HW 9 – December 5

Valence shell electron pair repulsion (VSEPR) theory

Chemical bonds and unbonded electron pairs or single electrons in a molecule repel, so they try to stay as far as possible from each other.

Linear combination of atomic orbitals (LCAO) – hybridization

1. Hybrid orbitals do not exist in isolated atoms. They are formed only in covalently bonded atoms.
2. Hybrid orbitals have shapes and orientations that are very different from those of the atomic orbitals in isolated atoms.
3. A set of hybrid orbitals is generated by combining atomic orbitals. The number of hybrid orbitals in a set is equal to the number of atomic orbitals that were combined to produce the set.
4. All orbitals in a set of hybrid orbitals are equivalent in shape and energy.

The hybridization of an atom is determined based on the number of regions of electron density that surround it. The geometrical arrangements characteristic of the various sets of hybrid orbitals are shown in the table. These arrangements are identical to those of the electron-pair geometries predicted by VSEPR theory. VSEPR theory predicts the shapes of molecules, and hybrid orbital theory provides an explanation for how those shapes are formed.

To find the hybridization of a central atom, we can use the following guidelines:

1. Determine the Lewis structure of the molecule (place the least electronegative atom in the middle, distribute the total number of valence electrons (the sum of valence electrons from the central atom and those bound to it)).
2. Determine the number of regions of electron density around an atom using VSEPR theory, in which single bonds, multiple bonds, radicals (one unbound electron), and lone pairs (a pair of unbound electrons) each count as one region.

Assign the set of hybridized orbitals from the table below that corresponds to this geometry.

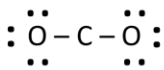
For example:

CO_2 molecule will have linear geometry. Carbon has 4 valence electrons; 2 oxygen atoms have 2x6 = 12 valence electrons. Total number of valence electrons is 12+4=16

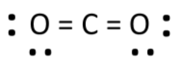
Carbon is less electronegative than oxygen, we place it in the center of the molecule and two oxygens on each side of the carbon:

O – C – O   each bond represents 2 electrons.

We have 16-4=12 electrons to distribute. Firstly, we assign to each oxygen a total of 8 electrons:



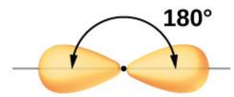
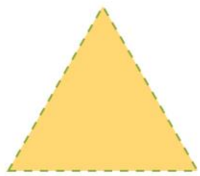
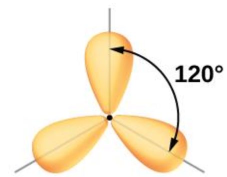
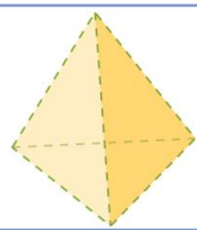
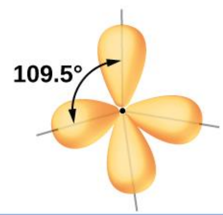
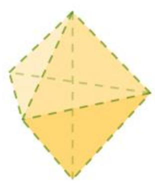
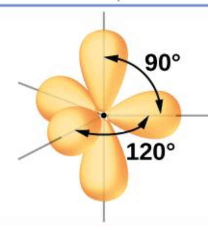
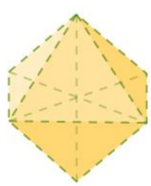
However, this leaves carbon with only 4 electrons from the two bonds. We make double bonds between carbon and oxygen for each atom to have 8 electrons:



There are two regions of electron density around carbon. The molecule is linear, it has “sp” hybridization.

Determine central atom hybridization and molecular geometry of the following molecules:

a) CH_4
b) ClNO
c) $HgCl_2$
d) $[SbF_6]^-$ (hint: disregard the charge)

Regions of Electron Density	Arrangement		Hybridization	
2		linear	*sp*	
3		trigonal planar	sp^2	
4		tetrahedral	sp^3	
5		trigonal bipyramidal	sp^3d	
6		octahedral	sp^3d^2