Chem 1045

## Chapter 10 Molecular Geometry and Chemical Bonding Theory

These Notes are to SUPPLIMENT the Text, They do NOT Replace reading the Text Material. Additional material that is in the Text will be on your tests! To get the most information, READ THE CHAPTER prior to the Lecture, bring in these lecture notes and make comments on these notes. These notes alone are NOT enough to pass any test!

The author is providing these notes as an addition to the students reading the text book and listening to the lecture. Although the author tries to keep errors to a minimum, the student is responsible for correcting any errors in these notes.

## Total Electron Pair

2
3

4

| Shape | Example |
| :--- | :--- |
| Linear | $\mathrm{BeF}_{2}$ |
| Trigonal Planar | $\mathrm{BF}_{3}$ |
| Tragonal Planar Bent | $\mathrm{SO}_{2} \quad$ [ Sulfur has one lone pair of electrons ] |
| Tetrahedral | $\mathrm{CH}_{4}$ |
| Trigonal Pyramidal | $\mathrm{NH}_{3} \quad$ [ Nitrogen has one lone pair of electrons ] |
| Tetrahedral Bent | $\mathrm{H} 2 \mathrm{O} \quad$ [ Oxygen has 2 lone pair of electrons ] |

Boron Trifluoride, $\mathrm{BF}_{3}$ is flat planar with $120^{\circ}$ angle between the bonds
Phosphorous Trifluoride, $\mathrm{PF}_{3}$ Tetrahedral, 3 Fluorine bonds and one electron lone pair, the P-F bonds are $96^{\mathbf{o}}$.
Structures tell more than molecular formulae. Look at the difference between cis and trans di-chloroethane Cis has a bp of $60^{\circ} \mathrm{C}$ and trans $48^{\circ} \mathrm{C}$.



Valence Shell Electron Pair Repulsion (VSEPR) Model predicts the shapes of molecules and ions by assuming that the valence shell electron pairs are arranged about each atom so that electron pairs are kept as far away from one another as possible, thus minimizing electron-pari repulsions.


See also the Trigonal Bipyramidal [ 5 bonds] and Octahedral [ 6 bonds].
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To determine the geometry, locate the direction in space of the bonding pair of electrons.

Two Electron Pair: $\quad \mathrm{BeF}_{2} \quad: \mathrm{F}: \mathrm{Be}: \mathrm{F}: \quad$ This is a linear arrangement

$$
\mathrm{CO}_{2} \quad: \mathrm{O}:: \mathrm{C}:: \mathrm{O}: \quad \text {-or- } \quad \mathrm{O}=\mathrm{C}=\mathrm{O}
$$

Three Electron Pair $\quad \mathrm{BF}_{3} \quad$ Trigonal Planar $-120^{\circ}$ between bonds

$$
\begin{gathered}
: F: \\
: F: B: F:
\end{gathered}
$$

Error on above pic, F should have 8 electrons around it!

Sulfur Dioxide $\quad \mathrm{SO}_{2}$


With 3 atoms, you can only arrange it as Trigonal Planer

## Four Electron Pair

$\mathrm{CH}_{4}$ Tetrahederal
$\mathrm{NH}_{3}$ Trigonal Pyramidal, sort of Tetrahedral, the nitrogen lone pair pushes the H down $\mathrm{H}_{2} \mathrm{O}$ Bent

Steps to predict the Geometry by the VSEPR Model

1. Write the electron dot formula
2. Determine the number of electron pair, include bonding and non-bonding pair
3. Determine the arrangement of electrons per Fig 10.2 p 374 or the table above
4. Obtain the molecular geometry from the directions of the bonding pair.

