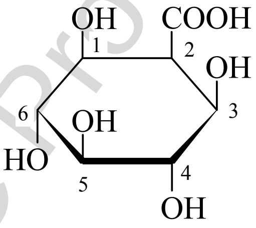
1L-1-amino-1-deoxy-*myo*-inositol (PIN)



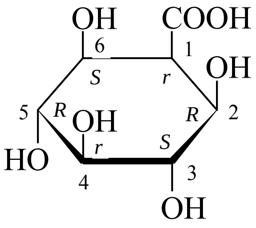
1L-1-deoxy-6-*O*-methyl-1-sulfanyl-*chiro*-inositol
(not 1L-6-*O*-methyl-1-thio-*chiro*-inositol)
(1*S*,2*S*,3*R*,4*S*,5*S*,6*S*)-6-methoxy-1-sulfanylcyclohexane-2,3,4,5-tetrol (PIN)



2-methyl-*myo*-inositol
(1*R*,2*S*,3*S*,4*R*,5*R*,6*S*)-2-methylcyclohexane-1,2,3,4,5,6-hexol (PIN)



I



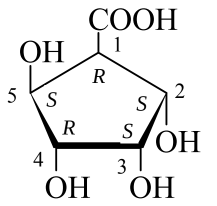
II

I 2-carboxy-2-deoxy-*myo*-inositol
II (1*r*,2*R*,3*S*,4*r*,5*R*,6*S*)-2,3,4,5,6-pentahydroxycyclohexane-1-carboxylic acid (PIN)

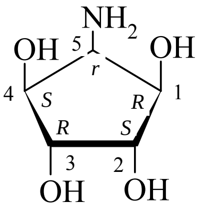
P-104.3.2 Derivatives of cyclitols other than inositols

Preferred names of derivatives of cyclitols other than inositols are all constructed by applying the principles, rules and conventions of substitutive nomenclature described in Chapters 1 to 9.

Examples:



(1*R*,2*S*,3*S*,4*R*,5*S*)-2,3,4,5-tetrahydroxycyclopentane-1-carboxylic acid (PIN)

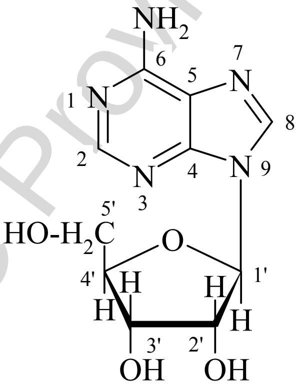


(1*R*,2*S*,3*R*,4*S*,5*r*)-5-aminocyclopentane-1,2,3,4-tetrol (PIN)

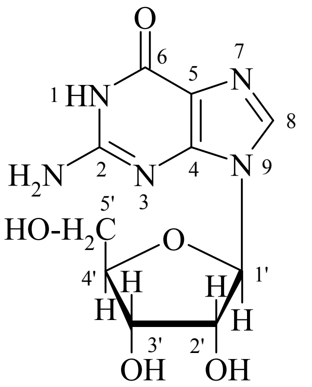
P-105 Nucleosides

Nucleosides are ribosyl or deoxyribosyl derivatives of the pyrimidine or purine bases adenine, guanine, xanthine, thymine, cytosine, and uracil, which are all retained names and are all preferred IUPAC names.

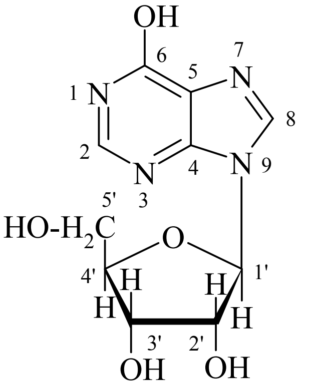
P-105.1 The following names are retained and recommended as preferred IUPAC names.



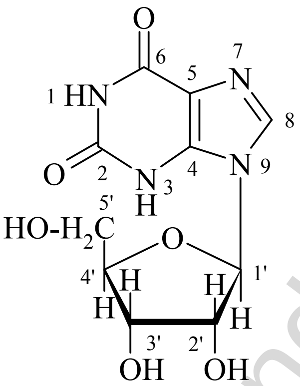
adenosine (PIN)



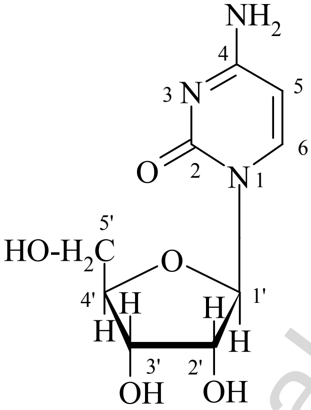
guanosine (PIN)



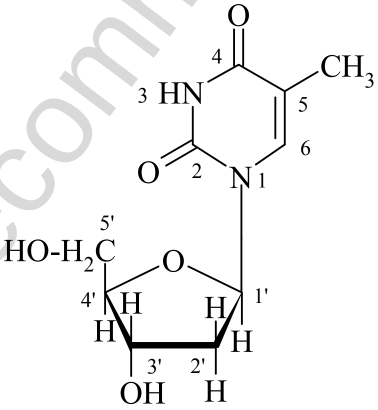
inosine (PIN)



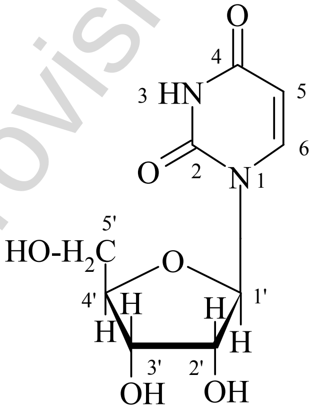
xanthosine (PIN)



cytidine (PIN)



thymidine (PIN)

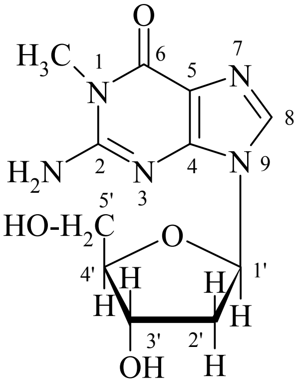


uridine (PIN)

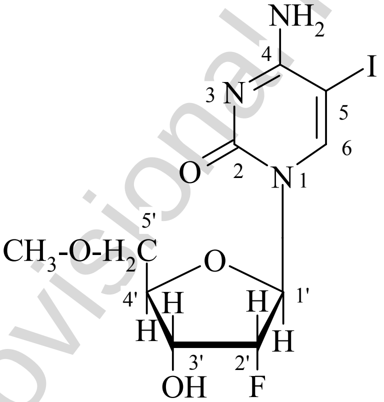
P-105.2 Substitution on nucleosides

P-105.2.1 Nucleosides having retained names can be fully substituted on the purine or pyrimidine ring. Replacement of oxo groups of nucleosides is described by functional replacement prefixes. The ribofuranosyl component may be modified as prescribed for carbohydrates (see P-102.5). 2′- and 3′- deoxyribose modificationsof the ribose component are allowed in preferred IUPAC names.

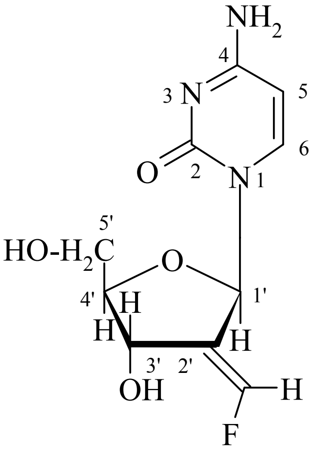
Examples:



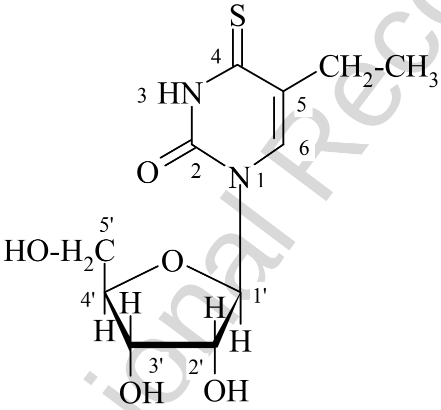
2′-deoxy-1-methylguanosine (PIN)



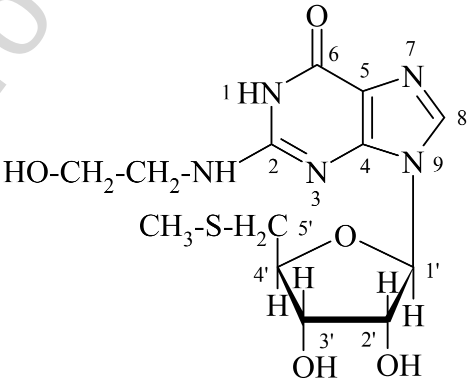
2′-deoxy-2′-fluoro-5-iodo-5′-*O*-methylcytidine
4-amino-1-[(2R,3R,4R,5R)-3-fluoro-4-hydroxy-5(hydroxymethyl)oxolan-2-yl]-5-iodopyrimidin-2(1*H*)-one (PIN)



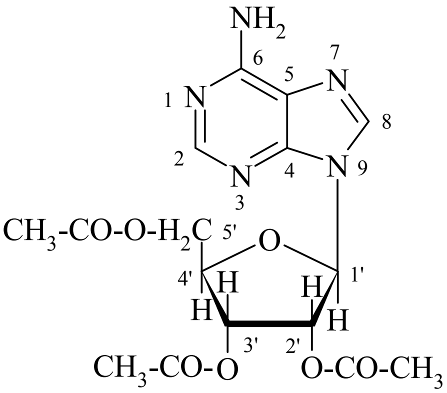
(2′*E*)-2′-deoxy-2′-(fluoromethylidene)cytidine (PIN)
4-amino-1-(2R,3*E*,4S,5R)-4-hydroxy-5(hydroxymethyl)-2-(fluoromethylidene)oxolan-2-yl]pyrimidin-2(1*H*)-one (PIN)



5-ethyl-4-thiouridine (PIN)



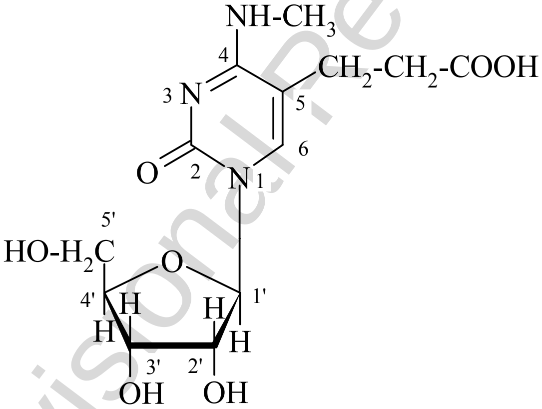
N-(2-hydroxyethyl)-5′-*S*-methyl-5′-thioguanosine (PIN)



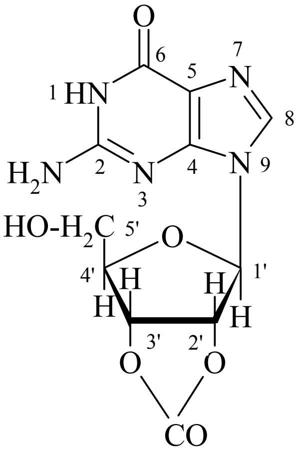
2′,3′,5′-tri-*O*-acetylguanosine (PIN)
guanosine 2′,3′,5′-triacetate

P-105.2.2 In the presence of a characteristic group higher than (pseudo) ketone, normal substitutive nomenclature principles are applied.

Example:



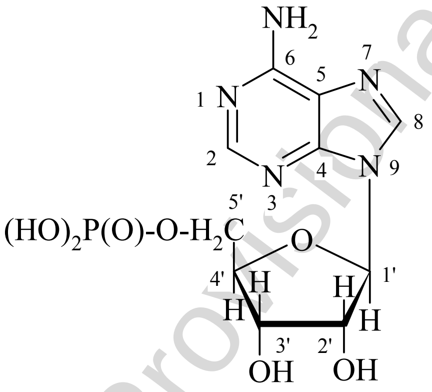
3-[4-(methylamino)-2-oxo-1-β-D-ribofuranosyl-1,2-dihydropyrimidin-5-yl]propanoic acid (PIN)



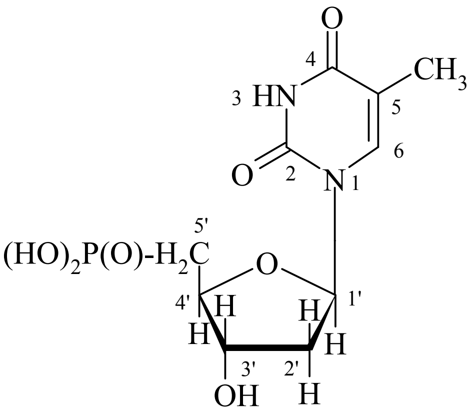
2′,3′-dideoxyguanosine-2′,3′-diyl carbonate (PIN, see P-101.7.4)
adenosine cyclic-2′,3′-carbonate

P-106 Nucleotides

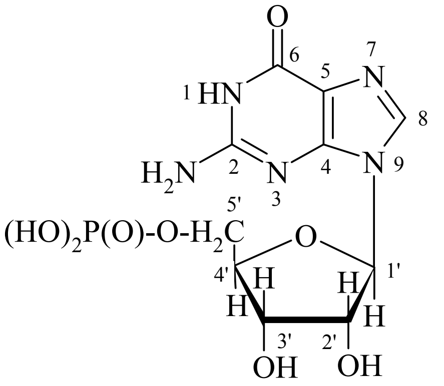
P-106.1 The following traditional names are retained to be used as preferred IUPAC names for esters of nucleosides with phosphoric acid. The primed locant of the ribosyl component is cited to locate the position of the phosphate group.



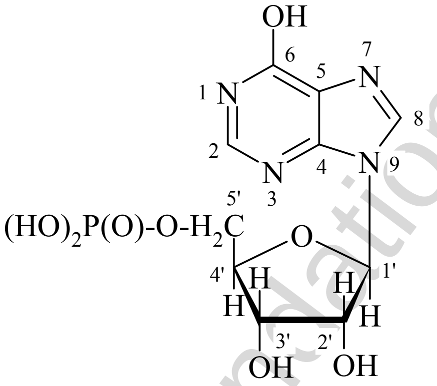
5′-adenylic acid (PIN)



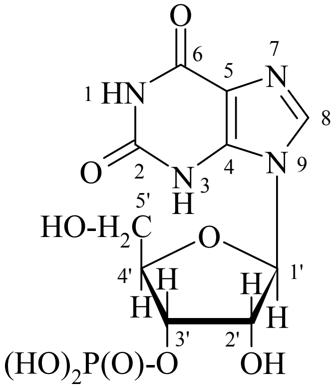
5′-thymidylic acid (PIN)



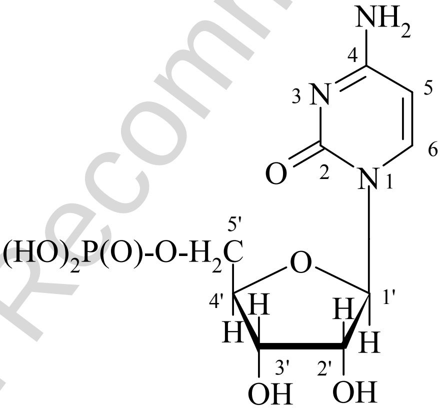
5′-guanylic acid (PIN)



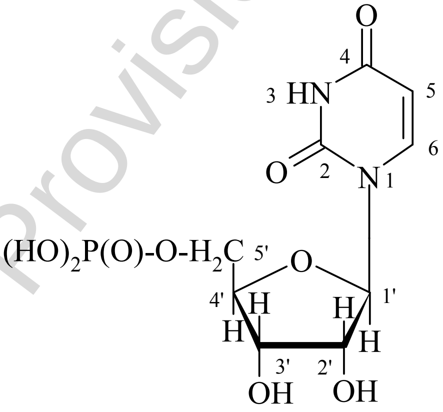
5′-inosinic acid (PIN)



3′-xanthylic acid (PIN)



5′-cytidylic acid (PIN)

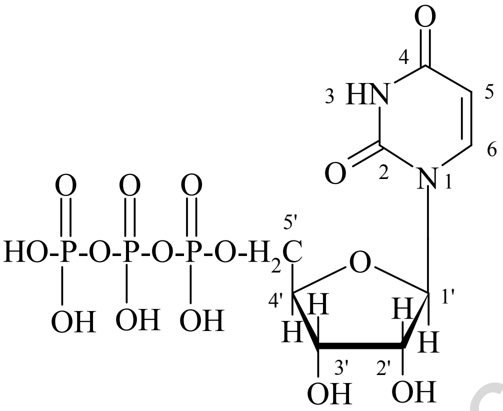


5′-uridylic acid (PIN)

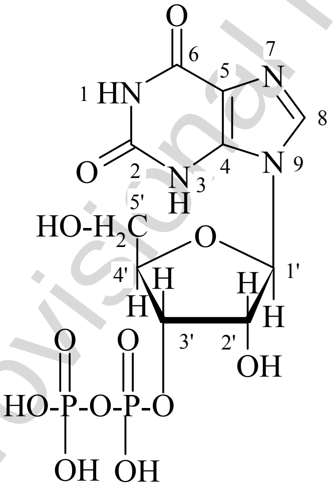
P-106.2 Nucleotide diphosphates and triphosphates

Diphosphate, triphosphate, etc. esters of nucleosides are named by citing a phrase such as diphosphate, after the name of the nucleoside. Preferred IUPAC names must indicate the presence of the hydrogen atoms on the diphosphate, triphosphate, etc. component of the molecule. Parentheses are used to avoid ambiguity.

Examples:



uridine 5′-(tetrahydrogen triphosphate) (PIN)

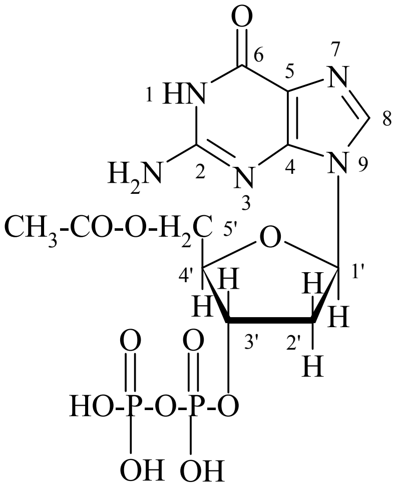


xanthine 3′-(trihydrogen phosphate) (PIN)

P-106.3 Derivatives of nucleotides

P-106.3.1. Derivatives of nucleotides having retained names are named in the same manner as the corresponding nucleoside, i.e., they can be fully substituted on the purine or pyrimidine ring and the ribofuranosyl component may be modified as prescribed for carbohydrates (see P-102.5). 2′- and 3′- deoxyribose modificationsof the ribose component are allowed in preferred IUPAC names.

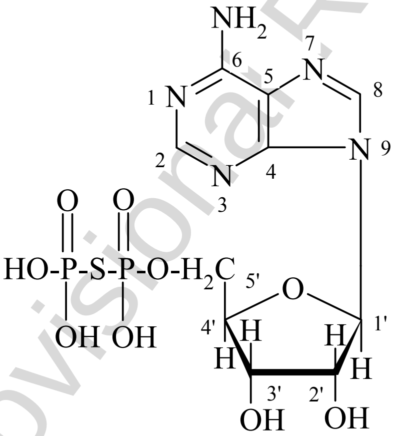
Examples:



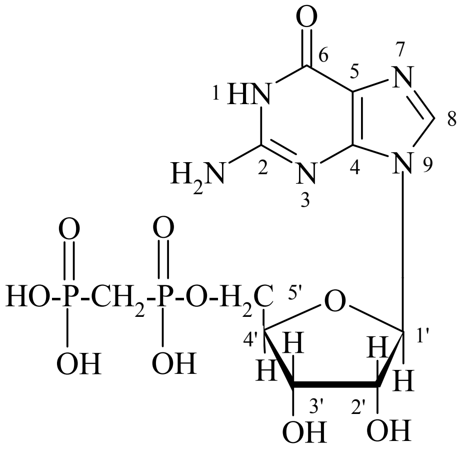
2′-deoxy-5′-*O*-acetylguanosine 3′-(trihydrogen diphosphate) (PIN)

P-106.3.2 Analogues of nucleoside di- and polyphosphates can be named by the functional replacement techniques applicable to di- and polyphosphoric acids (see P-67.2).

Examples:



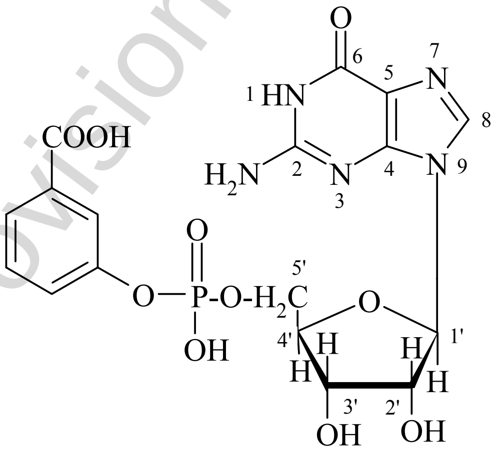
adenosine 5′-(trihydrogen 2-thiodiphosphate) (PIN)



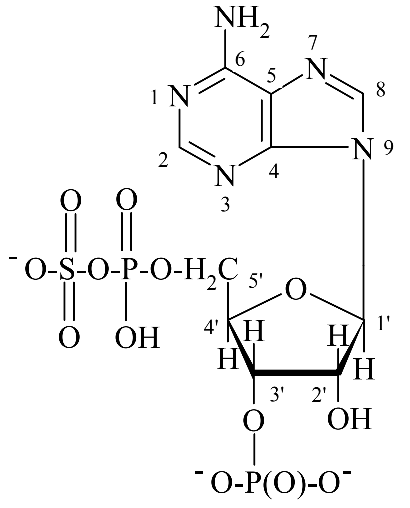
guanosine 5′-(trihydrogen methylenediphosphonate) (PIN)
guanosine 5′-(trihydrogen 2-carbadiphosphate)
(this name preserves the integrity of the nucleotide name; see P-101.4.3)

P-106.3.3 In the presence of a characteristic group higher than the phosphoric acid residue, normal substitutive nomenclature principles may be applied. Substitutive prefix names may be derived from the traditional names for the nucleotide monophosphates by replacing the 'ic acid' ending with 'yl', for example, adenylyl and cytidylyl. Note that the substituent prefix name from inosinic acid is an exception; it is named inosinylyl so that the ending is like the other substituent prefix names derived from the nucleotide monophosphates.

Examples:



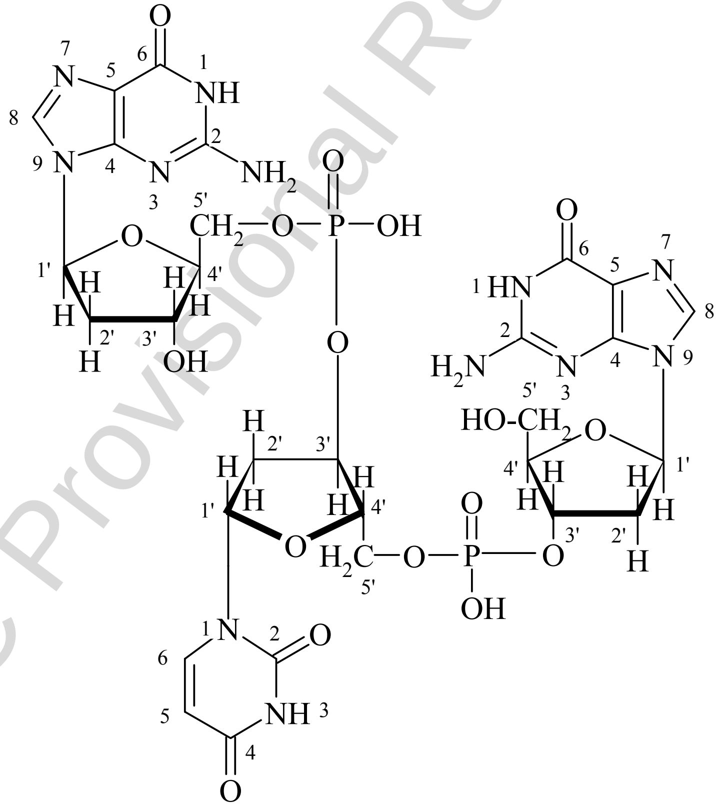
3-(5′-guanylyloxy)benzoic acid (PIN)



3′-*O*-phosphonato-5′-adenylyl sulfate (PIN)
3′-phospho-5′-adenylyl sulfate

P-106.3.4 Oligonucleotides are named using the prefix names derived from the traditional names for the nucleotides.

Example:



2′-deoxyguanylyl-(3′→5′)-2′-deoxyuridinylyl-(3′→5′)-2′-deoxyguanosine (PIN)

P-107 Lipids

P-107.1 Definitions

‘Lipids’ is a loosely defined term for substances of biological origin that are soluble in nonpolar solvents. They consist of saponifiable lipids, such as ‘glycerides’ (fats and oils) and ‘phospholipids’, as well as nonsaponifiable lipids, specifically ‘steroids’.

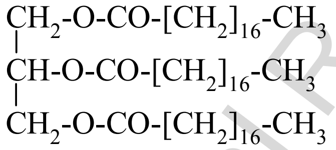
The nomenclature of glycerides, phospholipids and glycolipids has been published in 1976 (ref. 46); the nomenclature of glycolipids was revised in 1997 (ref. 47).

Preferred IUPAC names for individual substances are formed by using substitutive nomenclature with CIP stereodescriptors.

P-107.2 Glycerides

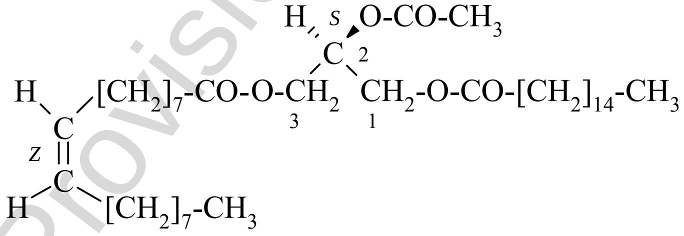
Glycerides are esters of glycerol (propane-1,2,3-triol) with fatty acids. They are by long established custom subdivided into triglycerides, 1,2- or 1,3-diglycerides, and 1- or 2-monoglycerides, according to the number and position of acyl groups. The recommended method for naming individual glycerides is mono-, di- or tri-*O*-acylglycerol. The name glycerol is allowed in general nomenclature to name organic compounds; it is however the preferred name in the field of natural products.

Examples:



$$\begin{array}{l} CH_2\text{-O-CO-}[CH_2]_{16}\text{-}CH_3 \\ | \\ CH\text{-O-CO-}[CH_2]_{16}\text{-}CH_3 \\ | \\ CH_2\text{-O-CO-}[CH_2]_{16}\text{-}CH_3 \end{array}$$

tri-*O*-octadecanoylglycerol
propane-1,2,3-triyl trioctadecanoate (PIN)



(2*S*)-2-*O*-acetyl-1-*O*-hexadecanoyl-3-*O*-(9*Z*)-octadec-9-enoylglycerol
(numbering shown)
(2*S*)-2-*O*-acetyl-1-*O*-oleoyl-3-*O*-palmitoylglycerol
(2*S*)-propane-1,2,3-triyl 2-acetate-1-hexadecanoate-3-[(9*Z*)-octadec-9-enoate] (PIN)

P-107.3 Phospholipids

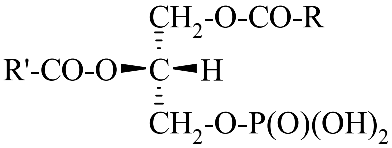
Phospholipids are lipids containing phosphoric acid as mono- or diesters, including ‘phosphatidic acids’ and ‘phosphoglycerides’.

Phosphatidic acids are derivatives of glycerol in which one hydroxyl group, commonly but not necessarily primary, is esterified with phosphoric acid, and the other two hydroxyl groups are esterified with fatty acids.

Phosphoglycerides are phosphoric diesters, esters of phosphatidic acids, generally having a polar head group (–OH or $-NH_2$) on the esterified alcohol which typically is 2-aminoethanol (not ethanolamine), choline, glycerol, inositol, serine. The term includes ‘lecithins’ and ‘cephalins’.

P-107.3.1 Phosphatidic acids

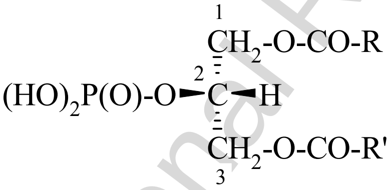
P-107-3.1.1 Phosphatidic acids have the following generic structure:



$$\begin{array}{c} CH_2\text{-O-CO-R} \\ \text{R'-CO-O}\blacktriangleright C \blacktriangleleft H \\ CH_2\text{-O-P(O)(OH)}_2 \end{array}$$

3-*sn*-phosphatidic acid
(for a discussion and examples of the symbol ‘*sn*’ see P-107.3.1.2)

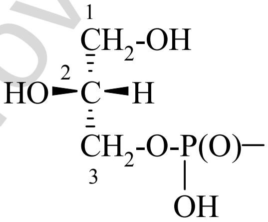
In general, the 3-*sn*-phosphatic acids are simply called phosphatidic acids.



$$\begin{array}{c} \overset{1}{C}H_2\text{-O-CO-R} \\ (HO)_2P(O)\text{-O}\blacktriangleright \overset{2}{C} \blacktriangleleft H \\ \underset{3}{C}H_2\text{-O-CO-R'} \end{array}$$

2-phosphatidic acid

The name of the monovalent acyl group:



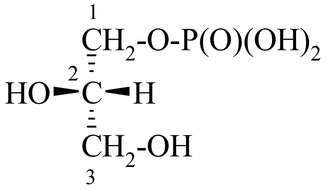
$$\begin{array}{c} \overset{1}{C}H_2\text{-OH} \\ HO\blacktriangleright \overset{2}{C} \blacktriangleleft H \\ \underset{3}{C}H_2\text{-O-}\underset{\displaystyle OH}{\underset{|}{P}}\text{(O)–} \end{array}$$

is ‘phosphatidyl’, a retained name used in general nomenclature.

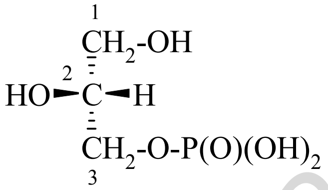
P-107.3.1.2 Configuration of phosphatidic acids

In order to designate the configuration of glycerol derivatives, the carbon atoms of glycerol are numbered stereospecifically. The carbon atom that appears on top of that Fischer projection that shows a vertical carbon chain with the hydroxy group at carbon 2 to the left is designated as C-1.

To differentiate such numbering from conventional numbering, which conveys no steric information, the stereodescriptor '*sn*' (for stereospecifically numbered) is used. This descriptor is written in lower case italic letters, even at the beginning of a sentence, immediately preceeding the glycerol term, from which it is separated by a hyphen. The stereodescriptor '*rac*' is used to describe racemates and the stereodescriptor '*X*' may be used if the configuration of the compound is unknown or unspecified.



sn-glycerol 1-phosphate
(2*S*)-1,2-dihydroxypropyl dihydrogen phosphate (PIN)

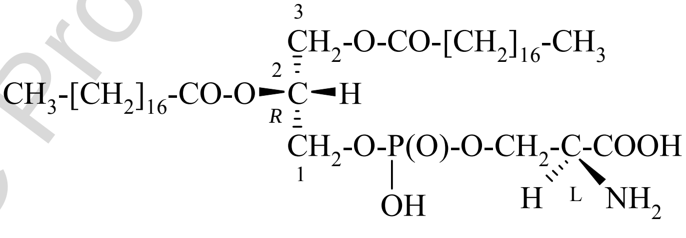


sn-glycerol 3-phosphate
(2*R*)-1,2-dihydroxypropyl dihydrogen phosphate (PIN)

P-107.3.1.3 Phosphatidylserines

The term 'phosphatidylserines' is used to describe the acyl derivatives of phosphatidic acids whose phosphorus acid component is esterified with the amino acid 'serine', usually L-serine. Preferred names of specific compounds are formed in accordance with the principles, rules and conventions of substitutive nomenclature.

Example:

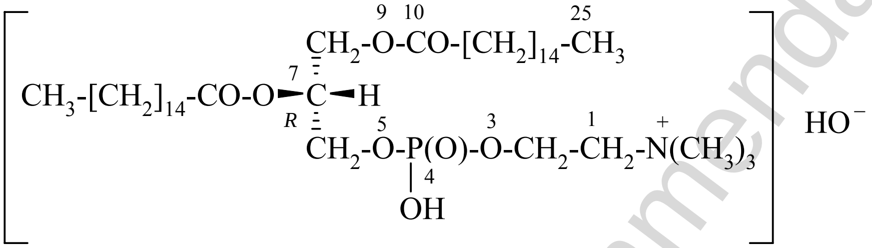


{[(2*R*)-2,3-bis(octadecanoyloxy)propoxy]hydroxyphosphoryl}-L-serine (PIN)
(2*R*)-2-*O*,3-*O*-bis(octadecanoyl)phosphatidyl-L-serine (traditional name)

P-107.3.1.4 Phosphatidylcholines

The term ‘phosphatidylcholines’ is used to describe the acyl derivatives of phosphatidic acids whose phosphorus acid component is esterified with choline. Preferred IUPAC names of specific compounds are formed in accordance with the principles, rules and conventions of substitutive nomenclature.

Example:



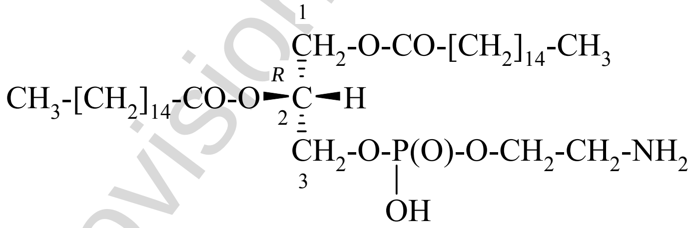
$$\left[\mathrm{CH_3\text{-}[CH_2]_{14}\text{-}CO\text{-}O\text{-}}\overset{\mathrm{CH_2\text{-}O\text{-}CO\text{-}[CH_2]_{14}\text{-}CH_3}}{\underset{\mathrm{CH_2\text{-}O\text{-}P(O)(OH)\text{-}O\text{-}CH_2\text{-}CH_2\text{-}\overset{+}{N}(CH_3)_3}}{\mathrm{C}}}\mathrm{\text{-}H}\right]\mathrm{HO^-}$$

(7*R*)-4-hydroxy-*N*,*N*,*N*-trimethyl-7-(hexadecanoyloxy)-4,10-dioxo-3,5,9-trioxa-4λ^5-phosphapentacosanaminium hydroxide (PIN)

P-107.3.1.5 Phosphatidylethanolamine

The term ‘phosphatidylethanolamines’ (more correctly ‘phosphatidyl(amino)ethanols) is used to describe the acyl derivatives of phosphatidic acids whose phosphorus acid component is esterified with 2-aminoethanol. Preferred IUPAC names of specific compounds are formed in accordance with the principles, rules and conventions of substitutive nomenclature.

Example:



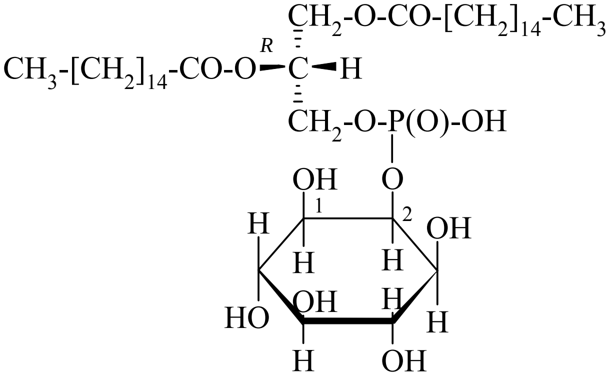
$$\mathrm{CH_3\text{-}[CH_2]_{14}\text{-}CO\text{-}O\text{-}}\overset{\mathrm{CH_2\text{-}O\text{-}CO\text{-}[CH_2]_{14}\text{-}CH_3}}{\underset{\mathrm{CH_2\text{-}O\text{-}P(O)(OH)\text{-}O\text{-}CH_2\text{-}CH_2\text{-}NH_2}}{\mathrm{C}}}\mathrm{\text{-}H}$$

(2*R*)-3-{[(2-aminoethoxy)hydroxyphosphoryl]oxy}propane-1,2-diyl dihexadecanoate (PIN)

P-107.3.2.6 Phosphatidylinositols

The term ‘phosphatidylinositols’ is used to describe the acyl derivatives of phosphatidic acids whose phosphorus acid component is esterified with an inositol molecule. Preferred IUPAC names of specific compounds are formed in accordance with the principles, rules and conventions of substitutive nomenclature.

Example:



(2*R*)-3-[({[(1*r*,2*R*,3*S*,4*r*,5*R*,6*S*)-(2,3,4,5,6-pentahydroxycyclohexyl]oxy}hydroxyphosphoryl)oxy]propane-1,2-diyl dihexadecanoate (PIN)
2-*O*-{[(2*R*)-2,3-bis(hexadecanoyloxy)propoxy]hydroxyphosphoryl}-*myo*-inositol

P-107.4 Glycolipids

P-107.4.1 Definitions

The term ‘glycolipid’ designates any compound containing one or more monosaccharide residues bound by a glycosidic linkage to a hydrophobic moiety such as an acyl glycerol, a sphingoid (a long chain aliphatic amino alcohol), a ceramide (an *N*-acyl-sphingoid) or a prenylphosphate.

Glycoglycerolipids are glycolipids containing one or more glycerol residues.

Glycosphingolipids designate lipids containing at least one monosaccharide residue and either a sphingoid or a ceramide.

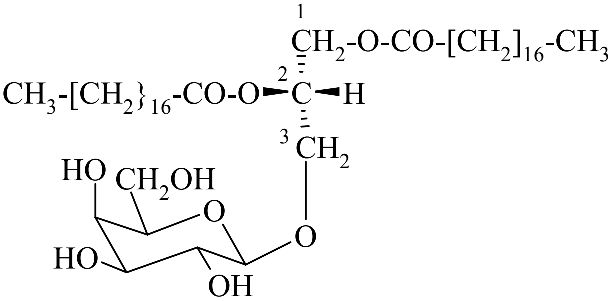
The term ‘glycophosphatidylinositol’ designates glycolipids which contain saccharides glycosidically linked to the inositol moiety of phosphatidylinositols.

Specific compounds are named systematically.

P-107.4.2 Glycoglycerolipids

Specific compounds are named on the basis of parent glycerol, whose configuration is specifically numbered as indicated in P-107.3.2.1.

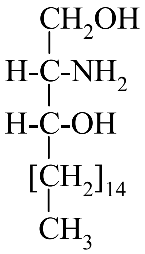
Example:



3-*O*-β-D-galactopyranosyl-1,2-di-*O*-octadecanoyl-*sn*-glycerol
(2*R*)-3-(*O*-β-D-galactopyranosyl)propane-1,2-diyl dioctadecanoate

P-107.4.3 Glycosphingolipids

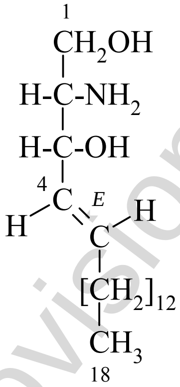
P-107.4.3.1 Names are formed by using the retained name ‘sphinganine’ for the aliphatic amino alcohol having the described absolute configuration. The retained name ‘sphinganine’ is preferred to the systematic name (2*S*,3*R*)-2-aminooctadecane-1,3-diol.



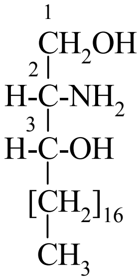
sphinganine (PIN)
(2*S*,3*R*)-2-aminooctadecane-1,3-diol

The retained name sphinganine is used to generate the names of unsaturated derivatives. Other derivatives, such as hydroxy, oxo and amino derivatives, as well as isomers with different chain length or other diastereoisomers are named systematically in accordance with the principles, rules and conventions of substitutive nomenclature.

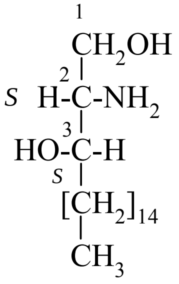
Examples:



(4*E*)- sphing-4-enine
(2S,3R,4*E*)-2-aminooctadec-4-ene-1,3-diol (PIN)



(2*R*,3*R*)-2-aminoicosane-1,3-diol (PIN)
icosasphinganine

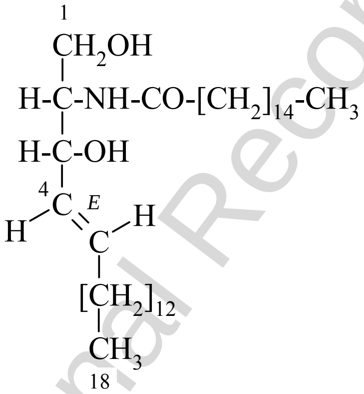


(2*S*,3*S*)-2-aminooctadecane-1,3-diol (PIN)

P-107.4.3.2 Ceramides

Ceramides are *N*-acylsphingoids.

Example:

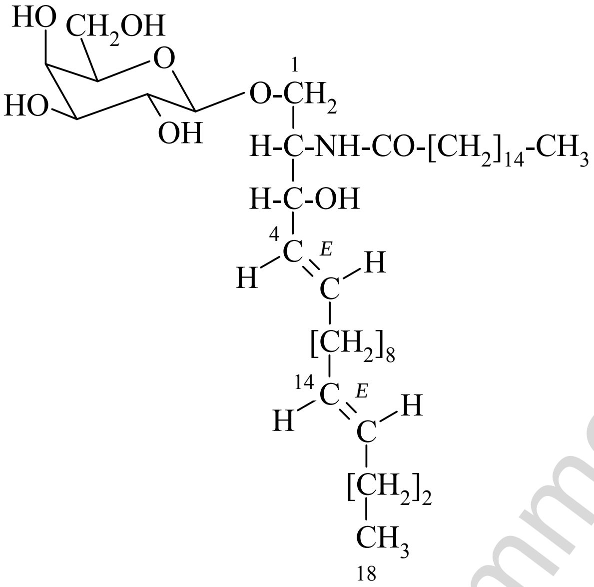


(4*E*)- *N*-hexadecanoylsphing-4-enine
N-[(2S,3R,4*E*)-1,3-dihydroxyoctadec-4-en-2-yl]hexadecanamide (PIN)

P-107.4.3.4 Neutral glycosphingolipids

A neutral glycosphingolipid is a carbohydrate containing derivative of a sphingoid or ceramide. It is understood that the carbohydrate residue is attached by a glycosidic linkage to 1-*O*-. Preferred systematic names must include all locants.

Example:



(4*E*,14*E*)-*N*-hexadecanoylsphinga-4,14-dienine (PIN)
N-[(4*R*,4*E*,14*E*)-1-(β-D-galactopyranosyloxy)-3-hydroxyoctadeca-4,14-dien-2-yl]hecadecanamide (PIN)

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APPENDIX 1

Seniority list of elements and ‘a’ terms used in replacement (‘a’) nomenclature, in decreasing order of seniority

Element	*‘a’ Term*
F	fluora
Cl	chlora
Br	broma
I	ioda
At	astata
O	oxa
S	thia
Se	selena
Te	tellura
Po	polona
N	aza
P	phospha
As	arsa
Sb	stiba
Bi	bisma
C	carba
Si	sila
Ge	germa
Sn	stanna
Pb	plumba
B	bora
Al	alumina
Ga	galla
In	inda
Tl	thalla
Zn	zinca
Cd	cadma
Hg	mercura
Cu	cupra
Ag	argenta
Au	aura
Ni	nickela
Pd	pallada
Pt	platina
Ds	darmstadta
Co	cobalta
Rh	rhoda
Ir	irida
Mt	meitnera
Fe	ferra
Ru	ruthena
Os	osma
Hs	hassa
Mn	mangana
Tc	techneta
Re	rhena
Bh	bohra
Cr	chroma
Mo	molybda
W	tungsta
Sg	seaborga
V	vanada
Nb	nioba
Ta	tantala
Db	dubna
Ti	titana
Zr	zircona
Hf	hafna
Rf	rutherforda
Sc	scanda

APPENDIX 1 (Cont'd)

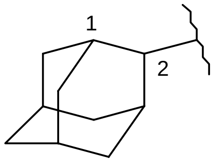
Element	*'a' Term*	*Element*	*'a' Term*
Y	yttra	Cf	californa
La	lanthana	Es	einsteina
Ce	cera	Fm	ferma
Pr	praseodyma	Md	mendeleva
Nd	neodyma	No	nobela
Pm	prometha	Lr	lawrenca
Sm	samara	Be	berylla
Eu	europa	Mg	magnesa
Gd	gadolina	Ca	calca
Tb	terba	Sr	stronta
Dy	dysprosa	Ba	bara
Ho	holma	Ra	rada
Er	erba	Li	litha
Tm	thula	Na	soda
Yt	ytterba	K	potassa
Lu	luteta	Rb	rubida
Ac	actina	Cs	caesa
Th	thora	Fr	franca
Pa	protactina	He	hela
U	urana	Ne	neona
Np	neptuna	Ar	argona
Pu	plutona	Kr	kryptona
Am	america	Xe	xenona
Cm	cura	Rn	radona
Bk	berkela		

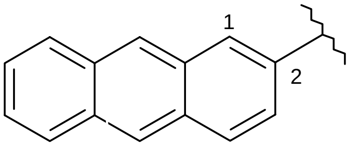
APPENDIX 2

Usual detachable prefixes used in substitutive nomenclature

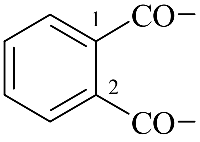
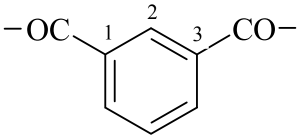
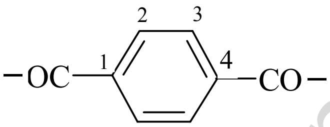
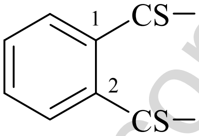
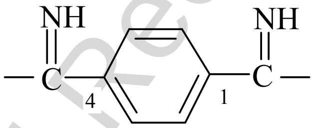
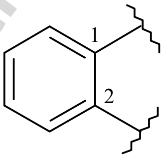
The symbol * designates the preferred IUPAC prefix name or preselected name, for example: acetamido* = acetylamino; acetylamino = acetamido*.

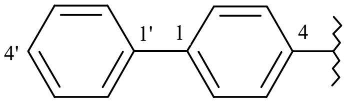
Prefixes that are not recommended are followed by the mention ‘see’ followed by the preferred prefix, for example ‘chloroxy: see chloryl*’. No formula is given for the entry ‘chloroxy’. As a counterpart, the preferred prefix is followed by the mention ‘not’ followed by the prefix that is not recommended, for example: chloryl* (not chloroxy).

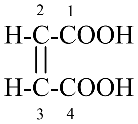
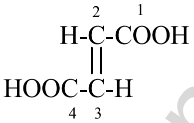
Name	Formula	
acetamido* = acetylamino	CH_3-CO-NH–	P-66.1.1.4.2
acetimidamido = acetimidoylamino = ethanimidamido*	CH_3-C(=NH)-NH–	P-66.4.1.3.5
acetimidoyl = ethanimidoyl*	CH_3-C(=NH)–	P-65.1.7.2.2
acetimidoylamino = acetimidamido = ethanimidamido*	CH_3-C(=NH)-NH–	P-66.4.1.3.5
acetohydrazido = 2-acetylhydrazin-1-yl*	CH_3-CO-NH-NH–	P-66.3.2.2
acetohydrazonoyl = ethanehydrazonoyl*	CH_3-C(=N-NH_2)–	P-65.1.7.2.2
acetohydroximoyl: see *N*-hydroxyethanimidoyl*		
acetonyl = 2-oxopropyl*	CH_3-CO-CH_2–	P-56.1.2; P-64.5.1
acetonylidene: see 2-oxopropylidene*		
acetonylidyne: see 2-oxopropylidyne*		
acetoxy = acetyloxy*	CH_3-CO-O–	P-65.6.3.2.2
acetoxysulfonyl = (acetyloxy)sulfonyl*	CH_3-CO-O-SO_2–	P-65.3.2.3
acetyl* = ethanoyl	CH_3-CO–	P-65.1.7.2.1
N-acetylacetamido* = diacetylamino	$(CH_3$-$CO)_2N$–	P-66.1.2.2
acetylamino = acetamido*	CH_3-CO-NH–	P-66.1.1.4.2
acetylazanediyl*	CH_3-CO-N<	P-66.1.1.4.3
2-acetylhydrazin-1-yl* = acetohydrazido	CH_3-CO-NH-NH–	P-66.3.2.2
acetyloxy* = acetoxy	CH_3-CO-O–	P-65.6.3.2.2
(acetyloxy)sulfonyl* = acetoxysulfonyl	CH_3-CO-O-SO_2–	P-65.3.2.3
acrylohydrazonoyl = prop-2-en-1-ylhydrazonoyl*	CH_2=CH-C(=NNH_2) –	P-65.1.7.3.2
acryloyl = prop-2-enoyl*	CH_2=CH-CO–	P-65.1.7.3.1
adamantan-2-yl* = 2-adamantyl 2-adamantyl = adamantan-2-yl*		P-29.6
adipoyl = hexanedioyl*	–CO-$[CH_2]_4$-CO–	P-65.1.7.3.1
allyl = prop-2-en-1-yl*	CH_2=CH-CH_2–	P-32.3
allylidene = prop-2-en-1-ylidene*	CH_2=CH-CH=	P-32.3

allylidyne = prop-2-en-1-ylidyne*	CH$_2$=CH-C≡	P-32.3
alumanyl*	H$_2$Al–	P-29.3.1; P-68.1.2
alumanylidene*	HAl=	P-29.3.1
amidino: see carbamimidoyl*		
amidochlorophosphoryl = phosphoramidochloridoyl*	–P(O)(NH$_2$)Cl	P-67.1.4.1.1
amidyl = azanidyl*	$^{-}$NH–	P-72.6.3
amidylidene = azanidylidene*	$^{-}$NH=	P-72.6.3
amino* (not azanyl)	H$_2$N–	P-62.2.1.1.3
aminocarbonimidoyl = carbamimidoyl*	H$_2$N-C(=NH)–	P-65.2.1.5; P-66.4.1.3.1
aminocarbonothioyl = carbamothioyl*	H$_2$N-CS–	P-65.2.1.5
aminocarbonyl = carbamoyl*	H$_2$N-CO–	P-65.2.1.5; P-66.1.1.4.1
[(aminocarbonyl)amino]carbonyl = carbamoylcarbamoyl*	H$_2$N-CO-NH-CO–	P-66.1.5.1.1.4
2-(aminocarbonyl)hydrazin-1-yl = 2-carbamoylhydrazin-1-yl* = semicarbazido	H$_2$N-CO-NH-NH–	P-68.3.1.2.4
aminodichlorosilyl*	(H$_2$N)Cl$_2$Si–	P-67.1.4.2
[amino(hydroxy)methylidene]amino* (not 3-isoureido)	H$_2$N-C(OH)=N–	P-66.1.5.1.2.2
2-(aminomethylidene)hydrazine-1-yl*	H$_2$N-CH=N-NH–	P-66.4.2.3.4
aminooxy* (not aminoxy)	H$_2$N-O–	P-68.3.1.1.1.5
amino(oxo)acetyl: see oxamoyl*		
aminooxoacetamido = oxamoylamino* = carbamoylformamido	H$_2$N-CO-CO-NH–	P-66.1.5.3
[(aminosulfanyl)methylidene]amino*	H$_2$N-C(SH)=N–	P-66.1.5.1.3.3
S-aminosulfinimidoyl*	H$_2$N-S(=NH)–	P-66.4.1.3.4
S-aminosulfonimidoyl*	H$_2$N-S(O)(=NH)–	P-66.4.1.3.4
S-aminosulfonodiimidoyl*	H$_2$N-S(=NH)$_2$–	P-66.4.1.3.4
aminosulfinyl* (not sulfinamoyl)	H$_2$N-SO–	P-66.1.1.4.1
aminosulfonyl = sulfamoyl*	H$_2$N-SO$_2$–	P-65.3.2.3
aminoxy: see aminooxy*		
amidyl = azanidyl*	$^{-}$NH–	P-72.6.3
ammonio = azaniumyl*	H$_3$N^{+}–	P-73.6
anilino* = phenylamino	C$_6$H$_5$-NH–	P-65.2.1.1.3
anthracen-1-yl* = 1-anthryl		P-29.6
anthracen-2-yl* = 2-anthryl		P-29.6
1-anthryl = anthracen-1-yl*		P-29.6
2-anthryl = anthracen-2-yl*		P-29.6
antimonyl: see stiboryl*		
arsanediyl* (not arsinediyl)	HAs<	P-68.3.2.4.2.2
arsanetriyl* (not arsinetriyl)	–As<	P-68.3.2.4.2.2
arsaniumyl* = arsonio	H$_3$As^{+}–	P-73.6
arsanyl* (not arsino)	H$_2$As–	P-29.3.1
λ^5-arsanyl* = arsoranyl	H$_4$As–	P-68.3.2.4.2.2
arsanylidene*	=AsH	P-29.3.1
arsenyl: see arsoryl*		
arsino: see arsanyl*		

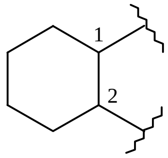
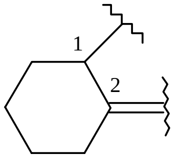
arsinoyl* (not arsinyl)	H_2As(O)–	P-67.1.4.1.1
arsinyl: see arsinoyl*		
arso*	O_2As–	P-61.5.5
arsonato*	($^{-}$O)As(O)–	P-72.6.1
arsonio = arsaniumyl*	H_3As^{+}–	P-73.6
arsono*	(HO)$_2$As(O)–	P-67.1.4.1.1
arsonoyl*	HAs(O)<	P-67.1.4.1.1
arsoranyl = λ^5-arsanyl*	H_4As–	P-68.3.2.4.2.2
arsorimidoyl* = imidoarsoryl	>As(=NH)–	P-67.1.4.1.1
arsoroso*	OAs–	P-61.5.5
arsoryl* (not arsenyl)	–As(O)<	P-67.1.4.1.1
azanediidyl*	$^{2-}$N–	P-72.6.3
azanediyl* (not imino)	HN<	P-62.2.1.2.3
azanetriyl: see nitrilo*		
azanidyl* = amidyl	$^{-}$ HN–	P-72.6.3
azanidylidene* = amidylidene	$^{-}$N=	P-72.6.3
azaniumyl* = ammonio	H_3N^{+}–	P-73.6
azanyl: see amino*		
azanylidene: see imino*		
azanylidyne (not nitrilo)	N≡	P-56.3.4
azanylylidene*	–N=	P-62.3.1.2
azido*	N_3–	P-61.6
azino: see hydrazinediylidene*	=N-N=	P-68.3.1.2.1
azinoyl* (not azinyl)	H_2N(O)–	P-67.1.4.1.1
azinyl: see azinoyl*		
azo = diazenediyl*	–N=N–	P-68.3.1.3.1.1; P-68.3.1.3.1
azonato*	($^{-}$O)$_2$N(O)–	P-68.6.1
azono*	(HO)$_2$N(O)–	P-67.1.4.1.1
azonothioyl* = thioazonoyl	>HN(S)–	P-67.1.4.1.1
azonoyl*	HN(O)<	P-67.1.4.1.1
azoryl* = nitroryl	>N(O)–	P-67.1.4.1.1
azoxy (general nomenclature only)	–N(O)=N–	P-68.3.1.3.2.1
benzal: see benzylidene*		
benzamido* = benzoylamino	C_6H_5-CO-NH–	P-66.1.1.4.2
benzenecarbohydroximoyl = *N*-hydroxybenzenecarboximidoyl* = *N*-hydroxybenzimidoyl	C_6H_5-C(=N-OH)–	P-65.1.7.2.2
benzenecarbonyl = benzoyl*	C_6H_5-CO–	P-65.1.7.2.1
benzenecarbothioamido* = benzenecarbothioylamino (not thiobenzamido)	C_6H_5-CS-NH–	P-66.1.3.1.2
benzenecarbothioyl* = thiobenzoyl	C_6H_5-CS–	P-65.1.7.2.3
benzenecarbothioylamino = benzenecarbothioamido* (not thiobenzamido)	C_6H_5-CS-NH–	P-66.1.3.1.2
benzenecarboximidoyl* = benzimidoyl	C_6H_5-C(=NH)–	P-65.1.7.2.2
2-benzenecarboximidoylhydrazin-1-yl* = benzenecarboximidohydrazido	C_6H_5-C(=NH)-NH-NH–	P-66.4.2.3.6
benzenecarboximidohydrazido = 2-benzenecarboximidoylhydrazin-1-yl*	C_6H_5-C(=NH)-NH-NH	P-66.4.2.3.6

benzene-1,2-dicarbonyl* = phthaloyl (not 1,2-phenylenedicarbonyl)		P-65.1.7.4.2
benzene-1,3-dicarbonyl* = isophthaloyl (not 1,3-phenylenedicarbonyl)		P-65.1.7.4.2
benzene-1,4-dicarbonyl* = terephthaloyl (not 1,4-phenylenedicarbonyl)		P-65.1.7.4.2
benzene-1,2-dicarbothioyl* (not dithiophthaloyl)		P-65.1.7.4.3
benzene-1,4-dicarboximidoyl* = terephthalimidoyl		P-65.1.7.2.2
benzene-1,2-diyl: see 1,2-phenylene		P-29.6
benzene-1,3-diyl: see 1,3-phenylene*		P-29.6
benzene-1,4-diyl: see 1,4-phenylene*		P-29.6
benzeneselenonyl* (not phenylselenonyl)	C_6H_5-Se(=O)$_2$–	P-63.6
benzenesulfinamido* = benzenesulfinylamino [not (phenylsulfinyl)amino]	C_6H_5-SO-NH–	P-66.1.1.4.2
benzenesulfinohydrazonamido* = benzenesulfinohydrazonoylamino	C_6H_5-S(=N-NH$_2$)-NH–	P-66.4.2.3.5
benzenesulfinohydrazonoylamino = benzenesulfinohydrazonamido*	C_6H_5-S(=N-NH$_2$)-NH–	P-66.4.2.3.5
benzenesulfinoselenoyl* [not phenyl(sulfinoselenoyl)]	C_6H_5-S(Se)–	P-65.3.2.2.2
benzenesulfinyl* (not phenylsulfinyl)	C_6H_5-SO–	P-63.6; P-65.3.2.2.2
benzenesulfonamido* = benzenesulfonylamino [not (phenylsulfonyl)amino]	C_6H_5-SO$_2$-NH–	P-66.1.1.4.2
benzenesulfonyl* (not phenylsulfonyl)	C_6H_5-SO$_2$–	P-63.6; P-65.3.2.2.2
benzhydroximoyl: see *N*-hydroxybenzenecarboximidoyl*		
benzimidoyl = benzenecarboximidoyl*	C_6H_5-C(NH)–	P-65.1.7.2.2
benzohydrazido = 2-benzoylhydrazinyl*	C_6H_5-CO-NHNH–	P-66.3.2.2.2
benzoyl* = benzenecarbonyl	C_6H_5-CO–	P-65.1.7.2.1

benzoylamino = benzamido*	C_6H_5-CO-NH–	P-66.1.1.4.2
benzoylazanediyl*	C_6H_5-CO-N<	P-66.1.1.4.3
2-benzoylhydrazinyl* = benzohydrazido	C_6H_5-CO-NH-NH–	P-66.3.2.2.2
benzoylimino*	C_6H_5-CO-N=	P-66.1.1.4.3
benzoyloxy*	C_6H_5-CO-O–	P-65.6.3.2.2
benzyl* = phenylmethyl	C_6H_5-CH_2–	P-29.6
benzylidene* = phenylmethylidene	C_6H_5-CH=	P-29.6
benzylidyne* = phenylmethylidyne	C_6H_5-C≡	P-29.6
benzyloxy = phenylmethoxy*	C_6H_5-CH_2-O–	P-63.2.2.1.1
[1,1'-biphenyl]-4-yl* = phenylphenyl		P-29.3.5
bis(acetyloxy)-λ^3-iodanyl*	$(CH_3\text{-CO-O})_2$I–	P-68.5.1
bismuthaniumyl* = bismuthonio	H_3Bi^+–	P-73.6
bismuthanyl* (not bismuthino)	H_2Bi–	P-68.3.3
λ^5-bismuthanylidene*	H_3Bi=	P-68.3.3
bismuthino: see bismuthanyl*		
bismuthonio = bismuthaniumyl*	H_3Bi^+–	P-73.6
bis(sulfanyl)phosphoryl*	$(H_2S)_2$P(O)–	P-67.1.4.1.1
boranediyl* (not borylene nor boranylidene)	HB<	P-68.1.2
boranetriyl*	–B<	P-68.1.2
boranuidyl*	^-H_3B–	P-72.6.3
boranyl* (not boryl)	H_2B–	P-29.3.1; P-68.1.2
boranylidene* (not borylidene)	HB=	P-29.3.1; P-68.1.2
boranylidyne* (not borylidyne)	B≡	P-29.3.1; P-68.1.2
borono* = dihydroxyboranyl	$(HO)_2B$–	P-67.1.4.2
boryl: see boranyl*		
borylene: see boranylidene*		
borylidene: see boranylidene*		
borylidyne: see boranylidyne*		
bromo*	Br–	P-61.3.1
bromocarbonothioyl = carbonobromidothioyl*	Br-C(S)–	P-65.2.1.5
bromosyl*	OBr–	P-61.3.2
bromyl*	O_2Br–	P-61.3.2
butanamido* = butanoylamino = butyramido = butyrylamino	CH_3-$[CH_2]_2$-CO-NH–	P-66.1.1.4.2
butanebis(thioyl)* = dithiosuccinyl	–SC-CH_2-CH_2-CS–	P-65.1.7.4.1; P-65.1.7.4.3
butanediimidoyl* = succinimidoyl	–(HN)C-CH_2-CH_2-C(NH)–	P-65.1.7.3.2
butanedioyl* = succinyl	–CO-CH_2-CH_2-CO–	P-65.1.7.3.1
butane-1,1-diyl*	CH_3-CH_2-CH_2-CH<	P-29.3.2.2
butane-1,4-diyl* (not tetramethylene)	–CH_2-CH_2-CH_2-CH_2–	P-29.3.2.2
butanethioyl* = thiobutyryl	CH_3-CH_2-CH_2-CS–	P-65.1.7.4.1
butanimidoyl* = butyrimidoyl	CH_3-CH_2-CH_2-C(=NH)–	P-65.1.7.4.1
butanoyl* = butyryl	CH_3-$[CH_2]_2$-CO–	P-65.1.7.3.1
butanoylamino = butanamido* =butyramido = butyrylamino	CH_3-$[CH_2]_2$-CO-NH–	P-66.1.1.4.2
butan-1-yl: see butyl*		
butan-2-yl* = 1-methylpropyl (not *sec*-butyl)	CH_3-CH_2-$CH(CH_3)$–	P-29.3.2.2

