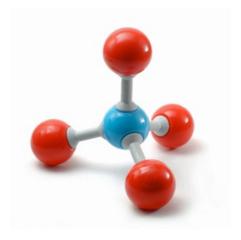
Ch11

Hydrocarbons

Getting to know organic molecules. Everything starts with Carbon.







Organic Compounds

- ▶ Atomic and elemental theories (review)
- Origin of organic classification
 - Living Essence (urea synthesis)
- Defining organic chemistry
 - ▶ Differences between organic & inorganic
- Representing Organic Compounds
 - Composition, Connectivity, Shape
 - ▶ Formulas
 - Structures
 - Sketches
 - ▶ Names/IUPAC
- Alkanes
 - Definition
 - Drawing Structures
 - ► Condensed, Expanded, Skeletal.
 - ▶ IUPAC Naming of Alkanes
 - ▶ It's not based on ions anymore.
 - ▶ Conformations
 - ▶ Same substance, different state



- Types of Alkanes
 - Chain Alkanes
 - Branched Alkanes
 - Cycloalkanes
- Structural Isomers
 - Same composition (formula) different connectivity (structure)
 - different substances!
- Substituted Alkanes
 - Substituents
 - alkane chains (alkyl groups)
 - ▶ isopropyl & tert-butyl
 - halogens
 - Naming (structure to name)
 - Drawing (name to structure)
- Properties of Alkanes
 - Uses
 - Density & Solubility
 - Reactivity
 - ▶ Combustion

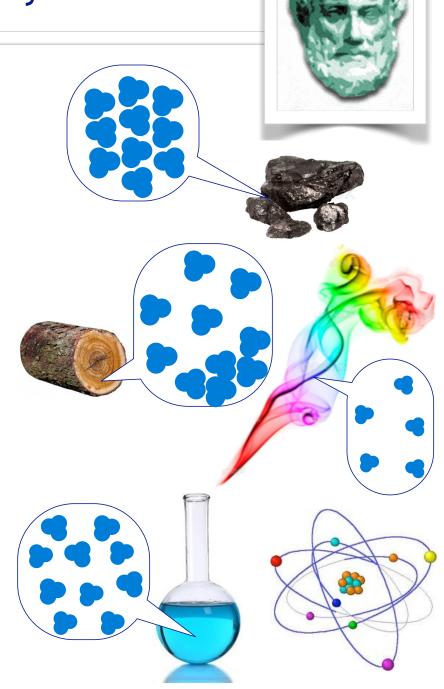






Atomic Theory

- The earliest concept of the atom came from the Greek philosopher/scientist Democritus between 460 and 370 BCE.
- Democritus thought of the world as being composed of very tiny "uncuttable" particles, which he called "atomoz." Which is where we get the word atoms.
- ► These tiny, invisible particles were thought to be separated by voids -- empty space.
 - Democritus explained different substances were caused by differences in the sizes of the particles and the amount of empty space between them.
- This original Atomic Theory explained many properties of matter:
 - Solid, liquid, and gas states
 - State changes
 - Density
 - Mass
 - Hardness
 - Heterogenous Mixtures

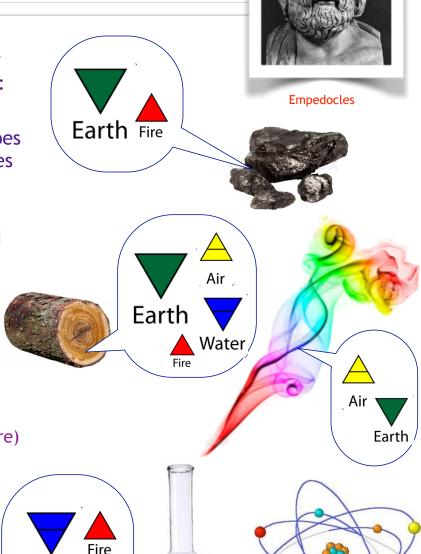


Democritus

Elemental Theory

- ► Empedocles (490-430 B.C.) offered a different explanation.
- He suggested matter was made up of four basic substances: the elements earth, air, fire, and water.
- Elemental theory explained the differences in different types of matter as arising from the proportion, form, and qualities of the four basic elements that each contained.
- It explained states of matter. Liquids contained mostly water, solids contained mostly earth, gases were composed of mostly air.
- Experiments supported elemental theory.
 - ▶ Earth and fire came out of coal.
 - Smoke contained mostly air with some earth.
 - Steam contained mostly air with some water.
 - Alcohol was mostly water, but it's fire could be released.
 - ▶ Burning wood liberates ashes (earth), smoke (air), flames (fire) and water.
- Aristotle (384-322 B.C.) rejected the atomic theory of Democritus and advanced the elemental theory of Empedocles.

Elemental theory became the dominant theory and guided science for the next 2000 years.

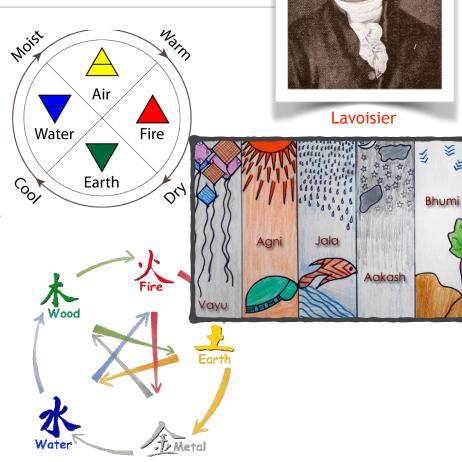


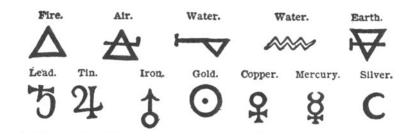
Water

Aristotle

Discovering Elements

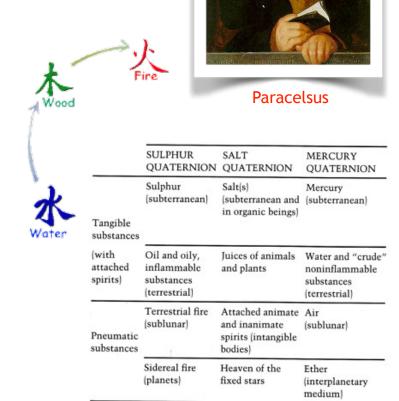
- For 2000 years scientists studied and compiled data from chemical reactions.
- Trying to isolate the four greek elements, chemists broke down all matter they found into simpler substances.
 - Materials were uniquely identified and categorized by the ratio of simpler substances they broke into.
- The substances that could not be broken down into any other substance were thought to have special significance.
 - Sulfur and Mercury were two of the first elements discovered.
 - ▶ Salt was thought to be one of the first elements, we were only able to break it down into the elements sodium and chloride in the 1700s.
 - Metals like copper, lead, iron, silver and gold were isolated early in history but treated differently.
- In 1789 Antoine Lavoisier redefined the term element to describe the twenty three pure substances that chemists had discovered but could not break down into simpler substances.
 - ▶ This was the the first time metals other than mercury were considered elements.





Organic Substances

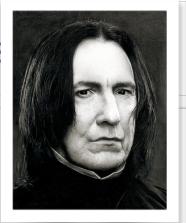
- ▶ Between 500 BC and 1800 AD alchemists studied the properties of matter and tried to break different kinds of matter down into the fundamental essences.
- ▶ They tried to organize useful substances into categories, based on the essences they were thought to contain.
 - The same way you make piles when you try to organize your taxes.
- Paracelsus, one of the founders of both Alchemy and Medicine, argued all matter should be classified into quaternions (major tribes) based on mercury, sulfur, and salt (what were then thought to be the three simplest substances in each category).
- Substances were further divided into those which had some animating spirit and those without spirit.
 - ▶ Fire danced, Water had currents, and plants grew. In contrast Earth, Air and crystals seemed inanimate.
 - Oils were thought to retain the spirit of fire, because you could ignite it and see the release of fire.
 - ▶ The tides ebbed and flowed, suggesting sea water contained a different, more ponderous and powerful animating spirit.
 - Likewise, many juices extracted from animals and plants demonstrated a kind of activity that we thought reflected a third animating spirit, one we thought might be the source of life.
- We described substances coming from living beings, ones which demonstrated this activity, as vital or organic.
- Everything else was described as inorganic.
- ▶ Paracelsus and those who followed his school, built much of what became the study of medicine on the study of organic substances.
- ▶ The caduceus, the modern symbol of medicine, is the symbol of alchemies universal solvent (alkahest). The spirit thought to be unique to organic substances.

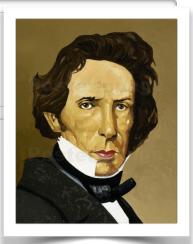




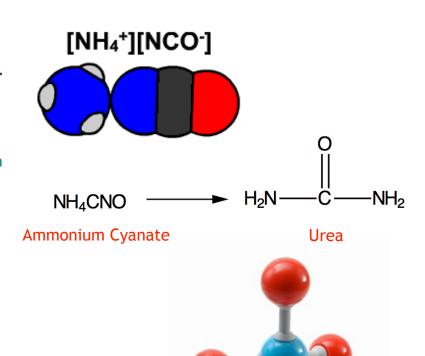
Organic Chemis

- Elemental theory led to observations it couldn't explain.
- These patterns without explanations became the three laws of stoichiometry:
 - The law of conservation of matter.
 - The law of constant composition.
 - ▶ The law of multiple proportions.
- To explain these laws John Dalton proposed an expanded atomic theory. One which returned us to thinking of substances being composed of grains of matter called atoms.
 - ▶ In Dalton's time we identified over 50 different flavors of atom (elements)
 - ▶ 118 elements are known today.
 - Organic substances were found to be composed always of carbon and hydrogen atoms; and often included oxygen, and nitrogen.
- In the 1700's we started questioning the idea of spirits being required to make organic compounds.
- Friedrich Wöhler heated an inorganic compound (ammonium cyanate) and it's atoms rearranged to form urea (an organic compound).
- This demonstrated that life wasn't necessary to make organic compounds.

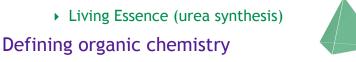




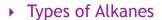
Wöhler



- Organic Compounds
 - ▶ Atomic and elemental theories (review)
 - Origin of organic classification



- Differences between organic & inorganic
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- Substituents
 - alkane chains (alkyl groups)
 - ▶ isopropyl & tert-butyl
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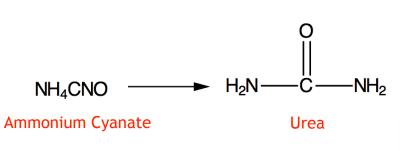


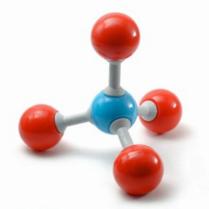


Organic Compounds

- We now consider organic compounds any compound based on carbon.
- Organic chemistry is the chemistry of carbon.
- Today there are over 22 million known organic substances.
- More than 99% of all substances synthesized and more than half the worlds chemists are organic.
- Organic substances are mostly molecular, while inorganic substances tend to be ionic.
- Organic compounds also differ from inorganic ones by:
 - melting point (lower)
 - boiling point (lower)
 - flammability (higher)
 - solubility in water (less)

Property	Organic	Example: C ₃ H ₈	Inorganic	Example: NaCl
Elements Present C and H, sometimes O, S, N, P, or Cl (F, Br, I)		C and H	Most metals and nonmetals	Na and Cl
Particles	Particles Molecules		Mostly ions	Na ⁺ and Cl ⁻
Bonding	Mostly covalent		Many are ionic, some covalent	Ionic
Polarity of Bonds	Nonpolar, unless a strongly electronegative atom is present		Most are ionic or polar covalent, a few are nonpolar covalent	Ionic
Melting Point	Melting Point Usually low		Usually high	801 °C
Boiling Point	Usually low	−42 °C	Usually high	1413 °C
Flammability	High	Burns in air	Low	Does not burn
Solubility in Water Not soluble, unless a polar group is present		No	Most are soluble, unless nonpolar	Yes





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 - ▶ Atomic and elemental theories (review)
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 - ▶ Differences between organic & inorganic



Representing Organic Compounds

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- Understanding organic compounds means understanding organic molecules.
- Molecules differ by:
 - Composition (what it's made of)
 - Connectivity (where bonds connect atoms)
 - Shape (the angle and directions of those bonds)
 - ... and some other things we'll save for later.
 - Molecular formulas communicate composition.
 - Always start organic formulas with C and H, then any other elements
 - ▶ Sometimes we may group common patterns of atoms together to suggest some connectivity.
- Molecular structures communicate composition and connectivity.
 - Lewis dot structures are the basis.
 - We generally write bonding pairs as a line.
 - We often omit non-bonding lone pairs.
 - Hydrogens can be:
 - Treated individual atoms (expanded form)
 - Annotated as being attached to other atoms (condensed form)
 - Omitted (skeletal form)
 - Where an atom isn't specified, it's a carbon.
- <u>Molecular models</u> or sketches communicate composition, connectivity, and shape.
 - ▶ There are many ways to model or sketch a molecule.
 - ▶ Ball and stick models
 - Space Filling models
 - Wedge-dash sketches (there are others)

 $C_{12}H_{22}O_{11}$

C7H5N3O6

 $C_6H_2(NO_2)_3CH_3$





For Simple Binary Inorganics

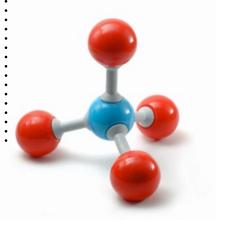
Anion Like Thing

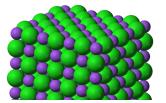
Cation Like Thing

NaCl P₂O₅



Carbon & Hydrogen, then N, O then the rest.





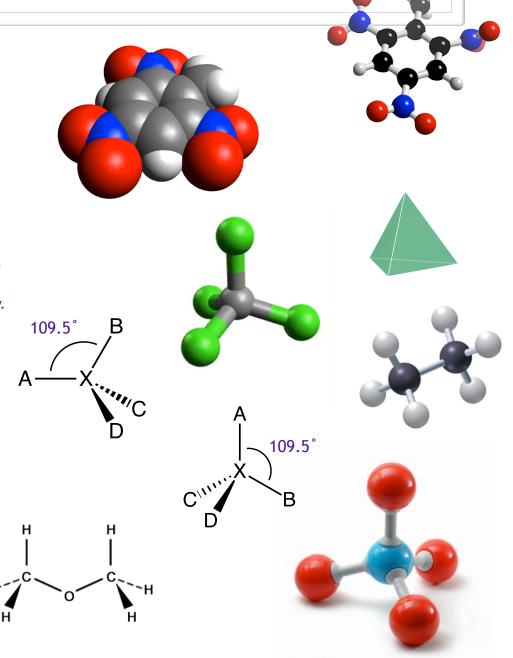
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$$O_2N$$
 NO_2
 NO_2

$$H_3C$$
 OH H_3C

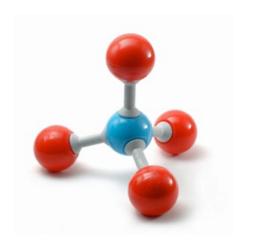


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- Naming organic compounds.
 - ▶ The name of an organic compound needs to clearly distinguish it from any other substance by all three of these considerations.
 - ▶ Composition
 - Connectivity
 - Shape
 - ▶ There are over 22 million different organic compounds known.
 - Coming up with a unique name for each is challenging.
 - ▶ IUPAC, the international union of pure and applied chemistry, is considered the authority in coming up with the systems by which we name different substances.
 - ► IUPAC releases color books, books that provide the rules for naming different types of substances.
 - ▶ The book that provides just lists the rules for naming organic substances is the "Blue" book.
 - ▶ Each year provisional (working) updates to these rules are released to deal with new classes of compounds discovered or created.
 - ▶ The "final" (non-provisional) version of these rules was released in 1979
 - ... then again in 1993
 - warning: it takes a long time to update the names of 22 million compounds, you will find compounds and even text books that are still using the 1979 rules!
 - ▶ The rules alone cover 1,376 pages.
 - We'll focus on a small part of these rules in this class.





