Lewis Structures and Molecular Shapes

Objectives

The objectives of this laboratory are to:

a) Practice drawing Lewis Structures for various covalently bonded molecules and polyatomic ions.
b) Use model kits to construct these molecules/ions in order to explore their structure and shapes.
c) Practice predicting molecular shapes (using VSEPR theory) and molecular polarity.

Background

Non-metal atoms bond covalently, resulting in the formation of either neutral molecules or polyatomic ions. A covalent bond is formed when non-metal atoms share their valence electrons, which they do in order to achieve filled valence orbitals like their nearest noble gas neighbor. This means that most bonded non-metal atoms will acquire a total of eight valence electrons via the sharing process – often referred to as the octet rule. A notable exception is hydrogen, which only needs to acquire two electrons to be like its nearest noble gas neighbor, helium.

Lewis Structures

A Lewis Structure is a representation of covalent molecules (or polyatomic ions) where all the valence electrons are shown distributed about the bonded atoms as either shared electron pairs (bond pairs) or unshared electron pairs (lone pairs). A shared pair of electrons is represented as a short line (a single bond). Sometimes atoms can share two pairs of electrons, represented by two short lines (a double bond). Atoms can even share three pairs of electrons, represented by three short lines (a triple bond). Pairs of dots are used to represent lone pair electrons.