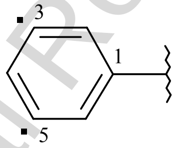
butan-1-ylidene: see butylidene*		
butan-2-ylidene* = 1-methylpropylidene (not *sec*-butylidene)	$CH_3-CH_2-C(CH_3)=$	P-29.3.2.2
butan-1-ylidyne: see butylidyne*		
butan-2-yloxy* = (1-methylpropyl)oxy = *sec*-butoxy	$CH_3-CH_2-(CH_3)CH-O$–	P-63.2.2.1.1
butan-2-yl-3-ylidene*	$CH_3-\overset{\vert}{C}H-\overset{\Vert}{C}-CH_3$	P-29.3.2.2
butan-3-yl-1-ylidene*	$CH_3-\overset{\vert}{C}H-CH_2-CH=$	P-29.3.2.2
(*Z*)-but-2-enedioyl* = maleoyl		P-65.1.7.3.1
(*E*)-but-2-enedioyl* = fumaroyl		P-65.1.7.3.1
but-1-enyl: see but-1-en-1-yl*		
but-1-en-1-yl* (formerly but-1-enyl)	$CH_3-CH_2-CH=CH$–	P-32.1.1
but-2-enyl : see but-2-en-1-yl*		
but-2-en-1-yl* (formerly but-2-enyl)	$CH_3-CH=CH-CH_2$–	P-32.1.1
but-3-en-2-yl* = 1-methylprop-2-en-1-yl	$CH_2=CH-\overset{\vert}{C}H-CH_3$	P-32.1.1
but-2-ene-1,4-diyl*	–$CH_2-CH=CH-CH_2$–	P-32.1.1
butoxy* = butyloxy	$CH_3-[CH_2]_2-CH_2-O$–	P-63.2.2.2
sec-butoxy = butan-2-yloxy* = (1-methylpropyl)oxy	$CH_3-CH_2-(CH_3)CH-O$–	P-63.2.2.1.1
tert-butoxy* (not *tert*-butyloxy)	$(CH_3)_3C-O$–	P-63.2.2.2
butyl* (not butan-1-yl)	$CH_3-CH_2-CH_2-CH_2$–	P-29.3.2.1
sec-butyl = butan-2-yl*	$CH_3-CH_2-CH(CH_3)$–	P-29.3.2.2
tert-butyl* =2-methylpropan-2-yl = 1,1-dimethylethyl	$(CH_3)_3CH$–	P-29.4; P-29.6
butylidene* (not butan-1-ylidene)	$CH_3-CH_2-CH_2-CH=$	P-29.3.2.1
butylidyne* (not butan-1-ylidyne)	$CH_3-CH_2-CH_2-C\equiv$	P-29.3.2.1
butyloxy: see butoxy*		
tert-butyloxy: see *tert*-butoxy*		
butyramido = butanamido* = butyrylamino = butanoylamino	$CH_3-[CH_2]_2-CO-NH$–	P-66.1.1.4.2
butyrimidoyl = butanimidoyl*	$CH_3-CH_2-CH_2-C(=NH)$–	P-65.1.7.4.1
butyryl = butanoyl*	$CH_3-CH_2-CH_2-CO$–	P-65.1.7.3.1
butyrylamino = butanamido* = butanoylamino = butyramido	$CH_3-[CH_2]_2-CO-NH$–	P-66.1.1.4.2
carbamimidamido* = carbamimidoylamino (not guanidino)	$H_2N-C(=NH)-NH$–	P-66.4.1.2.1.3
carbamimidoyl* = *C*-aminocarbonimidoyl	$H_2N-C(=NH)$–	P-65.2.1.5; P-66.4.1.3.1
carbamimidoylamino = carbamimidamido* (not guanidino)	$H_2N-C(NH)-NH$–	P-66.4.1.2.1.3
carbamohydrazonoyl*	$H_2N-C(=N-NH_2)$–	P-66.4.2.3.2

carbamothioyl* = aminocarbonothioyl (not thiocarbamoyl)	$\mathrm{H_2N}$-CS–	P-65.2.1.5
carbamothioylamino*	$\mathrm{H_2N}$-CS-NH–	P-66.1.5.1.3.3
carbamoyl* = aminocarbonyl	$\mathrm{H_2N}$-CO–	P-65.2.1.5; P-66.1.1.4.1
carbamoylamino* (not ureido)	$\mathrm{H_2N}$-CO-NH–	P-66.1.5.1.1.3
carbamoylcarbamoyl* = [(aminocarbonyl)amino]carbonyl	$\mathrm{H_2N}$-CO-NH-CO–	P-66.1.5.1.1.4
carbamoylcarbonyl: see oxamoyl*		
carbamoylformamido = oxamoylamino* = amino(oxo)acetamido	$\mathrm{H_2N}$-CO-CO-NH–	P-66.1.5.3
carbamoylformyl: see oxamoyl*		
carbonylbis(azanediyl)* (formerly ureylene)	–NH-CO-NH–	P-66.1.5.1.1.3
2-carbamoylhydrazin-1-yl* = 2-(aminocarbonyl)hydrazin-1-yl = semicarbazido	$\mathrm{H_2N}$-CO-NHNH–	P-68.3.1.2.4
2-carbamoylhydrazin-1-ylidene* = semicarbazono	$\mathrm{H_2N}$-CO-NHN=	P-68.3.1.2.5
carbazimidoyl: see hydrazinecarboximidoyl*		
carbazono: see 2-diazenecarbonylhydrazin-1-yl*		
carbazoyl: see hydrazinecarbonyl*		
carbethoxy: see ethoxycarbonyl*		
carbomethoxy: see methoxycarbonyl*		
carbonato*	–CO-O$^-$	P-72.6.1
carbonimidoyl*	HN=C<	P-65.2.1.5
carbonobromidothioyl* = bromocarbonothioyl	Br-C(S)–	P-65.2.1.5
carbonochloridoyl* = chlorocarbonyl	Cl-C(O)–	P-65.2.1.5
carbonochlorimidoyl* = *C*-chlorocarbonimidoyl	ClC(=NH)-	P-65.2.1.5
carbonocyanidoyl* = cyanocarbonyl	NC-C(O)–	P-65.2.1.5
carbonohydrazidoyl = hydrazinecarbonyl*	$\mathrm{H_2}$-N-NH-CO–	P-66.3.2.1
carbonohydrazonoyl*	>C(=$\mathrm{NNH_2}$)	P-65.2.1.5
carbonoperoxoyl* = hydroperoxycarbonyl	HOO-CO–	P-65.1.4.2; P-65.2.1.5
carbono(thioperoxoyl)* = (thiohydroperoxy)carbonyl	HOS-CO– or HSO-CO–	P-65.2.1.7
carbonothioyl* = thiocarbonyl	–CS–	P-65.2.1.5
carbonyl*	–CO–	P-65.2.1.5
carbonylbis(azanedyl)* (not ureylene)	–HN-CO-NH–	P-66.1.5.4.1.3
carboxy*	HO-CO–	P-65.1.2.2.3
carboxyamino*	HOOC-NH–	P-65.2.1.6
carboxycarbonothioyl: see 1-thiooxalo*		
(carboxycarbonothioyl)sulfanyl = 1-thiooxalylsulfanyl*	HO-CO-CS-S–	P-65.2.3.3
carboxycarbonyl = oxalo* (not carboxyformyl, nor hydroxyl(oxo)acetyl	HOOC-CO–	P-65.2.3.3
(carboxycarbonyl)amino = oxaloamino*	HO-CO-CO-NH–	P-65.2.3.3
(carboxycarbonyl)oxy = oxalooxy*	HO-CO-CO-O–	P-65.2.3.3
(carboxycarbonyl)sulfanyl = oxalosulfanyl*	HO-CO-CO-S–	P-65.2.3.3
carboxyformamido: see oxaloamino*		
carboxyformyl: see oxalo*		
(carboxyformyl)oxy; see oxalooxy*		
(carboxyformyl)sulfanyl; see oxalosulfanyl*		
carboxylato*	$^-$O-CO–	P-72.6.1
carboxyoxy*	HOOC-O–	P-65.2.1.6

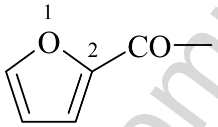
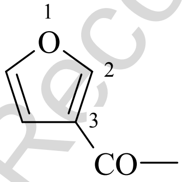
(carboxyoxy)formyl = (carboxyoxy)carbonyl*	HOOC-O-CO–	P-65.2.4.1.5
carboxysulfanyl*	HOOC-S–	P-65.2.1.6
chloro*	Cl–	P-61.3.1
chloroarsanyl*	–AsHCl	P-67.1.4.1.1
chloroboranyl*	Cl-BH–	P-68.1.2
C-chlorocarbonimidoyl = carbonochloridimidoyl*	Cl-C(=NH)–	P-65.2.1.5
chlorocarbonyl = carbonochloridoyl*	Cl-CO–	P-65.1.8.4 ; P-65.2.1.5
2-chloro-1,2-dioxoethyl = chlorooxalyl*	Cl-CO-CO–	P-65.2.3.3
chloroformyl: see carbonochloridoyl*		
chlorooxalyl* = 2-chloro-1,2-dioxoethyl	Cl-CO-CO–	P-65.2.3.3
2-chloro-2-oxo-1-thioxoethyl = 2-chloro-1-thiooxalyl*	Cl-CO-CS–	P-65.2.3.3
chloroso : see chlorosyl*		
chlorosulfinyl*	Cl-S(O)–	P-65.3.2.3; P-67.1.4.4.1
chlorosulfonyl* = sulfurochloridoyl	Cl-SO$_2$–	P-65.3.2.3; P-67.1.4.4.1
(chlorosulfonyl)oxy* = sulfurochloridoyloxy	Cl-SO$_2$-O–	P-67.1.4.4.2
chlorosyl* (not chloroso)	OCl–	P-61.3.2
2-chloro-1-thiooxalyl* = 2-chloro-2-oxo-1-thioxoethyl	Cl-CO-CS–	P-65.2.3.3
chloroxy: see chloryl*		
chloryl* (not chloroxy)	O_2Cl–	P-61.3.2
cinnamoyl = 3-phenylprop-2-enoyl*	C_6H_5-CH=CH-CO–	P-65.1.7.3.1
crotonyl: see but-2-enoyl*		
cyanato*	NCO–	P-65.2.2
cyano*	NC–	P-66.5.1.1.4
cyanocarbonyl = carbonocyanidoyl*	NC-CO–	P-65.2.1.5
cyano(isocyanato)(thiophosphoryl) = phosphorocyanidoisocyanatidothioyl*	–P(S)(CN)(NCO)	P-67.1.4.1.3
cyanosulfonyl* = sulfurocyanidoyl	NC-SO$_2$–	P-67.1.4.4.1
cyclohexanecarbonyl*	C_6H_{11}-CO–	P-65.1.7.4.2
cyclohexanecarboximidoyl* =*C*-cyclohexylcarboximidoyl	C_6H_{11}-C(=NH)–	P-65.1.7.4.2
cyclohexane-1,1-diyl*	C_6H_{10}<	P-29.3.3
cyclohexane-1,2-diyl* (and similarly for 1,3- and 1,4-isomers)		P-29.3.3
cyclohexanyl: see cyclohexyl*		
cyclohexan-1-yl-2-ylidene*		P-29.3.3
cyclohexanylidene: see cyclohexylidene*		
cyclohexyl* (not cyclohexanyl)	C_6H_{11}–	P-29.3.3
cyclohexylcarbonyl: see cyclohexanecarbonyl*		
1,4-cyclohexylene: see cyclohexane-1,4-diyl*		
cyclohexylidene* (not cyclohexanylidene)	C_6H_{10}=	P-29.3.3
cyclopentanecarboximidoyl*	C_5H_9-C(=NH)–	P-65.1.7.4.2
cyclopropanyl: see cyclopropyl*		

cyclopropanylidene: see cyclopropylidene*		
cyclopropyl* (not cyclopropanyl)	C_3H_7–	P-29.3.3
cyclopropylidene* (not cyclopropanylidene)	C_3H_6=	P-29.3.3
cyclotrisilan-1-yl: = trisiliran-1-yl*	Si_3H_7–	P-29.3.3
decanedioyl*	–CO-[CH$_2$]$_8$-CO–	P-65.1.7.4.1
decanoyl*	CH$_3$-[CH$_2$]$_8$-CO–	P-65.1.7.4.1
decan-1-yl: see decyl*		
decan-1-ylidene: see decylidene*		
decan-1-ylidyne: see decylidyne*		
decyl* (not decanyl)	CH$_3$-[CH$_2$]$_9$–	P-29.3.2.1
decylidene* (not decan-1-ylidene)	CH$_3$-[CH$_2$]$_8$-CH=	P-29.3.2.1
decylidyne* (not decan-1-ylidyne)	CH$_3$-[CH$_2$]$_8$-C≡	P-29.3.2.1
diacetoxyiodo: [see bis(acetyloxy)-λ^3-iodanyl*]		
diacetylamino = *N*-acetylacetamido*	(CH$_3$-CO)$_2$N–	P-66.1.2.2
diaminoboranyl*	(H$_2$N)$_2$B–	P-67.1.4.2.1
(diaminomethylidene)amino*	(H$_2$N)$_2$C=N–	P-66.4.1.2.1.3
diarsanyl*	H$_2$As-AsH–	P-29.3.2.2
diazane-1,2-diyl = hydrazine-1,2-diyl* (not hydrazo)	–HN-NH–	P-68.3.1.2.1.1
diazanediylidene = hydrazinediylidene* (not azino)	=N-N=	P-68.3.1.2.1.1
diazanyl = hydrazinyl* (not hydrazino)	H$_2$NNH–	P-68.3.1.2.1.1
diazanylidene = hydrazinylidene* (not ydrazono)	H$_2$NN=	P-68.3.1.2.1.1
diazenecarbohydrazido = 2-(diazenecarbonyl)hydrazin-1-yl* (not carbazono)	HN=N-CO-NHNH–	P-68.3.1.3.3
2-(diazenecarbonyl)hydrazin-1-yl* = diazenecarbohydrazido (not carbazono)	HN=N-CO-NHNH–	P-68.3.1.3.3
diazenediyl* = azo	–N=N–	P-68.3.1.3.1.2
diazenyl*	H$_2$N=N–	P-32.1.1; P-68.3.1.3.1.3
diazenyl(hydrazinylidene)methyl = formazan-3-yl*	HN=N-C(=NNH$_2$)–	P-68.3.1.3.4.2
(diazenylmethylidene)hydrazinyl = formazan-5-yl*	HN=N-CH=N-NH–	P-68.3.1.3.4.2
diazo*	N$_2$–	P-61.4
diazoamino: see triaz-1-ene-1,3-diyl*	–N=N-NH–	P-68.3.1.4.2
diazyn-1-ium-1-yl*	–N$^+$≡N	P-73.6
dibismuthane-1,2-diyl*	–HBi-BiH–	P-68.3.3
diborazan-1-yl*	H$_2$B-NH-BH–	P-68.1
diboroxanyl*	H$_2$B-O-BH–	P-68.1.2
dichloroboranyl* (not dichloroboryl)	Cl$_2$B–	P-67.1.4.2.1
dichloroboryl: see dichloroboranyl*		
dichloro-λ^3-iodanyl* (not dichloroiodo)	Cl$_2$I–	P-68.5.1
dichlorophosphoryl = phosphorodichloridoyl*	Cl$_2$P(O)–	P-67.1.4.1.1
dichlorophosphanyl* (not dichlorophosphino)	Cl$_2$P–	P-67.1.4.1.1
dichlorophosphino: see dichlorophosphanyl*		
dihydroarsoryl = arsinoyl*	H$_2$As(O)-	P-67.1.4.1.2
dihydronitroryl = azinoyl*	H$_2$N(O)–	P-67.1.4.1.2
dihydrophosphorimidoyl = phosphinimidoyl*	H$_2$P(=NH)–	P-67.1.4.1.2
dihydrophosphorothioyl = phosphinothioyl*	H$_2$P(S)–	P-67.1.4.1.2
dihydrophosphoryl = phosphinoyl*	H$_2$P(O)–	P-67.1.4.1.2
dihydrostiboryl = stibinoyl*	H$_2$Sb(O)–	P-67.1.4.1.2
dihydroxyboranyl = borono*	(HO)$_2$B–	P-67.1.4.2
dihydroxycarbonimidoyl*	HO-C(=N-OH)–	P-65.1.3.3.2

