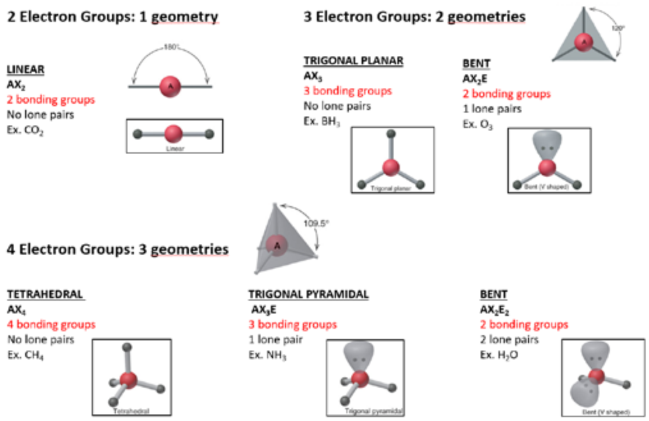
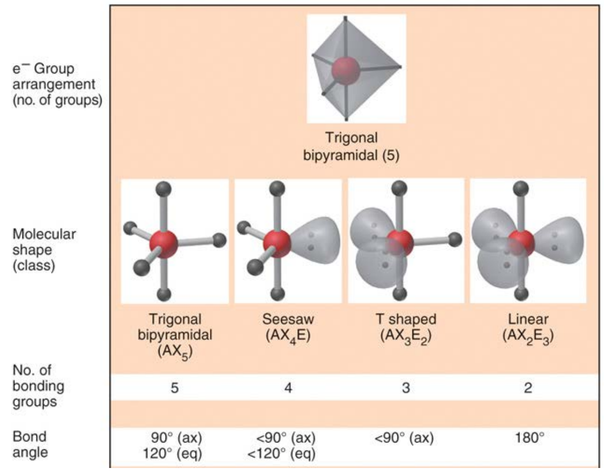
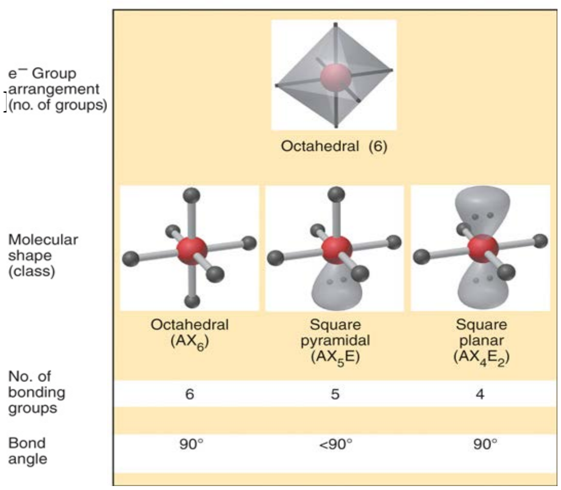
Major Concepts Covered – Lectures 15, 16 and 17

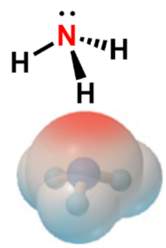
VSEPR (Valence Shell Electron Pair Repulsion) Theory



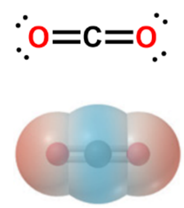




POLAR MOLECULES:
molecules with a net dipole moment (μ)
* "add up" the individual bond dipoles *



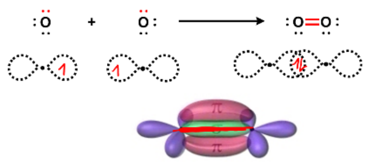
NONPOLAR MOLECULES:
molecules with **zero** net dipole moment (μ)
Either no individual bond dipoles or the individual bond dipoles cancel out



Theories of Covalent Bonding (Hybridization/VSEPR)

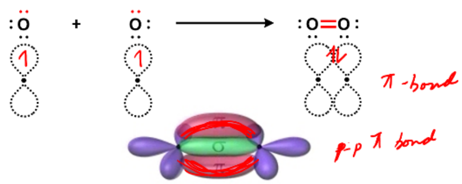
Formation of single and double bonds

A covalent bond forms when orbitals of two atoms overlap and a pair of electrons occupy the overlap region



σ-bond – **formed from overlap of two orbitals. Is cylindrically symmetrical around bond axis**

- The two electrons move over to the new **σ-bonding** orbital
- The two electrons in the bonding orbital have opposite spin (Pauli's exclusion principle still followed)



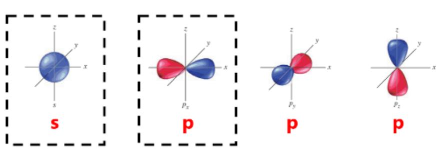
π-bond – **formed from overlap of two orbitals. Is not symmetrical around bond axis. Side to side overlap**