IUPAC Color Books

Chemical Terminology (Gold book)

▶ The IUPAC Compendium of Chemical Terminology is the definitive guide to chemical terminology; it now contains more than 7000 entries, is easy to browse, search, and navigate.

Quantities, Units and Symbols in Physical Chemistry (Green Book)

▶ This book provides a readable compilation of widely used terms and symbols from many sources together with brief understandable definitions. Full text pdf with with bookmark by chapters and sections is available. (PDF available)



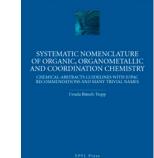
Nomenclature of Organic Chemistry (Blue book)

► HTML reproduction of the IUPAC Nomenclature of Organic Chemistry has been prepared by Advanced Chemistry Development, Inc and is searchable on the ACD website http://acdlabs.com/iupac/nomenclature. The most recent hardback edition has been published by RSC in December 2013. See corresponding project.



Compendium of Polymer Terminolgy and Nomenclature (Purple book)

▶ The second edition of the IUPAC Compendium of Polymer Terminology and Nomenclature (IUPAC Recommendations 2008) is an expansion and revision of the 1991 edition and contains 22 chapters. This new edition continues the significant contribution to clear and precise communication in polymer science made by its predecessor.(PDF available)



Analytical Terminology (Orange book)

▶ The Web edition of the IUPAC Compendium on Analytical Terminology provides ease of access to the extensive information contained in its recommendations.

Biochemical Nomenclature (White Book)

▶ The Biochemical Nomenclature and Related Documents (1992) presents IUPAC-IUBMB (International Union of Biochemistry and Molecular Biology) Joint Commissions' recommendations; it includes sections on amino acids, peptides and proteins, enzymes, nucleotides, nucleic acids and protein synthesis, carbohydrates, lipids, etc.



▶ The 'Red Book' clarifies and continues to update recommendations concerning the names and formulae of inorganic compounds and reflects major recent developments in inorganic chemistry.



IUPAC Blue Book

- The full version of the IUPAC Blue Book, including provisional rules, through 2004 is available on the class website (http://chem.ws/30B).
- An online version of both the 1979 non-provisional release, and the 1993 non-provisional release is available online at:
 - http://chem.ws/bluebook
- The rules we'll introduce in this class are based on the 1993 non-provisional release.
- We will only be covering a small, but important part of these rules.









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Alkanes

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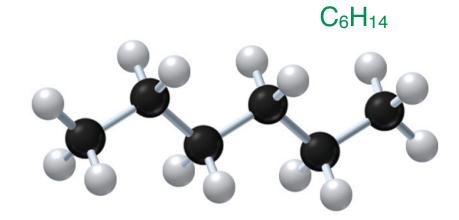


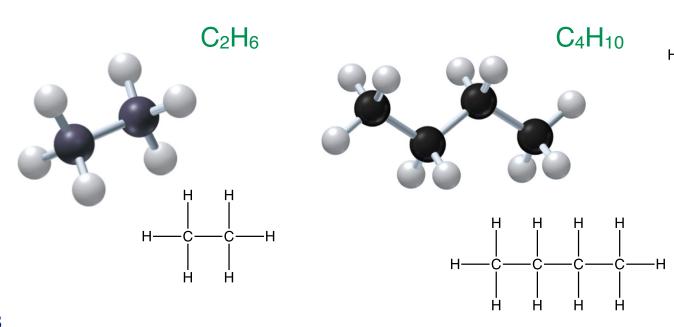


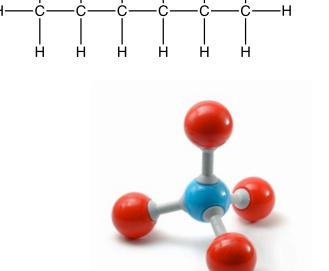


n-Alkanes

- Hydrocarbons are any organic compound that is made only of carbon and hydrogen.
- The simplest class of hydrocarbon are alkanes.
- Alkanes are hydrocarbons that have only single bonds between their atoms.
- The first kind of alkanes we will look at are n-Alkanes.
- n-Alkanes, also called chain alkanes or simple alkanes, are carbon atoms connected in series with single bonds between them.
- n-Alkanes have the molecular formula $C_nH_{(2n+2)}$ where n is the number of carbons in the chain.





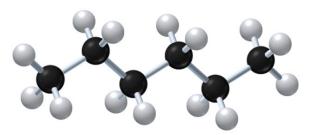


Condensed Structures

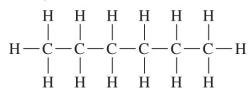
 $C_{6}H_{14}$

Alkane Name Molecular Formula Ball-and-Stick Model

Hexane Methane



Expanded Structural Formula

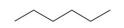


Condensed Structural Formulas

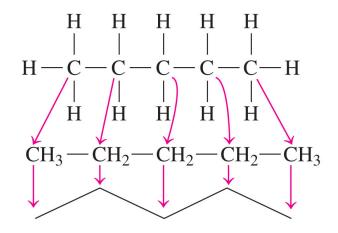
$$\begin{array}{cccc} CH_2 & CH_2 & CH_3 \\ CH_3 & CH_2 & CH_2 \end{array}$$

$$CH_3-CH_2-CH_2-CH_2-CH_2-CH_3$$

Skeletal Formula



- Organic structures are based on the same rules you learned for Lewis dot structures, there's just a lot more atoms involved.
- As Alkanes grow in size it becomes cumbersome to draw out the full
- The expanded structure is a complete depiction fo all atoms and all bonds in a molecule.
- As we look at larger molecular structures, it become cumbersome to use.
- The condensed structure shows all atoms, but eliminates the bonds between carbon and hydrogen.
- In a skeletal structures we omit hydrogen entirely and simply assume the open valence of carbon atoms is filled with hydrogens.
 - As a reminder, carbon has a valence of 4.



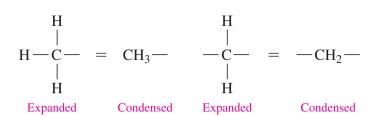
Expanded structural formula

Condensed structural formula

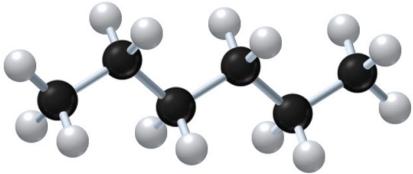
Skeletal formula

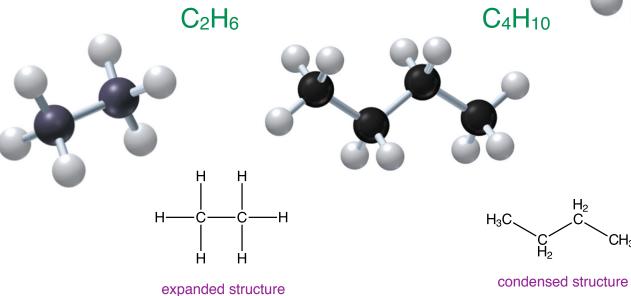
n-Alkanes

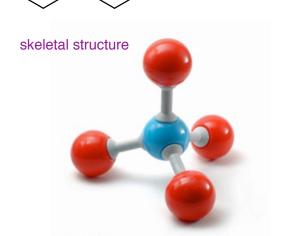
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- ightharpoonup n-Alkanes have the molecular formula $C_nH_{(n+2)}$