dihydroxy-λ^3-iodanyl* (not dihydroxyiodo)	$(HO)_2I$–	P-68.5.1
dihydroxyiodo : see dihydroxy-λ^3-iodanyl*		
dihydroxynitroryl = azono*	$(HO)_2N(O)$–	P-67.1.4.1.1
dihydroxyphosphanyl* (not dihydroxyphosphino)	$(HO)_2P$–	P-67.1.4.1.1
dihydroxyphosphino: see dihydroxyphosphanyl*		
dihydroxyphosphinothioyl: see dihydroxyphosphorothioyl*		
dihydroxyphosphorothioyl* (not dihydroxyphosphinothioyl)	$(HO)_2P(S)$–	P-67.1.4.1.1
dihydroxy(sulfanyl)silyl*	$(SH)(HO)_2Si$–	P-67.1.4.2
dimethoxyphosphoryl* = dimethoxy(oxo)phosphoranyl = dimethoxy(oxo)-λ^5-phosphanyl	$(CH_3O)_2P(O)$–	P-67.1.4.1.1
dimethoxyphosphoroselenoyl* = dimethoxy(selenoxo)phosphoranyl = dimethoxy(selenoxo) -λ^5-phosphanyl = dimethoxy(selenophosphoryl)	$(CH_3O)_2P(Se)$–	P-67.1.4.1.1
(dimethoxyphosphoryl)sulfanyl* = [dimethoxy(oxo)phosphoranyl]sulfanyl = [dimethoxy(oxo)-λ^5-phosphanyl]sulfanyl	$(CH_3O)_2P(O)$-S–	P-67.1.4.1.3
dimethoxy(selenophosphoryl) = dimethoxyphosphoroselenoyl*	$(CH_3O)_2P(Se)$–	P-67.1.4.1.1
(dimethylamido)phosphoryl = dimethylphosphoramidoyl*	$(CH_3)_2N$-$P(O)$<	P-67.1.4.1.1
dimethylammoniumylidene: see dimethylazaniumylidene*		
dimethylazaniumylidene* (not dimethylammoniumylidene)	$(CH_3)_2{}^+N$=	P-73.6
1,1-dimethylethyl = *tert*-butyl* (unsubstituted) = 2-methylpropan-2-yl	$CH_3)_3C$–	P-29.4; P-29.6
(1,1-dimethylethyl)oxy = (methylpropan-2-yl)oxy = *tert*-butoxy*	$(CH_3)_3$-C-O–	P-63.2.2.2
dimethylphosphinoselenoyl* = dimethyl(selenophosphinoyl)	$(CH_3)_2P(Se)$–	P-67.1.4.1.1
dimethylphosphoramidoyl* = (dimethylamido)phosphoryl	$(CH_3)_2N$-$P(O)$<	P-67.1.4.1.1
dimethyl(selenophosphinoyl) = dimethylphosphinoselenoyl*	$(CH_3)_2P(Se)$–	P-67.1.4.1.1
dioxoethane-1,2-diyl = oxalyl* = ethanedioyl	–CO-CO–	P-65.2.3.3
dioxo-λ^5-phosphanyl = phospho*	O_2P–	P-61.5.2
dioxy : see peroxy*		
diphosphanyl* (not diphosphino)	H_2PPH–	P-68.3.2.4.2.2
diphosphino : see diphosphanyl*		
diselanyl* = diselenohydroperoxy	HSeSe–	P-63.4.2.2
diselenohydroperoxy = diselanyl*	HSeSe–	P-63.4.2.2
disilane-1,1-diyl*	H_3Si-SiH<	P-29.3.2.2 ; P-68.2.2
disilanyl*	H_3Si-SiH_2–	P-29.3.2.2 ; P-68.2.2
disilazan-1-yl*	H_3Si-NH-SiH_2–	P-29.3.2.2; P-68.2.2
disilazan-2-yl*	$(H_3Si)_2$-N–	P-29.3.2.2; P-68.2.2
disiloxan-1-yl*	H_3Si-O-SiH_2–	P-29.3.2.2; P-68.2.2
disulfanediyl* (not dithio)	–SS–	P-63.1.5
disulfanidyl*	$^-$SS–	P-72.6.3

disulfanyl* = dithiohydroperoxy	HSS–	P-63.4.2.2
(disulfanylcarbonyl)oxy* = (dithiohydroperoxycarbonyl)oxy	HSS-CO-O–	P-65.2.1.7
ditellanyl* = ditellurohydroperoxy	HTeTe–	P-63.4.2.2
ditellurohydroperoxy = ditellanyl*	HTeTe–	P-63.4.2.2
dithio: see disulfanediyl*		
dithiocarboperoxoyl* (location of sulfur atoms unknown)	HOS$_2$C–	P-65.1.5.3
dithiocarboxy* = sulfanylcarbonothioyl	HSSC–	P-65.2.1.6
(dithiocarboxycarbonothioyl): see trithiooxalo*		
[(dithiocarboxy)sulfanyl]carbonothioyl* = [(sulfanylcarbonothioyl)sulfanyl]carbonothioyl = [(sulfanylthiocarbonyl)sulfanyl]thiocarbonyl {not [(dithiocarboxy)sulfanyl]thioformyl}	HS-CS-S-CS–	P-65.2.4.1.5
[(dithiocarboxy)sulfanyl]thioformyl}: see [(dithiocarboxy)sulfanyl]carbonothioyl*		
dithiohydroperoxy = disulfanyl*	HSS–	P-63.4.2.2
(dithiohydroperoxycarbonyl)oxy = (disulfanylcarbonyl)oxy*	HSS-CO-O–	P-65.2.1.7
dithiophthaloyl (see benzene-1,2-dicarbothioyl*)		
dithiosuccinyl [see butanebis(thioyl)*]		
dithiosulfo (unspecified)	HS$_3$O–	P-65.3.2.1
3,5-diylophenyl*		P-71.5
dodecanoyl*	CH$_3$-[CH$_2$]$_{10}$-CO–	P-65.1.7.4.1
dodecanyl: see dodecyl*		
dodecyl* (not dodecanyl)	CH$_3$-[CH$_2$]$_{11}$–	P-29.3.2.1
episeleno (ring formation)	–Se–	P-63.5
epitelluro (ring formation)	–Te–	P-63.5
epithio (ring formation)	–S–	P-63.5
epoxy (ring formation)	–O–	P-63.5
ethanedioyl = oxalyl* = dioxoethane-1,2-diyl	–CO-CO–	P-65.2.3.3
ethane-1,1-diyl*	CH$_3$-CH<	P-29.3.2.2
ethane-1,2-diyl* = ethylene	–CH$_2$-CH$_2$–	P-29.3.2.2; P-29.6
ethane-1,2-diylbis(oxy)* = ethylenebis(oxy) (not ethane-1,2-diyldioxy)	–O-CH$_2$-CH$_2$-O–	P-63.2.2.1.3
ethanehydrazonoyl* = acetohydrazonoyl	CH$_3$-C(=NNH$_2$)–	P-65.1.7.2.2
ethaneselenoyl* = selenoacetyl	CH$_3$-CSe–	P-65.1.7.2.3
ethanesulfinimidoyl* (not ethylsulfinimidoyl)	CH$_3$-CH$_2$-S(=NH)–	P-65.3.2.2.2
ethanesulfinyl* (not ethylsulfinyl)	CH$_3$-CH$_2$-SO–	P-63.6; P-65.3.2.2.2
ethanesulfonodiimidamido* =ethanesulfonodiimidoylamino	CH$_3$-CH$_2$-S(=NH)$_2$-NH–	P-66.4.1.3.5
ethanesulfonodiimidoylamino =ethanesulfonodiimidamido*	CH$_3$-CH$_2$-S(=NH)$_2$-NH–	P-66.4.1.3.5
ethanesulfonothioyl*	CH$_3$-CH$_2$-S(O)(S)–	P-65.3.2.2.2

ethanesulfonyl* (not ethylsulfonyl)	CH_3-CH_2-SO_2–	P-63.6; P-65.3.2.2.2
ethanethioamido* = ethanethioylamino (not thioacetamido)	CH_3-CS-NH–	P-66.1.3.1.2
ethanethioyl* = thioacetyl	CH_3-CS–	P-65.1.7.2.3
ethanethioylamino = ethanethioamido* (not thioacetamido)	CH_3-CS-NH–	P-66.1.3.1.2
ethanimidamido* = acetimidoylamino = acetimidamido	CH_3(=NH)-NH)–	P-66.4.1.3.5
ethanimidoyl* = acetimidoyl	CH_3-C(=NH)–	P-65.1.7.2.2
ethanoyl = acetyl*	CH_3-CO–	P-65.1.7.2.1
ethanyl: see ethyl*		
ethanylidene: see ethylidene*		
ethanylidyne: see ethylidyne*		
ethan-1-yl-2-ylidene*	–CH_2-CH=	P-29.3.2.2
ethene-1,2-diyl* (not vinylene)	–CH=CH–	P-32.1.1
ethenyl* = vinyl	CH_2=CH–	P-32.3
ethenylidene* = vinylidene	CH_2=C=	P-32.3
ethoxy* (not ethyloxy)	CH_3-CH_2-O–	P-63.2.2.2
ethoxycarbonyl* (not carbethoxy)	CH_3-CH_2-O-CO–	P-65.6.3.2.2
ethyl* (not ethanyl)	CH_3-CH_2–	P-29.3.2.1
ethylene = ethane-1,2-diyl*	–CH_2-CH_2–	P-29.3.2.2; P-29.6
ethylenebis(oxy) = ethane-1,2-diylbis(oxy)*	–O-CH_2CH_2-O–	P-63.2.2.1.3
ethylenedioxy: see ethane-1,2-diylbis(oxy)*		
ethylidene* (not ethanylidene)	CH_3-CH=	P-29.3.2.1
ethylidyne* (not ethanylidyne)	CH_3-C≡	P-29.3.2.1
ethyloxy: see ethoxy*		
1-ethylpropylidene = pentan-3-ylidene*	$(CH_3\text{-}CH_2)_2$C=	P-29.3.2.2
ethylstibinoyl*	CH_3-CH_2-Sb(O)–	P-67.1.4.1.1
ethylsulfanyl* (not ethylthio)	CH_3-CH_2-S–	P-63.2.5.1
ethylsulfinyl: see ethanesulfinyl*		
ethylsulfonimidoyl: see ethanesulfonimidoyl*		
ethylsulfonyl: see ethanesulfonyl*		
ethylthio: see ethylsulfanyl*		
fluoro*	F–	P-61.3.1
fluorosyl*	OF-	P-61.3.2
fluoryl*	O_2F-	P-61.3.2
formamido* = formylamino	HCO-NH–	P-66.1.1.4.2
formazan-1,5-diyl*	–HN-N=CH=N–	P-68.3.1.3.4.2
	|	
formazan-3,5-diyl*	HN=N-C=N-NH–	P-68.3.1.3.4.2
	|	
formazan-1,3-5-triyl*	–NH-N=C-N=N–	P-68.3.1.3.4.2
formazan-1-yl* = (hydrazinylidenemethyl)diazenyl	H_2N-N=CH-N=N–	P-68.3.1.3.4.2
formazan-3-yl* = diazenyl(hydrazinylidene)methyl	HN=N-C(=NNH_2)–	P-68.3.1.3.4.2
formazan-5-yl* = (diazenylmethylidene)hydrazinyl	HN=N-CH=N-NH–	P-68.3.1.3.4.2
formazan-1-yl-5-ylidene*	=N-N=CH-N=N–	P-68.3.1.3.4.2
	|	
formazan-3-yl-5-ylidene*	=N-NH-C-N=NH	P-68.3.1.3.4.2
formimidoyl = methanimidoyl*	HC(=NH)–	P-65.1.7.2.2

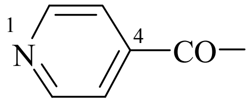
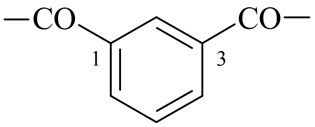
formimidoylamino = (iminomethyl)amino = methanimidamido*	HC(=NH)-NH–	P-66.4.1.3.3
formohydrazido = 2-formylhydrazin-1-yl*	OHC-NH-NH–	P-66.3.5.3
formohydrazonoyl = methanehydrazonoyl*	HC(=NNH$_2$)–	P-65.1.7.2.2
formyl* = methanoyl	HCO–	P-65.1.7.2.1; P-66.6.1.3
formylamino = formamido*	HCO-NH–	P-66.1.1.4.2
formylazanediyl*	HCO-N<	P-66.1.1.4.3
formylcarbonyl: see oxaldehydoyl*		
2-formylhydrazin-1-yl* = formohydrazido	OHC-NH-NH–	P-66.3.5.3
formylimino*	HCO-N=	P-66.1.1.4.3
formyloxy*	O=CH-O–	P-65.1.8.4
formylsulfanyl*	O=CH-S–	P-65.1.8.4
fulminato: see (oxo-λ^5-azanylidyne)methyl* and (λ^2-methylideneamino)oxy		
fumaroyl = (*E*)-but-2-enedioyl*	–OC-CH=CH-CO–	P-65.1.7.3.1
furan-2-carbonyl* = 2-furoyl		P-65.1.7.3.1
furan-3-carbonyl* = 3-furoyl		P-65.1.7.3.1
furan-3-yl* = 3-furyl		P-29.6
2-furoyl = furan-2-carbonyl*		
3-furoyl = furan-3-carbonyl*		
3-furyl = furan-3-yl* (same for isomer 2)		P-29.6

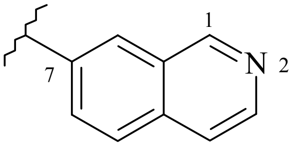
gallanyl*	H$_2$Ga–	P-68.1.2
germanediyl* (not germylene)	H$_2$Ge<	P-68.2.2
germanediylidene*	=Ge=	P-68.2.2
germanetetrayl*	>Ge<	P-68.2.2
germanetriyl*	–GeH<	P-68.2.2
germanyl: see germyl*		
germanylidene : see germylidene*		
germanylylidene*	–GeH=	P-68.2.2
germyl* (not germanyl)	H$_3$Ge–	P-29.3.1
germylidene* (not germanylidene)	H$_2$Ge=	
germylidyne* (not germanylidyne)	HGe≡	
germylene: see germanediyl*		
glutaryl = pentanedioyl*	–CO-[CH$_2$]$_3$-CO–	P-65.1.7.3.1
guanidino: see carbamimidamido*		

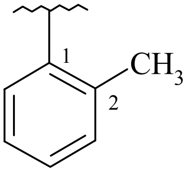
heptanoyl*	CH$_3$-[CH$_2$]$_5$-CO–	P-65.1.7.4.1
heptan-1-yl: see heptyl*		
heptan-1-ylidene: see heptylidene*		

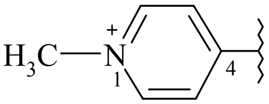
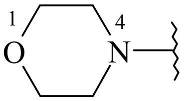
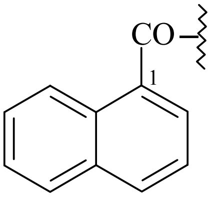
heptan-1-ylidyne: see heptylidyne*		
heptyl* (not heptan-1-yl)	$CH_3-[CH_2]_6-$	P-29.3.2.1
heptylidene* (not heptanylidene)	$CH_3-[CH_2]-CH=$	P-29.3.2.1
heptylidyne* (not heptanylidyne)	$CH_3-[CH_2]_5-C\equiv$	P-29.3.2.1
hexadecanoyl* = palmitoyl	$CH_3-[CH_2]_{14}-CO-$	P-65.1.7.3.1
hexadecan-1-yl: see hexadecyl*		
hexadecy* (not hexadecan-1-yl)	$CH_3-[CH_2]_{15}-$	P-29.3.2.1
hexamethylene: see hexane-1,6-diyl*		
hexanedioyl* = adipoyl	$-CO-[CH_2]_4-CO-$	P-65.1.7.3.1
hexane-1,6-diyl* (not hexamethylene)	$-CH_2-[CH_2]_4-CH_2-$	P-29.3.2.2
hexane-2,3,5-tricarbonyl*	$CH_3-CH(CO-)-CH(CO-)-CH_2-CH(CO-)-CH_3$	P-65.1.7.4.2
hexane-2,3,5-tricarbothioyl *	$CH_3-CH(CS-)-CH(CS-)-CH_2-CH(CS-)-CH_3$	P-65.1.7.4.2
hexanoyl*	$CH_3-[CH_2]_4-CO-$	P-65.1.7.4.1
hexan-1-yl: see hexyl*		
hexan-1-ylidene: see hexylidene*		
hexanylidyne: see hexylidyne*		
hexyl* (not hexan-1-yl)	$CH_3-[CH_2]_5-$	P-29.3.2.1
hexylidene* (not hexan-1-ylidene)	$CH_3-[CH_2]_4-CH=$	P-29.3.2.1
hexylidyne* (not hexanylidyne)	$CH_3-[CH_2]_4-C\equiv$	P-29.3.2.1
hydrazi: not to be used to form heterocycles		
hydrazidoimidophosphoryl = phosphorohydrazidimidoyl*	$>P(=NH)(NHNH_2)$	P-67.1.4.1.1
hydrazinecarbohydrazido = 2-(hydrazinecarbonyl)hydrazin-1-yl*	$H_2NNH-CO-NH-NH-$	P-66.3.5.3
hydrazinecarbohydrazonoyl* = *C*-hydrazinylcarbonohydrazonoyl	$H_2N-NH-C(=N-NH_2)-$	P-66.4.3.4.1
hydrazinecarbonyl* (not hydrazinylcarbonyl)	$H_2NNH-CO-$	P-66.3.2; P-68.3.1.2.1.1
2-hydrazinecarbonyldiazen-1-yl*	$H_2N-NH-CO-N=NH-$	P-68.3.1.3.3
2-hydrazinecarbonylhydrazin-1-yl* hydrazinecarbohydrazido	$H_2NNH-CO-NH-NH-$	P-66.3.5.3; P-68.3.1.2.6
2-hydrazinecarbonylhydrazine-1-ylidene*	$H_2NNH-CO-NH-N=$	P-68.3.1.2.6
hydrazinecarboximidoyl* (not carbazimidoyl, nor *C*-hydrazinocarbonimidoyl)	$H_2N-NH-C(=NH)-$	P-66.4.2.3.1
hydrazinediylidene* = diazanediylidene (not azino)	$=N-N=$	P-68.3.1.2.1.1
hydrazine-1,2-diyl* = diazane-1,2-diyl (not hydrazo)	$-NHNH-$	P-68.3.1.2.1.1
hydrazinesulfinyl* (not hydrazinosulfinyl)	$H_2N-NH-SO-$	P-66.3.2.1
hydrazinesulfonyl* (not hydrazinosulfonyl)	$H_2N-NH-SO_2-$	P-66.3.2.1
hydrazino: see hydrazinyl*		
C-hydrazinocarbonimidoyl: see hydrazinecarboximidoyl*		
hydrazinocarbonyl: see hydrazinecarbonyl*		
hydrazinosulfonyl: see hydrazinesulfonyl*		
hydrazinyl* = diazanyl (not hydrazino)	H_2N-NH-	P-68.3.1.2.1.1
C-hydrazinylcarbonohydrazonoyl = hydrazinecarbohydrazonoyl*	$H_2N-NH-C(=N-NH_2)-$	P-66.4.3.4.1
hydrazinylcarbonyl: see hydrazinecarbonyl*		
hydrazinylidene* = diazanylidene (not hydrazono)	$H_2N-N=$	P-68.3.1.2.1.1
(hydrazinylidenemethyl)diazenyl = formazan-1-yl*	$H_2N-N=CH-N=N-$	P-68.3.1.3.4.2
(2-hydrazinylidenemethyl)hydrazine-1-yl = 2-methanehydrazonoylhydrazine-1-yl*	$H_2N-NH=CH-NH-NH-$	P-66.4.3.4.2

