
Introduction to the Structures and Isomerism of Simple Organic Molecules: Description and Modeling

Objectives

The objectives for this lab are:

- **Part I:** To learn the structures of and construct models for simple organic molecules, and to draw their projection and perspective formulae.
- **Part II:** To classify, recognize and construct models of different types of isomers of organic compounds.

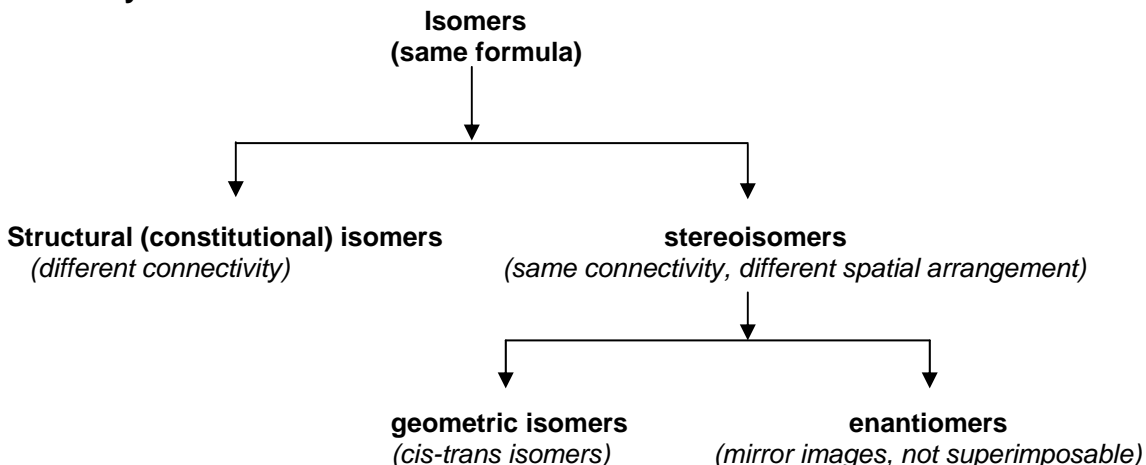
Background

Almost all compounds that contain carbon are known as **organic compounds**. Most organic compounds also contain hydrogen. Organic compounds that contain only carbon and hydrogen atoms are classified as **hydrocarbons**. The four classes of hydrocarbons are alkanes, alkenes, alkynes and aromatic hydrocarbons. Alkanes and alkenes and alkynes are further classified as aliphatic hydrocarbons. Structures and simple physical properties of hydrocarbons will be discussed in **Part I**.

Different arrangements of atoms in a set of molecules that *cannot* be interconverted by simple rotation around a single bond are called **isomers**. To convert one isomer to another requires enough energy to break and reform one or more π or σ bonds. Therefore, they are different compounds and exhibit different properties.

There are two main classes of isomers called constitutional (structural) isomers and stereoisomers. **Structural isomers** have the same molecular formula, but the atoms are bonded in a different order, or bonding connectivity. **Stereoisomers** have the same bonding connectivity, but have a different three dimensional arrangement. **Geometric isomers** have different orientations of atoms or groups across a double bond or a ring. **Enantiomers** are mirror images of each other, and therefore are not superimposable on their mirror image

Summary of Isomers



Molecular Models

Molecular models will be used to illustrate the three-dimensional structures of simple hydrocarbons and different types of isomers. The model kits contain different colored balls and different size sticks. Three-dimensional models will be constructed from these balls and sticks. Molecular models will be constructed for each molecule.

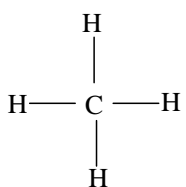
Different colored balls represent different atoms. The usual designation is:

Black – carbon	Orange – bromine
White – hydrogen	Purple - iodine
Red – oxygen	Blue – nitrogen
Green – chlorine	Yellow – sulfur

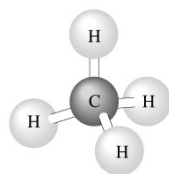
The plastic sticks in the kits represent bonds. There are two different sized sticks. The short, stiff sticks are used to represent single bonds and the long flexible sticks are used for double and triple bonds. In order to make one double bond two flexible sticks are needed to connect the two adjacent atoms and to make a triple bond three flexible sticks are used to connect the two adjacent atoms.