C₆H₁₄







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Alkanes

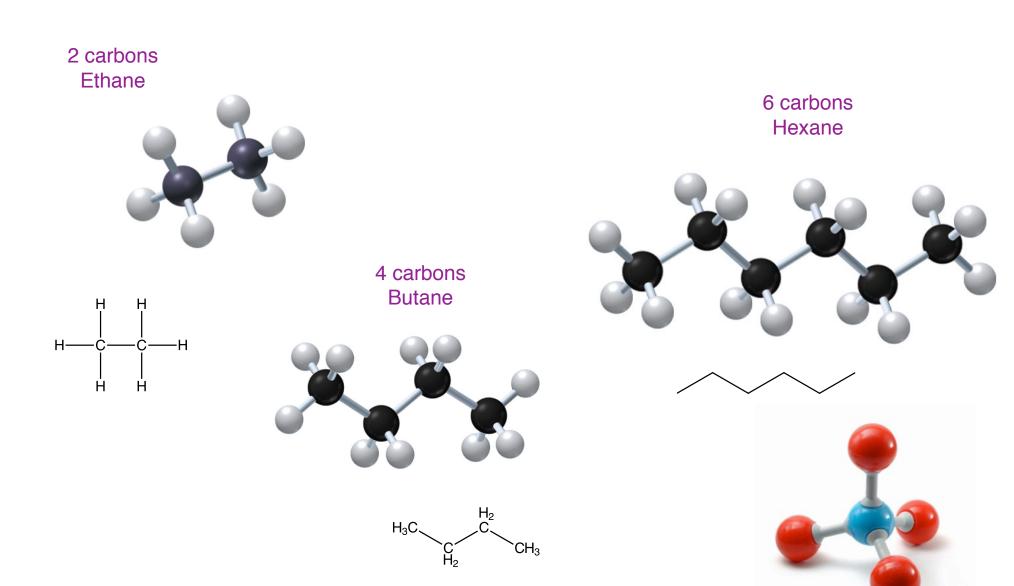
- IUPAC (International Union of Pure and Applied Chemistry) provides a system for naming organic compounds.
- Organic structures are mostly named based on this system.
- Alkanes structures are the starting point for naming most organic compounds.
 - ▶ Alkane chains are named using the number of carbons and ending with the suffix -ane.
 - ▶ Alkanes with 5 or more carbons use the greek prefix to indicated the number of carbons.
 - ▶ The alkanes with 1-4 carbons were named before we locked down their structure. Those names stuck and trump the greek prefixes for 1, 2, 3, and 4 carbon alkanes.

1 = meth—	6 = hex—
2 = eth—	7 = hept-
3 = prop—	8 = oct—
4 = but—	9 = non—
5 = pent—	10 = dec—

- ▶ Methane (CH₄) not mon-ane
- ▶ Ethane (C_2H_6) not di-ane
- ▶ Propane (C_3H_8) not tri-ane
- ▶ Butane (C_4H_{10}) not tetr-ane

Number of Carbon Atoms	Prefix	Name	Molecular Formula	Condensed Structural Formula	
1	Meth	Methane	CH ₄	CH ₄	You are responsible for knowing
2	Eth	Ethane	C_2H_6	CH ₃ —CH ₃	the names, formulas and structures of
3	Prop	Propane	C_3H_8	CH ₃ —CH ₂ —CH ₃	these 10 chain alkanes
4	But	Butane	C_4H_{10}	$CH_3-CH_2-CH_2-CH_3$	moso to onam amano
5	Pent	Pentane	C_5H_{12}	$CH_3-CH_2-CH_2-CH_2-CH_3$	
6	Hex	Hexane	C_6H_{14}	CH ₃ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -	-CH ₃
7	Hept	Heptane	C_7H_{16}	CH ₃ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -	-CH ₂ —CH ₃
8	Oct	Octane	C_8H_{18}	CH ₃ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -	$-CH_2-CH_2-CH_3$
9	Non	Nonane	C_9H_{20}	CH ₃ —CH ₂ —CH ₂ —CH ₂ —CH ₂ —	-CH ₂ -CH ₂ -CH ₃
10	Dec	Decane	$C_{10}H_{22}$	CH ₃ -CH ₂ -CH ₂ -CH ₂ -CH ₂ -	$-CH_2-CH_2-CH_2-CH_2-CH_3$

Alkanes



- Organic Compounds
 - ▶ Atomic and elemental theories (review)
 - Origin of organic classification
 - Living Essence (urea synthesis)
- Defining organic chemistry
 - ▶ Differences between organic & inorganic
- Representing Organic Compounds
 - Composition, Connectivity, Shape
 - ▶ Formulas
 - Structures
 - Sketches
- Alkanes
 - Definition
 - Drawing Structures
 - Condensed, Expanded, Skeletal.
 - ► IUPAC Naming
 - It's not based on ions anymore.



Conformations

▶ Same substance, different state



- Chain Alkanes
- Branched Alkanes
- Cycloalkanes
- Structural Isomers



– different substances!



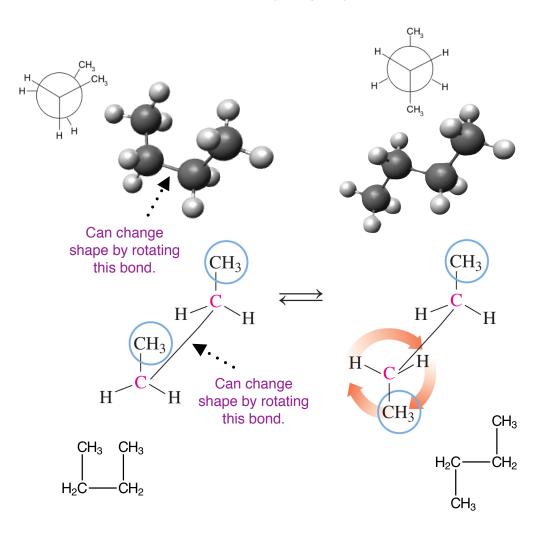
- Substituents
 - alkane chains (alkyl groups)
 - ▶ isopropyl & tert-butyl
 - halogens
- Naming (structure to name)
- Drawing (name to structure)
- Properties of Alkanes
 - Uses
 - Density & Solubility
 - Reactivity
 - Combustion





Conformations

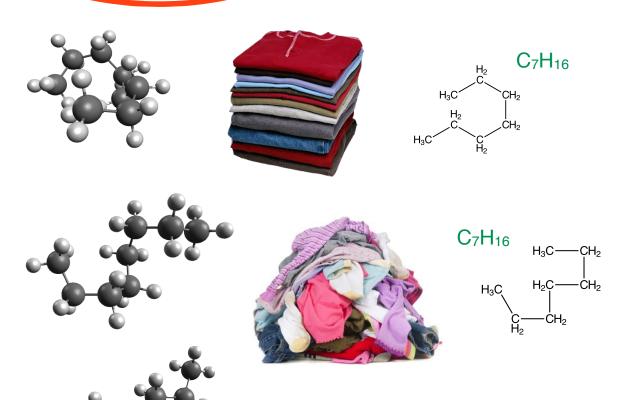
Two conformations (shapes) of Butane



- Alkanes have a dynamic shape.
- Each carbon-carbon single bond has free rotation.
- The different possible shapes resulting from these rotations are called conformations.
- Some conformations may be better than others, but for now just realize the organic molecules have the freedom to reshape themselves by rotating carbon carbon single bonds.
- Conformations are different states in which a molecule may find itself.
 - Similar to the way substances can find themselves in different states:
 - ▶ solid, liquid, gas
 - Water is water whatever state it's in.
 - A molecule in a different state is <u>still the same</u> molecule, it's still the same substance.
 - Changes in conformation are physical changes
 not chemical changes.

As long as the connectivity and composition is the same we're talking about the same substance.

