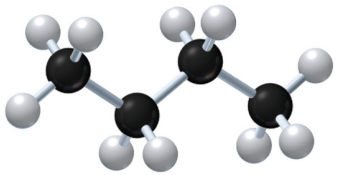
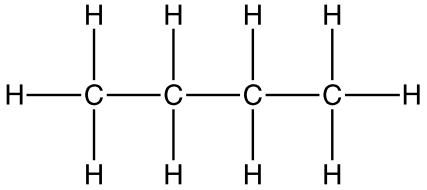
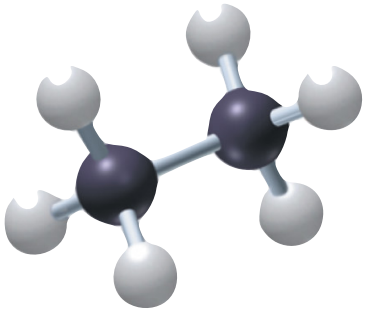
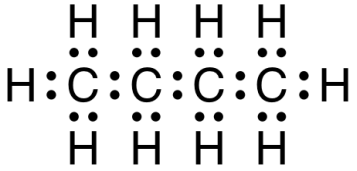
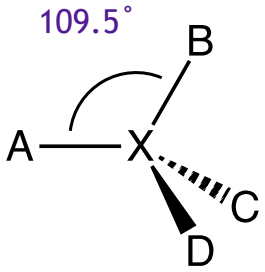
Exp 08: Organic Molecules

