MOLECULAR SHAPES

When bonds form between atoms molecules are created. Depending on how many bonds exist a molecule will take on different shapes. The bonds between atoms generally contain two electrons. These electron pairs will repulse each other, therefore the bonds will be equally spread around the surface of the atom.

The **Valence-Shell Electron Pair Repulsion theory (VSEPR)** states that in a small molecule, the pairs of electrons are arranged as far apart from each other as possible. (*of course there are always exceptions) The VSEPR effect helps determine the **bond angle**, the geometric angle between two bonds. This arrangement of bonds creates the shape of a molecule. Although bonds appear flat when drawn on paper we have to remember that a molecule is actually 3-dimensional.

There are seven basic shapes – linear, trigonal planar, tetrahedral, pyramidal, bent, trigonal bipyramidal, and octahedral. When determining the shape of a molecule you must first draw the Lewis Dot Diagram for the molecule or ion. Next, count the total number of regions of high electron density (bonding and unshared electron pairs) around the central atom.

Rules for determining high electron density:

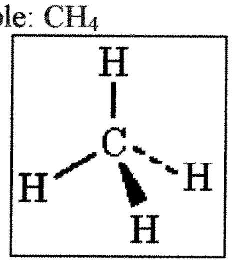
1. Double and triple bonds count as ONE REGION OF HIGH ELECTRON DENSITY.
2. An unpaired electron counts as ONE REGION OF HIGH ELECTRON DENSITY.
3. For molecules or ions that have resonance structures, you may use any one of the resonance structures.

Third, identify the most stable arrangement of the regions of high electron density as ONE of the following:

1. **linear** - molecules have bonds that form a straight line, the atoms are 180° apart. A molecule may be linear if it contains double or triple bonds that create a symmetry.
   - For example: O_2 O=O (diatomic)

     CO_2 O=C=O

2. **trigonal planar** - molecules form a flat triangle with the bond angle at 120°. Because the bond angle is greater than 90° the bonds may remain on the same plane.
3. **Tetrahedral** - molecules have four equal bonds. All bond angles are 109.5°.
   - For example: CH_4



4. **Pyramidal** – molecules have a central atom that contains an unshared pair of electrons. The unshared pair applies a greater repulsion force than the other bonds resulting in a tetrahedral with out the top 4^{th} bond. The bond angle is 107° between bonds.
5. **Bent** – is found in molecules with 2 unshared pairs of electrons. These two unshaired pairs repulse the bonded pairs resulting in a bond angle of 105°.

- For example: water

6. **Trigonal bipyramidal** – molecules are formed from a central atom with 5 bonds. The bonds will arrange in five directions, up, down and three pointing out from the middle.

7. **Octahedral** – molecules formed with 6 bonds around a central atom. The bond arrangement will be: up, down and four pointing out from the middle.

Fourth, determine the positions of the atoms based on the types of electron pairs present (i.e., bonding pairs vs. unshared pairs). For trigonal bipyramidal and octahedral arrangements, there can sometimes be more than one possible arrangement of the bonding and unshared pairs:

Trigonal bipyramidal - place any unshared pairs in the plane of the triangle.
Octahedral - if you have two unshared pairs, place them on opposite sides of the central atom.

Fifth, identify the molecular structure based on the positions of the ATOMS (NOT on the regions of high electron density).

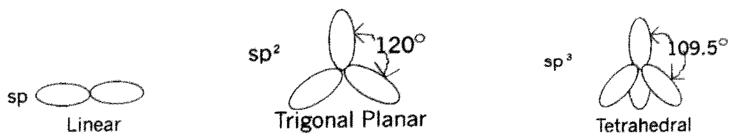
Practice: Draw the Lewis Dot Diagram, illustrate and identify the molecular shape of the following molecules.

1. HF

2. BF_3

3. CCl_4

To determine molecular shapes based on orbitals (**hybrid orbitals**) we must think about how atoms affect each other as they come together. The electron's *normal* orbits may be changed. When bonds form some chemists believe that the orbitals mix to form hybrid orbitals. Hybrid orbitals contain properties of both original orbitals. (Text figure 8-11, pg 263) **Be able to illustrate the following diagrams.



