Molecular Models

Experiment #1

Objective: To become familiar with the 3-dimensional structure of organic molecules, especially the tetrahedral structure of alkyl carbon atoms and the planar structure of alkenes.

Introduction

It is not possible to view molecules, even through the most powerful microscopes, except for a few extremely large polymeric molecules, whose images can be visualized with the electron microscope. The tunneling electron microscope can image atoms on the surface of materials, but it is not useful for visualizing small molecules. A nuclear magnetic resonance spectrometer (NMR) can provide important information about the relative position of atoms with respect to one another in a molecule, especially organic molecules. Consequently, chemists must resort to inferring a chemical structure from a variety of chemical and physical properties of a compound. Molecular models are useful in testing hypotheses about the structure of a molecule. In fact, Watson and Crick derived the double helix structure of DNA using a molecular model.

In this experiment you will use ball and stick models to represent atoms and bonds in molecules and build molecular structures using these models. In order to better understand chemical properties of molecules, it will help to be able to visualize the three dimensional structure.

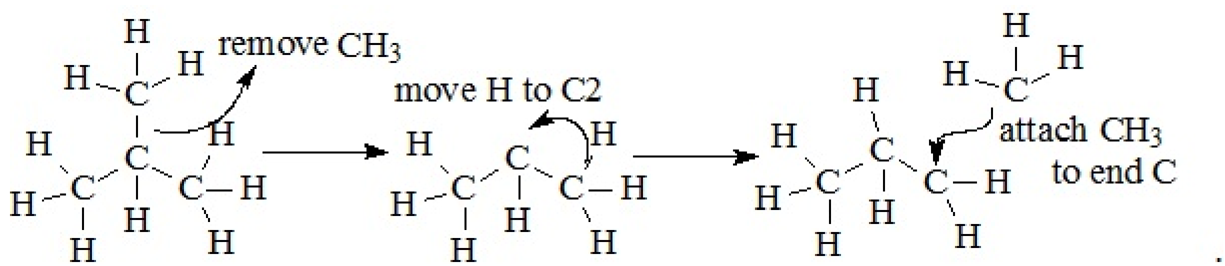
The model kits consist of different colored balls with holes for the pegs that connect them. The balls are color coded and the holes correspond to the number of bonds each atom normally has. We will not be using all of the different balls (atoms) provided in the kit. Notice that the number of holes in each ball corresponds to what chemists often refer to as the valence of an atom (in this case the usual valence for organic molecules). Hydrogen and the halogens, chlorine, bromine and iodine, have only one bond to carbon. Oxygen forms two covalent bonds, nitrogen usually forms three covalent bonds, and carbon always forms 4 covalent bonds. This gives rise to what is sometimes called the HONC rule; i.e., H has one bond, O has 2, N has 3 and C has 4 bonds in most neutral organic molecules.

Table of Atom Characteristics for Molecular Models

Color of Ball	Number of Holes	Atom Represented
Black	4	Carbon
White	1	Hydrogen
Red	2	Oxygen
Blue	4	Nitrogen
Green	1	Chlorine
Orange	1	Iodine or Bromine

The additional lone pair of electrons on the N atom allows it to form the ammonium ion if H^+ attaches, or quaternary amines if four carbons are attached. Oxygen may lose a proton in organic acids to form the negatively charged carboxylate ion (or phenolate ion from phenols). In summary, when O has only one bond to another atom it will carry a negative charge and when N has 4 bonds to other atoms it will carry a positive charge. You should also notice that there are different size pegs to connect the balls. In this exercise you will use only the gray pegs (some medium length, light gray and rigid, some longer, darker gray and flexible). The flexible pegs are used to make multiple bonds, *i.e.*, double bonds.

In this exercise you will construct different isomers of organic molecules. **Isomers** are molecules with the same chemical formula but different structures. **Structural isomers** are compounds with different connections among their atoms. You should be able to distinguish between different structural isomers and different conformations of the same isomer. You can form different **conformations** of a molecule by merely rotating groups around a bond without breaking any bonds. It is necessary to break bonds in order to form different structural isomers (see Fig 1 below).



2-methylpropane before removing methyl group | isopropyl radical before moving H to C2 | attach methyl radical to C3 of propyl to form n-butane

Figure 1. In this diagram it is necessary to break the C-C bond between C2 and the methyl C of 2-methylpropane (shown on the left) and transfer one H atom from C3 to C2 of that molecule (shown in the middle of the diagram) before connecting the methyl C to C3 (shown on the right) in transforming 2-methylpropane to n-butane; hence these are structural isomers. Is this perfectly clear?

Remember: It is necessary to break bonds in order to form a different isomer. It is also necessary to have the same number of atoms of each element for molecules to be isomers of one another.

In this exercise you will be frequently asked to describe the three dimensional structure of a molecule, sometimes drawing the molecule on paper (i.e., in two dimensions). Consequently, it is often necessary to describe the position of one atom relative to other atoms with respect to their distance from you in space. For example, if the methane model is placed on the bench, it will (due to gravity) have one hydrogen atom directly above the carbon atom. It will be necessary to draw structures to represent the relative positions of atoms in space. Some people find this difficult to do, but you must try to appreciate the spatial relationships of atoms in molecules.

Materials: Molecular model kits.

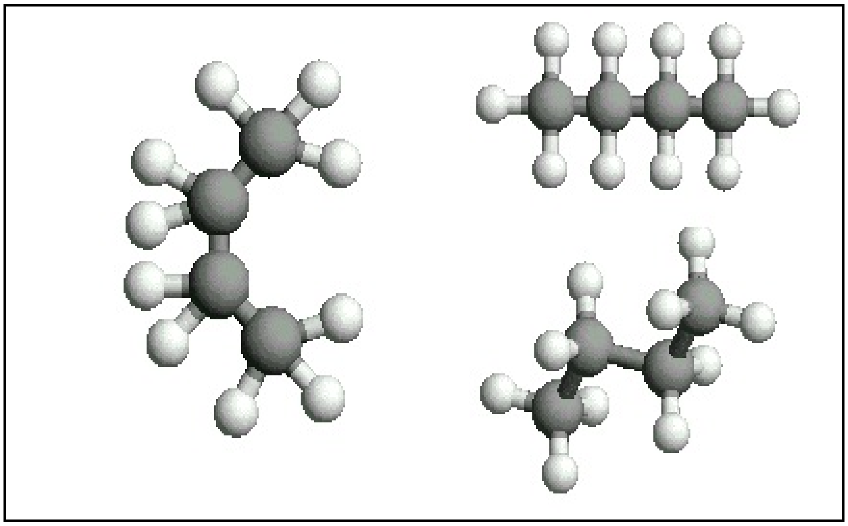


Figure 2. Different conformations of butane. Note: These different structures can be formed without breaking bonds. The shapes may be different and they may look different from different angles, but they are all identical molecules.

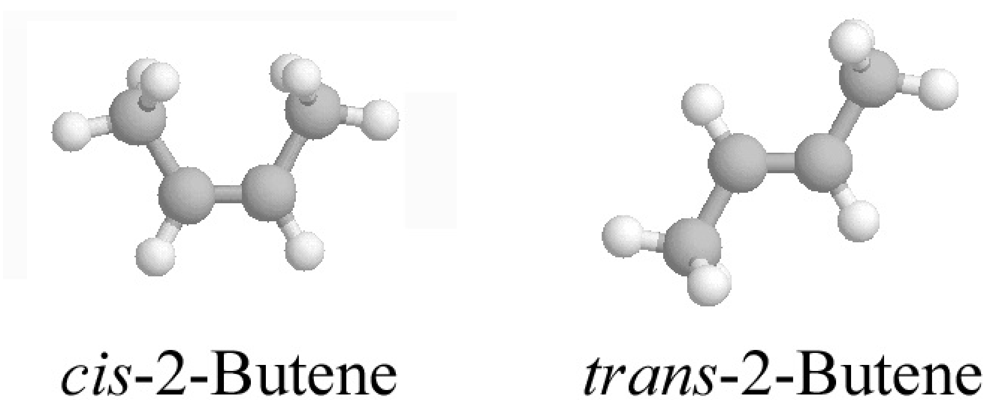


Figure 3. Different structural isomers of 2-butene. Note: bonds must be broken to convert *cis*-2-butene to *trans*-2-butene. The horizontal bond in the middle is a double bond.

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Molecular Models

Experiment #1 **Pre-Lab Exercise**

1. How many bonds are normally formed to atoms of each of the following elements when they are in most organic molecules.

	No. of Bonds		No. of Bonds		No. of Bonds
H		C		N	
O		Cl		Br	

2. Molecules can be represented by molecular formulas or by structural formulas. Write the molecular formula for butane below and show all the possible structural formulas for butane.

<u>Molecular Formula for Butane</u> <u>All (2) Possible Structural Formulas for Butane</u>

3. What is the difference between conformational structures of a molecule and different structural isomers? Give two examples of each to illustrate, *i.e.* two conformational structures and two structural isomers.

4. How would you describe the difference between a saturated hydrocarbon and an unsaturated hydrocarbon? Give an example of each to illustrate.

5. Give two examples of cycloalkanes and one example of a cycloalkene, showing the structural formula for each. Name the structures you have drawn.

6. What is meant by *cis*- and *trans*- isomers of alkenes. Give an example of each, making a structural formula and correctly naming it for each example.

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Molecular Models

Experiment #1 **Data & Report Sheet**

Part A. Simple Hydrocarbons.

1. Make a model of methane (CH_4) connecting four H atoms (white balls) to one C atom (black ball), using the light gray, rigid pegs. Place the model on the bench and notice the 3-dimensional structure. Write the structural formula for methane (using chemical symbols, *i.e.*, C and H) on the left below and draw a 3-dimensional diagram of the methane model on the right.