Examples:

```
H   N   H
|   H

bond pair (2 e−)
single bond
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```
O—S—O

lone pair
2 bond pairs (4 e−)
double bond
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The rules for drawing Lewis structures can be found in the Procedure Section of this handout.
Molecular Shapes

The shape of a molecule depends on the distribution of atoms in space about the central atom, and their bond angles. Bond pair electrons and lone pair electrons repel one another, thus they will be arranged around a central atom as far apart as possible in order to minimize repulsions. This is known as Valence Shell Electron Pair Repulsion theory, or VSEPR theory.

The following VSEPR table shows the most common molecular shapes that you will encounter. More molecular geometries do exist; however, they are beyond the scope of this course.

<table>
<thead>
<tr>
<th>Shape Name</th>
<th>Sketch</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linear</td>
<td><img src="linear.png" alt="Linear Sketch" /></td>
<td>Only two outer atoms surround the central atom. There are no lone pairs on the central atom. Outer atoms are arranged opposite to each other. The bond angles are exactly 180°.</td>
</tr>
<tr>
<td>Trigonal Planar</td>
<td><img src="trigonal-planar.png" alt="Trigonal Planar Sketch" /></td>
<td>Three outer atoms surround the central atom. There are no lone pairs on the central atom. The central and outer atoms all lie in the same plane (molecule is flat). Bond angles are exactly 120°.</td>
</tr>
<tr>
<td>Bent</td>
<td><img src="bent.png" alt="Bent Sketch" /></td>
<td>Two outer atoms and one lone pair surround the central atom. Bond angles are slightly less than 120°.</td>
</tr>
<tr>
<td>Tetrahedral</td>
<td><img src="tetrahedral.png" alt="Tetrahedral Sketch" /></td>
<td>Four outer atoms surround the central atom. There are no lone pairs on the central atom. The four outer atoms are evenly arranged in 3D around the central atom as if at the corners of a regular tetrahedron. The bond angles are exactly 109.5°.</td>
</tr>
<tr>
<td>Trigonal Pyramidal</td>
<td><img src="trigonal-pyramidal.png" alt="Trigonal Pyramidal Sketch" /></td>
<td>Three outer atoms and one lone pair surround the central atom. Here the central atom is located slightly above the three outer atoms, like a tripod. The bond angles are slightly less than 109.5°.</td>
</tr>
<tr>
<td>Bent</td>
<td><img src="bent.png" alt="Bent Sketch" /></td>
<td>Two outer atoms and two lone pairs surround the central atom. Bond angles are slightly less than 109.5°.</td>
</tr>
</tbody>
</table>
Electronegativity and Bond Polarity

Some atoms in molecules have the ability to pull shared electrons closer to themselves than other atoms, an ability referred to as electronegativity. Electronegativity increases going across a period and decreases going down a group.

If two bonded atoms have different electronegativities, then the bond pair electrons will be unequally shared. The atom with the greater electronegativity will pull the bond electrons closer towards itself, causing it to obtain a very slight negative charge (δ-). The atom with the lower electronegativity will have bond electrons pulled further away from it, causing it to obtain a very slight positive charge (δ+). The result is a polar covalent bond. However, if two bonded atoms have the same electronegativity, then the bond pair electrons will be equally shared. The result is a non-polar covalent bond.

Example:

\[
\begin{align*}
\text{H} & \rightleftharpoons \text{Cl} \\
\delta^+ & \text{H} \longrightarrow \text{Cl} : \delta^-
\end{align*}
\]

is better represented as

because the bond electrons are pulled closer to Cl due to its greater electronegativity. Thus, HCl contains a polar covalent bond.

Molecular Polarity

Molecular polarity results when the entire molecule (not just a bond in the molecule) ends up with an unequal distribution of electrons. In general, a molecule will be polar if it contains polar bonds that are distributed in a non-symmetrical arrangement around the central atom. A polar molecule is said to have a net dipole moment. A non-symmetrical arrangement typically results when there are lone pairs on the central atom, or, when different outer atoms surround the central atom.

Not surprisingly, a molecule will be non-polar if it contains all non-polar bonds. It will also be non-polar if it contains polar bonds distributed in a symmetrical arrangement around the central atom. The symmetry causes the individual bond polarities to cancel out, resulting in a net non-polar molecule. A symmetrical arrangement typically results when there are no lone pairs on the central atom, and if all the outer atoms are identical.

Examples:

Non-Polar  

Polar  

Polar
Procedure

Drawing Lewis Structures

1. Draw Lewis structures for each of the molecules and polyatomic ions given on your Report Form. Clearly show all bond pair electrons as lines and lone pair electrons as pairs of dots.

Rules for Drawing Lewis Structures

1. Total the number of valence electrons that each atom contributes to the molecule/polyatomic ion.
   - The quickest way is to find the group number for each atom.
   - For polyatomic anions, you must add electrons (equal to the negative charge) to the total number of valence electrons. For polyatomic cations, you must subtract electrons (equal to the positive charge) from the total number of valence electrons.

2. Draw a stick structure for the molecule.
   - Most molecules/polyatomic ions consist of one central atom bonded to 2, 3 or 4 other atoms.
   - The least electronegative atom is the central atom. Hydrogen is the only exception to this, as it forms only 1 bond. The central atom will usually need to form multiple bonds.
   - The other atoms are arranged around the central atom, and are attached to it via single bonds.

3. The octet rule must be obeyed for all elements except hydrogen (follows a “duet” rule).
   - Each bond in the stick structure contains two electrons, which must be subtracted from the total number of valence electrons.
   - Starting with the outside atoms, place the remaining electrons around each atom until it has a total of 8 electrons (except hydrogen – it only requires 2 electrons).
   - If there are not enough electrons available to obey the octet rule using single bonds, this indicates that double or triple bonds between two atoms are required in your structure. If short by two electrons, try a double bond, and if short by four electrons, try a triple bond or two double bonds.

Constructing Models, Determining Molecular Shapes and Molecular Polarity

1. Use your molecular model kit to construct a three-dimensional model of each of these molecules and polyatomic ions. Sketch a reasonably detailed picture of this model on your Report Form.

Rules for Constructing Molecules with the Model Kit

1. Each colored ball in your kit corresponds to different atom or different group of atoms. Refer to the inside of the container lid for the correct color key.

2. Use the short sticks for single bonds.

3. Use two long flexible sticks for a double bond and three long flexible sticks for a triple bond.

2. Compare each model constructed to the molecular shapes described in the Theory section. Then identify and record its correct shape name and its bond angles. If the molecule has no definite central atom, then only record the bond angles.

3. Evaluate the polarity of the bonds in each molecule as well as its overall symmetry in order to determine whether it is polar or non-polar.