MOLECULAR MODELS

OBJECTIVES

1. To learn to draw Lewis structures for common compounds
2. To identify electron pairs as bonding pairs or lone pairs
3. To use electron pair repulsion theory to predict electronic and molecular geometry

INTRODUCTION

Often in our attempts to comprehend bonding theory, we become so accustomed to pushing a pen across two dimensional paper that we forget that molecules are three dimensional. Molecules are made up of atoms occupying space in a definite pattern, which is quite often symmetrical and definitely three dimensional. In this experiment, we will attempt to overcome this tendency by using molecular models to represent our predictions of electronic and molecular geometry.

Lewis structures show the valence, or outer shell, electrons that are used to form bonds in a molecule or polyatomic ion. A **single bond** consists of one pair of electrons that is shared between two atoms. Two shared pairs of electrons form a **double bond**, and three shared pairs form a **triple bond**. Valence electrons that are not shared are called **nonbonding electrons** or **lone pairs**.

One method used to draw Lewis structures is called the "**N-A = S**" rule. It will be discussed further below. This method is very useful when working with compounds formed from the representative elements that follow the **octet rule,** including those normally encountered in Chemistry 105. There are exceptions to the octet rule, such as expanded octets, that you may encounter in other chemistry classes. The "**N-A = S**" rule will not work for these exceptions. There are also other methods that may be used to draw Lewis structures, but they all have the same goal: to obtain a valid structure.

A valid Lewis structure in conjunction with valence shell electron pair repulsion theory, or VSEPR, is used to predict the electronic and molecular shape around a central atom in a compound. VSEPR expands Lewis structures to a three-dimensional picture, using the simple concept that like charges repel each other. Therefore, electron regions around an atom will tend to separate as much as possible. A single, double, or triple bond each comprise one bonding region. Each lone pair of electrons comprises a separate region. Thus the number of bonding regions and lone pairs around each central atom determines the electronic and molecular geometry around that atom.

Before the LABORATORY REPORT section you will find a description of the "**N-A = S**" rule and a table describing the various geometries studied in this class.

To draw a Lewis structure:

1. Start with a "skeletal" structure for the molecule or polyatomic ion. First, pick the central atom. Usually the first atom in the formula is central, unless it is hydrogen. Surround the central atom with the other atoms. Hydrogens will always be on the outside. Molecules are usually symmetrical.
2. Find **N**, the total number of valence shell electrons needed by all the atoms in the molecule or polyatomic ion to obtain a noble gas configuration. **N** will be 2 for each hydrogen and 8 for each other type of atom. For the compounds covered in this laboratory,

N = 8 x number of elements other than hydrogen plus 2 x number of hydrogen atoms (1)

3. Find **A**, the total number of electrons available in the valence shells of all the atoms. For representative elements, the number of valence shell electrons is equal to the group number. For negative ions, add to **A** the number of electrons equal to the charge. For positive ions, subtract from **A** the number of electrons equal to the charge.

4. Find **S**, the total number of electrons shared.

N - **A** = **S**. (2)

5. Connect the atoms by placing the **S** electrons into the "skeletal" structure as shared pairs. **S**/2 will give you the number of bonds in the structure. Connect with single bonds first, forming double or triple bonds with the remaining **S** electrons only when it is necessary. Remember: Hydrogen can never have more than one bond, and halogens rarely do.

6. The remaining electrons (**A - S**) will be used as **lone pairs** to complete the octet of every representative element. Remember: Hydrogen will not have any lone pairs!

For example, for the compound CO_2:

Skeletal structure: O C O

Find **N**: **N** = 3 x 8 = 24

Find **A**: **A** = 4 + 6 + 6 = 16

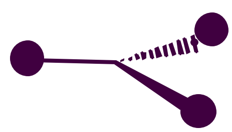
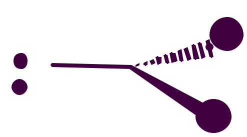
Find **S**: **N - A = S** = 24 - 16 = 8

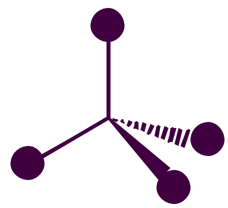
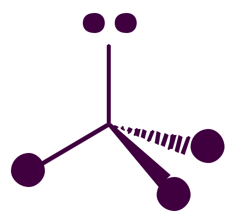
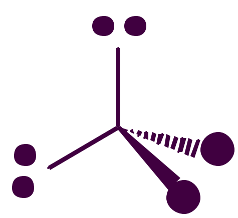
Thus there must be 4 bonds (8 shared electrons). O=C=O

Complete the octets with the remaining electrons. **A - S** = 16 - 8 = 8.

Thus there will be 4 lone pairs, and the correct Lewis structure for CO_2 is: O=C=O

ELECTRONIC AND MOLECULAR GEOMETRIES

Bonding Electron Regions	Lone Electron Pairs	VSEPR Model Arrangements	Examples
2	0	 Electronic Shape: Linear Molecular Shape: Linear	$BeCl_2$ CO_2
3	0	 Electronic Shape: Trigonal Planar Molecular Shape: Trigonal Planar	BCl_3 NO_3^-
2	1	 Electronic Shape: Trigonal Planar Molecular Shape: Angular	NO_2^- SO_2

Bonding Electron Regions	Lone Electron Pairs	VSEPR Model Arrangements	Examples
4	0	 Electronic Shape: Tetrahedral Molecular Shape: Tetrahedral	CCl_4 CH_4 SO_4^{-2} ClO_4^-
3	1	 Electronic Shape: Tetrahedral Molecular Shape: Trigonal Pyramid	NH_3 PCl_3
2	2	 Electronic Shape: Tetrahedral Molecular Shape: Angular	H_2O H_2S

Compound	Lewis Structure	Bonding Regions on Central Atom	Lone Pairs on Central Atom	Electronic Geometry on Central Atom	Molecular Geometry on Central Atom
H_2					
F_2					
H_2O					
N_2					

Compound	**Lewis Structure**	**Bonding Regions on Central Atom**	**Lone Pairs on Central Atom**	**Electronic Geometry on Central Atom**	**Molecular Geometry on Central Atom**
NH_3					
NH_4^+					
NO_2^-					
NO_3^-					

Compound	Lewis Structure	Bonding Regions on Central Atom	Lone Pairs on Central Atom	Electronic Geometry on *Central Atom	Molecular Geometry on *Central Atom
PCl_3					
C_2H_2					
* CH_3-O-CH_3					
* CH_3CH_2OH					