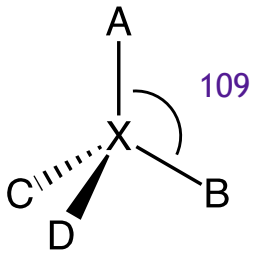


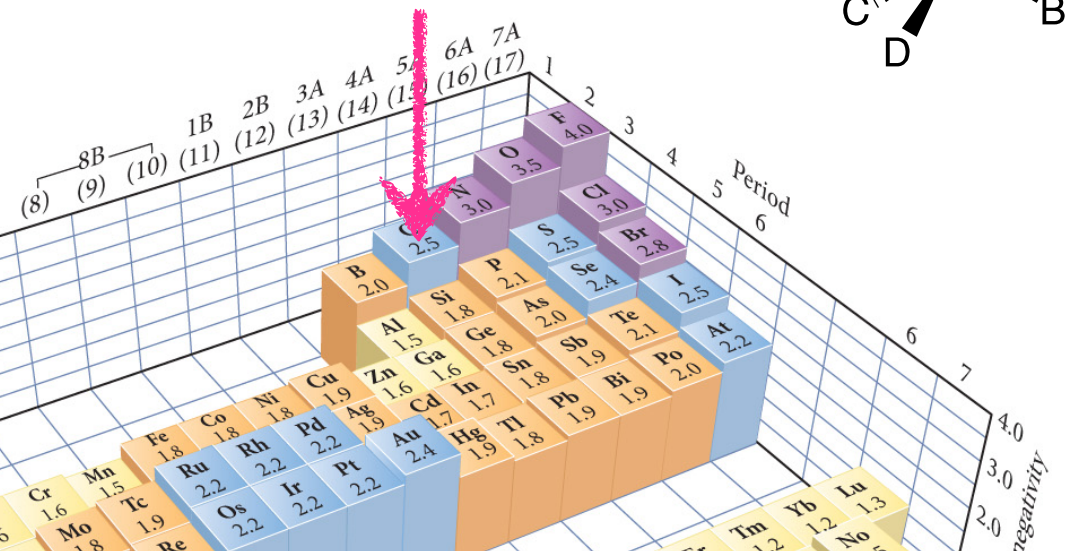


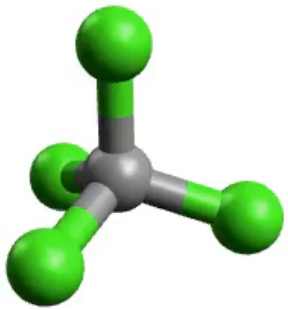


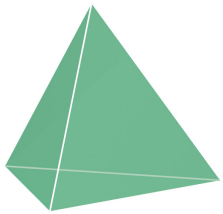


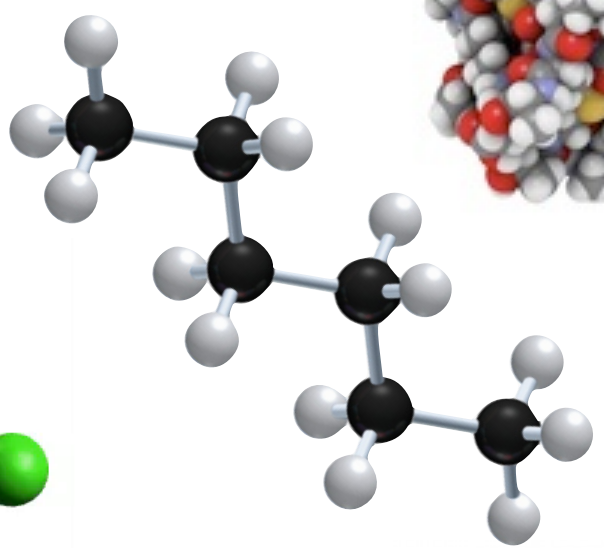








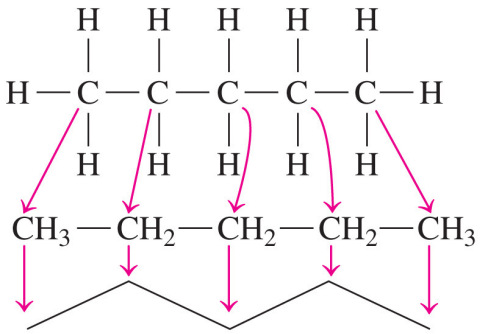




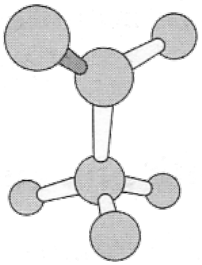
Exp 08: Organic Molecules

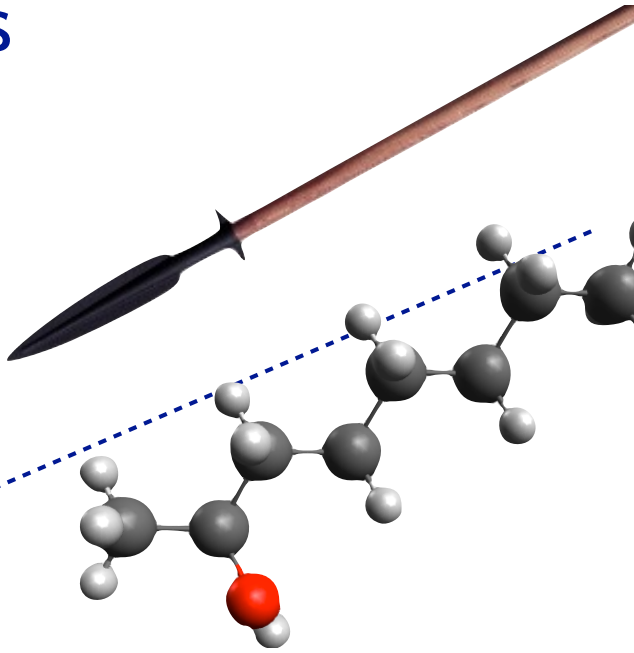
Part A: Representing Organic Molecules

Explore different ways to draw and sketch, to represent organic molecules.



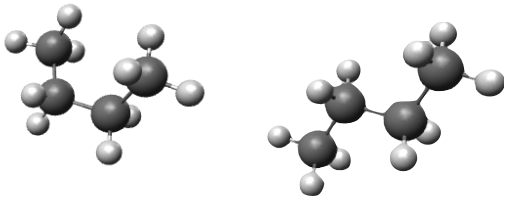
Part E: Functional Groups — Formula to Model



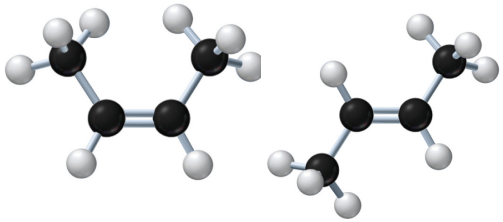


Part B: Structural Isomers and Conformer Relationships

Understand isomers and explore how structural formulas can have the same composition, but display other differences.



Part C: Structural Isomer and Stereo Isomer Relationships



Explore the idea of stereo isomers, a more subtle difference between structures.

Part D: Functional Groups — Formula to Model

Building more complex molecules by adding small groups of atoms that entirely change the function of molecules. Beginning the discussion of functonalization and families of organic compounds.

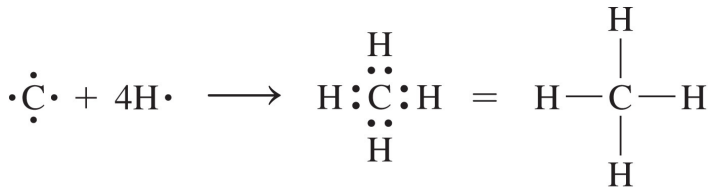
Objective: Determine the relationship between provided structures.

A Representing Organic Molecules

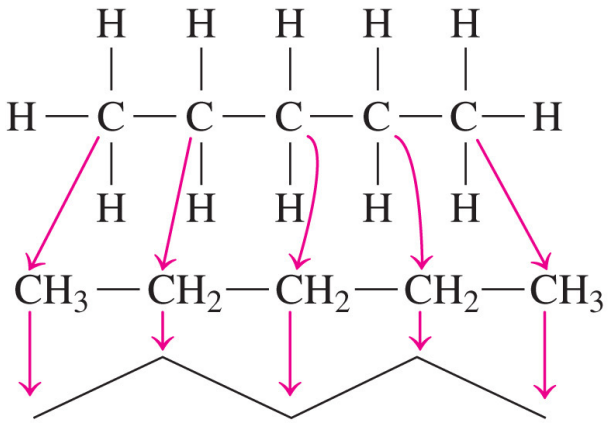
Practice representing organic molecules.

For each of the six formulas provided, draw each of the following representations.

1. Condensed Structural Formula
2. Full Structural Formula
3. Stick (Skeleton) Structural Formula



Methane

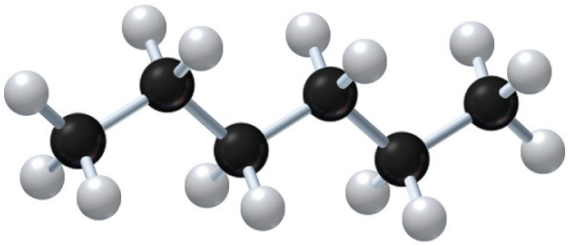


Expanded structural formula

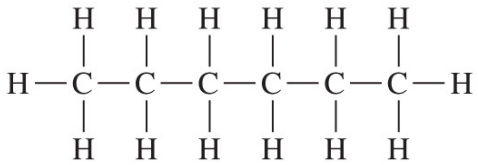
Condensed structural formula

Skeletal formula

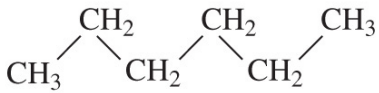
Alkane Name	Hexane
Molecular Formula	C_6H_{14}
Ball-and-Stick Model	



Expanded Structural Formula



Condensed Structural Formulas



$CH_3—CH_2—CH_2—CH_2—CH_2—CH_3$

Skeletal Formula

B Structural Isomer and Conformer Relationships

1. Build models B1 and B2
    1. See data section for a step by step walk though.
2. Draw a stick structure to represent each model.
3. Explore the models, compare their:
    1. Composition
    2. Connectivity
    3. Shape
        1. Can you duplicate the shape by bond rotation?
4. Decide what the relationship of these models is.
    1. Are they conformers or structural isomers?
5. Repeat with models B2 and B3

Isomers are substances that have the same composition.