- The two electrons move over to the new **π -bonding** orbital
- The two electrons in the bonding orbital have opposite spin (Pauli's exclusion principle still followed)

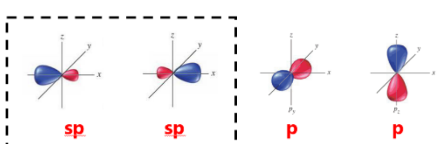
Hybridization

sp

Atomic Be
Valence Orbitals:

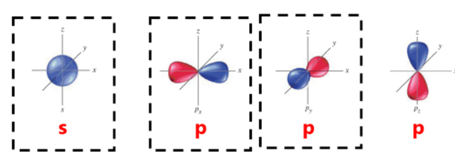


Be atoms in $BeCl_2$
Valence Orbitals:

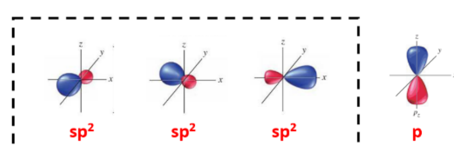


sp^2

Atomic B
Valence Orbitals:



B atoms in BF_3
Valence Orbitals:

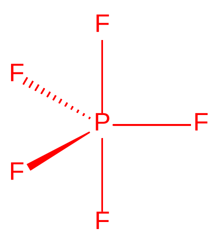


1) Which of the following molecules are polar? Explain your choice.

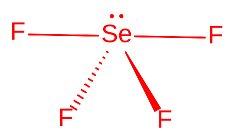
a. COF_2 POLAR (trigonal planar. Asymmetric)
b. SiF_4 NONPOLAR (tetrahedral – Symmetric)
c. PF_3 POLAR (trigonal pyramidal)
d. CS_2 NONPOLAR (linear – Symmetric)

2) For each of the following compare the electron geometry (based on total electron groups) and molecular geometry (shape of the molecule) around:

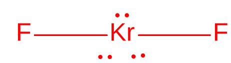
Central atom for: PF_5, SeF_4, KrF_2



Electron geometry: Trigonal Bipyramidal
Molecular geometry: Trigonal Bipyramidal



Electron geometry: Trigonal Bipyramidal
Molecular geometry: Seesaw

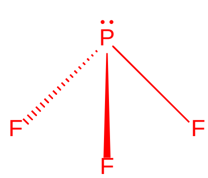


Electron geometry: Trigonal Bipyramidal
Molecular geometry: Linear

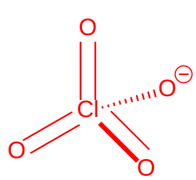
3) Arrange the following (Explain your answer – show Lewis structures and geometry where applicable)

From lowest to highest bond angle

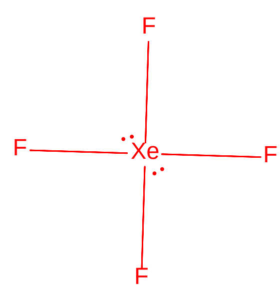
PH_3, ClO_4^-, XeF_4, SCl_2



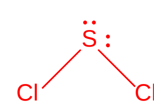
Trigonal pyramidal
Bond angle <109.5



Tetrahedral
Bond angle = 109.5



Sqaure Planar
Bond angle = 90



Bent
Bond angle < <109.5

$XeF_4 < SCl_2 < PF_3 < ClO_4^-$

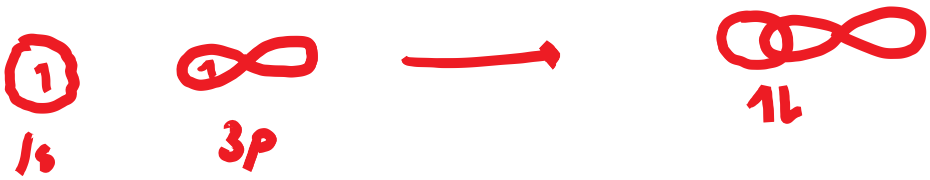
4) Describe the bonding for the following molecules using **valence bond theory**:

a. HBr b. H_2O

Using only valence bond theory here (no hybridization)

