Molecular Models
Experiment #5

Molecular Models

Experiment #5

Objective: To become familiar with the 3-dimensional structure of molecules and their relationship to Lewis structures.

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. 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 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, hence the fourth hole in the blue ball to represent N. Oxygen may lose a proton in acids to form a negatively charged ion. 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. 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 make models of some simple molecules, such as water, methane, ammonia and carbon dioxide, in order to observe the 3-D structure. You will write the Lewis dot structures for these molecules to understand why they are considered polar or nonpolar molecules. You will also construct several different organic molecules and determine whether they should be polar or nonpolar. Polarity is an important concept to understand with regard to biological molecules and biological processes. Some of the organic molecules you make will have double bonds connecting the carbon atoms. In some cases, the double bonds may be designated *cis*- or *trans*- double bonds. You may be familiar with the term *trans* in relation to the types of double bonds in certain fatty acids of fats. You will also make models of cyclic hydrocarbons, including cyclohexane, cyclohexene and benzene. Benzene is classified as an aromatic hydrocarbon because of its alternating double bonds and single bonds in a cyclic structure. The hydrocarbons are nonpolar molecules that do not mix with or dissolve in water, which is a polar molecule. Polar and nonpolar molecules tend to repel one another (oil and water don't mix), whereas polar molecules will mix with other polar molecules and nonpolar molecules mix with other nonpolar molecules. These chemical properties are one of the foundations of living organisms and life.

Materials: Molecular model kits

Procedure

The procedure is described on the report sheet.

Name ___________________________________ Section ____________

Molecular Models

Experiment #5 **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, such as Lewis structures. For each of the following molecular formulas, write an appropriate Lewis structure for that molecule showing any nonbonding valence electrons. Indicate below each Lewis structure whether the molecule would be polar or nonpolar.

H_2O CH_4

NH_3 CH_3NH_2

3. Write the chemical structures for ethylene/ethene (C_2H_4) and acetylene/ethyne (C_2H_2) below, showing any double or triple bonds where appropriate and label each structure with its correct name.

Name ____________________________________ Section ____________

4. Draw the Lewis structures for ethane (C_2H_6), ethanol (C_2H_5OH) and acetic acid ($CH_3C(O)OH$), where -C(O)- is another way of writing C=O to form a carboxylic acid. Label each structure with its correct name.

5. Write the chemical structures for cyclohexane (C_6H_{12}) and benzene (C_6H_6) below and label each.

Name ___________________________________ Section ____________

Molecular Models
Experiment #5 **Data & Report Sheet**

Part A. Structures of some simple molecules

1. Make a model of a water molecule using one red ball and attaching two white balls to it using the rigid gray pegs. Draw a diagram of the molecule model you have just made below on the left and write a Lewis structure for the molecule on the right, including the nonbonding electron pairs.

2. Do you expect water to be a polar or a nonpolar molecule, based on the structure?___________ Explain your answer.

3. Make a model of an ammonia molecule using one blue ball and attaching three white balls to it using the rigid gray pegs. Draw a diagram of the model and a Lewis structure of ammonia below.

4. Do you expect ammonia to be a polar or a nonpolar molecule, based on the structure? ________ Explain your answer.

5. Make a model of a methane molecule using one black ball and attaching four white balls to it using the rigid gray pegs. Draw a diagram of the model and a Lewis structure of methane below.

Name ___________________________________ Section ____________

6. Do you expect methane to be a polar or a nonpolar molecule, based on the structure? _________
Explain your answer.

7. Make a model of carbon dioxide (CO_2) by inserting 4 flexible gray pegs into the 4 holes of a C atom (black ball). Attach an O atom (red ball with 2 holes) to two of the flexible pegs in the C atom forming a double bond between C and O. Attach another O atom to the remaining two flexible pegs of the C atom to form another double bond between C and the second O.

   Do carbon and oxygen have the appropriate number of bonds for each? _______________

8. Draw a diagram of the model below on the left and a Lewis structure below on the right.

9. Are there any nonbonding pairs of electrons in the CO_2 molecule (yes or no)? _____________

10. Is carbon dioxide a polar or a nonpolar molecule? ____________________
Explain your answer.

B. Saturated vs unsaturated hydrocarbons

1. Make a model of butane (C_4H_{10}) by connecting 4 black balls together with 3 rigid gray pegs. Fill all the holes with rigid gray pegs and place white balls on each one. Count the carbon and hydrogen atoms in the model to make sure it is complete. Notice that the model is somewhat flexible and you can rotate around the C-C bonds to get different shapes. Draw at least two diagrams that illustrate the different shapes, such as a linear zig-zag shape (\/\) or a more or less ⊔ shape.

Name ____________________________________ Section ____________

2. Do you expect butane to be a polar or a nonpolar molecule, based on the structure? _________ Explain your answer.

3. Remove the rigid gray peg connecting the second C atom to the third C atom of butane and replace it with a flexible gray peg. Remove one H atom from the second C atom and one H atom from the third C atom and fill those holes with a second flexible gray peg. You should now have a double bond connecting the second and third C atoms. This molecule is called 2-**butene** (the 2- designates a double bond beginning at C number two of the molecule and the *-ene* ending indicates a C=C double bond). Can you make different shapes of the molecule by rotating around the C=C (double bond)? Draw a diagram of this model of 2-butene below on the left.

4. Remove a CH_3 group from one end of the 2-butene molecule and move the H atom on that same C to the hole where the CH_3 group was and place the CH_3 group where the H atom was.

5. Is the shape of the molecule any different? (yes or no)

6. Can you rotate the molecule around the C=C (double bond)? (yes or no)

7. Draw a diagram of this model of 2-butene above step 4 on the right. If the H atoms on the second and third C atoms of 2-butene are on the same side of the plane of the double bond, this would be a *cis*- double bond and the molecule is called *cis*-2-butene. If the H atoms on the second and third C atoms are on opposite sides of the plane of the double bond (across the plane) it is a *trans*- double bond and the molecule is *trans*-2-butene. Write the appropriate name for each of the structures of 2-butene below the diagrams you have drawn above.

Name ___________________________________ Section ____________

C. Organic functional groups

1. Make models of the following organic compounds, draw a diagram of the molecular model for each below and show the chemical structure for each next to it. Name each structure and indicate whether it is a polar or nonpolar molecule. The compounds are: ethane (C_2H_6), ethanol (C_2H_5OH), ethanamine ($C_2H_5NH_2$), ethanal ($CH_3C(O)H$, acetaldehyde), and ethanoic acid ($CH_3C(O)OH$, acetic acid). All of these have 2 C atoms. [Remember -C(O) is -C=O)]

Name ___________________________________ Section ____________

D. Cyclic hydrocarbons

1. Connect 6 carbon atoms (black balls) together with rigid gray pegs and connect the first and last C atoms to one another with a rigid gray peg. Fill any empty holes in the C atoms with rigid gray pegs and add H atoms (white balls) to each of them. Write a chemical structural formula, showing all H atoms for cyclohexane below on the left above its name.

   Can you rotate the molecule around the C-C bonds to form a different shape? ___________

Cyclohexane Cyclohexene

2. Remove a rigid gray peg connecting two C atoms of cyclohexane and replace it with a flexible gray peg. Remove one H atom from a C on each side of the flexible peg and fill the holes with another flexible peg to make a double bond connecting those two C atoms. This molecule is **cyclohexene**, where the -ene ending means there is a C=C double bond. Write a chemical structural formula showing all H atoms for cyclohexene above on the right above its name.

3. Are either of these structures polar molecules? ____________

4. Leave a rigid gray peg connecting the C atoms that have a double bond between them to their next neighboring C atoms and remove two rigid gray pegs from the second C atom away from each side of the double bond. Form double bonds that are alternating with single bonds around the cyclic structure. You should finish with six C atoms forming a ring and each C atom has a single bond to another C atom on one side of it and a double bond to a C atom on the other side of it, resulting in 3 double bonds and 3 single bonds going around the ring with each double bond having a single bond on either side of it. The compound you have formed is **benzene**. Write the chemical structural formula showing all H atoms for benzene on the next page above its name.

   Is benzene a polar or a nonpolar molecule? __________________

Name ___________________________________ Section ____________

Benzene