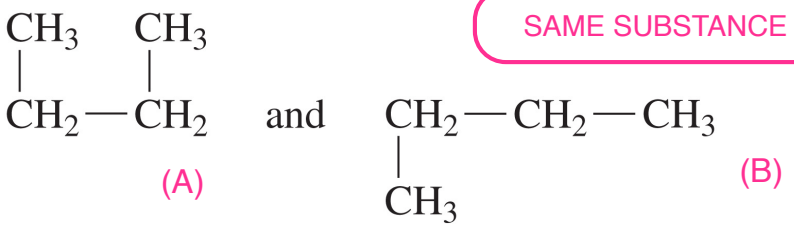
They have many similarities (molar mass, molecular formula, …)
— but are not the same substance.

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.

The same substance or structural isomers?

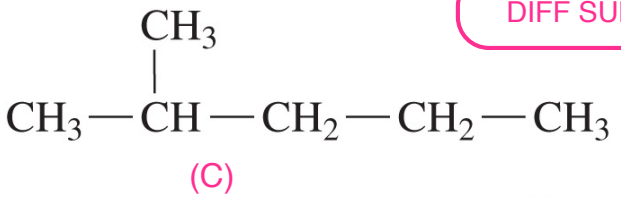
SAME SUBSTANCE



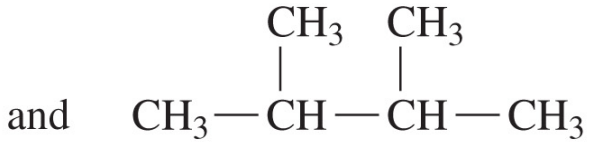
(A) (B)

The same substance or structural isomers?

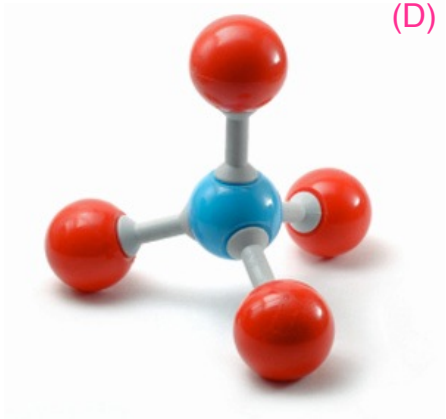
DIFF SUBSTANCES



(C)



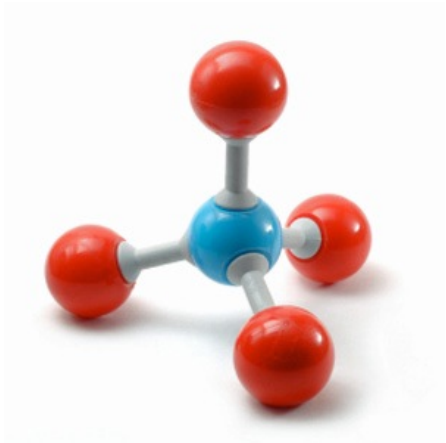
(D)



Possible Relationships

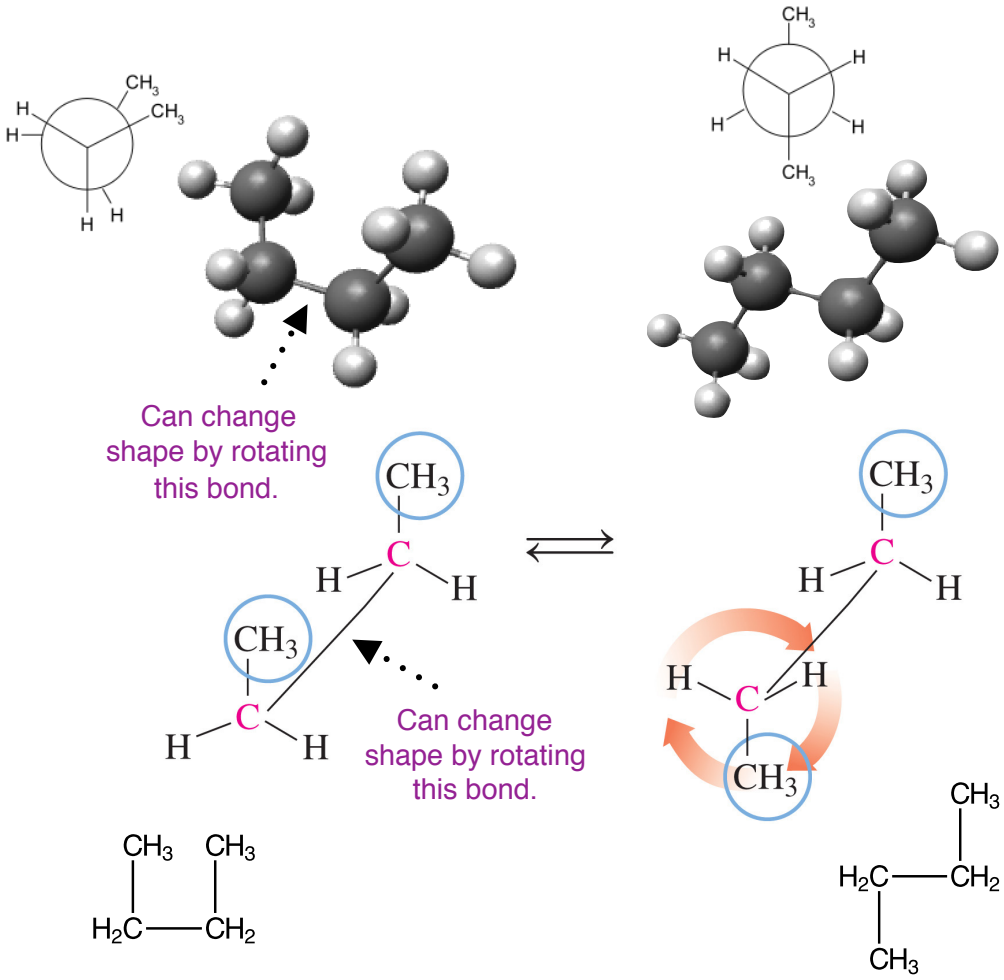
	no relation	isomers		same substance	
		structural		conformer	identical
composition	X	✔		✔	✔
connectivity	X	X		✔	✔
shape	X	X		X	✔
sense	X	X			✔