Conformations



- Rotating around those carbon carbon single bonds can produce new shapes of the whole molecule. The shape around the carbon atoms isn't changed, but these larger molecules can adopt different relative positions of of the carbon atoms. Different conformations.
- ► Conformations are different states in which a molecule may find itself.
 - ▶ In the same way your shirt can be neatly folded up, wadded in a ball, or stretched thin across a hanger but still be your shirt.
 - ► A molecule in a different state is <u>still the same</u> <u>molecule</u>, it's still the same substance.
 - Changes in conformation are physical changesnot chemical changes.
- Conformations can best be described with models or sketches, but we'll sometimes try to indicate a rough conformation with a structure drawing.



 C_7H_{16} H_2 H_2 H_2 H_3 H_4 H_5 H_6 H_7 H_8 H_8



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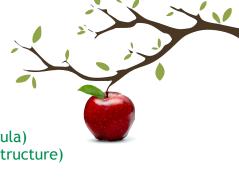




Types of Alkanes

- Chain Alkanes
- Branched Alkanes
- Cycloalkanes
- Structural Isomers
 - Same composition (formula) different connectivity (structure)
 - different substances!
- Substituted Alkanes
 - Substituents
 - alkane chains (alkyl groups)
 - ▶ isopropyl & tert-butyl
 - halogens
 - Naming (structure to name)
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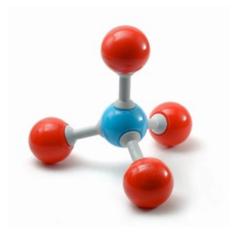


- Some alkanes are just a line of carbon atoms.
- They are called simple alkanes or alkane chains or n-alkanes.
- Like a tree, other alkanes have branches that split off of that chain.
- The longest chain in an alkane is it's backbone or parent chain.
- The smaller chains that sprout off of the backbone are branches.
- Branched alkanes are alkanes with more than one carbon chain.

skeletal structure of a branched alkane

$$\begin{array}{c|ccccc} & CH_3 & & \\ & CH_3 & & H_2C & & \\ & & & & \\ & & & & \\ & & & & \\ H_3C & & & C & \\ & & & & \\ & & & & \\ H_2 & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & \\ & & & \\$$

condensed structure

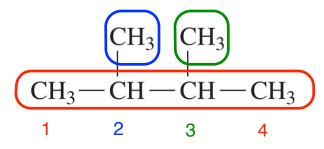


- A carbon branch is also called an alkyl group.
- An alkyl group is an alkane with one less hydrogen.
- Alkyl groups are named as if they were alkanes, replacing the -ane with -yl.
 - ▶ A CH₃— group is a methyl group.
 - ▶ The first four groups don't use standard greek prefixes!
 - ▶ A CH₃CH₂CH₂CH₂CH₂— group is a pentyl group.
- To name a branched alkane:
 - 1. Find the backbone (the longest chain).
 - 2. Number the carbons of the backbone
 - ▶ Start with the end that gives you the smallest numbers.
 - ▶ If both ends give you the same numbers, start with the end that gives your the name that comes first alphabetically.
 - 3. Write the location and name for each branch.
 - When there are different branches, list them in alphabetical order.
 - When there are identical branches use the greek prefixes (di, tri, tetra, penta, hexa etc) and write the branch name once.

(These prefixes do not count for alphabetizing!)

4. End with the name of the backbone.

1 = meth—	6 = hex—
2 = eth—	7 = hept-
3 = prop—	8 = oct-
4 = but—	9 = non—
5 = pent—	10 = dec-



2,3-dimethylbutane



- To name a branched alkane:
 - 1. Find the backbone (the longest chain).
 - 2. Number the carbons of the backbone
 - > Start with the end that gives you the smallest numbers.
 - ▶ If both ends give you the same numbers, start with the end that gives your the name that comes first alphabetically.
 - 3. Write the location and name for each branch.
 - ▶ When there are different branches, list them in alphabetical order.
 - 4. End with the name of the backbone.

$$_{\rm CH_2-CH_3}^{\rm CH_2-CH_3}^{\rm CH_3-CH-CH_3}^{\rm CH_3-CH-CH_3}^{\rm CH_3-CH_3-CH_3}$$

3,3-Diethylhexane

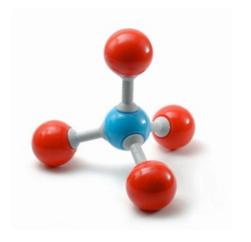
CH3-CH2

2,3,4-Trimethylhexane

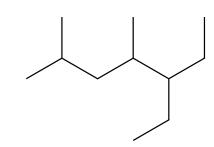
Take the time to be sure you found the longest chain for your backbone.

$$_{\mathrm{CH_{3}}}$$
 $_{\mathrm{CH_{3}}}$ $_{\mathrm{CH_{3}}}$ $_{\mathrm{CH_{2}}}$ $_{\mathrm{CH}}$ $_{\mathrm{CH}}$ $_{\mathrm{CH_{2}}}$ $_{\mathrm{CH_{3}}}$ $_{\mathrm{CH_{2}}}$ $_{\mathrm{CH_{3}}}$

3,4-Dimethylhexane



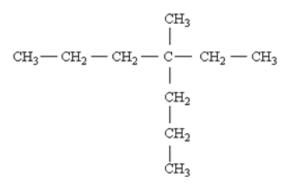
- To name a branched alkane:
 - 1. Find the backbone (the longest chain).
 - 2. Number the carbons of the backbone
 - ▶ Start with the end that gives you the smallest numbers.
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 - 4. End with the name of the backbone.



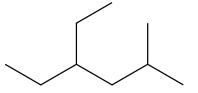
5-Ethyl-2,4-dimethyheptane not 2,4-Dimethyl-5-ethylheptane

(alphabetically ethyl before methyl, the "di" doesn't count for alphabetizing

-di is not part of the branches name it just describes it)

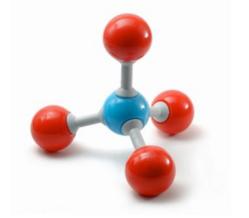


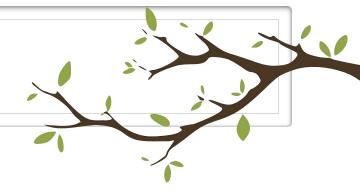
4-Ethyl-4-methylheptane (alphabetically ethyl before methyl)

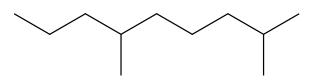


4-Ethyl-2-methylhexane not 2-Methyl-4-ethylhexane

(write the branch names not in order of their address, but alphabetically by their name)

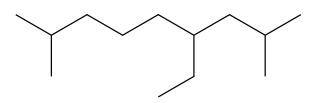






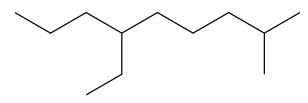
2,6-Dimethylnonane not 4,8-Dimethylnonane

(start numbering from the end that gives you the smallest numbers)



4-Ethyl-2,8-dimethylnonane not 6-Ethyl-2,8-dimethylnonane

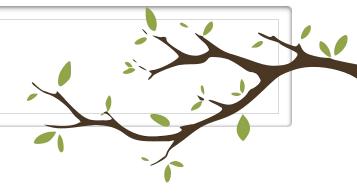
(if the first branch is the same distance from either end, look at the next branch)

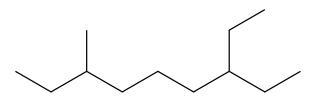


6-Ethyl-2-methylnonane not 2-Methyl-6-ethylnonane

(include the branches not in order of their address, but alphabetically by their name)

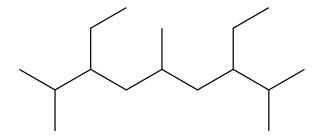






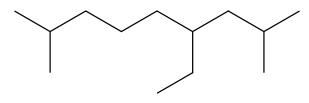
3-ethyl-7-methylnonane not 3-methyl-7-ethylnonane

(if numbering from either side gives you the same numbers, assign addresses alphabetically)



3,7-diethyl-2,5,8-trimethylnonane

(if they're symmetric, number from either side —you'll get the same name)



4-ethyl-2,8-dimethylnonane not 6-ethyl-2,8-dimethylnonane

(if the first branch is the same distance from either end, look at the next branch)



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- Chain Alkanes
- Branched Alkanes



- Structural Isomers
 - Same composition (formula) different connectivity (structure)
 - different substances!