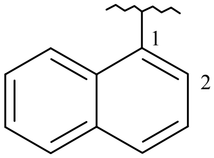
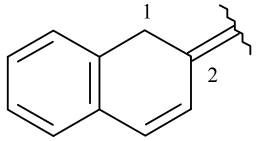
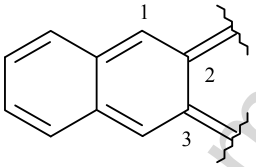
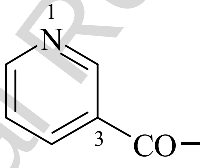
(hydrazinylmethylidene)amino*	H$_2$N-NH-CH=N–	P-66.4.2.3.3
hydrazinylsulfonyl: see hydrazinesulfonyl*		
hydrazo = hydrazine-1,2-diyl* = diazane-1,2-diyl	–NHNH–	P-68.3.1.2.1.1
hydrazono: see hydrazinylidene*		
hydrazonomethylidene = hydrazinylidenemethylidene *	H$_2$N-N=C=	P-65.2.1.8
hydrazonostiboryl = stiborohydrazonoyl*	>Sb(=NNH$_2$)–	P-67.1.4.1.1
C-hydroxycarbonohydrazonoyl*	HO-C(=NNH$_2$)–	P-65.1.3.2.2
(hydrazinylidenemethyl)diazenyl = formazan-1-yl*	H$_2$N-N=CH-N=N–	P-68.3.1.3.4.2
hydroarsoryl = arsonoyl*	HAs(O)<	P-67.1.4.1.2
hydronitroryl = azonoyl*	HN(O)<	P-67.1.4.1.2
hydrooxalyl = oxaldehydoyl* (not formylcarbonyl)	HCO-CO–	P-65.2.3.3
hydroperoxy*	HOO–	P-63.4.2.2
hydroperoxycarbonyl = carbonoperoxoyl*	HOO-CO–	P-65.1.4.2; P-65.2.1.5
hydrophosphoryl = phosphonoyl*	HP(O)<	P-67.1.4.1.2
hydroseleno: see selanyl*		
hydroselenonyl*	H-Se(O)–	P-65.3.2.3
hydrostiboryl = stibonoyl*	HSb(O)<	P-67.1.4.1.2
hydrosulfinyl*	H-S(O)–	P-65.3.2.3
hydrosulfonyl*	H-SO$_2$–	P-65.3.2.3
hydrotelluro: see tellanyl*		
hydroxy*	HO–	P-63.1.4
N-hydroxyacetimidoyl = *N*-hydroxyethanimidoyl* (not acetohydroximoyl)	CH$_3$C(=N-OH)–	P-65.1.3.3.1; P-65.1.7.4.1
hydroxyamino*	HO-NH–	P-68.3.1.1.1.5
hydroxyarsanyl*	HAsOH)–	P-67.1.4.1.1
hydroxyarsoryl*	HO-As(O)<	P-67.1.4.1.1
hydroxyazanediyl*	HO-N<	P-68.3.1.1.1.5
hydroxyazanylidene = hydroxyimino*	HO-N=	P-68.3.1.1.1.5
hydroxyazonoyl*	HN(O)(OH)–	P-67.1.4.1.1
N-hydroxybenzenecarboximidoyl* = *N*-hydroxybenzimidoyl = benzenecarbohydroximoyl	C$_6$H$_5$-C(=N-OH)–	P-65.1.7.2.2
N-hydroxybenzimidoyl = *N*-hydroxybenzenecarboximidoyl* = benzenecarbohydroximoyl	C$_6$H$_5$-C(=N-OH)–	P-65.1.7.2.2
hydroxyboranyl*	(HO)HB–	P-67.1.4.2.1
C-hydroxycarbonohydrazonoyl*	HO-C(=NNH$_2$)–	P-65.1.3.2.2
C-hydroxycarbonimidoyl*	HO-C(=NH)–	P-65.1.3.1.2
(*C*-hydroxycarbonimidoyl)amino* (not 1-isoureido)	HN=C(OH)-NH–	P-66.1.5.1.2.2
hydroxycarbonothioyl*	HO-CS–	P-65.1.5.1
(hydroxycarbonothioyl)carbonyl: see 2-hydroxy-2-thiooxalyl*		
hydroxyimino* = hydroxyazanylidene	HO-N=	P-68.3.1.1.1.5
hydroxy(methy)lphosphonoyl*	CH$_3$-P(O)(OH)–	P-67.1.4.1.1
hydroxy(oxo)-λ^5-azanylidene* (not *aci*-nitro)	HO-N(O)=	P-61.5.4; P-67.1.6
hydroxy(oxo)acetyl: see oxalo*		
hydroxy(oxo)-λ^5-arsanylidene*	HO-As(O)=	P-67.1.4.1.1
hydroxy(oxo)-λ^5-azanylidene* (not *aci*-nitro)	HO-N(O)=	P-61.5.4; P-67.1.4.1.4
hydroxy(oxo)-λ^5-phosphanylidene*	HO-P(O)=	P-67.1.4.1.1
hydroxy(oxo)-λ^5-stibanylidene*	HO-Sb(O)=	P-67.1.4.1.1

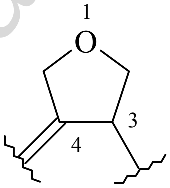
hydroxyphosphanylidene*	HO-P=	P-67.1.4.1.1
hydroxyphosphoryl*	HO-P(O)<	P-67.1.4.1.1
hydroxyselanyl* = seleneno	HO-Se–	P-63.4.2.2
(hydroxyselanyl)methyl* = (*OS*-selenohydroperoxy)methyl	HO-Se-CH_2–	P-63.4.2.2
hydroxystibanediyl*	(OH)Sb<	P-67.1.4.1.1
hydroxystiboryl* = hydroxy(oxo)-λ^5-stibanediyl	HO-Sb(O)<	P-67.1.4.1.1
hydroxysulfanyl* (not sulfeno; nor hydroxythio)	HO-S–	P-63.4.2.2
(hydroxysulfanyl)carbonoselenoyl* = (*OS*-thiohydroperoxy)carbonoselenoyl	HO-S-CSe–	P-65.2.1.7
(hydroxysulfanyl)carbonyl* = (*OS*-thiohydroperoxy)carbonyl	HO-S-CO–	P-65.1.5.3
(hydroxysulfanyl)phosphorothioyl* = (*OS*-thiohydroperoxy)phosphorothioyl	(HO-S)P(O)<	P-67.1.4.1.1
hydroxy(sulfanyl)phosphoryl* [not hydroxy(mercapto)phosphoryl]	(HO)(HS)P(O)–	P-67.1.4.1.1
hydroxysulfonothioyl*	HO-S(O)(S)–	P-65.3.2.3
hydroxytellanyl*	HO-Te–	P-63.4.2.2
2-hydroxy-2-thiooxalyl* [not (hydroxycarbonothioyl)carbonyl]	HO-CS-CO–	P-65.2.3.3
imidoarsoryl = arsorimidoyl*	>As(=NH)–	P-67.1.4.1.1
imidophosphinoyl = phosphinimidoyl*	H_2P(=NH)–	P-67.1.4.1.1
imino* (not azanylidene)	HN=	P-62.3.1.2
(iminomethyl)amino = methanimidamido* formimidoylamino	HN=CH-NH–	P-66.4.1.3.3
iminomethylidene*	HN=C=	P-65.2.1.8
indiganyl*	H_2In–	P-29.3.1; P-68.1.2
iodo*	I–	P-61.3.1
iodoso: see iodosyl*		
iodosyl* (not iodoso)	OI–	P-61.3.2
iodyl*	O_2I–	P-61.3.2
isocyanato*	OCN–	P-61.7
isocyano*	CN–	P-61.8
isonicotinoyl* = pyridine-3-carbonyl		P-67.1.7.3.1.2.
isophthaloyl = benzene-1,3-dicarbonyl*		P-65.1.7.4.2
isopropenyl = prop-1-en-2-yl* = 1-methylethen-1-yl	CH_2=C(CH_3)–	P-32.1.1
isopropoxy = (propan-2-yl)oxy*	$(CH_3)_2$CH–	P-63.2.2.2
isopropyl = propan-2-yl* = 1-methylethyl	$(CH_3)_2$CH–	P-29.4; P-29.6
isopropylidene = propan-2-ylidene* = 1-methylethylidene	$(CH_3)_2$C=	P-29.6

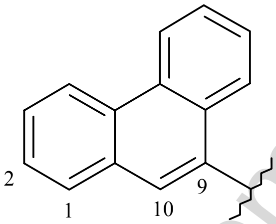
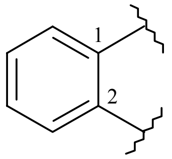
isoquinolin-7-yl* = 7-isoquinolyl (and 1-, 3-, 4-, 5-, 6-, and 8-isomers)		P-29.6
.		
7-isoquinolyl = isoquinolin-7-yl*		P-29.6
isoselenocyanato*	SeCN–	P-61.7
isotellurocyanato*	TeCN–	P-61.7
isothiocyanato*	SCN–	P-61.7
isothiocyanatosulfonothioyl* = sulfuro(isothiocyanatido)thioyl	SCN-S(O)(S)–	P-67.1.4.4.1
isothiocyanatosulfonyl* = sulfuroisothiocyanatidoyl	SCN-SO$_2$–	P-67.1.4.4.1
1-isoureido: see (*C*-hydroxycarbonimidoyl)amino*		
3-isoureido: see [amino(hydroxy)methylidene]amino*		
keto (not to be used): see oxo*		
maleoyl = (*Z*)-but-2-enedioyl*	–CO-CH=CH-CO–	P-65.1.7.3.1
malonimidoyl = propanediimidoyl*	–(HN)C-CH$_2$-C(NH)–	P-65.1.7.4.1
malonyl = propanedioyl*	–CO-CH$_2$-CO–	P-65.1.7.3.1
mercapto: see sulfanyl*		
mercaptocarbonyl: see sulfanylcarbonyl*		
mercaptooxy: see sulfanyloxy*		
methacryloyl = 2-methylprop-2-enoyl*	CH$_2$=C(CH$_3$)-CO–	P-65.1.7.3.1
methanediyl: see methylene*		
methanehydrazonoyl* = formohydrazonoyl	HC(=NNH$_2$)–	P-65.1.7.2.2
2-methanehydrazonoy)hydrazine-1-yl* = (2-hydrazinylidenemethyl)hydrazine-1-yl	H$_2$N-NH=CH-NH-NH–	P-66.4.3.4.2
methaneseleninyl* (not methylseleninyl)	CH$_3$-Se(O)–	P-65.3.2.2.2
methaneselenoyl* = selenoformyl	SeHC–	P-65.1.7.2.3
methanesulfinamido* = methanesulfinylamino	CH$_3$-SO-NH–	P-65.1.1.4.2
methanesulfinyl* (not methylsulfinyl)	CH$_3$-SO–	P-65.3.2.2.2
methanesulfinylamino = methanesulfinamido*	CH$_3$-SO-NH–	P-65.1.1.4.2
methanesulfonamido* = methanesulfonylamino	CH$_3$-SO$_2$-NH–	P-66.1.1.4.2
methanesulfonyl* (not methylsulfonyl)	CH$_3$-SO$_2$–	P-65.3.2.2.2
methanesulfonylamino = methanesulfonamido*	CH$_3$-SO$_2$-NH–	P-66.1.1.4.2
methanesulfonylimino*	CH$_3$-SO$_2$-N=	P-66.1.1.4.3
methanetelluroyl* = telluroformyl	TeHC–	P-65.1.7.2.3
methanetetrayl*	>C<	P-29.3.2.2
methanethioamido* = methanethioylamino (not thioformamido)	CH$_3$-CS-NH–	P-66.1.3.1.2
methanethioyl* = thioformyl	SHC–	P-65.1.7.2.3
methanethioylamino = methanethioamido* (not thioformamido)	CH$_3$-CS-NH–	P-66.1.3.1.2
methanetriyl*	–CH<	P-29.3.2.2
methanidyl*	$^{-}$CH$_2$–	P-72.6.3
methanimidamido* = (iminomethyl)amino formimidoylamino	HN=CH-NH–	P-66.4.1.3.3
methanimidoyl* = formimidoyl	HC(=NH)–	P-65.1.7.2.2
methanoyl = formyl*	HCO–	P-65.1.7.2.1

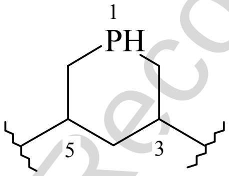
methanyl: see methyl*		
methanylidene: see methylidene*		
methanylidyne: see methylidyne*		
methanylylidene*	–CH=	P-29.3.2.2
methoxy* (not methyloxy)	CH_3-O–	P-63.2.2.2
C-methoxycarbonimidoyl*	CH_3-O-C(=NH)–	P-65.6.3.3.1
methoxycarbonothioyl*	CH_3-O-CS–	P-65.6.3.3.1
methoxycarbonyl* (not carbomethoxy)	CH_3-O-CO–	P-65.6.3.2.2
methoxy(isocyanato)phosphoryl*	CH_3-P(O)(NCO)–	P-67.1.4.1.1
methoxysulfanyl* (not methoxythio)	CH_3-O-S–	P-63.3.2
S-methoxysulfinimidoyl*	CH_3-O-S(=NH)–	P-65.3.2.3
(methoxysulfinyl)oxy*	CH_3O-SO-O–	P-67.1.4.4.2
methoxysulfonyl* = methoxysulfuryl	CH_3-O-SO_2–	P-65.3.2.3; P-67.1.4.4.1
(methoxysulfonyl)amino*	CH_3O-SO_2-NH–	P-67.1.4.4.2
methoxysulfuryl = methoxysulfonyl*	CH_3-O-SO_2–	P-65.3.2.3; P-67.1.4.4.1
methoxythio: see methoxysulfanyl*		
methyl* (not methanyl)	CH_3–	P-29.3.1
(methylamino)sulfinyl*	CH_3-NH-SO–	P-66.1.1.4.1
1-methylbutyl = pentan-2-yl*	CH_3-CH_2-CH_2-CH(CH_3)–	P-29.4
2-methylbutyl*	CH_3-CH_2-CH(CH_3)-CH_2–	P-29.4
3-methylbutyl* (not isopentyl)	$(CH_3)_2$CH-CH_2-CH_2–	P-29.4
methyldioxy: see methylperoxy*		
methyldiselanyl*	CH_3-SeSe–	P-63.3.1
methyldisulfanyl*	CH_3-SS–	P-63.3.1
methylditellanyl*	CH_3-TeTe–	P-63.3.1
methylene* (not methanediyl)	–CH_2–	P-29.6
methylenebis(oxy)* (not methylenedioxy)	–O-CH_2-O–	P-63.2.2.1.3
methylenebis(sulfanediyl)*	–S-CH_2-S–	P-63.2.2.1.3
1-methylethenyl = prop-1-en-2-yl* =isopropenyl	CH_2=C(CH_3)–	P-32.1.1
1-methylethyl = propan-2-yl* = isopropyl	$(CH_3)_2$CH–	P-29.4; P-29.6
1-methylethylidene = propan-2-ylidene* = isopropylidene	$(CH_3)_2$C=	P-29.4; P-29.6
(1-methylethyl)oxy = propan-2-yloxy*	$(CH_3)_2$C-O–	P-63.2.2.1.1
methylidene* (not methanylidene)	CH_2=	P-29.3.1
(λ^2-methylideneamino)oxy* (not fulminato)	C=N-O–	P-61.9
methylidyne* (not methanylidyne)	CH≡	P-29.3.1
methylperoxy* (not methyldioxy)	CH_3-OO–	P-63.3.1
methyloxy (see methoxy*)		
2-methylphenyl* = *o*-tolyl		P-29.6
3-methylphenyl* = *m*-tolyl		P-29.6
4-methylphenyl* = *p*-tolyl		P-29.6
methyl(phenyl)arsinoyl*	$(C_6H_5)(CH_3)$As(O)–	P-67.1.4.1.1

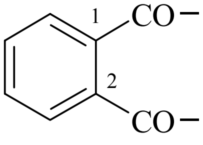
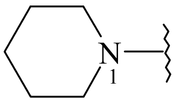
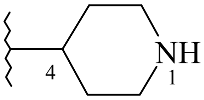
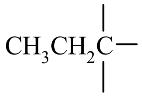
methylphosphonoyl*	$CH_3-P(O)<$	P-67.1.4.1.1
2-methylpropan-2-yl = *tert*-butyl* (unsubstsituted) = 1,1-dimethylethyl	$(CH_3)_3C-$	P-29.4; P-29.6
(2-methylpropan-2-yl)oxy = *tert*-butoxy*	$(CH_3)_3C-O-$	P-63.2.2.2
2-methylpropan-2-ylium-1-yl*	$\underset{1}{C}H_3-\underset{2}{C}^+(CH_3)-\underset{3}{C}H_2-$	P-73.6
2-methylprop-2-enoyl* = methacryloyl	$CH_2=C(CH_3)-CO-$	P-65.1.7.3.1
1-methylprop2-en-1-yl = but-3-en-2-yl*	$CH_2=CH-\overset{\vert}{C}H-CH_3$	P-32.1.1
1-methylpropyl = butan-2-yl*	$CH_3-CH_2-C(CH_3)-$	P-29.3.2.2
(1-methylpropyl)oxy = butan-2-yloxy* = *sec*-butoxy	$CH_3-CH_2-(CH_3)CH-O-$	P-63.2.2.1.1
1-methylpyridin-1-ium-4-yl*		P-73.6
methylselanyl* (not methylseleno)	CH_3-Se-	P-63.2.2.1.2; P-63.2.5
methylseleninyl: see methaneseleninyl*		
methylseleno: see methylselanyl*		
methylsulfaniumdiyl* = methylsulfoniumdiyl	$CH_3-{}^+S<$	P-73.6
methylsulfanyl* (not methylthio)	CH_3-S-	P-63.2.2.1.2
(methylsulfanyl)oxy*	CH_3-S-O-	P-63.3.2
S-methylsulfinimidoyl: see methanesulfinimidoyl*	$CH_3-S(=NH)-$	P-65.6.3.2.2.2
methylsulfinyl: see methanesulfinyl*		
S-methylsulfonimidoyl: see methanesulfonimidoyl*	$CH_3-S(=NH)(O)-$	P-65.6.3.2.2.2
methylsulfoniumdiyl = methylsulfaniumdiyl*	$CH_3-{}^+S<$	P-73.6
methylsulfonyl: see methanesulfonyl*		
methyltellanyl* (not methyltelluro)	CH_3-Te-	P-63.2.2.1.2; P-63.2.5
methyltelluro: see methyltellanyl*		
1-methyltetrasilan-1-yl*	$SiH_3-SiH_2-SiH_2-SiH(CH_3)-$	P-29.4
methylthio: see methylsulfanyl*		
(methylthio)oxy: see methylsulfanyl)oxy*		
(methylthio)sulfonyl = (methylsulfanyl)sulfonyl*	CH_3-S-SO_2-	P-65.6.3.3.1
methyltrisulfanyl* = methyltrithio	CH_3-SSS-	P-68.4.1.3
(λ^2-methylideneamino)oxy*	$C=N-O-$	P-61.9
morpholino: see morpholin-4-yl*		
morpholin-4-yl* (not morpholino)		P-29.3.3
naphthalene-1-carbonyl* = 1-naphthoyl		P-65.1.7.4.2
naphthalene-2-carbonyl* = 2-naphthoyl		P-65.1.7.4.2

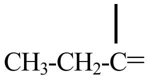
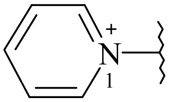
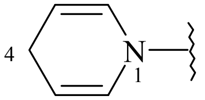
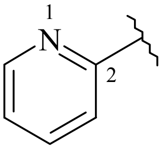
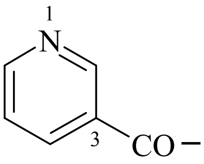
naphthalen-1-yl* - 1-naphthyl		P-29.3.4.1;P-29.6
naphthalen-2-yl* = 2-naphthyl		
naphthalene-2(1*H*)-ylidene* (also 1(2*H)-isomer)*		P-29.3.4.1
naphthalene-2,3-diylidene*		P-29.3.4.2
1-naphthoyl = naphthalene-1-carbonyl*	$C_{10}H_7$-CO–	P-65.1.7.3.1
2-naphthoyl = naphthalene-2-carbonyl*	$C_{10}H_7$-CO–	P-65.1.7.3.1
1-naphthyl = naphthalen-1-yl*	$C_{10}H_7$–	P-29.3.4.1; P-29.6
2-naphthyl = naphthalen-2-yl*	$C_{10}H_7$–	P-29.3.4.1; P-
nicotinoyl = pyridine-3-carbonyl*		P-65.1.7.3.1
nitramido*	O_2N-NH–	P-67.1.4.3
nitridophosphoryl = phosphoronitridoyl*	P(≡N)<	P-67.1.4.1
nitrilo* (not azanetriyl)	–N<	P-62.2.1.2.3
nitro*	O_2N–	P-61.5.1
aci-nitro: see hydroxy(oxo)-λ^5-azanylidene*		
nitrooxy*	O_2N-O–	P-67.1.4.3
nitroryl = azoryl*	–N(O)<	P-67.1.4.1.1
nitroso*	O=N–	P-61.5.1
nonanoyl*	CH_3-[CH_2]$_7$-CO–	P-65.1.7.4.1
nonan-1-yl: see nonyl*		
nonan-1-ylidene: see nonylidene*		
nonan-1-ylidyne: see nonylidyne*		
nonyl* (not nonan-1-yl)	CH_3-[CH_2]$_8$–	P-29.3.2.1
nonylidene* (not nonan-1-ylidene)	CH_3-[CH_2]$_7$-CH=	P-29.3.2.1
nonylidyne* (not nonanylidyne)	CH_3-[CH_2]$_7$-C≡	P-29.3.2.1
octadecanoyl* = stearoyl	CH_3-[CH_2]$_{16}$-CO–	P-65.1.7.3.1
octadecan-1-yl: see octadecyl*		
(*Z*)-octadec-9-enoyl* = oleoyl	CH_3-[CH_2]$_7$-CH=CH-[CH_2]$_7$-CO-	P-65.1.7.3.1
octadecyl* (not octadecan-1-yl)	CH_3-[CH_2]$_{17}$–	P-29.3.1
octanoyl*	CH_3-[CH_2]$_7$-CO–	P-65.1.7.4.1
octan-1-yl: see octyl*		