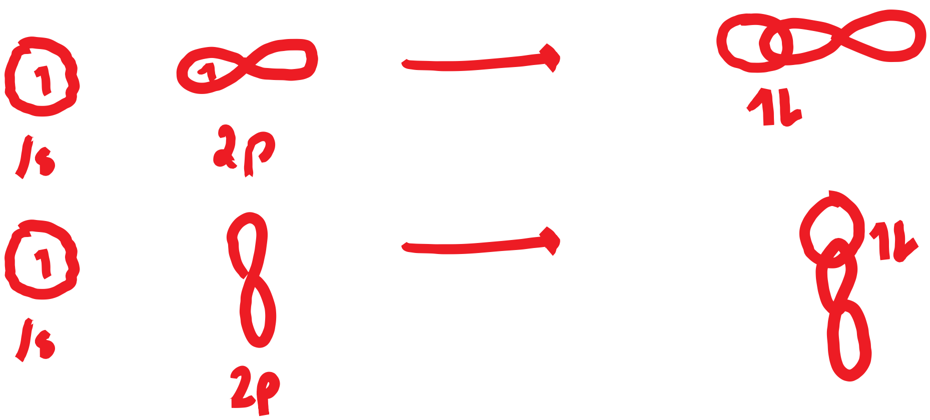
In HBr

H valence orbital (1s) overlaps with Br (3p) orbital, creating a sigma bond



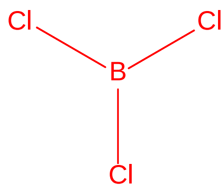
In H_2O

Each H's valence orbital (1s) overlap with Oxygen's partially filled (2p) orbital – creating 2 sigma bonds



5) For the underlined atom in the following molecules, predict the electron geometry, the molecular geometry, and the hybridization of the atom

a. **<u>B</u>**Cl_3

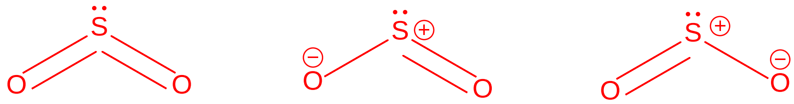


Electron Geometry: Trigonal Planar; 3 electron groups
Molecular Geometry: Trigonal Planar
Hybridization = sp^2
(number of electron groups = number of hybridized orbitals)

b. **<u>C</u>**O_2

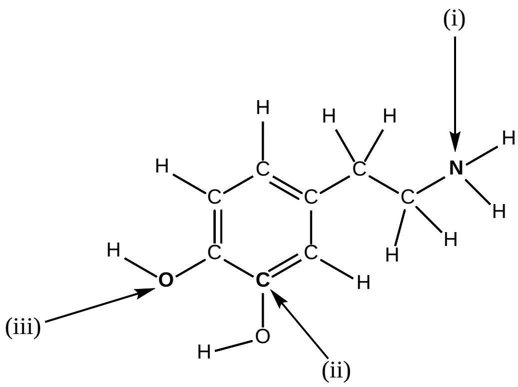
Electron Geometry: Linear; 2 electron groups
Molecular Geometry: Linear
Hybridization = sp
(number of electron groups = number of hybridized orbitals)

c. **<u>S</u>**O_2 (for the central oxygen atom) – try doing this for all resonance structures (the hybridization of the central atom should be the same for each resonance structure



Electron Geometry: Trigonal Planar; 3 electron groups
Molecular Geometry: Bent
Hybridization = sp^2
(number of electron groups = number of hybridized orbitals)

6)



For the indicated atoms (denoted with an arrow), (i) to (iii), answer the following questions. Lone pairs are **not** indicated in the structure. Consider the structure as given (no need to consider resonance structures). All atoms have formal charge of 0. (Use valence bond theory and hybridization to describe the bonding.)

a) For (i)

1. What is the electron **and** molecular geometry at N?

Electron geometry: Tetrahedral; Molecular Geometry: Trigonal Pyramidal

2. Circle the one value that best describes the H-N-H bond angle.

>90° to <109.5° 109.5° 120° >120° to <180

b) For (ii)

1. What is the molecular geometry at C (ii).

Trigonal Planar

2. Circle the one value that best describes the O-C-C bond angle.

>90° to <109.5° 109.5° 120° >120° to <180

3. Using principles of hybridization, describe all the orbitals involved in the various sigma and pi bonds formed by C (ii) with the adjacent carbons.

sp^2-sp^2 sigma bond and p-p pi bond with carbon on the right.

sp^2-sp^2 sigma bond with carbon on the left

c) **For (iii)**

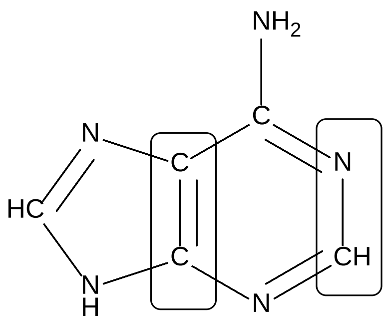
1. What is the electron **and** molecular geometry at O (iii).

Electron geometry: Tetrahedral; Molecular Geometry: Bent

2. Circle the one value that best describes the H-O-C bond angle.

>90° to <109.5° 109.5° >109.5° to <120° 120° >120° to <180

7) Below is the structure of Adenine (this is the building block of nucleic acids), determine the orbitals (using Valence bond theory + hybridization) involved in bonding between the highlighted atoms



Adenine
Nucleobase

a. C=C: sp^2-sp^2 sigma bond and p-p pi bond

b. N-C sp2-sp2 sigma bond.

C-H sp2-s sigma bond