- Substituents
 - alkane chains (alkyl groups)
 - ▶ isopropyl & tert-butyl
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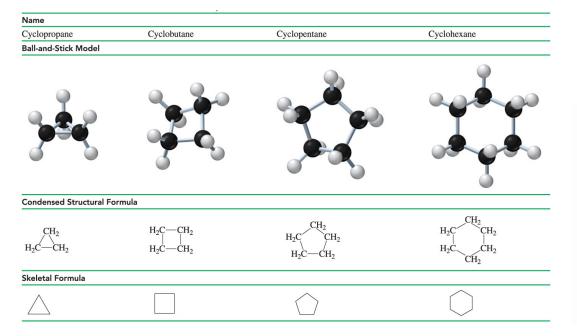


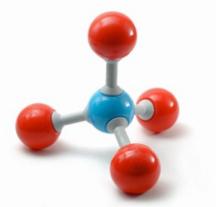


Cycloalkanes

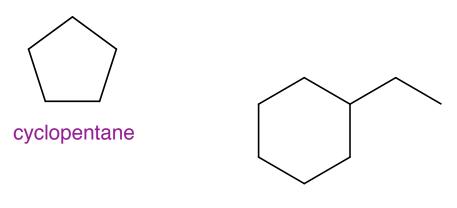
- Alkanes form chains, they can also form cyclic or ring structures.
- Cylcoalkanes or alkane rings are named the same as straight chain alkanes, with a cyclo- prefix.
 - Hexane in a ring is cyclohexane.
 - Pentane in a ring is cyclopentane.
- ▶ A cycloalkane as a molecular formula of C_xH_x where X equals the number of carbons.
- ▶ 5 and 6 membered rings most easily allow carbon it's preferred 109.5° bond angle, and those are the most common cycloalkanes.
- Smaller and larger rings are possible, but less frequently observed.

(annit make a mine	
(can't make a ring with one atom)	6 = hex—
(can't make a ring with two atoms)	7 = hept-
3 = prop—	8 = oct—
4 = but—	9 = non—
5 = pent—	10 = dec-

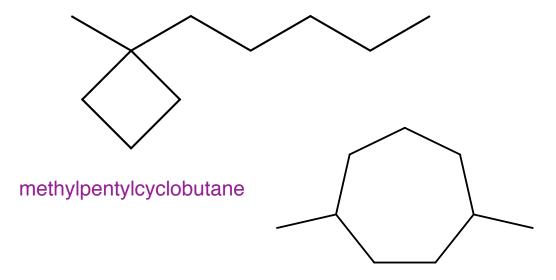




Naming Cycloalkanes



ethylcyclohexane



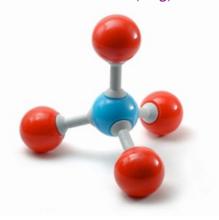
1,4-dimethylcycloheptane

- ▶ To name a cycloalkane:
 - 1. The ring is your backbone
 - ▶ Even if there is longer chain attached to the ring.
 - 2. Number the atoms of the ring.
 - ▶ If there is less than two atoms with branches, there is no need to give an address.
 - ▶ Number the ring starting from the carbon with the branch that comes first in the alphabet.
 - Number in the direction that give the lower overall numbers.
 - If both directions give you the same numbers, start with the end that gives your the name that comes first alphabetically.
 - 3. Write the location and name for each branch.
 - ▶ When there are different branches, list them in alphabetical order.
 - When there are identical branches use the greek prefixes (di, tri, tetra, penta, hexa etc) and write the branch

(These prefixes do not count for alphabetizing!)

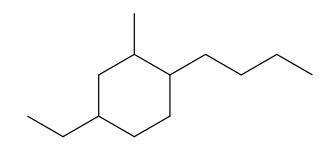
4. End with the name of the backbone (ring).

name once.



Assigning Addresses in Rings

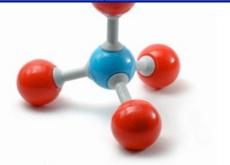
- ▶ With a chain backbone we give addresses from one end or the other.
- We decide which end based on which gives us simpler addresses (smaller numbers).
 - We're just looking at two possibilities.
- With a ring, you can't do that. There isn't just two ends, any atom could be the "end" so it would get very complicated, very quickly.
 - ▶ With this structure we would have six possibilities...
- We need a way to agree on the "end".
- With rings we add an extra step, to find that end:
 - We list all the branches.
 - ▶ Find the one that comes first in the alphabet.
 - ▶ Take that atom as the "start" of our chain.
- ▶ Then continue like a chain (number the rest in whichever direction gives us the smallest numbers).
- We still have two choices to decide from, but it's better than six (or more).



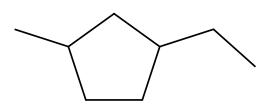
There are too many combinations to reliably come up with the "smallest numbers" quickly using the rules for chains.

propyl	ethyl	butyl
1	3	4
1	5	4
5	1	2
5	1	3
4	2	1
4	5	1

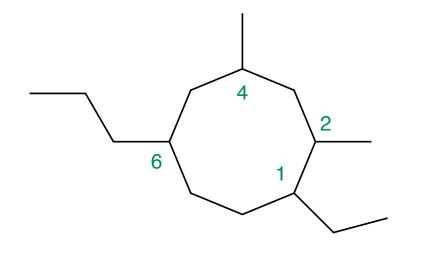
butyl 1-butyl-4-ethyl-2-methylcyclohexane ethyl 1-butyl-4-ethyl-5 methylcyclohexane



Naming Cycloalkanes



1-Ethyl-3-methylcyclopentane

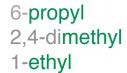


propyl methyl methyl ethyl

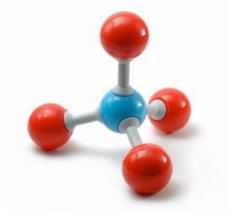
- ▶ To name a cycloalkane:
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 - When there are identical branches use the greek prefixes
 (di, tri, tetra, penta, hexa etc) and write the branch name once.

(These prefixes do not count for alphabetizing!)

4. End with the name of the backbone (ring).



1-Ethyl-2,4-dimethyl-6-propylcyclooctane



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- Chain Alkanes
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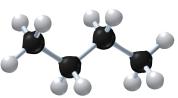


 Same composition (formula) different connectivity (structure)

– different substances!



- Substituents
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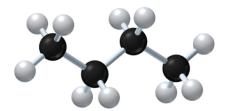


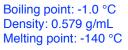




Structural Isomers

- Alkanes with more than three carbon atoms can have more than one arrangement of atoms.
 - The same combination of atoms can have different connectivity.
- Isomers are substances that have the same molecular formula but other differences.
- Structural isomers have the same molecular formula but different connectivity.
 - Structural isomers are different substances.
 - ▶ A chemical change is required to convert between structural isomers — you have to break and make bonds.
 - ➤ This is not the same a conformational change where you just rotate along bonds.
 - Structural isomers may have different properties:
 - Different boiling point.
 - Different density.
 - Different melting point.
 - ▶ Structural isomers have the same composition, so they do have some things in common.
 - The same chemical formula.
 - ▶ The same molar mass.

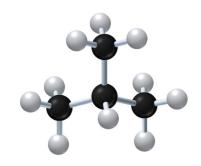




C₄H₁₀

Molar mass: 58.12 g/mol

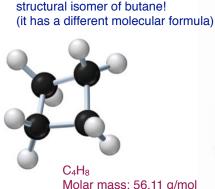
$$CH_3 - CH_2 - CH_2 - CH_3$$



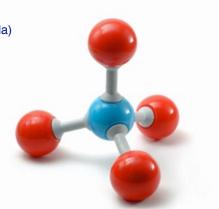
Boiling point: -11.7 °C Density: 2.064 g/mL Melting point: -159.6 °C

 C_4H_{10}

Molar mass: 58.12 g/mol



Note: cyclobutane is **not** a



Structural Isomers

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 - The same chemical formula.
 - The same molar mass.

