Models of Molecular Structure

Molecular model kits are designed to give a reasonably accurate picture of how atoms are arranged in molecules. They follow common bonding patterns and produce the geometric shapes typical of many typical molecules. However, there are types of bonds and examples of geometries that they can not accurately depict.

Most model kits follow a commonly accepted color scheme for atoms. Using the instructions for your model kit, fill in the following information:

Atom	Color	Number of holes (possible bonds)
Hydrogen		
Carbon		
Nitrogen		
Oxygen		
Halogens		
Sulfur (if present)		
Phosphorus (if present)		

Models also depict bonds by using connectors. (The length of the connectors may or may not give proportional bond lengths.) What type of connector is used in your kit for the following:

A single bond (other than to Hydrogen)
A single bond (specifically to Hydrogen)
A double bond
A triple bond

The number of holes also represents the number of bonds that an atom commonly forms. If non-bonding pairs (also known as lone pairs) are present, the number of bonds will be fewer. For atoms that form molecules with octets, one of the following will normally hold:

4 bonding pairs (4 bonds) and zero non-bonding pairs	Example: Carbon
3 bonding pairs (3 bonds) and one non-bonding pair	Example: Nitrogen
2 bonding pairs (2 bonds) and two non-bonding pairs	Example: Oxygen
1 bonding pair (1 bond) and three non-bonding pairs	Example: Halogens

The most powerful way to use these relationships is to memorize common bonding patterns of these atoms, and apply these patterns to deduce molecular structure. For example, in the molecule CF_2Cl_2, the fluorine and the chlorine atoms must be on the outside of the molecule (since they are halogens) and the carbon must be in the middle for common bonding patterns to hold.

The most common exceptions are:

Hydrogen does not form an octet; it holds one bonding pair.
Boron, Sulfur and Phosphorus often do not have octets.
At least one atom in polyatomic ions does not follow common bonding patterns.
There are other exceptions.

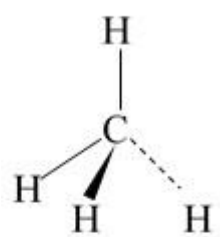
<u>Where exceptions exist, the number of holes in the model kit may not match the number of bonds!</u>

Drawing Structures

Electron-dot structures do not normally show the three-dimensional relationship of the atoms in a molecule or ion. To draw a three-dimensional structure, you need to know its bonding scheme and the arrangement in space of the atoms. The style of drawing a structure depends on what you are trying to communicate:

- To emphasize the distribution of electrons a Lewis (electron-dot) structure is used.
- To emphasize the location of chemical bonds, electron pairs in bonds are replaced by single lines.
- To emphasize the locations of lone pairs of electrons, a mixture of straight lines and dots is used.
- To emphasize the three-dimensional structure, either a perspective drawing or a "dash-wedge" notation is used.

The "dash-wedge" notation places three atoms in the plane of the paper, and single (or double) lines indicate bonds in the plane of the paper. Then, atoms behind the plane of the paper are connected by a dashed line indicating its bond, and atoms in front of the plane of the paper are connected by a narrow wedge with the wide end pointing outward. An example is methane, CH_4, which shows the carbon and two of the four hydrogen atoms in the plane, one in front, and one behind:



If double bonds or lone pairs (non-bonding pairs) are present they are usually placed in the plane of the paper wherever possible.

Name ______________________________
Lab Day _________

Procedure
For each molecule in the table below, count valence electrons and draw Lewis (electron-dot) structures following common bonding patterns and the octet rule. Then build the molecule and draw a "dash-wedge" drawing of the molecule, including lone pairs. Enter each dot structure and its drawing in your lab notebook. Count the number of bonds (bonding pairs) and the number of non-bonding pairs on the central atom only and enter these below.