Example 10.1 Predict the geometry of the following: $\begin{array}{lllll}\mathrm{BeCl}_{2} & \mathrm{NO}_{2}{ }^{-} & \mathrm{SiCl}_{4}\end{array}$
See page 379 for the answer
$\mathrm{Cl}: \mathrm{Be}: \mathrm{Cl} \quad$ Linear
$[\mathrm{O}-\mathrm{N}=\mathrm{O}]^{-} \quad$ Has resonance of double bond. Trigonal Planar Bent
$\mathrm{SiCl}_{4}$ is like Carbon Tetrahedral

## Bond Angles and Lone Electron Pair

A lone pair tends to require more space than a corresponding bonding pair: See pg 380
$\mathrm{CH}_{4} \quad 109.5^{\circ} \quad \mathrm{CH}_{3} \mathrm{Cl} \quad 110^{\circ}$ between H
$\mathrm{NH}_{3} \quad 107^{\circ}$ between $\mathrm{H} \quad \mathrm{H}_{2} \mathrm{O} \quad 105^{\circ}$ between H

## Bond Angles with C-C double bonds




Central Atom with 5 or 6 Valence Shell Electrons
Examples BSOC

## 5 Trigonal Bipyramidal <br> 6 Octahedral

Left and Right handed Molecules. Carbon molecules that have 4 different groups on a central Carbon atom are optically active and have $\mathrm{L} \& \mathrm{R}$ shapes. This is very important in biochemistry. Build two molecular models of carbon with 4 different groups on it. It's just like your left and right hand are mirror images of each other.

Dipole Moment is a quantitative measure of the degree of charge separation in a molecule. Upper right side of the Periodic Table is most electronegative. Example is water - it's a polar molecule
$\mathrm{H}-\mathrm{Cl} \quad$ Electronegative Chlorine pulls the electron from hydrogen HCl has a large dipole moment.
$\mathrm{NF}_{3}$
CO2
$\mathrm{O}=\mathrm{C}=\mathrm{O}$ Linear
Net Zero Dipole Moment
$\mathrm{H}_{2} \mathrm{O}$
$109^{\circ}$ angle for Hydrogen
Large Dipole Moment
Formula Molec Geom Dipole Moment
AX Linear
$\mathrm{AX}_{2}$
Linear
Bent
$\mathrm{AX}_{3} \quad$ Trigonal Planer
Trigonal Pyramidal
Trigonal T-Shaped
AX4-6 BSOC

Can be non-zero [ $\mathrm{H}-\mathrm{Cl}$ ]
Zero
Can be non-zero
Zero
Can be non-zero
Can be non-zero

Cis and Trans DiChloroEthane above. The Cis, with both Chlorine on the same side has a dipole moment. The Trans does not.
Hybrid Orbitals:
Chloride


Oxygen


Carbon and its Hybrid Orbital

## Carbon



A Hybrid Orbital describes bonding that is obtained by taking combinations of atomic orbitals of the isolated atoms.

The shapes of the Carbon Orbital actually changes from the expected 3s beach ball shapped and the 3 dumball shapped $\mathrm{Px}, \mathrm{Py}$, and Pz .

The shape of the hybrid orbitals also changes. It is not the normal round S and 3 figure 8 ps . It forms a tetrahedral - see page 390.
$\mathrm{Sp}^{3}$ forms 4 bonds Tetrahedral, 109.5 degrees
$\mathrm{Sp}^{2}$ forms 3 bonds Trigonal Planer, 120 degrees
Sp forms 2 bonds Linear, 180 degrees
$\mathrm{CH}_{4}$
$\mathrm{BF}_{3}$ or ethylene
Be in $\mathrm{BeF}_{2}$ or acetylene
$\mathbf{H}_{\mathbf{2}} \mathbf{O}$ Oxygen has 2 lone pair of electrons and 2 bonds. 4 Bonds $=$ Tetrahederal or $\mathrm{Sp}^{3}$ hybrid instead of a 2 s and 2 p .

Multiple Bonds Ethylene


Ethylene has 3 bonding pair. It Is hybridized to Sp 2 with a 2 p electron available for the double bond.


Sigma Bond: The Carbon to Hydrogen bond in ethylene is the cylindrical shaped electron cloud.

Pi Bond: is an electron distribution above and below the $\mathrm{C}-\mathrm{C}$ bond axis.
The triple bond is Acetylene is

$$
\begin{aligned}
& \mathrm{H}-\mathrm{C} \equiv \mathrm{C}-\mathrm{H} \\
& \mathrm{C} \text { in Acetylene }
\end{aligned}
$$



## Practice Questions:

Review Questions: All Example Problems in the chapter
Concept Questions:
Practice Problems:

