BUILDING MOLECULAR MODELS

LAB MOLECULAR GEOMETRY 1

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INTRODUCTION

Most molecules in this activity obey the octet rule. Their Lewis-dot structures are straightforward. Recall that to draw the Lewis-dot structure of a molecule obeying the octet rule, eight electrons on each atom (except hydrogen and a few others) are arranged in four pairs. Each pair either participates in a covalent bond or is present as a lone pair. Some molecules may have an odd number of valence electrons or may have more than four pairs on the central atom. If any of these are encountered, your teacher will provide the necessary information.

According to the electron pair repulsion rule, the regions of high electron density (two, three, or four electron pairs) around an atom move as far apart as possible without leaving the atom. Double and triple covalent bonds are treated as a single electron pair or region of high electron density determing molecular shape. Lone pairs are considered when determing electron distribution, but only the geometric distribution of atoms dictates molecular shape.

When four electron pairs around a central atom form single bonds, the pairs can be arranged tetrahedrally. This arrangement assures that the electron pairs are as far apart as possible, satisfying the pair repulsion rule. Three electron pairs can be arranged to form a triangular plane, two to form a straight line, *etc.*

Molecular shape is determined by the positions of the atoms in a molecule, not the electrons. For a central atom with four tetrahedrally arranged electron pairs, bonding to four other atoms will yield a molecule with tetrahedral geometry; bonding to three other atoms results in a triangular pyramid with one lone pair, and bonding to two other atoms yields a bent shape with two lone pairs.

The following table summarizes these ideas.

Electron pairs	Bond pairs	Lone pairs	Example	Angle	Shape
4	4	0	CCl_4	109.5°	Tetrahedral
4	3	1	PCl_3	$<109.5^\circ$	Pyramidal
4	2	2	SCl_2	$<109.5^\circ$	Bent
3	3	0	BCl_3	120°	Triangular
3	2	1	$SnCl_2$	$<120^\circ$	Bent
2	2	0	$BeCl_2$	180°	Linear

Remember that the "repulsive effect" of a double or triple bond is counted the same as that of a single electron pair.

Knowing the geometry of a molecule allows one to predict whether it is polar or nonpolar. A bond between unlike atoms is usually polar with a positive end and a negative end. The symmetry of the molecule determines polarity. Formal rules are available for this determination, but the easiest way for beginning chemistry students is to decide whether each polar bond is countered by another identical bond in the molecule.

A diatomic molecule containing two different atoms is polar. Examples are HF, CO, and ICl. N_2 and O_2 are nonpolar since both ends of the molecules are equivalent. A polyatomic molecule may be nonpolar even if it contains polar bonds because, in such cases, the polar bonds are counteracting each other. CO_2 and CH_4 are nonpolar because of this geometric (symmetrical arrangement) effect.

Ball-and-stick models will be used to represent the shapes of molecules in this activity. Several molecular models will be built. The molecular formulas, the Lewis-dot structures, sketches of the molecules, the names of the molecular shapes, the approximate bond angles, and the polarities will be recorded in a data table.

Purpose

To predict shapes, bond angles, and polarities of some molecules and to build models of these molecules confirming the predictions.

Safety

There are no unusual hazards in this activity.

Materials

1 Molecular Visions Molecular Model Kit

Procedure

1. Construct a data table having eight columns with headings as follows: molecular formula, Lewis-dot structure, number of bond pairs, number of lone pairs, molecule sketch, molecular shape, bond angle, and polarity. Use the page's long axis for the column labels. Record data for each of the assigned molecules in the data table as the procedure is followed.

2. Write the molecular formula, and draw the Lewis-dot structure for each of the following molecules: CH_4, H_3O^+, N_2, C_2H_2, CH_2Cl_2, HF, Cl_2, SO_2, CH_4O, NH_3, C_2H_4, SO_4^{2-}, H_2, H_2O_2, CH_2O, CO_2.

   The formula should be in the first column and the Lewis-dot structure in the second column.

3. Using ball-and-stick models, build a model for each of the assigned molecules after completing Step 2 above. After completing each model, take it to your teacher to be checked. Draw a sketch of each model as soon as it is checked; then complete the remaining five entries in the data table.

4. After completing your table, your teacher will give you formulas for two unfamiliar molecules. Predict the shape, bond angle, and polarity after recording the formula and the Lewis-dot structure. Take your data table to your teacher to be initialed.
5. After your teacher has initialed your predictions, build the models to confirm them.
6. Return the model sets as your teacher directs.

Data Analysis

1. Did your prediction of the geometry of the unknowns prove valid? Why or why not?
2. Did your prediction of the polarity of the unknowns prove valid? Why or why not?

Implications and Applications

1. CO_2 is nonpolar, but SO_2 is polar. Explain.
2. Describe the electronic similarities between NH_3 and H_3O^+. These species are called isoelectronic. Why?
3. Using your data table try to write some rules of thumb that would allow predictions of molecular geometry. These rules of thumb are generalizations and should include the total number of electron pairs, the number of bonding pairs, and the number of lone pairs on the central atom. Develop a table having columns containing number of electron pairs, number of bond pairs, number of lone pairs, molecular shape, and an example. The table should summarize the rules of thumb.
4. Develop some rules of thumb to help with determining molecular polarity. These rules should be in terms of the shape of the molecule and the kinds of atoms bonded to the central atom (all alike or some different, *etc.*).
5. Relate the Lewis-dot structure to the geometry of molecules.

Reference

Doing Chemistry. (1988). Washington, DC: American Chemical Society.