Chapter 10 Molecular Geometry and Chemical Bonding Theory

These Notes are to <u>SUPPLIMENT</u> 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, <u>READ THE</u> <u>CHAPTER</u> 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	Shape	Example	
2	Linear	BeF ₂	
3	Trigonal Planar	BF ₃	
	Tragonal Planar Bent	O ₂ [Sulfur has one lone pair	of electrons]
4	Tetrahedral	CH ₄	
	Trigonal Pyramidal	NH ₃ [Nitrogen has one lone p	air of electrons]
	Tetrahedral Bent	I2O [Oxygen has 2 lone pair	of electrons]

Boron Trifluoride, BF₃ is flat planar with 120° angle between the bonds

Phosphorous Trifluoride, PF₃ Tetrahedral, 3 Fluorine bonds and one electron lone pair, the P-F bonds are 96°.

Structures tell more than molecular formulae. Look at the difference between cis and trans di-chloroethane Cis has a bp of 60 °C and trans 48 °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].

To determine the geometry, locate the direction in space of the bonding pair of electrons.

Two Electron Pair: BeF_2 : F : Be : F :
 $: CO_2$ This is a linear arrangement
: O :: C :: O :
: O :: C :: O :
: O = C = O
: O :: C :: O :
<math>: O = C = OThree Electron Pair BF_3 Trigonal Planar – 120° between bonds
: F :

:F:B:F:

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



Sulfur Dioxide SO₂

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

Four Electron Pair

CH₄ Tetrahederal

NH₃ Trigonal Pyramidal, sort of Tetrahedral, the nitrogen lone pair pushes the H down

H₂O 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: $BeCl_2$ $NO_2^ SiCl_4$ See page 379 for the answer

Cl : Be : Cl	Linear
$[O - N = O]^{-1}$	Has resonance of double bond. Trigonal Planar Bent
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

CH_4	109.5°	CH ₃ Cl	110° between H
~ 4	10710	011301	110 000000000000

 NH_3 107° between H H_2O 105° between H

Bond Angles with C-C double bonds



Central Ator	n with 5 or 6 Valence Shell Electrons	Examples BSOC
5	Trigonal Bipyramidal	
6	Octahedral	

Left and Right handed Molecules. Carbon molecules that have 4 different groups on a central Carbon atom are optically active and have L & 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

H-Cl	Electronega HCl has a la	tive Chlorine p arge dipole mor	Chlorine pulls the electron from hydrogen lipole moment.			
NF ₃	with a lone	pair has a small	ir has a small dipole moment.			
CO2	O = C = O	Linear	Net Zero Dipole Moment			
H_2O	109° angle f	for Hydrogen	Large Dipole Moment			
Formula	Molec Geom	Dipole Mome	ent			
AX	Linear	Can be	non-zero [H-Cl]			
AX_2	Linear	Zero				
	Bent	Can be	non-zero			
AX_3	Trigonal Planer	Zero				
	Trigonal Pyramida	al Can be	non-zero			
	Trigonal T-Shaped	d Can be	non-zero			
AX4 – 6	BSOC					

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

Chlorine						
<u>1s</u>	<u>2s</u>	<u>2p</u>	<u>3s</u>	<u>3p</u>		
		<u>-1 0 +1</u>		<u>-1 0 +1</u>		
$\downarrow \uparrow$	$\downarrow \uparrow$	$\downarrow\uparrow\downarrow\downarrow\uparrow\downarrow\uparrow$	$\downarrow\uparrow$	$\downarrow\uparrow\downarrow\downarrow\uparrow$		

Oxygen

Oxygen						
<u>1s</u>	<u>2s</u>	<u>2p</u>	<u>3s</u>	<u>3p</u>		
		<u>-1 0 +1</u>		<u>-1 0 +1</u>		
$\downarrow\uparrow$	$\downarrow \uparrow$		$\downarrow \uparrow$	$\downarrow\uparrow\uparrow\uparrow\uparrow$		

Carbon and its Hybrid Orbital

		Carbo	n		
<u>1s</u>	<u>2s</u>	<u>2p</u>	<u>3s</u>	<u>3p</u>	
		<u>-1 0 +1</u>		<u>-1 0 +1</u>	
$\downarrow\uparrow$	$\downarrow\uparrow$	$\downarrow\uparrow\downarrow\downarrow\uparrow\downarrow\uparrow$	$\downarrow \uparrow$	\uparrow \uparrow	
$\downarrow\uparrow$	$\downarrow \uparrow$		\uparrow	$\uparrow \uparrow \uparrow$	Hybrid Orbital

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 Px, 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.

Sp ³ forms 4 bonds Tetrahedral, 109.5 degrees	CH_4
Sp ² forms 3 bonds Trigonal Planer, 120 degrees	BF ₃ or ethylene
Sp forms 2 bonds Linear, 180 degrees	Be in BeF ₂ or acetylene

Ch 10 Molec Geometry

H₂**O** Oxygen has 2 lone pair of electrons and 2 bonds. 4 Bonds = Tetrahederal or Sp³ hybrid instead of a 2s and 2p.

Multiple Bonds Ethylene



Ethylene has 3 bonding pair. It Is hybridized to Sp2 with a 2p electron available for the double bond.

C in Ethylene					
<u>1s</u>	<u>sp</u> 2	<u>2p</u>	<u>)</u>		
	-	<u>-1</u>	<u>0</u>	<u>+1</u>	
$\downarrow \uparrow$	\uparrow	\uparrow	\uparrow	\uparrow	

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 C-C bond axis.

The triple bond is Acetylene is

 $H - C \equiv C - H$ C in Acetylene

 $\downarrow\uparrow \uparrow \uparrow \uparrow \uparrow \uparrow$

Practice Questions:

Review Questions: All Example Problems in the chapter

Concept Questions:

Practice Problems: