Chapter 9: Covalent Bonding: Orbitals

9.1: Hybridization and the Localized Electron Model

Hybridization: - the combining of orbitals of different atomic subshells into new orbitals.
- the new hybridized orbitals tend to have minimized energy levels.

Effective Electron Pairs: - the number of pairs of electrons including lone pairs and bonding pairs (however, multiple bonds are counted as one bonding pair).

Sigma (σ) Bond: - a bonding electron pair localized in the area centred along a line between the two nuclei.

Pi (π) Bond: - a bonding pair that utilizes a *p* orbital that is not involved in the hybridization process.
- it exists away from the centred line between the two nuclei.

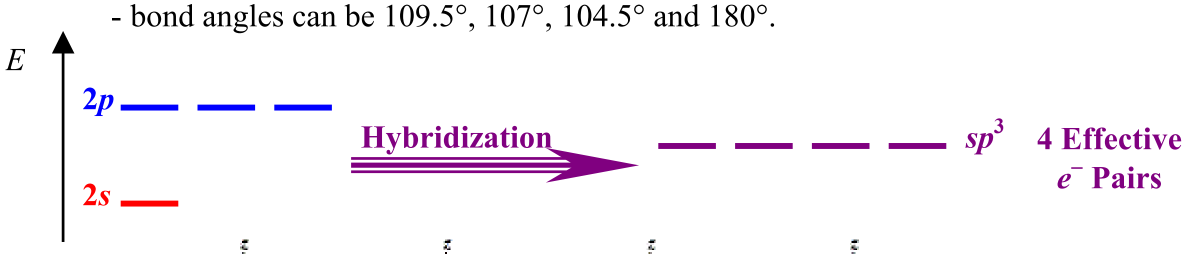
3 Steps to Describe using the Localized Electron Model

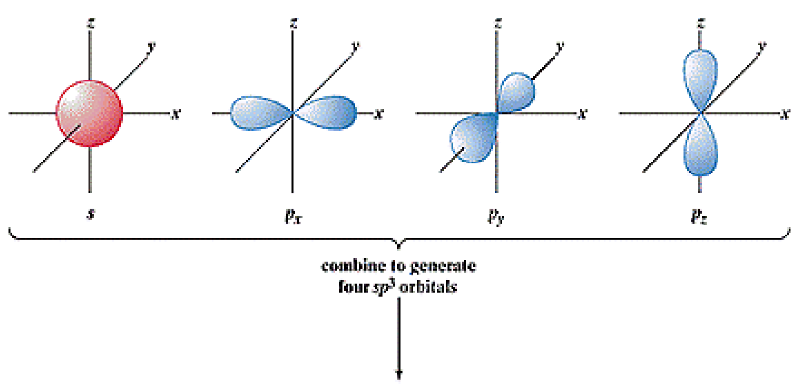
1. Write the Lewis Structures and Account for Minimization of Formal Charges.
2. Using the VSEPR model, determine the electron pairs arrangement.
3. State the type of hybrid atomic orbital for all bonding and lone pairs.

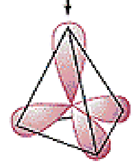
Different Types of Hybridization

(Check out this website: http://www.mhhe.com/physsci/chemistry/essentialchemistry/flash/hybrv18.swf)

1. **sp^3 Hybridization**: - characterized by **4 effective electron pairs** where one *s* and three *p* orbitals are mixed.
   - possible orbital shapes around the atom involved are tetrahedral, trigono pyramid, V-shape, and linear.
   - all bonding electron pairs form σ bonds.
   - bond angles can be 109.5°, 107°, 104.5° and 180°.



