MOLECULAR MODELS: CHEMICAL BONDING AND SHAPE

INTRODUCTION

The properties of chemical compounds are directly related to the ways in which atoms are bonded together into molecules. Chapter 1 in Klein's Organic Chemistry presents the basic ideas of chemical bonding, while Chapter 2 shows how organic chemists represent molecular structures. In this exercise, you will have the opportunity to visualize molecular structures by constructing simple ball-and stick models for some common organic molecules. The models should help your understanding of atom arrangements in molecules and the resulting shapes of the molecules. You will investigate a number of small molecules containing carbon, nitrogen, oxygen and hydrogen. These are mostly substances that are discussed in Chapters 1, 2, and 3 of *Organic Chemistry* by David Klein. In the process of doing this exercise you will see how "models" become very useful to chemists in understanding and predicting chemical properties.

BACKGROUND INFORMATION: ELECTRONS AND MOLECULES

A **single bond** consists of one shared pair of electrons; a **double bond** is two shared pairs (i.e., 4 electrons), and a **triple bond** is three shared pairs (6 electrons). On paper the bonds are represented by single, double, or triple lines, respectively (-, =, ≡). In model kits, straight sticks represent single bonds, while pairs or triplets of curved sticks or springs represent double and triple bonds. Electrons not involved in bonding are termed *unshared electrons*.

An important part of this exercise involves identifying the *3-dimensional shapes* of molecules. (Molecular shapes are discussed in the text in Chapter 5 of Klein's.) Molecules have certain shapes depending on their component atoms and the ways in which they are bonded to each other. The important shapes encountered in this exercise are *linear, trigonal planar, or tetrahedral*. Several factors contribute to determining molecular shape: (1) Electron pairs (both shared and unshared) try to keep as far away from each other as possible, while still remaining "attached" to atoms. (After all, they are all negatively charged and electrical charges of the same type will repel each other.) (2) Electron pairs tend to be symmetrically arranged around each atom in a 3-dimensiional manner. (3) Electron pairs *not* involved in the bonding ("unshared pairs" or "lone pairs") are as important as bonding electron pairs (shared pairs) in determining the overall molecular shape and arrangement of atoms.

MODEL BUILDING BASICS

Molecular model kits vary; therefore, your instructor will explain the particular models that

you will use. The kit probably contains balls (used for atoms), sticks (for single bonds and unshared electron pairs), and springs or curved sticks (for double and triple bonds). Each stick or spring represents two electrons. Hydrogen atoms are usually represented by small light-colored balls (yellow, white, or pale blue) that have only one hole. The color code for other atoms will vary. A common set of colors is shown in the table on the next page.

Typical Color Code for Molecular Model Sets

Atom	Color
Hydrogen	White
Carbon	Black
Nitrogen	Blue
Oxygen	Red
Fluorine	Green
Chlorine	Purple or Orange
Sulfur	Blue

THE ASSIGNMENT

1. Each pair of students should have a model kit. First, get acquainted with the components of the kit. Note the holes in the various colored balls and their positions. If there are two lengths of sticks, the shorter gray ones are for single bonds. The longer, flexible gray ones are for double and triple bonds.
2. Build models for each of the molecules listed on the data sheet.
    a. Gather the kind and number of atoms required. (For example, to make the CH_4 molecule you will need one black ball and four white ones.)
    b. To determine how many sticks (pairs of electrons) you will need, refer to your Lewis structure and notice if the bonds are single, double, or triple.
    c. Assemble the model by connecting the balls and sticks to match the arrangement in your Lewis structure.
3. Use the models to fill in the information in the last column "Geometry". You should take time to think about (and write down in words and a diagram) the shape of each molecule before proceeding to the next one. If you have questions, ask your instructor or teaching assistant for help.
4. Save each model for reference (until you've completed the assignment.) When you're done with them, dissemble the models and return the pieces to the kit.

Question to be Answered After Completing the Models

The tetrahedral shape is one of the most fundamental shapes in chemical compounds. How would you describe it in words to someone who has not seen it?

Name _____ Date_____
Partner _____ Section _____

Data Sheet- Molecular Models

Molecule	**Classification** (1) linear (2) branched (3) cyclic	**Hybridization of carbons** (1) Sp3 (2) Sp2 (3) Sp	**Geometry of the Atoms** (1) linear (2) trigonal planar (3) tetrahedral
Butane $CH_3CH_2CH_2CH_3$			
2-Methylpropane $CH_3CH(CH_3)_2$			
1-Butene $CH_2=CHCH_2CH_3$			
2-Methylpropene $CH_2=C(CH_3)_2$			
Cyclopropane $(CH_2)_3$			
Cyclohexane $(CH_2)_6$			
1-Butyne $HC\equiv CCH_2CH_3$			

Name _____ Date _____
Partner _____ Section _____

Data Sheet- Molecular Models (cont.)

Molecule	**Classification** (1) linear (2) branched (3) cyclic	**Hybridization of carbons** (1) Sp3 (2) Sp2 (3) Sp	**Sketch of the model** (1) linear (2) trigonal planar (3) tetrahedral
Cis-2-butene			
Trans-2-butene			
Cis-1,2-dimethyl-cyclobutane			
Trans-1,2-dimethyl-cyclobutane			
Cyclohexane			
Cis-1,2-Dimethyl-cyclohexane			
Trans-1,2-Dimethyl-cyclohexane			