The same substance or structural isomers?

$$\begin{array}{c|ccccc} CH_3 & CH_3 & & & & & \\ & | & & | & & \\ CH_2-CH_2 & \text{and} & CH_2-CH_2-CH_3 & & \\ & & | & & | & \\ (A) & & & CH_3 & & \\ \end{array}$$

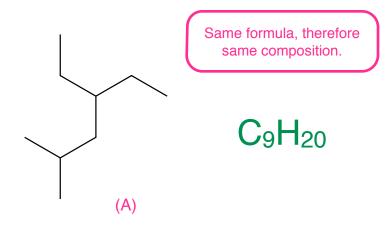
The same substance or structural isomers?

$$\begin{array}{c} \text{CH}_3 \\ \text{CH}_3 - \text{CH} - \text{CH}_2 - \text{CH}_2 - \text{CH}_3 \\ \text{(C)} \\ \text{and} \quad \text{CH}_3 - \text{CH} - \text{CH}_3 \\ \text{and} \quad \text{CH}_3 - \text{CH} - \text{CH} - \text{CH}_3 \\ \end{array}$$

Exploring Isomerism

If two substances have the same composition but different connectivity, the are structural isomers of each other.

What's the relationship between these structures?
 (are they the same substance, structural isomers or is there no relationship)



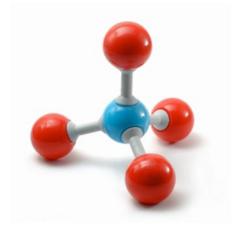
Same name, therefore same connectivity.

4-Ethyl-2-methylhexane

C₉H₂₀

4-Ethyl-2-methylhexane

These two structures describe the same substance.



Exploring Isomerism

If two substances have the same composition but different connectivity, the are structural isomers of each other.

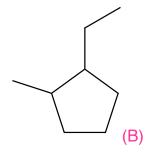
What's the relationship between these structures?
 (are they the same substance, structural isomers or is there no relationship)

Same formula, therefore same composition.

Same name, therefore same connectivity.

C₈H₁₆

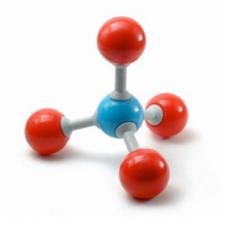
1-Ethyl-2-methylcyclopentane



C₈H₁₆

1-Ethyl-2-methylcyclopentane

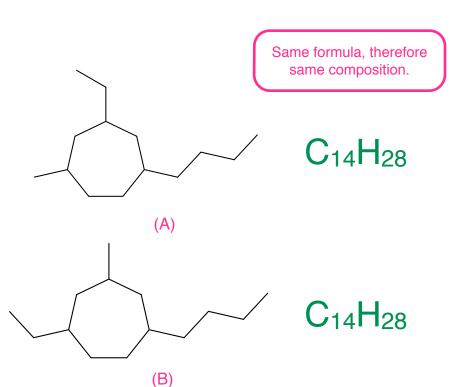
These two structures describe the same substance.



Exploring Isomerism

If two substances have the same composition but different connectivity, the are structural isomers of each other.

What's the relationship between these structures?
 (are they the same substance, structural isomers or is there no relationship)



Different name, therefore different connectivity.

1-Butyl-3-ethyl-5-methylcycloheptane

1-Butyl-5-ethyl-3-methylcycloheptane

These two structures describe different substances.

They do share the same composition.

They have different structure.

The two substances are **structural isomers** of each other.

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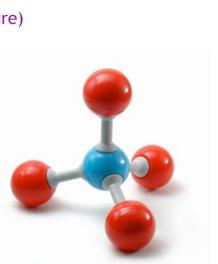
- Chain Alkanes
- Branched Alkanes
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Substituted Alkanes

- Substituents
 - alkane chains (alkyl groups)
 - ▶ isopropyl & tert-butyl
 - halogens
- Naming (structure to name)
- Drawing (name to structure)
- Properties of Alkanes
 - Uses
 - Density & Solubility
 - Reactivity
 - Combustion

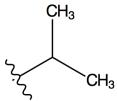




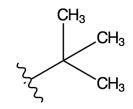


- ▶ Substituted alkanes are alkanes which have a hydrogen substituted with another type or group of atoms.
- Substituted alkanes can have backbones of carbon chains or of carbon rings.
- Branched alkanes are one kind of substituted alkane, where a hydrogen has been substituted with a simple alkane.
- ▶ Branched alkanes can become more intricate if those branches, *have* branches of their own.
 - Complex alkanes are branched alkanes, whose branches have their own branches.
 - These types of alkanes are beyond the scope of this class.
- ▶ There are some simple cases that occur frequently, that we do have to deal with.
- Instead of using the rules for a branch on a branch, we will use the following names for these common groups of atoms.
 - ▶ The **isopropyl** group: a propyl group attached by it's <u>central</u> carbon.
 - ▶ Isopropyl is a common name (slang).
 - ▶ The name of this group begins with "i" so it's alphabetized under "i."
 - Just like "water" is alphabetized under "w."
 - ▶ The tert-butyl group: a structural isomer of a butyl group.
 - ▶ The 'tert-' is an IUPAC prefix (like di-, tri, etc).
 - ▶ These prefixes are not part of the name, they describe the name.
 - ▶ tert-butyl is alphabetized under "b" like "tri-butyl" is alphabetized under "b."

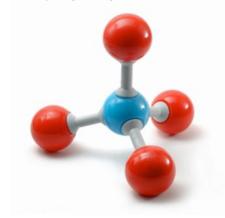




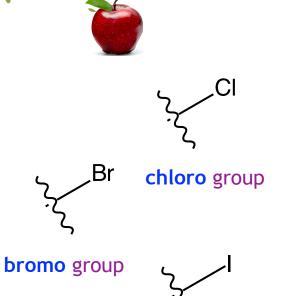
isopropyl group



tert-butyl group



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- Branched alkanes are one kind of substituted alkane, where a hydrogen has been substituted with a simple alkane.
- Haloalkanes are substituted alkanes where a halogen is the substituent.
 - Halo groups are named with the halogen stem followed by "o"
 - ▶ Fluorine atoms are "flouro" groups.
 - ▶ Chlorine atoms are "chloro" groups.
 - ▶ Bromine atoms are "bromo" groups.
 - ▶ lodine atoms are "iodo" groups.





iodo group

hexane

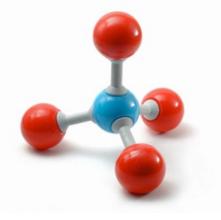
$$\begin{array}{cccc} CH_{3} & Br \\ | & | \\ CH_{3}-CH-CH_{2}-C-CH_{2}-CH_{3} \\ | & CH_{3} \end{array}$$

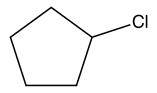
CH₃ Br CH₃ CH₃ CH₃ CH₃ CH₃ CH₃ CH₃ CH₃ CH₃

To name a substituted alkane:

- 1. Find the backbone.
 - 1. Number the carbons of the backbone, give addresses to the substituents.
 - 2. Choose the numbers that give you the smallest address first.
 - 3. If it's a tie, use alphabetical order to choose who get's the first address.
- 2. Group any common substituents using greek prefixes to show how many times they appear.
- 3. Write the substituents with their addresses in alphabetical order.
 - 1. Ignore prefixes including "tert-" and "di-", "tri-" etc when ordering them.
- 4. End with the name of the backbone.

4-bromo-2,4-dimethylhexane





chlorocylcopentane

With rings, no number is needed if only one substituent.