Bond length is the distance between the nuclei of two bonded atoms. Bond length distance depends upon the repulsion of the nuclei . If you have larger nuclei the repulsion is larger. If you add more electrons to a bond (double or triple bonds) the electrons act to pull the nuclei together and shorten the bonds. This can be summarized in these trends:

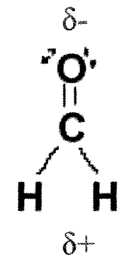
1. As you move down a group the atoms form larger bonds.
2. Multiple bonds are shorter than single bonds.
3. The shorter the bond length the higher the energy.

Bond energy is the energy required to break a chemical bond and form neutral atoms, measured in kJ/mole.

POLARITY IN MOLECULES

Like polar and non-polar bonds, molecules can be polar and non-polar also. Polar molecules have a positive end and a negative end, also referred to as **dipoles**. Non-polar molecules do not have charged ends. The shape of a molecule and the polarity of its bonds together determine whether the molecule is polar or non-polar. (again we will refer to the δ+ and δ-) The shape of large molecules are determined in part by their polarity.

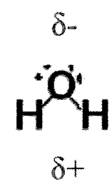
-For example: CH_2O (polar)



CO_2 (non-polar)

(all sides are equal)

H_2O (polar)



Name: ____________________________ **Period:** ___ **Date:** ____________________

Homework: Molecular Shapes

1-5. Draw the Lewis Dot Diagram, illustrate and indentify the molecular shape of the following, and then indicate if it is a polar or non-polar molecule.

	Lewis Dot Diagram	Illustrate	Shape	Polar/Non-polar
1. BFI_2				
2. NH_2Cl				
3. C_2H_4				
4. CBr_4				
5. NH_3				

6. Illustrate the hybrid orbitals for the sp^3.

7. Which has longer bonds H_2O or CO_2? Why?

8. In a polar bond, electrons are shared (equally/unequally) between two atoms.

9. A molecule that is composed of only one kind of atom is a(n) ____________.

10. Compare the bonds in C_2H_4 and C_2H_2, which bonds would require more energy to break?

11. Why is HCl a polar molecule while Cl_2 is a non-polar molecule?

12. The __________________ of a large molecule helps determine its shape.

Choose the best answer for the following multiple choice questions.

_____ 13. The distance between the nuclei of two bonded atoms is referred to as:

a. bond energy
b. ionic radii
c. molecular radii
d. bond length

_____ 14. When the bonds result in partial charges on the ends of a molecule, the molecule is referred to as:

a. ionic compound
b. non-polar molecule
c. polar molecule
d. none of the above

_____ 15. Which of the following is the correct Lewis Dot Diagram for hydrogen chloride?

a. H$\overset{x}{\cdot}$Cl   b. H$\overset{x}{\cdot}$$\ddot{\underset{\cdot\cdot}{Cl}}$:   c. $\overset{x}{\underset{x}{\cdot H}}$$\overset{x}{\cdot}$$\dot{\underset{\cdot}{Cl}}\cdot$ d. ×H:$\ddot{\underset{\cdot\cdot}{Cl}}\cdot$

_____ 16. Which of the following is a major determining factor of molecular shape?

a. repulsive forces between shared and unshared electron pairs
b. attractive forces between shared and unshared electron pairs
c. repulsive forces between adjacent nuclei
d. attractive forces between adjacent nuclei

_____ 17. What is the bond angle in a molecule whose central atom has formed three bonds?

a. 90°   b. 109.5°   c. 120°   d. 180°

_____ 18. Which of the following is a result of merging orbitals from different sublevels to form new orbitals?

a. resonance
b. hybrid orbitals
c. isomerism
d. polyvalence

_____ 19. In a triple bond how many electron pairs are shared?

a. 1   b. 2   c. 3   d. 4

_____ 20. In the hybrid orbital sp^3 what is the bond angle?

a. 90°   b. 109.5°   c. 120°   d. 180°

_____ 21. A molecule of water has how many unshared electron pairs?

a. 1   b. 2   c. 3   d. 4

_____ 22. The repulsion of an unshared pair of electrons is _____ a shared pair of electrons.

a. more than   b. less than   c. equal to   d. not comparable

_____ 23. Which type of bond has the highest bond energy?

a. single   b. double   c. triple   d. they are equal

_____ 24. A polar molecule is referred to as a:

a. dipole   b. hybrid   c. anion   d. cation