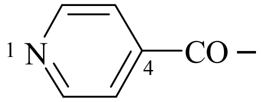
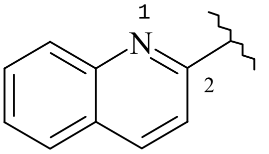
octan-1-ylidene: see octylidene*		
octan-1-ylidyne: see octylidyne*		
octyl* (not octan-1-yl)	CH_3-[CH_2]$_7$–	P-29.3.2.1
octylidene* (not octan-1-ylidene)	CH_3-[CH_2]$_6$-CH=	P-29.3.2.1
octylidyne* (not octan-1-ylidyne)	CH_3-[CH_2]$_6$-C≡	P-29.3.2.1
oleoyl = (*Z*)-octadec-9-enoyl*	CH_3-[CH_2]$_7$-CH=CH-[CH_2]$_7$-CO–	P-65.1.7.3.1
oxaldehydoyl* = hydrooxalyl (not formylcarbonyl)	HOC-CO–	P-65.2.3.3
oxalo* = carboxycarbonyl (not carboxyformyl, nor hydroxyl(oxo)acetyl)	HO-CO-CO–	P-65.2.3.3
oxaloamino* = (carboxycarbonyl)amino	HO-CO-CO-NH–	P-65.2.3.3
oxalooxy* = (carboxycarbonyl)oxy	HO-CO-CO-O–	P-65.2.3.3
oxalosulfanyl* = (carboxycarbonyl)sulfanyl	HO-CO-CO-S–	P-65.2.3.3
oxalyl* = ethanedioyl = dioxoethane-1,2-diyl	–CO-CO–	P-65.2.3.3
oxalylbis(azanediyl)*	–HN-CO-CO-NH–	P-66.1.5.3
oxalylbis(azanediylidene)*	=N-CO-CO-N=	P-66.1.5.3
oxalyldinitrilo*	>N-CO-CO-N<	P-66.1.5.3
oxamoyl* (not carbamoylcarbonyl, nor carbamoylformyl, nor amino(oxo)acetyl)	H_2N-CO-CO–	P-65.2.3.3
oxamoylamino* = carbamoylformamido = aminooxoacetamido	H_2N-CO-CO-NH–	P-66.1.5.3
oxamoylazanediyl*	H_2N-CO-CO-N<	P-66.1.5.3
oxamoylimino*	H_2N-CO-CO-N=	P-66.1.5.3
oxido*	$^{-}$O–	P-72.6.2
oxo* (not keto)	O=	P-64.5
oxoacetyl: see hydrooxalyl*		
oxo-λ^5-azanyl*	O=NH_2–	P-62.5
(oxo-λ^5-azanylidyne)methyl* (not fulminato)	ONC–	P-61.9; P-66.5.3
oxolan-3-yl-4-ylidene*	 	P-29.3.3
oxomethylidene*	=C=O	P-65.2.1.8
oxo-λ^5-phosphanylidene*	HP(O)=	P-67.1.4.1.1
oxo-λ^5-phosphanylidyne*	P(O)≡	P-67.1.4.1.1
2-oxopropyl* = acetonyl	CH_3-CO-CH_2–	P-56.1.2; 64.5.1
2-oxopropylidene* (not acetonylidene)	CH_3-CO-CH=	P-56,1,2
2-oxopropylidyne* (not acetonylidyne)	CH_3-CO-C≡	P-56.1.2
oxy*	–O–	P-63.2.2.1.1
palmitoyl = hexadecanoyl*	CH_3-[CH_2]$_{14}$-CO–	P-65.1.7.3.1
pentanedioyl* = glutaryl	–CO-CH_2-CH_2-CH_2-CO–	P-65.1.7.3.1
pentanoyl*	CH_3-CH_2-CH_2-CH_2-CO–	P-65.1.7.4.1
pentan-1-yl: see pentyl*		
pentan-2-yl* = 1-methylbutyl	CH_3-CH_2-CH_2-CH(CH_3)–	P-29.4
pentan-1-ylidene: see pentylidene*		
pentan-3-ylidene* = 1-ethylpropylidene	(CH_3-CH_2)$_2$C=	P-29.3.2.2; P-29.4
pentan-1-ylidyne: see pentylidyne*		

pent-2-enoyl*	CH_3-CH_2-CH=CH-CO–	P-65.1.7.4.1
pentyl* (not pentan-1-yl)	CH_3-CH_2-CH_2-CH_2-CH_2–	P-29.3.2.1
pentylidene* (not pentan-1-ylidene)	CH_3-CH_2-CH_2-CH_2-CH=	P-29.3.2.1
pentylidyne* (not pentan-1-ylidyne)	CH_3-CH_2-CH_2-CH_2-C≡	P-29.3.2.1
pentyloxy*	CH_3-$[CH_2]_3$-CH_2-O–	P-63.2.2.1.1
perbromyl*	O_3Br–	P-61.3.2
perchloryl*	O_3Cl–	P-61.3.2
perfluoryl*	O_3F–	P-61.3.2.
periodyl*	O_3I–	P-61.3.2
peroxy* (not dioxy)	–OO–	P-63.3.1
peroxycarboxy: see carbonoperoxoyl*		
peroxyphosphoryl = phosphoroperoxoyl*	P(O)(OOH)<	P-67.1.4.1.1
phenanthren-9-yl* =9-phenanthryl (also 1-, 2-, 3-, and 4- isomers)		P-29.3.4.1;P-29.6
phenoxy* (not phenyloxy)	C_6H_5-O–	P-63.2.2.2
phenyl*	C_6H_5–	P-29.6
phenylamino = anilino*	C_6H_5-NH–	P-62.2.1.1.3
(phenylamino)sulfonyl = phenylsulfamoyl*	C_6H_5-NH-SO_2–	P-66.1.1.4.1
phenylazo = phenyldiazenyl*	C_6H_5-N=N–	P-68.3.1.3.1.2
phenylcarbonyl = benzoyl*	C_6H_5-CO–	P-65.1.7.1.2
phenyl(chlorophosphonoyl) = phenylphosphonochloridoyl*	C_6H_5-P(O)Cl–	P-67.1.4.1.1
phenyldiazenyl* = phenylazo	C_6H_5-N=N–	P-68.3.1
1,2-phenylene* (not benzene-1,2-diyl)		P-29.6
1,3-phenylene* (not benzene-1,3-diyl)		P-29.6
1,4-phenylene* (not benzene-1,4-diyl)		P-29.6
2-phenylethenyl* = 2-phenylvinyl = styryl	C_6H_5-CH=CH–	P-29.6
phenyloxy: see phenoxy*		
phenylmethyl = benzyl*	C_6H_5-CH_2–	P-29.6
phenylmethylidene =benzylidene*	C_6H_5-CH=	P-29.6
phenylmethylidyne = benzylidyne*	C_6H_5-C≡	P-29.6
phenylphosphonochloridoyl* = phenyl(chlorophosphonoyl)	$C_6H_5P(O)(Cl)$–	P-67.1.4.1.1
3-phenylprop-2-enoyl* = cinnamoyl	C_6H_5-CH=CH-CO–	P-67.1.7.3.1
phenylselanyl* (not phenylseleno)	C_6H_5-Se–	P-63.2.2.1.2; P-63.2.5
(phenylselanyl)oxy*	C_6H_5-Se-O–	P-63.4.2
phenylseleno: see phenylselanyl*		
phenylselenonyl: see benzeneselenonyl*		

phenylsulfamoyl* = (phenylamino)sulfonyl =anilinosulfonyl	C_6H_5-NH-SO_2–	P-66.1.1.4.1
phenylsulfanyl* (not phenylthio)	C_6H_5-S–	P-63.2.2.1.2
(phenylsulfanyl)oxy*	C_6H_5-Se-O–	P-63.4.2
phenylsulfinoselenoyl: see benzenesulfinoselenoyl*		
phenylsulfinyl; see benzenesulfinyl*		
phenylsulfonyl: see benzenesulfonyl*		
phenyltellanyl* (not phenyltelluro)	C_6H_5-Te–	P-63.2.2.1.2
(phenyltellanyl)oxy*	C_6H_5-Te-O–	P-63.4.2
phenyltelluro: see phenyltellanyl*		
phenylthio: see phenylsulfanyl*		
2-phenylvinyl = 2-phenylethenyl* = styryl	C_6H_5-CH=CH–	P-29-6
phosphanediyl* (not phosphinediyl)	HP<	P-68.3.2.4.2.2
phosphanetriyl* (not phosphinetriyl)	–P<	P-68.3.2.4.2.2
phosphaniumyl* = phosphonio	H_3P^+–	P-73.6
phosphanyl* (not phosphino)	H_2P–	P-29.3.1
λ^5-phosphanyl* = phosphoranyl	H_4P–	P-68.3.2.4.2.2
phosphanylidene*	HP=	P-68.3.2.4.2.2
phosphanylylidene*	–P=	P-68.3.2.4.2.2
phosphinane-3,5,diyl*		P-29.3.3
phosphinimidoyl* = imidophosphinoyl	H_2P(=NH)–	P-67.1.4.1.1
phosphino: see phosphanyl*		
phosphinothioyl*	H_2P(S)–	P-67.1.4.1.1
phosphinoyl*	H_2P(O)–	P-67.1.4.1.1
phospho*	PO_2P–	P-61.5.5
phosphonato*	$(^{-}O)P(O)$–	P-72.6.1
phosphonio = phosphaniumyl*	H_3P^+–	P-73.6
phosphono*	$(HO)_2P(O)$–	P-67.1.4.1.1
phosphonooxy*	$(HO)_2P(O)$-O–	P-67.1.4.1.3
phosphonothioyl* = hydro(thiophosphoryl)	>PH(S)	P-67.1.4.1.1, P-67.1.4.1.2
phosphonoyl* = hydrophosphoryl	HP(O)<	P-67.1.4.1.1, P-67.1.4.1.2
phosphooxy*	O_2P-O–	P-67.1.4.3
phosphoramidochloridoyl* = chloroamidophosphoryl	$P(O)(NH_2)Cl$–	P-67.1.4.1.1
phosphoranyl = λ^5-phosphanyl*	H_4P–	P-68.3.2.4.2.2
phosphorodichloridoyl* = dichlorophosphoryl	$P(O)Cl_2$–	P-67.1.4.1.1
phosphoronitridoyl* = nitridophosphoryl	P(≡N)<	P-67.1.4.1.1
phosphorocyanidoisocyanatidothioyl* = cyano(isocyanato)phosphorothioyl = cyano(isocyanato)(thiophosphoryl)	–P(S)(CN)(NCO)	P-67.1.4.1.1
phosphorohydrazidimidoyl* = hydrazidimidophosphoryl	$>P(=NH)(NHNH_2)$	P-67.1.4.1.1
phosphoroperoxoyl* = peroxyphosphoryl	>P(O)(OOH)	P-67.1.4.1.1
phosphoroso*	–PO	P-61.5.5
phosphoro(thioperoxoyl)* = (thioperoxy)phosphoryl	>P(O)(OSH) or >P(O)(SOH)	P-67.1.4.1.1
phosphorothioyl* = thiophosphoryl	>P(S)–	P-67.1.4.1.1

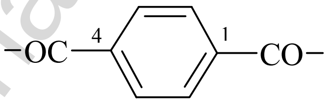
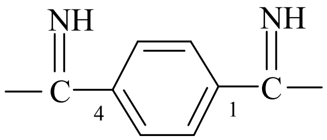
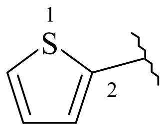
phosphoryl*	$-P(O)<$	P-67.1.4.1.1
phthaloyl = benzene-1,2-dicarbonyl* (not 1,2-phenylenedicarbonyl)		P-65.1.7.3.1
piperidino: see piperidin-1-yl*		
piperidin-1-yl* = 1-piperidyl (not piperidino)		P-29.6
piperidin-4-yl* = 4-piperidyl (and 2- and 3- isomers)		P-29.6
1-piperidyl = piperidin-1-yl* (not piperidino)		P-29.6
4-piperidyl = piperidin-4-yl*		P-29.6
plumbanediyl* (not plumbylene)	$H_2Pb<$	P-68.2.2
plumbanediylidene*	$=Pb=$	P-68.2.2
plumbanetetrayl*	$>Pb<$	P-68.2.2
plumbanetriyl*	$-PbH<$	P-68.2.2
plumbanyl:see plumbyl*		
plumbanylidene : see plumbylidene*		
plumbanylidyne: see plumbylidyne*		
plumbanylylidene*	$-PbH=$	P-68.2.2
plumbyl* (not plumbanyl)	H_3Pb-	P-68.2.2
plumbylene: see plumbanediyl*		
plumbylidene* (not plumbanylidene)	$H_2Pb=$	P-68.2.2
plumbylidyne* (not plumbanylidyne)	$HPb\equiv$	P-68.2.2
propanamido* = propanoylamino = propionamido = propionylamino	CH_3-CH_2-CO-NH–	P-66.1.1.4.2
propanediimidoyl* = malonimidoyl	–(HN)C-CH_2-C(NH)–	P-65.1.7.4.1
propanedioyl* = malonyl	–CO-CH_2-CO–	P-65.1.7.3.1
propane-1,3-diyl* (not trimethylene)	–CH_2-CH_2-CH_2–	P-29.3.2.2
propane-1,2-diyl* = 1-methylethane-1,2-diyl (not propylene)	–CH_2-CH(CH_3)–	P-29.3.2.2
propane-1-1-1-triyl	 $CH_3CH_2\overset{\vert}{\underset{\vert}{C}}-$	P-29.3.2.2
propanethioyl* = thiopropionyl	CH_3-CH_3-CS–	P-65.1.7.4.1
propanimidoyl* = propionimidoyl	CH_3-CH_2-C(=NH)–	P-65.1.7.4.1
propanoyl* = propionyl	CH_3-CH_2-CO–	P-65.1.7.3.1
propanoylamino = propanamido* = propionamido = propionylamino	CH_3-CH_2-CO-NH–	P-66.1.1.4.2
propanoyloxy* = propionyloxy	CH_3-CH_2-CO-O–	P-65.6.3.2.2
propan-1-yl: see propyl*		
propan-2-yl* = isopropyl = 1-methylethyl	$(CH_3)_2CH-$	P-29.4; P-29.6
propan-1-ylidene: see propylidene*		

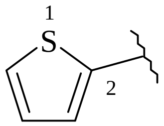
propan-2-ylidene* = 1-methylethylidene = isopropylidene	$(CH_3)_2C=$	P-29.4; P-29.6
propan-2-yloxy* = isopropoxy	$(CH_3)_2CH$-O–	P-63.2.2.2
propan-1-yl-1-ylidene*	 $CH_3\text{-}CH_2\text{-}\overset{|}{C}=$	P-29.3.2.2
propan-1-ylidyne: see propylidyne*		
prop-2-enehydrazonoyl* = acrylohydrazonoyl	CH_2=CH-C(=NNH_2)–	P-65.1.7.3.2
prop-2-enoyl* = acryloyl	CH_2=CH-CO–	P-65.1.7.3.1
prop-2-eneselenoyl* = selenoacryloyl	CH_2=CH-CSe–	P-65.1.7.3.3
prop-1-en-1-yl*	CH_3-CH=CH–	P-32.3
prop-1-en-2-yl* = 1-methylethen-1-yl = isopropenyl	CH_2=C(CH_3)–	P-32.1.1
prop-2-en-1-yl* = allyl	CH_2=CH-CH_2–	P-32.3
prop-2-en-1-ylidene* = allylidene	CH_2=CH-CH=	P-32.3
prop-2-en-1-ylidyne* = allylidyne	CH_2=CH-C≡	P-32.3
propionamido= propanamido* = propionylamino = propanoylamino	CH_3-CH_2-CO-NH–	P-66.1.1.4.2
propionimidoyl = propanimidoyl*	CH_3-CH_2-C(=NH)-	P-65.1.7.4.1
propionyl = propanoyl*	CH_3-CH_2-CO–	P-65.1.7.3.1
propionylamino = propanamido* = propanoylamino = propionamido	CH_3-CH_2-CO-NH–	P-66.1.1.4.2
propionyloxy = propanoyloxy*	CH_3-CH_2-CO-O–	P-65.6.3.2.2
propoxy* (not propyloxy)	CH_3-CH_2-CH_2-O–	P-63.2.2.2
propyl* (not propan-1-yl)	CH_3-CH_2-CH_2–	P-29.3.2.1
propylidene* (not propan-1-ylidene)	CH_3-CH_2-C=	P-29.3.2.1
propylidyne* (not propan-1-ylidyne)	CH_3-CH_2-C≡	P-29.3.2.1
propyloxy: see propoxy*		
piperidino = piperidin-1-ium-1-yl*		P-73.6
pyridin-1-ium-1-yl* = pyridinio		P-73.6
pyridin-1(4*H*)-yl*		P-29.3.4.1
pyridin-2-yl* = 2-pyridyl (and 3- and 4- isomers)		P-29.3.4.1; P-29.6
pyridine-3-carbonyl* = nicotinoyl		P-65.1.7.3.1

