Experiment 13: Molecular Models

Skills/Concepts

- Molecular Structure
- Lewis Dot Structures
- Electronegativity
- Covalent Bonds

Relevant Reading

Hein & Arena 11.2–11.11

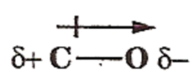
Introduction

Bonds

Chemists are interested in the nature of the chemical bond. Linus Pauling won his first Nobel Prize for his pioneering work in this area. He has contributed significantly to our understanding of the covalent bond. Chemical bonds are strong attractions that hold atoms together in compounds. Covalent bonds are formed when two atoms share electrons between them. Ionic bonds are formed by the transfer of electrons between ions of opposing charge (a molecule with any ionic bonds is ionic, otherwise the molecule is covalent) This lab focuses on the covalent bond.

If two atoms with the same electronegativity (a measure of electron attraction) form a covalent bond, the atoms will equally shared the electrons in the bond. The bond is said to be "nonpolar." Diatomic elements, such as O_2, N_2, and F_2, are nonpolar molecules. To be considered nonpolar, the difference in electronegativity should be less than 0.6 units.

As the electronegativity difference increases, the bond becomes polar. This means that the electrons are unevenly shared. The electrons spend more time at the more electronegative atom. The more electronegative atom has a partial negative charge (not a full ionic charge) and the less electronegative atom has a partial positive charge. We draw the bond as



where δ is the symbol for a partial charge. The arrow denotes a dipole, or a separation of charge.

If the electronegativity difference is greater than 1.6 units, the electron actually transfers to the more electronegative atom. That atom becomes an ion and the bond is ionic. Ionic compounds are not polar because they carry a full charge.

A molecule containing polar bonds may or may not be a polar molecule. The polarity of a molecule depends on the distribution and symmetry of the molecule. Carbon dioxide is nonpolar because the two dipoles cancel each other out.

O=C=O

Lewis Structures

In most molecules, atoms strive to achieve a noble gas electron structure, an octet. Each atom contributes its outermost electrons to form bonds. These chemically active electrons are called valence electrons. The number of valence electrons on an atom increases as you go across the periodic table. Molecules can also have unshared electrons called lone pairs. They are shown as a pair of dots on the electron to which they belong. A line between atoms represents a single covalent bond, two lines a double bond, and three lines a triple bond.

```
 H
 |
:S:
 |
 H
```

There are exceptions. The first 5 elements, H–B, and Al seldom form complete octets and do not form multiple bonds.

Writing Lewis Structures

Here is a general approach to drawing Lewis structures:

1. Draw a skeleton of the non-hydrogen atoms with single bonds (lines) between each one. Consider the following three hints in drawing your skeleton
    a. normal covalency number or number of bonds that each atom forms. For the major atoms these are:

Hydrogen	1 bond
Boron	3 bonds
Aluminum	3 bonds
Carbon	4 bonds
Nitrogen	3 bonds
Oxygen	2 bonds
Halogens	1 bond

    Exceptions:
    NH_4^+ ion, nitrogen has 4 bonds
    H_3O^+ ion, oxygen has 3 bonds

    b. Hydrogen, boron, aluminum, and the halogens seldom form multiple bonds.
    c. In molecules with multiple oxygen atoms, the oxygen atoms usually do not bond to each other. For example, carbon dioxide has two oxygens bonded to carbon and not to each other.
2. Add in hydrogens and lone pairs to give the non-hydrogen atoms octets.
3. Looking at the formula of your compound, count the total number of valence electrons in your molecule. Adjust this count for ionic charge. If the molecule has a negative charge, add electrons. Subtract electrons if it has a positive charge.

4. Looking at your structure, count all your electrons both in bonds and as lone pairs.
5. If the counts from steps 3 and 4 match, you are done. If your structure shows too many electrons, remove lone pairs of electrons from adjacent atoms and add a multiple bond.

When dealing with organic compounds, the following technique may prove easier. To illustrate this technique, the example of C_3H_8O will be used.

1. Draw a skeleton of the carbon atoms and then add the oxygens. Draw in single bonds.

   C – C – C – O

2. Add the hydrogens to the carbon-oxygen skeleton.

```
    H   H   H
    |   |   |
H – C – C – C – O – H
    |   |   |
    H   H   H
```

3. Complete the structure by adding lone pairs to the oxygen.

```
    H   H   H
    |   |   |   ..
H – C – C – C – O – H
    |   |   |   ..
    H   H   H
```

One complication with this method is that multiple formations, or isomers, are possible. For example, in the molecule above, the oxygen could be placed between two carbons.

One tricky organic structure is –COOH. Remember not to bond the oxygens together. Rather have the oxygens bond to the carbon. Try having a double bond for one of the carbon-oxygen connections.