Lewis structure and three dimensional perspective diagrams will be drawn. **Three dimensional** drawings can be either done as ball and stick or projection drawings. Projection drawings require a different drawing technique to identify bond orientation. A solid straight lines (—) represent bonds lying in the plane of the paper, a wedge-shaped line constructed of hatch marks (▨) represents bonds that project down into the paper, and solid wedge-shaped line (▴) represents bonds that project up out of the paper, toward the viewer.

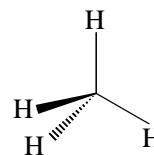
- Lewis and 3D diagram of CH₄



Lewis Structure



3D
ball and stick



projection

It is important to be able to visualize these three-dimensional structures in your mind without the aid of molecular models. If you need further practice with these models you can purchase them or you can be creative and make home made models using materials that are available in your home.

Lab Report for Introduction to the Structures and Isomerism of Simple Organic Molecules: Description and Modeling

Part I: Hydrocarbons

Alkanes

1. Construct a model of C_2H_6 name: _____

Lewis Structure:	3D Drawing:
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- Predict the HCH and HCC bond angles.
- Name of carbon geometry.
- Name the hybridization of the carbons.

2. Construct a model of CH_3CH_3 name: _____

Lewis Structure:	3D Drawing:
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- Predict the HCH and HCC bond angles.
- Name of carbon geometry.
- Name the hybridization of the carbon.

Alkenes

3. Construct a model of CH_2CH_2 name: _____

Lewis Structure:	3D Drawing:
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- Predict the HCH and HCC bond angles.
- Name of carbon geometry.
- Name the hybridization of the carbon.

4. Construct a model of CH_2CHCH_3 name: _____

Lewis Structure:	3D Drawing:
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- Predict the angle HCH (the first carbon).
- Predict the angle HCC (the first and the second carbon).
- Predict the angle HCH (the third carbon).

Alkynes

5. Construct a model of CHCH name: _____

Lewis Structure:	3D Drawing:
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- Predict the angle HCC.
- Name the molecular geometry about each carbon.
- Name the hybridization of the carbon atoms.

6. Construct a model of CHCCH₃ name: _____

Lewis Structure:	3D Drawing:
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- Predict the angel HCC (the first carbon).
- Predict the molecular geometry around each carbon.

Aromatic hydrocarbons

7. Construct a model of C_6H_6 name: _____

Lewis Structure:	3D Drawing:
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- Predict the angle HCC.
- Predict the angle CCC.
- Name the geometry around each carbon atom.
- Name the hybridization of each carbon.

8. Construct a model of $o\text{-}C_6H_4Cl_2$ (1,2-dichlorobenzene).

Lewis Structure:	3D Drawing:
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- Predict the angle CCC.
- Predict the angle ClCC.
- Indicate the position of the two chlorine atoms on the benzene ring.

Part II: Isomers

9. Construct models of the alkane C_4H_{10} .

Lewis structures of all isomers of C_4H_{10} ; name each.

- How many possible isomers exist?
- What type of isomerism do they represent?

10. Construct models of the alkane C_5H_{12} .

Lewis structures of all isomers of C_5H_{12} ; name each.

- How many possible isomers exist?
- What type of isomerism do they represent?

11. Construct models of the hydrocarbon C_4H_8 .

Lewis structures of all isomers of C_4H_8 ; name each.

- How many possible isomers exist?
- What type of isomerism do they represent?

12. Construct models of $C_6H_4Cl_2$ (dichlorobenzene).

Lewis structures of all isomers of $C_6H_4Cl_2$ (dichlorobenzene); name each.

- How many isomers exist?
- Can you convert one into another without breaking any bonds?
- What type isomerism do these represent?

13. Construct models of the isomers of $\text{ClCH}=\text{CHCl}$ (1,2-dichloroethene)

Lewis structures of both isomers; name each.

- Make two models that have different spatial arrangement of the substitutions (the two Cl atoms) across the double bond.
- What type of isomerism do these represent?

14. Construct models of the geometric isomers of C_4H_8 . (There are geometric isomers for one of the isomers drawn in question 11.)

Lewis structures of both isomers; name each.

15. Construct models of the enantiomers of CHBrIF

3D drawings of both enantiomers (make one model then make its mirror image):

- Can the two models be superimposed?
- What type of isomerism do these models represent?