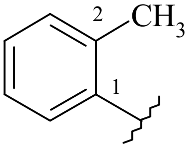
pyridin-4-carbonyl* = isonicotinoyl		P-65.1.7.3.1
2-pyridyl = pyridin-2-yl* (and 3-, 4-isomers)		P-29.3.4.1; P-29.6
pyruvoyl: see 2-oxopropanoyl*	CH_3-CO-CO–	P-65.1.7.4.1
quinolin-2-yl* = 2-quinolyl (and 3-, 4-, 5-, 6-, 7-, and 8- isomers)		P-29.6
2-quinolyl = quinolin-2-yl*		P-29.6
selanediyl* (not seleno)	–Se–	P-63.1.5
selaniumyl* = selenonio	H_2^+Se–	P-73.6
selanyl* (not hydroseleno)	HSe–	P-63.1.5
selanylphosphinoyl*	HP(O)(SeH)–	P-67.1.4.1.1
selanylidene* = selenoxo	Se=	P-64.6.1
seleneno: see hydroxyselanyl*		
selenino* (preferred when unmodified)	HO-SeO–	P-65.3.2.1
seleninyl*	>Se=O	P-65.3.2.3
seleno: see selanediyl*		
selenoacetyl = ethaneselenoyl*	CH_3-CSe–	P-65.1.7.2.3
selenoacryloyl = prop-2-enselenoyl*	CH_2=CH-CSe–	P-65.1.7.3.3
selenocyanato*	NC-Se–	P-65.2.2
selenoformyl = metahnetelluroyl*	SeHC–	P-65.1.7.2.3
selenohydroperoxy = hydroxyselanyl*	HO-Se–	P-63.4.2.2
(*OS*-selenohydroperoxy)methyl (hydroxyselanyl)methyl* =	HO-Se-CH_2–	P-63.4.2.2
selenonimidothioyl*	Se(=NH)(=S)<	P-65.3.2.3
selenonio = selaniumyl*	H_2^+Se–	P-73.6
selenono* (preferred when unmodified)	HO-SeO_2–	P-65.3.2.1
selenonohydrazonoyl*	Se(O)(=NNH_2)–	P-65.3.2.3
selenonyl*	SeO_2<	P-65.3.2.3
selenoxo = selanylidene*	Se=	P-64.6.1
semicarbazido = 2-carbamoylhydrazin-1-yl* = 2-(aminocarbonyl)hydrazin-1-yl	H_2N-CO-NHNH–	P-68.3.1.2.4
semicarbazono = 2-carbamoylhydrazin-1-ylidene*	H_2N-CO-NHN=	P-68.3.1.2.5
silanediyl* (not silylene)	H_2Si<	P-68.2.2
silanediyldiethane-1,2-diyl* = silanediyldiethylene	–CH_2-CH_2-SiH_2-CH_2-CH_2–	P-29.5
silanediyldiethylene = silanediyldiethane-1,2-diyl*	–CH_2-CH_2-SiH_2-CH_2-CH_2–	P-29.5
silanediylidene*	=Si=	P-68.2.2
silanetetrayl*	>Si<	P-68.2.2
silanetriyl*	–SiH<	P-68.2.2
silanyl: see silyl*		
silanylidene : see silylidene*		
silanylidyne: see silylidyne*		

silanylylidene*	$-\mathrm{SiH}=$	P-68.2.2
siloxy: see silyloxy*		
silyl* (not silanyl)	$\mathrm{H_3Si}-$	P-68.2.2
silylene: see silanediyl*		
silylidene* (not silanylidene)	$\mathrm{H_2Si}=$	P-68.2.2
silylidyne* (not silanylidyne)	$\mathrm{HSi}\equiv$	P-68.2.2
silyloxy* (not siloxy)	$\mathrm{H_3Si\text{-}O}-$	P-68.2.6.2
3-silyltetrasilan-1-yl*	$\mathrm{SiH_3\text{-}SiH(SiH_3)\text{-}SiH_2\text{-}SiH_2}-$	P-29.4
stannanediyl* (not stannylene)	$\mathrm{H_2Sn}<$	P-68.2.2
stannanediylidene*	$=\mathrm{Sn}=$	P-68.2.2
stannanetetrayl*	$>\mathrm{Sn}<$	P-68.2.2
stannanetriyl*	$-\mathrm{SnH}<$	P-68.2.2
stannanyl: see stannyl*		
stannanylidene : see stannylidene*		
stannanylidyne: see stannylidyne*		
stannanylylidene*	$-\mathrm{SnH}=$	P-68.2.2
stannyl* (not stannanyl)	$\mathrm{H_3Sn}-$	P-68.2.2
stannylene: see stannanediyl*		
stannylidene* (not stannanylidene)	$\mathrm{H_2Sn}=$	P-29.3.1
stannylidyne* (not stannanylidyne)	$\mathrm{HSn}\equiv$	P-68.2.2
stearoyl = octadecanoyl*	$\mathrm{CH_3\text{-}[CH_2]_{16}\text{-}CO}-$	P-65.1.7.3.1
stibanediyl* (not stibinediyl)	$\mathrm{HSb}<$	P-68.3.2.4.2.2
stibanetriyl* (not stibinetriyl)	$-\mathrm{Sb}<$	P-68.3.2.4.2.2
stibaniumyl* = stibonio	$\mathrm{H_3Sb^{+}}-$	P-73.6
stibanyl* (not stibino)	$\mathrm{H_2Sb}-$	P-68.3.2.4.2.2
λ^5-stibanyl* = stiboranyl	$\mathrm{H_4Sb}-$	P-68.3.2.4.2.2
stibanylidene*	$\mathrm{HSb}=$	P-68.3.2.4.2.2
stibanylylidene*	$-\mathrm{Sb}=$	P-68.3.2.4.2.2
stibinediyl : see stibanediyl*		
stibinetriyl : see stibanetriyl*		
stibinimidoyl* = dihydrostiborimidoyl	$\mathrm{H_2Sb(=NH)}-$	P-67.1.4.1.1
stibino: see stibanyl*		
stibinothioyl* = dihydrostiborothioyl	$\mathrm{H_2Sb(S)}-$	P-67.1.4.1.1
stibinoyl*	$\mathrm{H_2Sb(O)}-$	P-67.1.4.1.1
stibonato*	$(^{-}\mathrm{O})\mathrm{Sb(O)}-$	P-72.6.1
stibonio = stibaniumyl*	$\mathrm{H_3Sb^{+}}-$	P-73.6
stibono*	$\mathrm{(HO)_2Sb(O)}-$	P-67.1.4.1.1
stibonoyl*	$\mathrm{HSb(O)}<$	P-67.1.4.1.1
stiboranyl = λ^5-stibanyl*	$\mathrm{H_4Sb}-$	P-68.3.2.4.2.2
stiboronitridoyl*	$\mathrm{Sb(\equiv N)}<$	P-67.1.4.1.1
stiborodiamidothioyl*	$\mathrm{(H_2N)_2Sb(S)}-$	P-67.1.4.1.1
stiborohydrazonoyl* = hydrazonostiboryl	$>\mathrm{Sb(=NNH_2)}-$	P-67.1.4.1.1
stiboryl* (not antimonyl)	$>\mathrm{Sb(O)}-$	P-67.1.4.1.1
styryl = 2-phenylethen-1-yl* = 2-phenylvinyl	$\mathrm{C_6H_5\text{-}CH=CH}-$	P-29.6
succinyl = butanedioyl*	$-\mathrm{CO\text{-}CH_2\text{-}CH_2\text{-}CO}-$	P-65.1.7.3.1
succinimidoyl = butanediimidoyl*	$\mathrm{(HN=)C\text{-}CH_2\text{-}CH_2\text{-}C(=NH)}-$	P-65.1.7.3.2
sulfamoyl* = aminosulfonyl	$\mathrm{H_2N\text{-}SO_2}-$	P-65.3.2.3
sulfanediyl* (not thio)	$-\mathrm{S}-$	P-63.1.5
sulfanediylbis(methylene)* = sulfanediyldimethylene	$-\mathrm{CH_2\text{-}S\text{-}CH_2}-$	P-63.2.2.1.3
sulfanediyldimethylene = sulfanediylbis(methylene)*	$-\mathrm{CH_2\text{-}S\text{-}CH_2}-$	P-63.2.2.1.3

sulfaniumyl* = sulfoniumyl = sulfonio	H$_2$S$^+$–	P-73.6
sulfanyl* (not mercapto)	HS–	P-63.1.5
sulfanylboranyl*	(HS)BH–	P-67.1.4.2.1
(*C*-sulfanylcarbonimidoyl)amino*	HN=C(SH)-NH–	P-66.1.5.1.3.3
sulfanylcarbonothioyl = dithiocarboxy*	HS-CS–	P-65.2.1.6
[(sulfanylcarbonothioyl)sulfanyl]carbonothioyl = [(dithiocarboxy)sulfanyl]carbonothioyl* = [(sulfanylthiocarbonyl)sulfanyl]thiocarbonyl {not [(dithiocarboxy)sulfanyl]thioformyl}	HS-CS-S-CS–	P-65.2.4.1.5
sulfanylcarbonyl*	HS-CO–	P-65.1.5.1; P-65.2.1.6
(sulfanylcarbonyl)oxy*	HS-CO-O–	P-65.2.1.6
sulfanylidene* = thioxo	S=	P-64.6.1
sulfanylidenemethylidene* = thioxomethylidene	S=C=	P-65.2.1.8
sulfanyloxy* = *SO*-thiohydroperoxy (no longer mercaptooxy)	HS-O–	P-63.4.2.2
[(sulfanyloxy)carbonyl]oxy* =[(*SO*-thiohydroperoxy)carbonyl]oxy	HS-O-CO-O–	P-65.2.1.7
(sulfanyloxy)phosphoryl* = (*SO*-thioperoxy)phosphoryl	P(O)(O-SH)<	P-67.1.4.1.1
sulfanylphosphinothioyl* =sulfanyl(thiophosphinoyl)	PH(S)(SH)–	P-67.1.4.1.1
(sulfanylsulfinyl)oxy*	HS-SO-O–	P-65.3.2.3
[(sulfanylthiocarbonyl)sulfanyl]thiocarbonyl = [(dithiocarboxy)sulfanyl]carbonothioyl* = [(sulfanylcarbonothioyl)sulfanyl]carbonothioyl {not [(dithiocarboxy)sulfanyl]thioformyl}	HS-CS-S-CS–	P-65.2.4.1.5
sulfanyl(thiophosphinoyl) = sulfanylphosphinothioyl*	PH(S)(SH)–	P-67.1.4.1.1
sulfeno: see hydroxysulfanyl*		
sulfide*	$^-$S–	P-72.6.2
sulfimidoyl*	S=(NH)<	P-65.3.2.3
sulfinamoyl: see aminosulfinyl*		
sulfino* (preferred when unmodified)	HO-S(O)–	P-65.3.2.1
sulfinothioyl*	–S(S)–	P-65.3.2.3
sulfinyl* = thionyl	–SO–	P-65.3.2.3
sulfo* (preferred when unmodified)	HO-SO$_2$–	P-65.3.2.1
sulfonato *	$^-$O-SO$_2$–	P-72.6.1
sulfonimidoyl* = sulfurimidoyl	–S(O)(=NH)–	P-67.1.4.4.1
sulfonio = sulfoniumyl = sulfaniumyl*	H$_2$S$^+$–	P-73.6
sulfoniumyl = sulfaniumyl* = sulfonio	H$_2$S$^+$–	P-73.6
sulfonodihydrazonoyl* = sulfurodihydrazonoyl	–S(=NNH$_2$)$_2$–	P-67.1.4.4.1
sulfonodiimidoyl* = sulfurodiimidoyl	–S(=NH)$_2$–	P-67.1.4.4.1
sulfonodithioyl* = sulfurodithioyl	–S(S)$_2$–	P-65.3.2.3; P-67.1.4.4.1
sulfonohydrazonoyl* = sulfurohydrazonoyl	–S(O)(=NNH$_2$)–	P-65.3.2.3 ;P-67.1.4.4.1
sulfonothioyl* = sulfurothioyl	–S(O)(S)–	P-65.3.2.3; P-67.1.4.4.1
sulfonyl* = sulfuryl	–SO$_2$–	P-65.3.2.3; P-67.1.4.4.1
sulfonylbis(methylene)* (not sulfonyldimethylene)	–CH$_2$-SO$_2$-CH$_2$–	P-65.3.2.3
sulfonylbis(oxy)* (not sulfonyldioxy)	–O-SO$_2$-O–	P-65.3.2.3
sulfonylbis(sulfanediyl)*	–S-SO$_2$-S–	P-65.3.2.3
sulfonyldimethylene: see sulfonylbis(methylene)*		

sulfonyldioxy: see sulfonylbis(oxy)*		
sulfooxy*	HO-SO$_2$-O–	P-65.3.2.3; P-67.1.4.4.2
sulfuramidoyl = aminosulfonyl = sulfamoyl*	H$_2$N-SO$_2$–	P-65.3.2.3
sulfurimidoyl = sulfonimidoyl*	–S(O)(=NH)–	P-67.1.4.4.1
sulfurochloridoyl = chlorosulfonyl*	Cl-SO$_2$–	P-67.1.4.4.1
sulfurochloridoyloxy = (chlorosulfonyl)oxy*	Cl-SO$_2$-O–	P-67.1.4.4.2
sulfurocyanidoyl = cyanosulfonyl*	NC-SO$_2$–	P-67.1.4.4.1
sulfurodihydrazonoyl = sulfonodihydrazonoyl*	–S(=NNH$_2$)$_2$–	P-67.1.4.4.1
sulfurodiimidoyl = sulfonodiimidoyl*	–S(=NH)$_2$–	P-67.1.4.4.1
sulfonodithioyl* = sulfurodithioyl	–S(S)$_2$–	P-65.3.2.3; P-67.1.4.4.1
sulfurohydrazonoyl = sulfonohydrazonoyl*	–S(O)(=NNH$_2$)–	P-65.3.2.3; P-67.1.4.4.1
sulfuro(isothiocyanatido)thioyl = isothiocyanatosulfonothioyl*	SCN-S(O)(S)–	P-67.1.4.4.1
sulfuroisothiocyanatidoyl = isocyanatosulfonyl*	SCN-SO$_2$–	P-67.1.4.4.1
sulfurothioyl = sulfonothioyl*	–S(O)(S)–	P-65.3.2.3; P-67.1.4.4.1
sulfuryl = sulfonyl*	–SO$_2$–	P-65.3.2.3
tellanediyl* (not telluro)	–Te–	P-63.1.5
tellanyl* (not hydrotelluro)	HTe–	P-63.1.5
tellanylidene* = telluroxo	Te=	P-64.6.1
tellurino* (preferred when unmodified)	HO-TeO–	P-65.3.2.1
tellurinyl*	OTe<	P-65.3.2.3
telluro: see tellanediyl*		
tellurocyanato*	NC-Te–	P-65.2.2
telluroformyl = methanetelluroyl*	HTeC–	P-65.1.7.2.3
tellurono* (preferred when unmodified)	HO-TeO$_2$–	P-65.3.2.1
telluronyl*	O$_2$Te<	P-65.3.2.3
telluroxo = tellanylidene*	Te=	P-64.6.1
terephthaloyl = benzene-1,4-dicarbonyl*		P-65.1.7.3.1
terephthalimidoyl = benzene-1,4-dicarboximidoyl*		P-65.1.7.2.2
tetradecanoyl*	CH$_3$-[CH$_2$]$_{12}$-CO–	P-65.1.7.4.1
tetramethylene: see butane-1,4-diyl*		
tetrasulfanediyl*	–S-S-S-S–	P-68.4.1.2
thallanyl *	H$_2$Tl–	P-68.1.2
2-thienyl = thiophene-2-yl*		P-29.6
thio: see sulfanediyl* (not sulfenyl)		
thioacetamido: see ethanethioamido*		
thioacetyl = ethanethioyl*	CH$_3$-CO–	P-65.1.7.2.3
thioazonoyl = azonothioyl*	>NH(S)–	P-67.1.4.1.1

thiobenzamido: see benzenecarbothioamido*		
thiobenzoyl = benzenecarbothioyl*	C_6H_5-CS–	P-65.1.7.2.3
thiobutyryl = butanethioyl*	CH_3-CH_2-CJH_2-CS–	P-65.1.7.4.1
thiocarbamoyl: see carbamothioyl*		
thiocarbonyl = carbonothioyl*	–CS–	P-65.2.1.5
thiocarboxy* (unspecified)	H{S/O}C–	P-65.1.5.1; P-65.2.1.6
(thiocarboxy)carbonyl: see 2-thiooxalo*		
thiochlorosyl*	S=Cl–	P-67.1.4.5
thiocyanato*	NCS–	P-65.2.2
thiodimethylene: see sulfanediylbis(methylene)*		
thioformamido: see methanethioamido*		
thioformyl = methanethioyl*	HCS–	P-65.1.7.2.3
OS-thiohydroperoxy = hydroxysulfanyl*	HO-S–	P-63.4.2.2
SO-thiohydroperoxy = sulfanyloxy*	HS-O–	P-63.4.2.2
(*OS*-thiohydroperoxy)carbonoselenoyl = (hydroxysulfanyl)carbonoselenoyl*	HO-S-CSe–	P-65.2.1.7
(thiohydroperoxy)carbonyl = carbono(thioperoxoyl)*	HO-S-CO– or HSO-CO–	P-65.1.5.3; P-65.2.1.7
(*OS*-thiohydroperoxy)carbonyl = (hydroxysulfanyl)carbonyl*	HOS-CO–	P-65.1.5.3
[(*SO*-thiohydroperoxy)carbonyl]oxy = [(sulfanyloxy)carbonyl]oxy*	HS-O-CO-O–	P-65.2.1.7
(thiohydroperoxy)phosphoryl = phosphoro(thioperoxoyl)*	P(O)(OSH)< or P(O)(SOH)<	P-67.1.4.1.1
(*SO*-thiohydroperoxy)phosphoryl = (sulfanyloxy)phosphoryl*	P(O)(O-SH)<	P-67.1.4.1.1
(*OS*-thiohydroperoxy)phosphorothioyl = (hydroxysulfanyl)phosphorothioyl*)	(HO-S)P(S)<	P-67.1.4.1.1
thionitroso*	S=N–	P-67.1.4.3
thionitrososulfanyl*	S=N-SH–	P-67.1.4.3
thionyl = sulfinyl*=	–SO–	P-65.3.2.3
1-thiooxalo* (not carboxycarbonothioyl)	HOOC-CS–	P-65-2.3.3
2-thiooxalo* (not (thiocarboxy)carbonyl	H{O/S}C-CO–	P-65.2.3.3
1-thiooxalylsulfanyl* = (carboxycarbonothioyl)sulfanyl	HO-CO-CS-S–	P-65.2.3.3
(thioperoxy)phosphoryl = (phosphorothioperoxoyl)*	>P(O)(OSH) or >P(O)(SOH)	P-67.1.4.1.1
thiophene-2-yl* = 2-thienyl		P-29.6
thiophosphinoyl = phosphinothioyl*	$H_2P(S)$–	P-67.1.4.1.1
thiophosphono* (unspecified)	$H_2\{O_2S\}P$–	P-67.1.4.1.1
thiophosphoryl = phosphorothioyl*	>P(S)–	P-67.1.4.1.1
thiopropionyl = propanethioyl*	CH_3-CH_2-CS–	P-65.1.7.4.1
thiosulfeno: see disulfanyl*		
thiosulfino* (unspecified	H{O/S}S	P-65.3.2.1
thiosulfo* (unspecified)	HO_2S_2–	P-65.3.2.1
thioxo = sulfanylidene*	S=	P-64.6.1
thioxomethylidene = sulfanylidenemethylidene*	S=C=	P-65.2.1.8

o-tolyl = 2-methylphenyl*		P-29.6
m-tolyl = 3-methylphenyl*		P-29.6
p-tolyl = 4 methylphenyl*		P-29.6
triazano: see triazan-1-yl*		
triazan-1-yl* (not triazano)	$H_2N\text{-}NH\text{-}NH–$	P-29.3.2.2; P-68.3.1.4.1
2-triazeno: see triaz-2-en-1-yl*		
triaz-2-en-1-io = traz-2-en-1-ium-1-yl*	$\overset{3}{NH_2}\text{-}\overset{2}{N}=\underset{1}{\overset{+}{NH}}-$	P-73.6
triaz-2-en-1-ium-1-yl* = triaz-2-en-		
triaz-2-en-1-ium-1-yl* = tria-2-en-1-io	$\overset{3}{NH_2}\text{-}\overset{2}{N}=\underset{1}{\overset{+}{NH}}-$	P-73.6
triaz-2-en-1-yl* (not 2-triazeno)	HN=N-NH–	P-32.1.1; P-68.3.1.4.1
triborane(5)-1-yl*	$H_2B=BH\text{-}B–$	P-68.1.2
trihydroxysilyl*	$(HO)_3Si–$	P-67.1.4.2
triphenylmethyl = trityl*	$(C_6H_5)_3C–$	P-29.6
trioxidanyl*	HOOO–	P-68.4.1.3
trioxidanediyl*	–OOO–	P-68.4.1.2
trisilan-2-yl*	$(CH_3)_2SiH–$	P-29.3.2.2
trisilazan-3-yl*	$(SiH_3\text{-}NH)_2SiH–$	P-29.3.2.2
triselanyl*	HSeSeSe–	P-68.4.1.3
triselanediyl*	–SeSeSe–	P-68.4.1.2
trisulfanediyl* (not trithio)	–SSS–	P-68.4.1.2
tritellanyl*	HTeTeTe–	P-68.4.1.3
tritellanediyl*	–TeTeTe–	P-68.4.1.2
trithio: see trisulfanediyl*		
trithiooxalo* [(not (dithiocarboxy)carbonothioyl]	HS-CS-CS–	P-65.2.3.3
trithiophosphono*	$(HS)_2P(S)$-	P-67.1.4.1.1
trithiosulfo = sulfanylsulfonodithioyl*	$HS\text{-}S(S)_2–$	P-65.3.2.1
trityl* = triphenylmethyl	$(C_6H_5)_3C–$	P-29.6
undecan-1-yl: see indecyl*		
undecyl* (not undecan-1-yl)	$CH_3\text{-}[CH_2]_9\text{-}CH_2–$	P-29.3.2.1
ureido: see carbamoylamino*		
ureylene: see carbonylbis(azanediyl)*		
vinyl = ethenyl*	$CH_2=CH–$	P-32.3
vinylene: see ethene-1,2-diyl*		
vinylidene = ethenylidene*	$CH_2=CH=$	P-32.3
yloamino*	$–NH^{\bullet}$	P-71.5
ylocarbonyl*	$–\underset{\bullet}{\overset{\bullet}{C}}=O$	P-71.5

ylomethyl*	$-CH_2$	P-71.5
ylooxy* (not ylohydroxy)	$-O^\bullet$	P-71.5
(ylooxy)carbonyl*	$-CO\text{-}O^\bullet$	P-71.5