2. Remove an H atom and replace it with a C atom forming a C-C bond. Complete the model by adding bonds (light gray, rigid pegs) to H atoms to fill all the holes in the two C atoms.

   What is the name of the molecule you have just formed? ____________________________

   Write the chemical formula for this molecule. ______________
   Notice it is possible to rotate the molecule about the C-C bond. Place it on the bench with four H atoms in contact with the bench and two H atoms pointing straight up. Draw a diagram of this model below on the left. Then rotate the molecule about the C-C bond so there are two H atoms from one C in contact with the bench and only one H atom from the other C pointing straight down in contact with the bench. Draw a diagram of this form of the model below on the right.

   Are these different isomers? (yes or no) _________________
   Did you break any bonds when you rotated the molecule about the C-C bond? _______________

3. Remove one H atom from the molecule above.
   What is the name of the C_2H_5 radical (group) you have just formed? _____________

   Attach a C atom where the H atom was, and fill in the remaining holes with bonds to H atoms.

   What is the name of this three carbon molecule? ____________________

   Is it still possible to rotate the molecule about both of the C-C bonds? (yes or no) ____________

Remove an H from the central C and remove one -CH_3 group from this C and place it where the H was. Place the H where the -CH_3 group was.
Have you formed a different isomer? (yes or no) _______

Does the molecule look any different? (yes or no) ____________
Write the structural formula (using chemical symbols) for this molecule below on the left and draw a diagram of this model (ball and stick) below on the right.

4. Remove an H atom from an end C of the three carbon molecule above and replace it with a -CH_3 group.
What is the name of the molecule you have formed? ____________________________
We will now use numbering to represent the order of the C atoms (*i.e.*, C1, C2, C3, and C4 in this case). Place the molecule on the bench so two H atoms from C2 and two H atoms from C3 are in contact with the bench. Write the structural formula (using chemical symbols) for this molecule (as you see it) in the space below on the left. After drawing that structure, rotate the molecule about the bond connecting C2 and C3 to get two H atoms from C1 in contact with the bench and two H atoms from C3 in contact with the bench. Write the structural formula (using chemical symbols) for this molecule (as you see it) in the space below on the right.

Have you broken any bonds to change the shape? (yes or no) ______
Is this the same molecule or a different molecule after rotating it? (same or different)_________

5. Remove an H atom from C2 and remove C4 (as a -CH_3 group) from C3. Place the -CH_3 group on C2 and place the H atom on C3.
Is this the same molecule or a different molecule than the one you had in step 4? _____________

What is the common name for the molecule you have just formed? ________________________

What is the IUPAC name for this molecule? ____
(See the text book if you need help naming this compound)

Write the structural formula for this molecule in the space to the right.

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Part B. Unsaturated Hydrocarbons.

6. Make a model of 2-butene using two of the longer, flexible (dark gray) pegs to connect C2 and C3, forming a double bond. The remainder of the molecule should have single bonds (rigid, light gray pegs).
What is the molecular formula for 2-butene? ________________________
Be sure you have made the correct model for 2-butene.
Can you rotate the molecule about the double bond connecting C2 and C3? (yes or no) _______
Notice the general shape of the molecule and notice that all **atoms** connected to C2 and C3, as well as C2 and C3 are in a plane (*i.e.*, this part of the molecule is planar). Place the model on the bench and write the structural formula (using chemical symbols) for the molecule you have just made in the space below. Is this the *cis*- or *trans*- isomer of 2-butene? ______________

7. Now make the other structural isomer (*cis*- or *trans*-) of 2-butene.
Does it look different from the model you made in step 6? (Yes or no) _______
Place the model on the bench and write the structural formula (using chemical symbols) for the molecule in the space below.

Part C. Alkanes vs Cycloalkanes

8. Make a continuous chain (no branching, no double bonds) of six C atoms and make the model of the saturated hydrocarbon by filling all the remaining holes with bonds (rigid pegs) to H atoms.

What is the name of this molecule? ___________________________________
Notice you can now rotate the molecule about all of the C-C bonds to form many different shapes.

Do the different shapes result in different molecules or different isomers? (yes or no) _________

Have you broken any bonds when you rotate about C-C bonds to give different shapes? ______
Draw structural diagrams for at least four of the possible **structural isomers** of hexane below.

9. Remove one H atom (white ball only) from C1 and remove one H atom (with its bond) from C6 of n-hexane and connect C1 to C6 with a single bond (light gray, rigid peg).

Write the chemical formula for this molecule. __________ Is this an isomer of n-hexane? ______

What is the name of this compound? _____________________________________

Is it possible to rotate the molecule about the C-C bonds? ______
Draw the structure for this molecule below using both the condensed structural formula and the line angle structural formula.