Molecule and Count of Valence electrons	Lewis Dot Structure	Drawing	Count of Central Atom Bonds	Count of Central Atom Non-bonding pairs
CH_4 Count of valence electrons: _____				
CH_3Cl Count of valence electrons: _____				
NH_3 Count of valence electrons: _____				
H_2O Count of valence electrons: _____				
H_2S Count of valence electrons: _____				
CO_2 Count of valence electrons: _____				
CH_2O Count of valence electrons: _____				

Since ions contain either extra or fewer electrons than the atoms, you must add or subtract electrons before drawing a Lewis structure. Build and draw the following ions, where one atom does not follow common bonding patterns, but all atoms obey the octet rule:

Ion and Count of Valence electrons	Lewis Dot Structure	Drawing	Count of Central Atom Bonds	Count of Central Atom Non-bonding pairs
OH^- Count of valence electrons: _____				
CO_3^{2-} (use one C=O double bond) Count of valence electrons: _____				
NH_4^+ Count of valence electrons: _____				

Build and draw the following ions, which do not follow common bonding patterns, and do not obey the octet rule. (Some models of these may also not follow the structure predicted by VSEPR theory; see the last question on the last page.) Count the number of central atom bonds and non-bonding pairs:

Ion and Count of Valence electrons	Lewis Dot Structure	Drawing	Count of Central Atom Bonds	Count of Central Atom Non-bonding pairs
SO_4^{2-} (use two S=O double bonds) Count of valence electrons: _____				
PO_4^{3-} (use one P=O double bond) Count of valence electrons: _____				

For PO_4^{3-} , was a ball with the correct number of holes available? __________
If not, how does that affect the structure you built?

Some molecular formulas present two or more true possibilities for a molecule, and some represent one true and one false possibility. Sulfur dioxide could be drawn in a three-membered ring, or in a chain; each follows common bonding patterns. Draw both. (Experimental evidence shows it is not a ring.) You will find it is difficult to make a model of the ring structure.

Molecule and Count of Valence electrons	Lewis Dot Structure	Drawing	Number of bonds on each atom	Number of lone pairs on each atom
SO_2 Count of valence electrons: _____			O S	O S
SO_2 Count of valence electrons: _____			O S	O S

The same principles apply to molecules that do not have a single central atom. Apply common bonding patterns to the atoms one at a time. Build and draw the following carbon compounds; count bonds and non-bonding pairs:

Molecule and Count of Valence electrons	Lewis Dot Structure	Drawing	Count of Each Carbon's Bonds	Count of Each Carbon's Non-bonding pairs
C_2H_6 Count of valence electrons: _____				
C_2H_4 Count of valence electrons: _____				
$C_2H_2Cl_2$ Count of valence electrons: _____				
$C_2H_2Cl_2$ (second possibility) Count of valence electrons: _____				

Build and draw the following Nitrogen compounds; count bonds and non-bonding pairs:

Molecule and Count of Valence electrons	Lewis Dot Structure	Drawing	Count of Each N's Bonds	Count of Each N's Non-bonding pairs
N_2 Count of valence electrons: _____				
N_2H_4 Count of valence electrons: _____				
HCN Count of valence electrons: _____				
CH_3NH_2 Count of valence electrons: _____				

Answer the following questions:

1. Look at all the structures above for situations where oxygen "violates" common bonding patterns by having only one bond and three non-bonding pairs. What is in common for all these situations?

2. Look at all the atoms and ions above that contain S. How many bonds to S are possible in the various structures?

3. There are two real isomers of C_2H_4O, both of which follow common bonding patterns, but neither has a C=C bond. In each, the oxygen and both carbon atoms are in the same plane. Draw a dash-wedge structure for each. (If you get stuck, try the Merck Index's formula index.)

4. After you have studied the Valence Shell Electron Pair Repulsion Theory (VSEPR Theory) in class, you may discover that some of your drawings of the molecular models do not match this theory. If there are any that you would like to change, place an asterisk next to your drawing in the "drawing" column, and re-draw that structure in the margin to match VSEPR.

Name ________________________

Prelaboratory Assignment –

Molecular Models

1. How many electrons comprise a bond?

2. Define a “lone pair”.

3. What is the “octet rule”?

4. How does the octet rule apply to H?

5. How many bonds does each of the following atoms normally form in molecules?

   H C O N F

6. Draw dot diagrams for S and for P. These can form several numbers of bonds because paired electrons in the atoms can “unpair” before forming bonds.

   S P

   For P, how many bonds will it form (two possibilities)? _______ _______

7. Make Lewis (electron-dot) drawings of ammonia (NH_3) and hydrogen peroxide (H_2O_2).