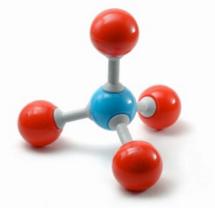
1-chloro-2-methylcylcopentane

With rings, carbon connected to the alphabetically first substituent is #1.

- To name a cycloalkane:
 - 1. The ring is your backbone
 - ▶ Even if there is longer chain attached to the ring.
 - 2. Number the atoms of the ring, give addresses to the substituents.
 - ▶ If there is less than two atoms with branches, there is no need to give an address.
 - ▶ Number the ring starting from the carbon with the branch that comes first in the alphabet.
 - Number in the direction that give the lower overall numbers.
 - If both directions give you the same numbers, start with the end that gives your the name that comes first alphabetically.
 - 3. Write the location and name for each branch.
 - When there are different branches, list them in alphabetical order.
 - ▶ When there are identical branches use the greek prefixes (di, tri, tetra, penta, hexa etc) and write the branch name once.

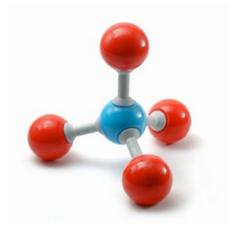
(These prefixes do not count for alphabetizing!)

4. End with the name of the backbone (ring).



1-bromo-3-isopropylhexane

3-Bromo-6-tert-butyl-5-methylnonane



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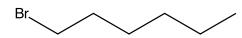
Drawing Alkanes

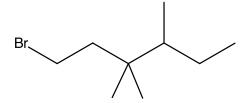
- Drawing a structure from it's name is easier than going the other way.
 - Start with the backbone or ring.
 - ▶ Then hang each substituent or branch onto the structure at it's numbered position.
 - Any remaining valence spots on carbon are filled with hydrogen.

1-bromo-3,3,4-trimethylhexane

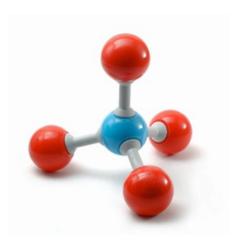


1-bromo-3,3,4-trimethylhexane





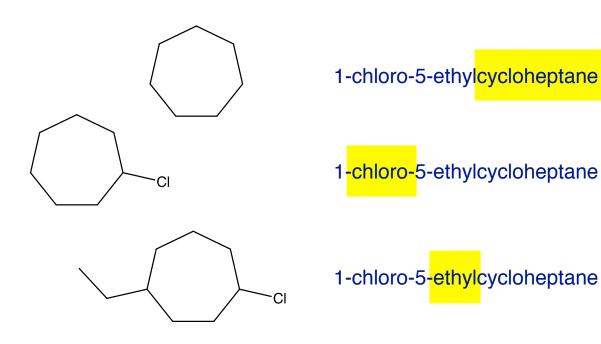
1-bromo-3,3,4-tr<mark>imethylh</mark>exane

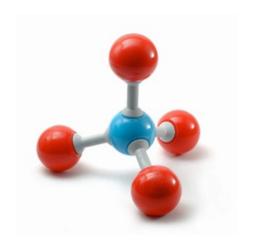


Drawing Alkanes

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1-chloro-5-ethylcycloheptane





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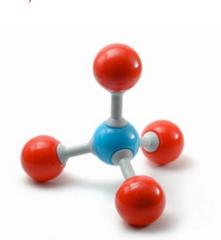
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Properties of Alkanes

- Uses
- Density & Solubility
- Reactivity
- Combustion











Properties of Alkanes

- Carbon-carbon bonds are strong, difficult to break, but release a lot of energy when you do.
- Alkanes are good fuels.
- At room temperature:
 - ▶ Alkanes with 1-4 carbons are gases and are burned when light weight, efficient fuel is required.
 - Methane is "natural gas."
 - Propane and butane gas are used as fuel in camp stoves.
 - Easiest to ignite.
 - Alkanes with 5-8 carbons are liquids, they're used for vehicle fuels.
 - ▶ Think of the "octane rating" in gasoline.
 - Harder to ignite, but more rich in energy.
 - ▶ Alkanes with 9-17 carbons tend to be liquids and are used as bulk fuels and lubricants.
 - ▶ Kerosene, diesel, jet fuel, and mineral oil are mixtures of these alkanes.
 - "Crude" oil, containing many different hydrocarbons.
 - ▶ Alkanes with 18-24 carbons tend to be waxy solids.
 - ▶ Paraffins are used to seal preserves, make candles, and coat fruit.
 - Alkanes with more than 25 carbons are semi solids.
 - ▶ Petroleum jelly or vaseline is an example.











Properties of Alkanes

- Oil and water don't mix.
 - ... alkanes are non-polar, water is polar.
- Alkanes tend to be less dense than water.
 - Alkanes tend to float on water.
 - Oil spills form slicks on the surface of the ocean.
 - Many things that float on water, can't float in oil.
 - Which is one reason animals drown in tar pits.
 - Swimming in oil, requires floating in oil.







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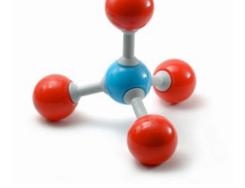


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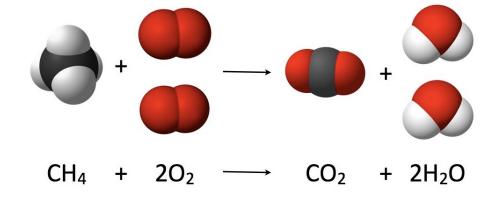


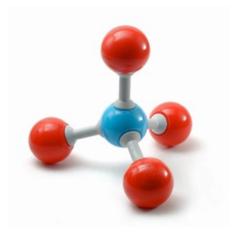


Reactions of Alkanes

$$X + O_2 \rightarrow H_2O + CO_2 + NO_2 + P_2O_5 + ...$$

- Carbon-carbon bonds aren't easy to break.
- Alkanes are flammable (they burn).
- Burning something is causing it to combust.
- Combustion reactions are reacting any substance with oxygen to form the most stable binary compounds of it's elements and oxygen.
- The most common products are CO₂ and H₂O. Other common products are NO₂ and P₂O₅.
- Combustion reactions are red-ox reactions, in which oxygen is reduced.
- The driving force in combustion reactions is oxygens fierce demand for electrons. Harnessing that property of oxygen is what gave us the internal combustion engine and is at the heart of most of fuels humans use.





Combustion Reactions

Write the balanced equation for the combustion of pentane.



$$C_5H_{12}$$

$$C_5H_{12} + O_2$$

$$C_5H_{12} + O_2 \rightarrow H_2O + CO_2$$

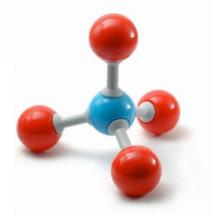
$$C_5H_{12} + O_2 \rightarrow H_2O + 5 CO_2$$

$$C_5H_{12} + O_2 \rightarrow 6 H_2O + 5 CO_2$$

$$C_5H_{12} + 8 O_2 \rightarrow 6 H_2O + 5 CO_2$$

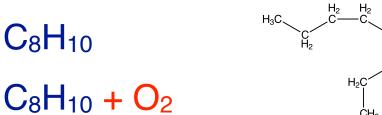


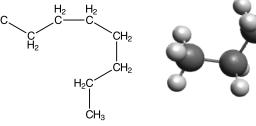




Combustion Reactions

Write the balanced equation for the combustion of octane.









$$C_8H_{10} + O_2 \rightarrow H_2O + 8 CO_2$$

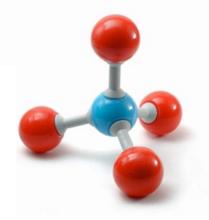
$$C_8H_{10} + O_2 \rightarrow 5 H_2O + 8 CO_2$$

$$C_8H_{10} + \frac{21}{2}O_2 \rightarrow 5 H_2O + 8 CO_2$$

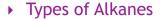


 $2 C_8H_{10} + 21 O_2 \rightarrow 10 H_2O + 16 CO_2$





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Questions?