bond rotation
can make same

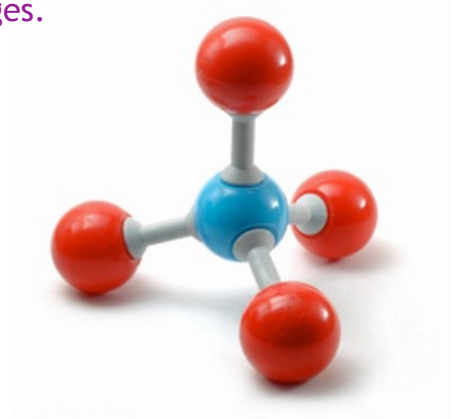


Conformations

Two conformations (shapes) of Butane

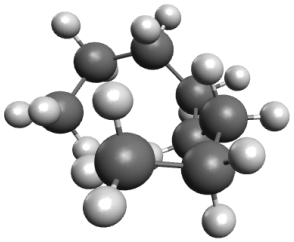


- Alkanes have a dynamic shape.
- Each carbon-carbon single bond has free rotation.
- The different possible shapes resulting from these rotations are called conformations.
- Some conformations may be better than others, but for now just realize the organic molecules have the freedom to reshape themselves 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 still the same molecule, it's still the same substance.
  - Changes in conformation are physical changes — not chemical changes.

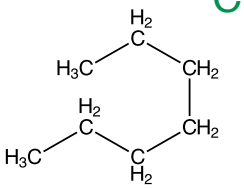


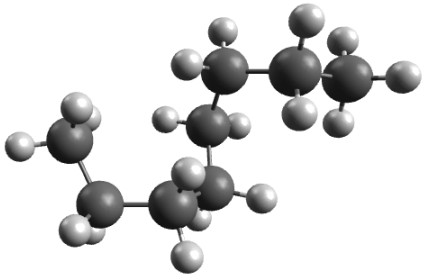
As long as the connectivity and composition is the same we're talking about the same substance.

Conformations

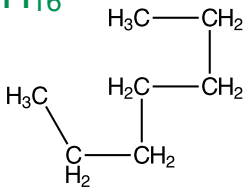


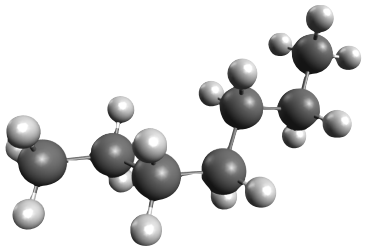
C_7H_{16}



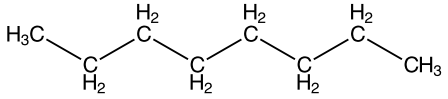


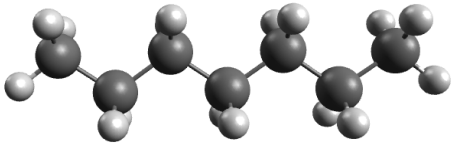
C_7H_{16}



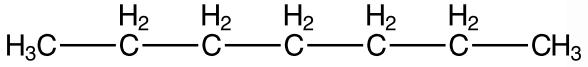


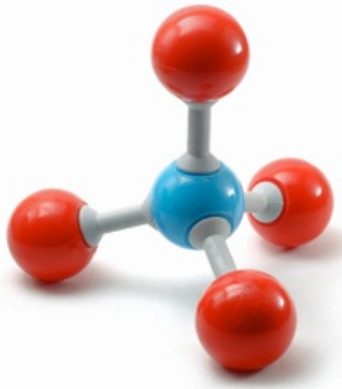
C_7H_{16}





C_7H_{16}



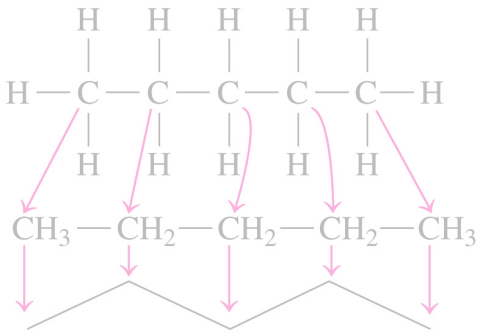


- Rotating around those carbon carbon single bonds can produce new shapes of the whole molecule. The shape around the carbon atoms isn't changed, but these larger molecules can adopt different relative positions of of the carbon atoms. Different conformations.
- Conformations are different states in 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 still the same molecule, it's still the same substance.
  - Changes in conformation are physical changes – not 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.

