9B Model Building with Covalent Molecules

The most common way that chemists represent structures of covalent molecules is in two dimensions. This is because of the need to show them on paper or another flat surface. There are two main methods for showing molecular structure in two dimensions. These are the electron-dot (Lewis) formula and the structural formula. The electron-dot formula shows a covalent bond as a pair of dots representing the two electrons in the bond, whereas the structural formula shows the covalent bond as a straight line joining the two atoms.

In order to understand the three-dimensional nature of a compound, we need to make a model and there are a number of different types that can be used. A ball-and-stick model shows the spatial arrangement of the atoms and the angles between the bonds. If a spring is used instead of a stick, this enables the stretching and bending of the bond to be visualized as well. The advantage of both of these is that the models can be easily taken apart and reassembled into other molecules. However, neither of these makes any attempt to show the relative sizes of the atoms. A space-filling model can show the relative sizes as well as the orientation of the atoms. Increasingly in recent years, chemists have been making excellent use of the advances in computer graphics technologies, to make computer simulations of the structure of many molecules. This is especially true with the very complicated three-dimensional structures of biological molecules such as proteins and deoxyribonucleic acid (DNA).

In making models in this experiment, you need to be aware that atoms which require more than one bond will sometimes have double or triple bonds between two atoms. In addition, sometimes molecular formulas may have a number of different structural formulas called isomers which represent completely different compounds. As an example, C_2H_6O is the molecular formula for both ethyl alcohol (ethanol) and dimethyl ether, which belong to two completely different classes of compounds.

OBJECTIVES

1. to construct molecular models of some simple and more complicated molecules, in order to visualize their shape
2. to construct all possible structures for some molecules that have different structural isomers
3. to draw structural formulas for all the molecules studied

SUPPLIES

Equipment
molecular model kit

PROCEDURE

1. Obtain a molecular model kit and separate the atoms by color. Using the chart below, decide which color to represent each atom by. Record them in your notebook.

Atom	Nnumber of Bonding Sites (Holes or Extensions)
hydrogen fluorine chlorine bromine iodine	1
oxygen sulfur	2
nitrogen phosphorus	3
carbon silicon	4

2. Make models of the following molecules. There is only one structural formula for each one. If you think you have another structure, try rotating the molecule to various different positions and you will find it is not in fact new. Sketch the structure of each model in your notebook.
   a. water H_2O
   b. methane CH_4
   c. methanol CH_4O
   d. ethane C_2H_6
   e. silicon tetrachloride $SiCl_4$
   f. ammonia NH_3
   g. hydrazine N_2H_4
   h. hydrogen sulfide H_2S
3. For the following molecular formulas there are two or more arrangements of the atoms. For each one, try to find all the different structural isomers that exist. Draw the structural formula for each isomer in your notebook.
   a. C_4H_{10}
   b. C_3H_8O
   c. $C_2H_4Br_2$
   d. $C_2H_3Cl_2Br$

4. Elements that have two or more bonding sites can sometimes form double or triple bonds. All the following molecules contain one or more double or triple bonds in their structure. Make a model of each and draw the structural formula in your notebook.
   a. carbon dioxide CO_2
   b. nitrogen N_2
   c. oxygen O_2
   d. ethene (ethylene) C_2H_4
   e. ethyne (acetylene) C_2H_2
   f. hydrogen cyanide HCN
   g. carbon disulfide CS_2
   h. methanal (formaldehyde) CH_2O

5. If you still have time available your instructor may suggest other molecules for you to try. Draw their structural formulas in your notebook.

POST LAB CONSIDERATIONS

Using models is a great aid in enabling you to visualize molecules in three dimensions. Often when using a two-dimensional representation it may appear that there are several possible structures for a molecule. However, when using a model that can be turned upside-down, end-over-end, or viewed from the opposite side, it soon becomes apparent that seemingly different structures are in fact identical. Models will be very useful later in your studies when you must learn how to name structures, especially the many possible structures of compounds of carbon (called organic compounds). When there are four single bonds attached to a carbon atom, the bonds arrange themselves as far away from one another a possible, in what is called a tetrahedral arrangement. The angle between adjacent bonds is 109.5°. For simplicity, single bonds in carbon compounds (especially larger ones) are often shown as though the molecule has been squashed flat. See Figure 9B-1(a) for an example, using carbon tetrafluoride, CF_4. Here, the bond angles appear to be 90°, but it is understood that they are at 109.5°. Diagrams like this are still very useful because they still indicate how the atoms are connected in the molecule. If an attempt at a three-dimensional diagram is required, it can be done as shown in Figure 9B-1(b):

Figure 9B-1 *Structural Formulas for CF_4.*
(a) two-dimensional
(b) three-dimensional

In the three-dimensional diagram, the ordinary line represents a bond in the plane of the paper, the solid wedge represents a bond coming forward from the plane of the paper, and the broken wedge represents a bond going backwards behind the plane of the paper.

EXPERIMENTAL RESULTS

Your observations in this experiment may be recorded in table form. However, it will be difficult to prepare the table for Procedure 3 in advance as you do not know how many structures there are for each substance. Just list the compound and then draw all of the structures you find for that compound.

ANALYSIS OF RESULTS

1. How many different structures did you write for (a) C_4H_{10} (b) C_3H_8O (c) $C_2H_4Br_2$ (d) $C_2H_3Cl_2Br$?
2. The class of carbon compounds that contain the hydroxyl group (O directly attached to H, –O–H) is called the alcohols. Review the structures that you sketched for C_3H_8O. How many have a hydroxyl group? (These are isomers of the alcohol propanol.) Any structures remaining are not alcohols and belong to a completely different class of compound. How many do you have?

FOLLOW-UP QUESTIONS

Using your new understanding of bonding and structural formulas, draw structural formulas for the following:

1. Br_2
2. HCl
3. H_2O_2
4. C_3H_6
5. Si_2H_6
6. S_2Cl_2

CONCLUSION

What is the advantage of representing molecules by means of three-dimensional models?