Electron Pair and Molecular Geometries

The Valence Shell Electron Pair Repulsion theory (VSEPR) is useful for predicting the geometries of molecules. The key premise is that electron pairs whether in pairs or bonds repel each other. Accordingly electron pairs and bonds want to be spaced as far away from each other as possible.

To determine the shape of molecules, we will use a 2-step process:

1. Draw the Lewis dot structure to determine the electron geometry.
2. Determine the molecular shape from the shape the bonded atoms form.

Lone pairs determine geometry by repelling bonds away. However, they are not included in the final geometry. For example, consider water. Without considering the lone pairs, one may think the molecule is linear: H–O–H. The two lone pairs on the oxygen affect the geometry. Think of the molecule as tetrahedral. The lone pairs on the oxygen push bonds down to a 109˚ angle. When naming the final molecular structure do not include the lone pairs. Include only what you would see with a ball-and-stick model, as you will be building for this lab. With the ball-and-stick models, we do not see lone pairs. For the model of water, we would have just a bent structure. The final molecular structure of water is "bent."

See Table 11.6 in Hein and Arena for a listing of electron pair arrangements and molecular structures. Below is an equivalent summary.

In determining the shape, think of in terms of sets of bonds. A set of bonds is either a multiple bond or a single bond.

Sets of Bonds	**Lone Pairs**	**Electron Pair Geometry**	**Molecular Geometry**	**Bond Angle**	**Example**
2	0	Linear	Linear	180˚	BeCl
3	0	Trigonal Planar	Trigonal Planar	120˚	BF_3
3	1	Trigonal Planar	Bent	120˚	SO_2
4	0	Tetrahedral	Tetrahedral	109˚	CH_4
4	1	Tetrahedral	Trigonal Pyramidal	109˚	NH_3
4	2	Tetrahedral	Angular (bent)	109˚	H_2O

Name: ___________________

Pre-Lab

1. How many electrons form an octet?

2. How many electrons are in a single bond?

3. How many electrons does a neutral atom of oxygen have?

4. How many valence electrons does a neutral atom of oxygen have?

5. How many bonds does an oxygen atom want to form?

6. Is the bond in hydrogen chloride non-polar covalent, polar covalent or ionic?

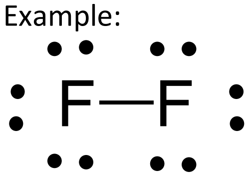
7. Is lithium fluoride a covalent or ionic molecule?

Name: ___________________ Lab Partner: ___________________

Procedure

(1) Each student should take one each of the small models from the kit (the small tetrahedral, trigonal planar, and linear models).
(2) Draw out the Lewis structures for the molecules listed in the post-lab table and fill in the geometry and bond information. (Draw out the Lewis structure on scratch paper before drawing your final structure in the post-lab table.) The example F_2 is done for you.
(3) Consider the underlined atom. Look at the three small models and decide which one best matches the underlined atom. Hint: consider the number of electron sets around the atom.
(4) Choose the model that best describes the underlined atom. The white caps around that atom represent the atoms attached to it. The spokes coming out of the central atom represent the sets of electrons around the central atom. Remove enough of the white caps so the model matches your Lewis dot structure. Now, considering only the atoms—what shape do the white atoms make around the central atom? Write the name of this shape in the molecular geometry column.
(5) What is the angle between the two white atoms in your model?
(6) Do you think the molecule you are modeling is polar? Are the white atoms pulling on the central atom canceling each other out? Be careful, not all atoms pull with equal strength—some are more electronegative than others. Write N or P in the Polar or Non-Polar column.
(7) Finally, ask yourself if the molecule is ionic or not. Hint: If any bond in the molecule is ionic, the whole molecule is considered ionic.

Part A

Formula	Lewis Structure	Electron Pair Geometry	Molecular Geometry	Bond Angle	Polar(P) or Nonpolar(N)	Ionic? (yes or no)
$\underline{F}_2$	Example: 	Tetrahedral	Linear	180°	N (non polar)	No (not ionic)
$H\underline{Cl}$						

$H_2\underline{O}$					
$\underline{N}H_3$					
$\underline{B}Cl_3$					
$\underline{C}O_2$					
$\underline{I}O_2^-$					
$\underline{P}O_4^{3-}$					

The following molecules are more challenging! Many contain double or triple bonds, to see how double and triple bonds are made with your models, look at the examples in your model kit. You may want to use red atoms for oxygen and black ones for carbon in your models. Be careful to get the electronic geometry correct for each atom before connecting them. You may want to work on these models as a group (you instructor has extra model parts if you need them).

Part B

$\underline{C}_2H_6$					
$\underline{C}_2H_4$					
$\underline{C}_2H_2$					
$C_2H_5\underline{O}H$					

H<u>C</u>HO					
$CH_3\underline{O}CH_3$					
H<u>C</u>OOH					
$HC_2H_3\underline{O}_2$ (the O with single bonds)					