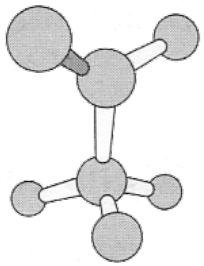
Exp 08: Organic Molecules

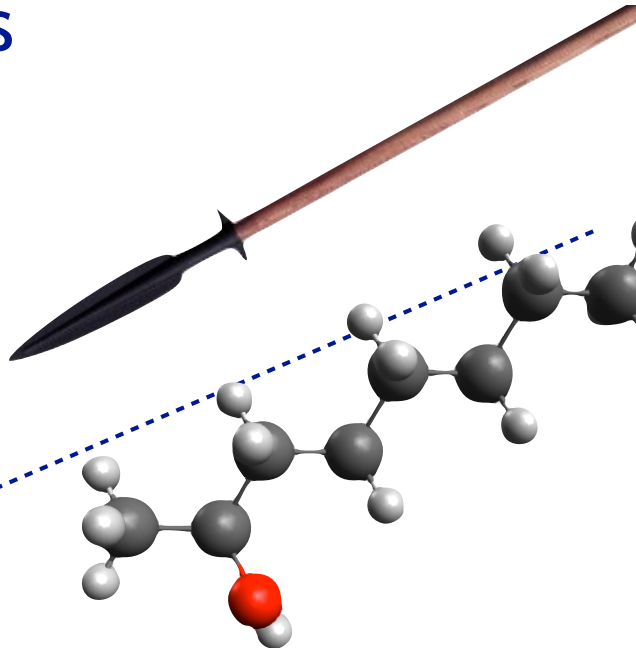
Part A: Representing Organic Molecules

Explore different ways to draw and sketch, to represent organic molecules.



Part E: Functional Groups — Formula to Model

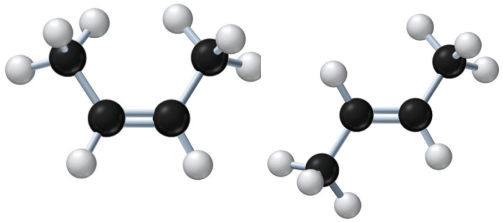




Part B: Structural Isomers and Conformer Relationships

Understand isomers and explore how structural formulas can have the same composition, but display other differences.

Part C: Structural Isomer and Stereo Isomer Relationships



Part D: Functional Groups — Formula to Model

Building more complex molecules by adding small groups of atoms that entirely change the function of molecules. Beginning the discussion of functonalization and families of organic compounds.

Explore the idea of stereo isomers, a more subtle difference between structures.

Objective: Determine the relationship between provided structures.

C Structural Isomer and Stereo Isomer Relationships

1. Build models C1 and C2
    1. See data section for a step by step walk though.
2. Draw a full structure to represent each model.
3. Explore the models, compare their:
    1. Composition
    2. Connectivity
    3. Shape
        1. Can you duplicate the shape by bond rotation?
4. Decide what the relationship of these models is.
    1. Are they conformers or structural isomers?

6. Build models C3 and C4
7. Explore these models, decide the relationship

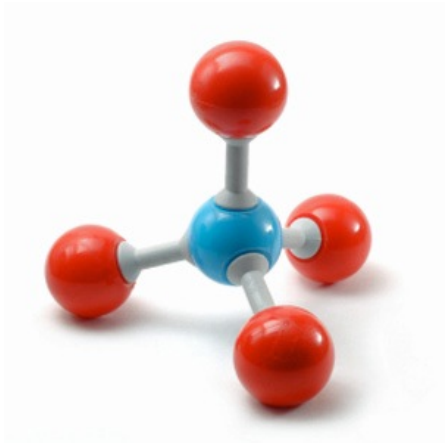
9. Build models C5 and C6
10. Explore these models, decide the relationship

Possible Relationships

	no relation	isomers		same substance	
		structural	stereo	conformer	identical
composition	x	✔	✔	✔	✔
connectivity	x	x	✔	✔	✔
shape	x	x	x	x	✔
sense	x	x	x		✔

