Lab 2: Molecular Models

Objectives: To practice drawing Lewis Dot Structures, to apply VSEPR theory to predict molecular geometry, and to build models of the structures and compare them to the theoretical predictions.

Materials: Molecular model kit including units for 5 electron pairs (trigonal bipyramidal) and 6 electron pairs (octahedral).

INTRODUCTION

The physical and chemical behavior of compounds depends on the types of bonds that exist within the molecule and on the overall shape of the molecules. The branch of chemistry that investigates how molecules are put together is called Structural Chemistry. Analytical techniques such as x-ray crystallography and mass spectrometry can help verify the structure and geometry of a molecule.

Gilbert N. Lewis was one of the more prolific chemists of the twentieth century, with contributions ranging from thermodynamics to acid-base theory. He is best known, at least to chemistry students, for his work dealing with the electronic structure of molecules including Lewis dot structures and the "rule of eight," or octet rule. The Lewis dot structure is elegant in its simplicity—it uses dots to represent valence electrons—but it provides us with a model to predict the type of bonding present in molecules. Knowledge of the bonding and shape of molecules is needed to explain the physical properties of molecules and how they react.

In this lab exercise you will draw Lewis dot structures of a wide variety of molecules and build three dimensional molecular models to determine the shape of the molecules using Valence Shell Electron Pair Repulsion Theory (VSEPR).

Lewis Dot Structures

A Lewis dot structure is a two-dimensional sketch of a molecule that uses dots to represent valence electrons. The Lewis dot structure helps us identify the type of bonding that may be present in a molecule based on the number of valence electrons available and the octet rule. The **octet rule** states that atoms will gain, lose, or share electrons to attain a completely filled valence shell electron configuration (i.e., eight electrons). In molecular compounds, this is accomplished by sharing electrons to form covalent bonds.

Lewis dot structures for most molecules can be drawn by following a simple strategy:

1. *Determine the total number of valence electrons in the molecule or polyatomic ion.* Simply add up the number of valence electrons for each atom in the molecular formula, based on electronic configuration. For polyatomic ions, add an electron for each negative charge and subtract one electron for each positive charge.
2. *Draw a skeleton structure for the molecule.* Connect the atoms using single lines to represent a covalent bond. Usually, the least electronegative element is the central atom. Hydrogen is always on the outside since it can only form one bond. Halogens are often on the outside as well but can be in the center if paired with a more electronegative atom such as oxygen.
3. *Calculate the number of remaining electrons.* Subtract the number of electrons involved in covalent bonding from the total valence electrons in the molecule.
4. *Distribute the remaining electrons.* Typically, these electrons are distributed around the outside atoms until each atom has a complete octet, and then any remaining electrons are placed on the central atom(s).
5. *If you run out of electrons before every atom has a complete octet, form multiple bonds.* Use pairs of non-bonding electrons from an outside atom to form double or triple bonds until each atom has a complete octet.

There are many exceptions to the octet rule. Beryllium and boron, for example, only have two and three valence electrons to share, respectively. As a result, these elements form compounds in which the Be or B atom has less than eight valence electrons. Elements in the third rows and higher ($n \geq 3$) can often form compounds in which the central atom has an **expanded octet**; because these elements have empty *d*-orbitals available, they can accommodate more than eight electrons in their valence shell.

Valence Shell Electron Pair Repulsion Theory (VSEPR)

Many chemical and physical properties depend on molecular shape or geometry. The Lewis dot structure can show us the basic structure in two dimensions, but it cannot tell us the shape of the molecule. The three-dimensional arrangement of bonding and non-bonding electron pairs can be predicted using VSEPR theory. The basis for VSEPR theory is that negatively charged electron clouds (i.e., bonding and non-bonding e^- pairs) will arrange themselves around the central atom in order to minimize repulsive energies. In VSEPR, the electrons in a covalent bond count as one pair, regardless of whether it is a single, double, or triple bond. This makes sense, given that all the electrons in these covalent bonds are essentially oriented between the two atoms involved in the covalent bond. Non-bonding e^- pairs also count as an electron cloud.

The geometric orientation of electron clouds will depend on the number of electron clouds around the central atom. Two electron clouds, for example, will arrange themselves on opposite sides of the atom to form a linear geometry. Three electron clouds will form a triangular or trigonal planar configuration. Four electron clouds will assume a tetrahedral configuration. **Molecular geometry**, however, depends only on the arrangement of bonding electron clouds and may be different from the electronic geometry. Molecular geometries based on VSEPR theory are summarized in Figure 2.1.

There is a difference, however, between the **molecular geometry** and the **electron pair geometry**. The electron pair geometry is determined by the total number of electron clouds (i.e., bonds or non-bonding e^- pairs) and how they are arranged according to VSEPR theory to

minimize repulsive energies. The molecular geometry is determined only by the arrangement of bonding electrons around the central atom. This difference can be seen in Figure 2.1. For example, four electron clouds will result in a tetrahedral electron cloud geometry (column 1). If all four electron clouds involve bonding electrons, then the molecular geometry is also tetrahedral. When one of the bonding electron clouds is replaced by a non-bonding e^- pair (column 2), the molecular geometry becomes trigonal pyramidal. Replacement of additional bonding electrons with non-bonding e^- pairs results in bent (two non-bonding e^- pairs) or linear (three non-bonding e^- pairs) respectively.

These concepts are illustrated in the example below.

Example BH_3 and NH_3 both have the general formula AB_3, yet they have very different shapes and properties. Explain these facts by determining the molecular shapes.

Solution: *Details are provided in the table below.*

Molecule	**Total Valence Electrons**	**Bonding e^- Pairs**	**Non-Bonding e^- Pairs**	**Molecular Shape (From Fig. 2.1)**
*BH_3	B = 3; 3H = 3; total = 6	3	0	Trigonal planar
NH_3	N = 5; 3H = 3, total = 8	3	1	Trigonal pyramid

*Remember that boron compounds are often exceptions to the octet rule.

The purpose of this lab exercise is to provide practice in drawing Lewis Dot Structures and to observe how these dot structures translate into three-dimensional structures by constructing molecular models. Seeing the molecular geometry will help you understand the physical properties of these molecules, such as whether they are polar or non-polar.

# Of electron clouds		1 non-bonding e⁻ pair	2 non-bonding e⁻ pair	3 non-bonding e⁻ pair
2	Linear	Linear with atom-atom electron group		
3	Trigonal planar	Angular or bent	Linear (with two electron groups)	
4	Tetrahedral	Trigonal pyramidal	Angular or bent (with two electron groups)	Linear (with three electron groups)
5	Trigonal bipyramidal	See-saw	T-shaped	Linear (with three electron groups)
6	Octahedral	Square pyramid	Square planar	

Figure 2.1. Electron cloud geometries based on VSEPR theory (Column 1) for 2, 3, 4, 5, and 6 electron clouds. Columns 2, 3, and 4 show molecular geometries when bonding electron clouds are replaced by non-bonding lone e^- pairs.

Pre-Lab Questions

1. What does the acronym *VSEPR* represent, and how is this model useful in predicting molecular geometry?

2. What is the *octet rule*, and how is it useful in drawing Lewis Dot Structures?

3. List two common exceptions to the octet rule and provide an example of each.

4. Draw the Lewis Dot Structures for CS_2 and $SiCl_4$. Use VSEPR rules to predict the geometry of each molecule.

PROCEDURE

The model kits have color-coded atom centers with pegs to represent electron pairs arranged in the more common geometries. The contents of your model kit are listed below, including color codes for specific atoms and the types of connectors used to represent bonds.

Black = Carbon (4-bond center)
Red = Oxygen (2-bond center)
Light purple = Phosphorus (5-bond center)
Orange= Fluorine (1-bond center)
Dark blue= Bromine (5-bond center)
Gray = Variable (3-bond and 6-bond centers)
White plastic connector = single bonds

White = Hydrogen (1-bond center)
Blue = Nitrogen (3-bond center)
Dark purple = Iodine (5-bond centers)
Green = Chlorine (1-bond center)
Yellow = Sulfur (6-bond center)
Light blue flexible connector = multiple bonds

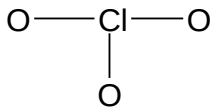
Assemble into groups as directed by the instructor. You may need to share modeling kits or to share/trade pieces with your neighbors in order to complete all the models in the assignment. Take the time to construct models of <u>all</u> the molecules assigned and have them inspected by your lab instructor.

First, draw Lewis Dot Structures for each molecule. A step-by-step method has been provided here. You may wish to use the instructions in your textbook or to follow an alternative method if provided by your instructor.

1. Calculate the total number of valence electrons in the molecule or ion based on the number and location of the individual atoms in the periodic table. For a polyatomic ion, be sure to add or subtract the appropriate number of electrons based on the ionic charge. For example, the polyatomic ion ClO_3^- (chlorate) has 26 valence electrons as demonstrated below:

   # valence electrons = 7 (for chlorine) + [3 x 6 (for 3 oxygens)] + 1 (for ionic charge)
   = 7 + 18 + 1 = 26 total valence electrons

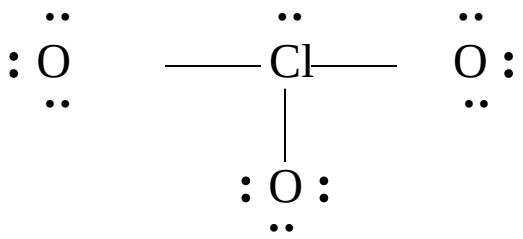
2. Decide how the atoms are connected, and draw single lines between the central atom and the outer atoms to represent covalent single bonds:



3. Determine the number of valence electrons remaining by subtracting the number of bonding electrons (2 per single bond) from the total valence electrons.

   26 total valence electrons – 6 electrons (in 3 covalent bonds) = 20 e^- remaining

4. Starting with the outer atoms, distribute the remaining electrons as lone pairs (non-bonding e^- pair) until each atom satisfies the octet rule. In other words, each atom will have eight electrons (except H, which gets only two).



5. From the remaining number of electrons, subtract the number of electrons distributed as lone pairs. Ideally, there will be none left over. If there <u>are</u> electrons left over, place them on an atom that can accommodate an *expanded octet* (i.e., a third-row element such as sulfur or phosphorus).

    20 remaining electrons – 10 x 2 (for 10 lone pairs) = 0 electrons left over

6. If all the remaining electrons have been distributed and there are still atoms that do not have a complete octet, you can use lone pairs of electrons to make multiple bonds. For example, if you are 2 electrons short of a complete octet, make a double bond; if you are 4 electrons short, make a triple bond. Keep in mind that you can only form multiple bonds to atoms that will form more than one bond; hydrogen, for example, will only form one bond. As a general rule you will never place multiple bonds on a halogen.

Once Lewis Dot Structures are constructed, use the VSEPR model to predict the geometry (i.e., the orientation of electron charge clouds) around the central atom, using the following method.

1. Count the total number of electron clouds (i.e., bonds and lone pairs) around the central atom.

2. The *electron pair geometry* (i.e., the orientation of electron clouds) is determined based on the number of the electron clouds identified in step one. Refer to column 1 in Figure 2.1.

3. The *molecular geometry* is based on the orientation of <u>atoms</u> in the molecule. In this case, we are only interested in the bonding electron clouds and can ignore the non-bonding electron pairs. As an example, the ClO_3^- ion presented previously included four electron clouds around the central Cl atom (3 bonds + 1 lone pair). The electronic geometry, therefore, is tetrahedral. Ignoring the lone pair, we see that the molecular geometry is trigonal pyramidal. Molecular geometries can be determined from columns 2, 3, and 4 in Figure 2.1.

Use pencil to draw your structures so corrections can be accomplished easily as needed.

Molecular Models
Data Sheets

Black = C Blue = N Yellow = S Red = O
White = H Green = Cl Orange = F

Geometry. Draw Lewis Dot Structures for each of the molecules listed and then draw the structures, indicating the geometry as accurately as you can. Describe the correct geometry around the central atom.

Molecule	**Lewis dot structure**	**Electron pair geometry**	**Molecular geometry**
NH_3			
CO_2			
CF_4			
BeF_2 (You may have to use a 6-bond center to obtain the correct geometry.)			

Molecular Models
Data Sheets

Molecule	Lewis dot structure	Electron pair geometry	Molecular geometry
O_3			
OCl_2			
BF_3 (Use the three-hole unit for B.)			
ClO_4^-			
PCl_5			

Molecular Models
Data Sheets

Molecule	Lewis dot structure	Electron pair geometry	Molecular geometry
SF_6			
ClF_3			
ClF_5			
XeF_4			
XeF_2			

Post-Lab Questions

1. What is special about the 5- and 6-coordinate geometries?

2. Draw the Lewis Dot Structure for SF_4. What is the electronic geometry? What is the molecular geometry?

3. Why is it difficult to construct a Lewis Dot Structure for the molecule NO?

4. The geometry that chemists call "octahedral" is sometimes called "square bipyramidal" by mineralogists. Explain why this is logical.

5. A general rule in Lewis Dot Structures is to avoid double bonds to halogens. Draw two different Lewis Dot Structures for the molecule BF_3—one that has only single bonds between B and F (in which the B is electron deficient), and one that contains a double bond between B and one of the F atoms. Explain why this rule is valid based on the electronegativity of the halogens.