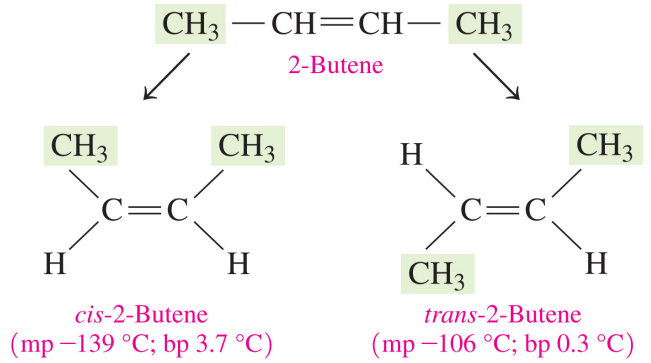
bond rotation
cannot make same

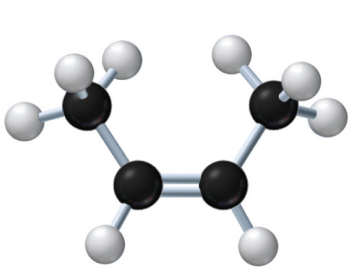
bond rotation
can make same

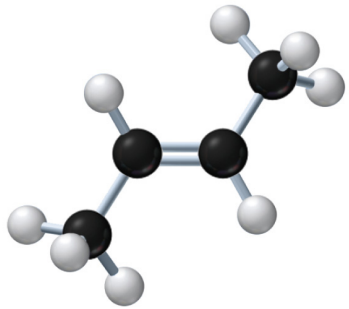


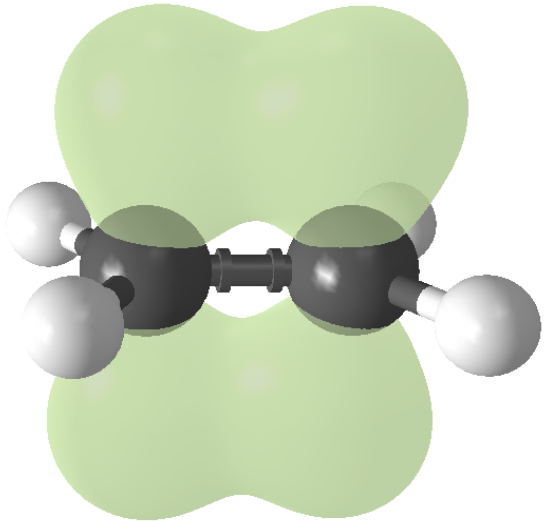
cis-trans Stereo Isomers

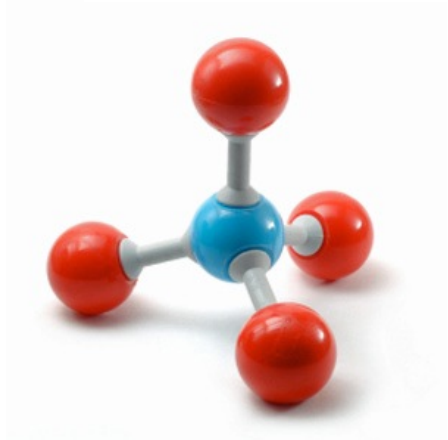
- Alkenes with double substituted bonds can have more than one arrangement of atoms.
- A chemical change is required to convert between substituents arranged on a double bond next to each other (*cis*) or opposite each other (*trans*).
- A double bond cannot rotate without breaking.




cis-2-Butene

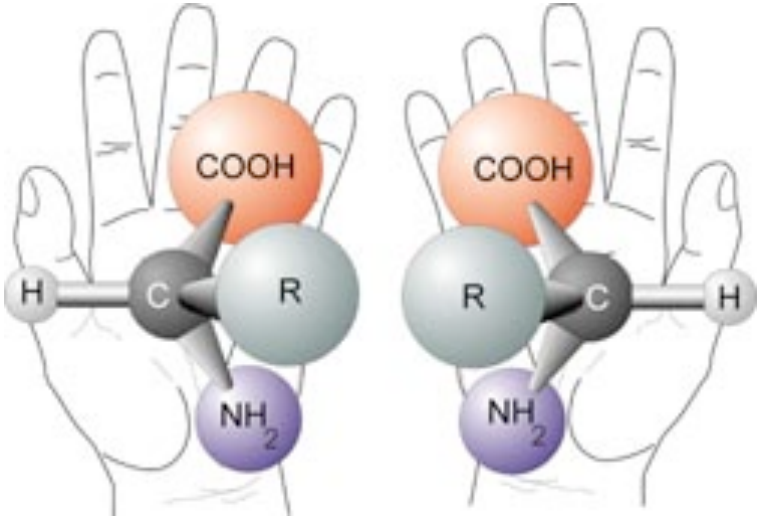

trans-2-Butene

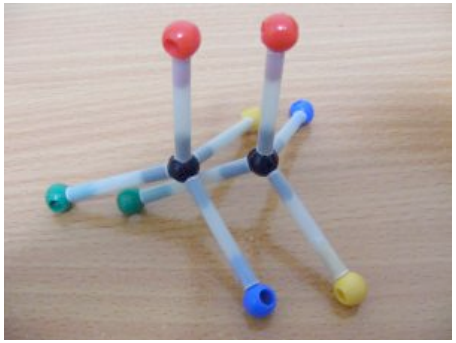


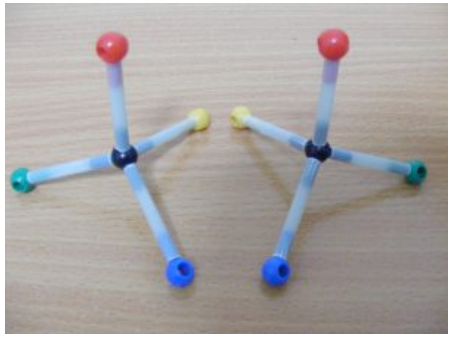


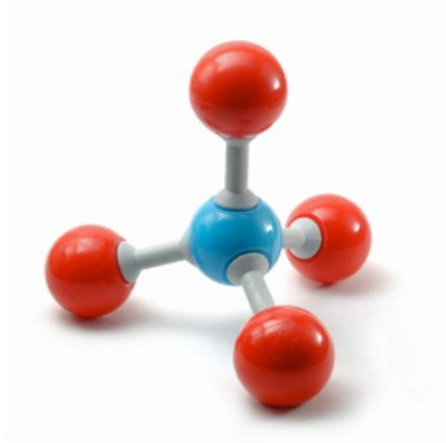
R/*S* Stereo Isomers

	(*R*)–lactic acid **(1)**	(*S*)–lactic acid **(2)**
molecular formula	$C_3H_6O_3$	$C_3H_6O_3$
structural formula	CH_3CHCO_2H, OH	CH_3CHCO_2H, OH
configuration	CH_3, C, HO_2C, H, OH	CH_3, C, H, HO, CO_2H





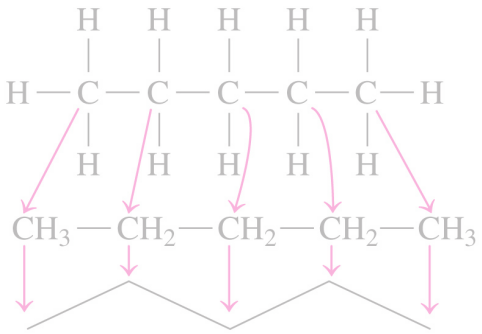




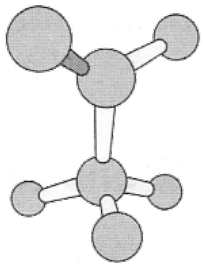
Exp 08: Organic Molecules

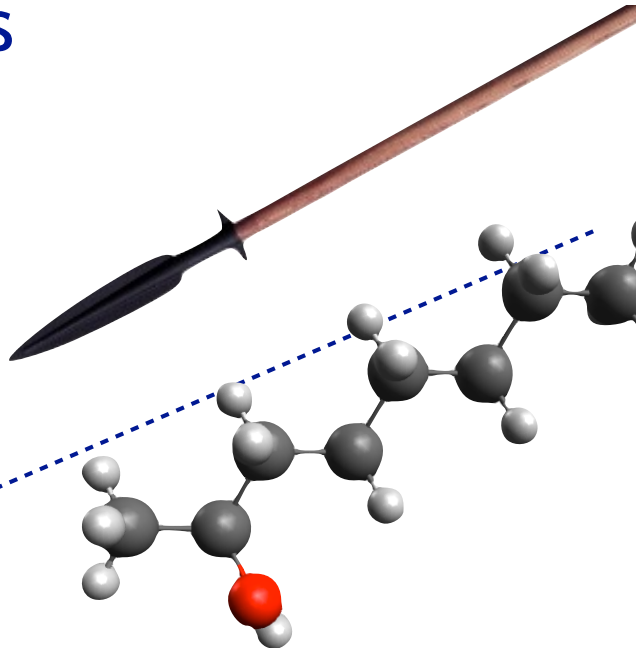
Part A: Representing Organic Molecules

Explore different ways to draw and sketch, to represent organic molecules.



Part E: Functional Groups — Formula to Model

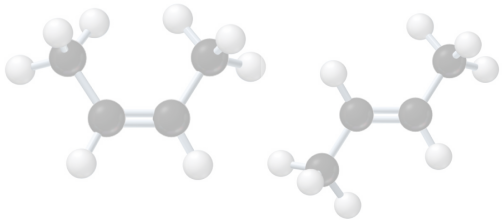




Part B: Structural Isomers and Conformer Relationships

Understand isomers and explore how structural formulas can have the same composition, but display other differences.

Part C: Structural Isomer and Stereo Isomer Relationships



Part D: Functional Groups — Formula to Model

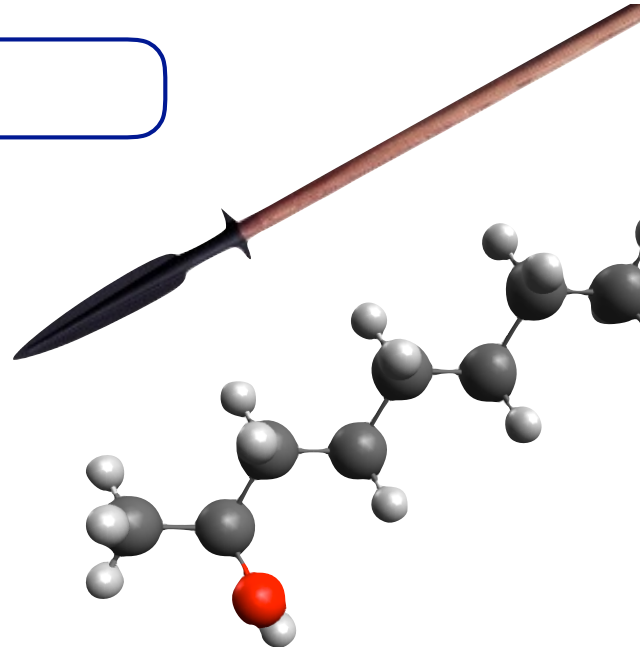
Building more complex molecules by adding small groups of atoms that entirely change the function of molecules. Beginning the discussion of functonalization and families of organic compounds.

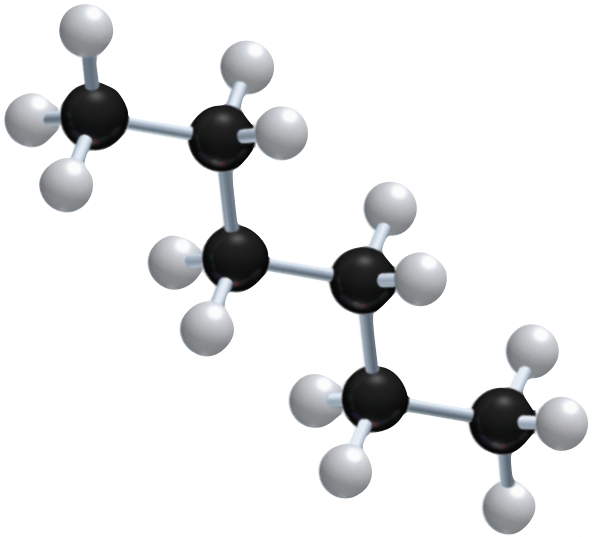
Explore the idea of stereo isomers, a more subtle difference between structures.

Objective: Determine the relationship between provided structures.

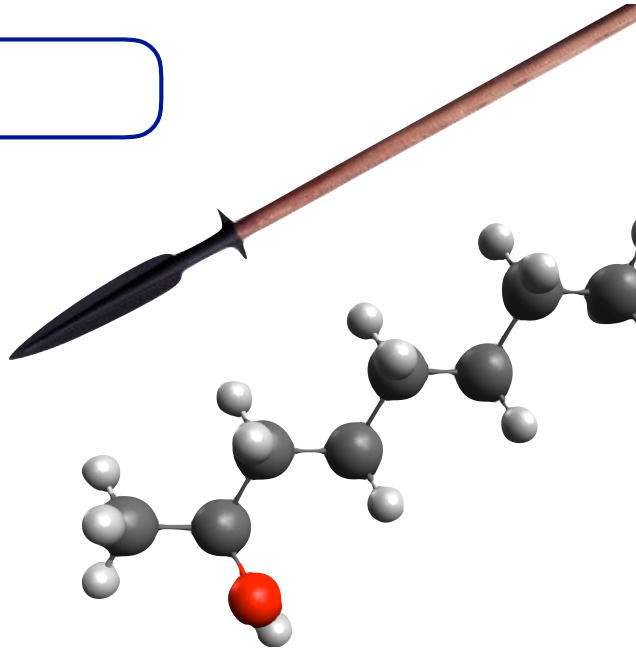
D Functional Groups — Formula to Model

1. Build models D1 and D2
    1. See data section for a step by step walk though.
2. Draw a skeleton (stick) structure to represent each model.
3. Explore the models, compare their:
    1. Composition
    2. Connectivity
    3. Shape
        1. Can you duplicate the shape by bond rotation?
4. Decide what the relationship of these models is.
    1. Are they conformers or structural isomers?

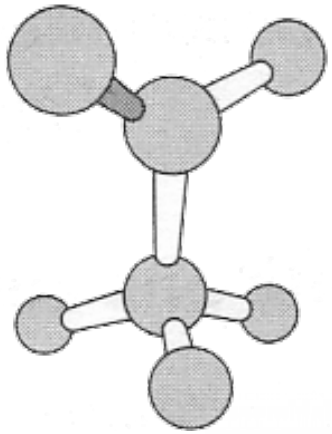




E Functional Groups — Model to Formula



1. For each of the models shown in section E determine what substance is being represented.
2. Write it's condensed and stick formulas.
3. Identify the functional group (group of atoms that indicate it's family) and the family of compounds it belongs to. Include this information in the table below.
4. To make your determination consider the valence of each atom shown in the model.
5. Assume any atom that forms four bonds is carbon, with three is nitrogen, with two oxygen, and with one hydrogen.
    1. Remember that double bond will count as two bonds for satisfying the atoms valence.



6. Identify the characteristic group of atoms, the functional group, for each molecule.
7. Identify the family of substances defined by this functional group.

Functional Groups to Families

Functional Group	Structure	Compound Classification
Halogen (–X is F, Cl, Br, I)	R –X	Halocarbon
Hydroxyl (–OH)	R – OH	Alcohol
Carboxyl –C(=O)–OH	R–C(=O)–OH	Carboxylic acid
Carbonyl (– C=O)	R– C=O	Aldehyde
	R – C(=O) – R	Ketone
Ester –C(=O)–O–	R –C(=O) –O– R	Ester

Exp 08: Organic Molecules

Part A: Representing Organic Molecules

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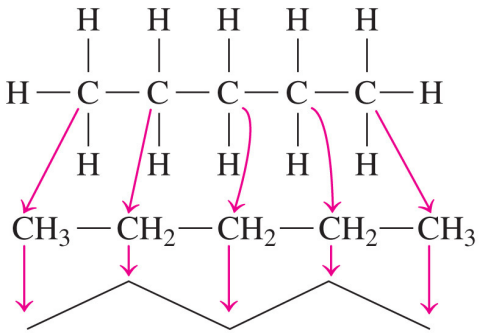
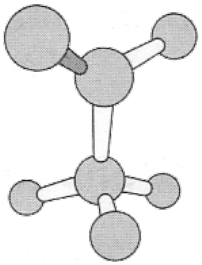
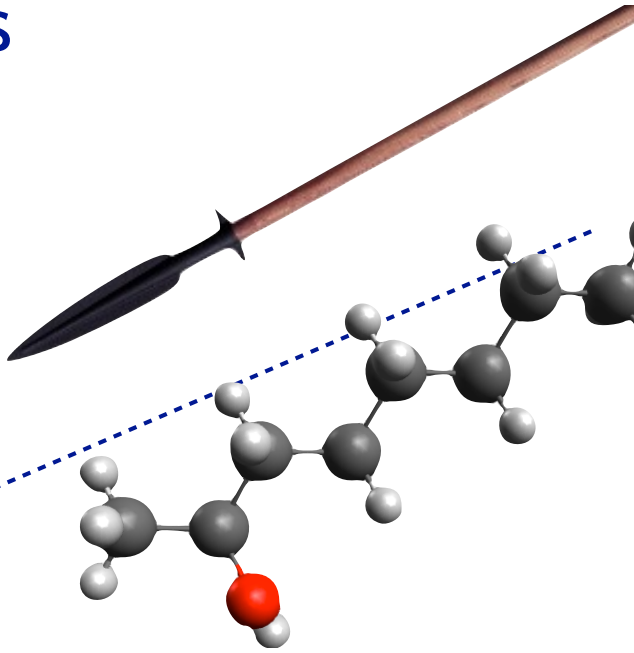


Part E: Functional Groups — Formula to Model





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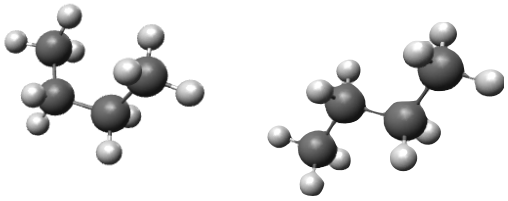
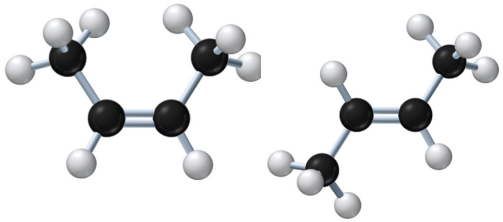


Part C: Structural Isomer and Stereo Isomer Relationships



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Questions?