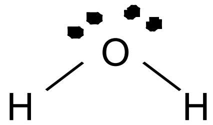




4 Effective e^- Pairs (for lone pairs or σ bonds)

Example 1: Describe the bonding of H_2O using the LE model.

a. Lewis Structure and Formal Charges:

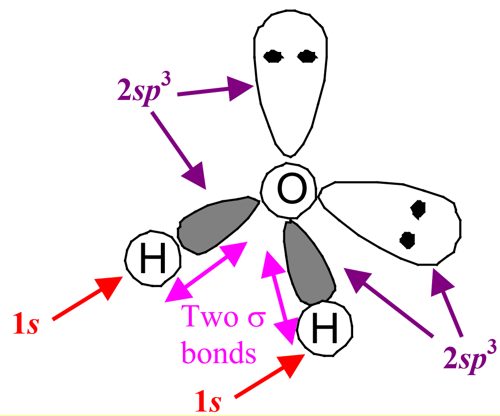


Minimize Formal Charges
O = 6 – 4 – ½(4) = 0
H = 1 – 0 – ½(2) = 0

b. VSEPR model:

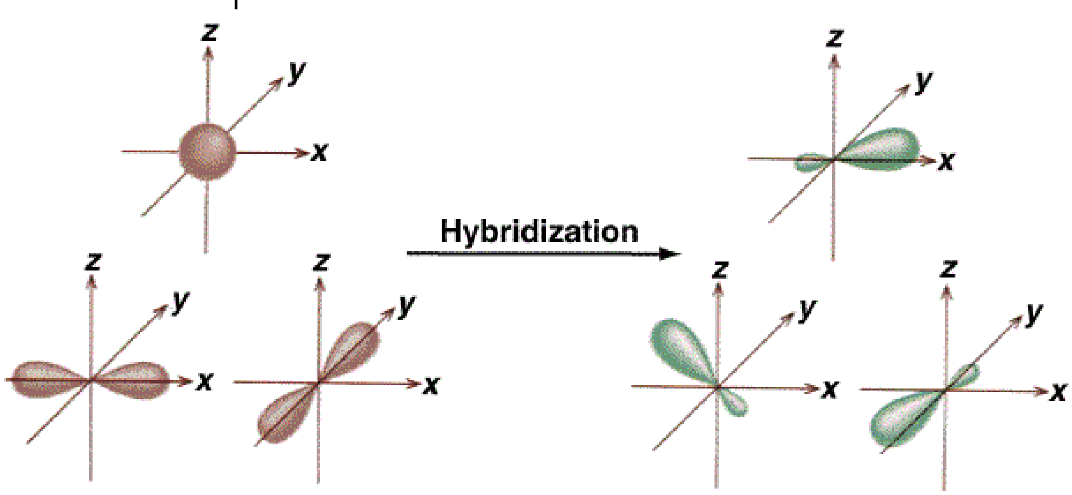
H_2O is **V-shape** because of 4 effective e^- pairs around oxygen with two lone pairs and 2 bonding pair. Due to two lone pair repulsions, **bond angle is 105°**.

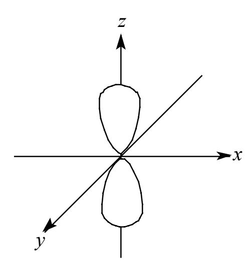
c. State the type hybrid orbitals



All e^- pairs around the oxygen atom have $2sp^3$ orbitals. Both hydrogen atoms have $1s$ orbitals.

2. sp^2 Hybridization: - characterized by **3 effective electron pairs** where one s and two p orbitals are mixed. One set of p orbital remains unmixed and becomes the π bond.
- orbital shapes around the atom involved are trigono planar and linear.
- there is at least one bonding electron pair that is a σ bond, one other bonding pair is a π bond. (together they make a double bond)
- the notable exception is boron compounds. Boron has 3 valance electrons. Even with sp^2 hybridization (due to the trigono planar geometry), there are no electrons in the unmixed p orbital. Thus, no π bond and no double bond.
- bond angles can be 120° and 180°.



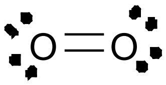


p_z orbital for π bond

3 Effective e^- Pairs (for lone pairs or σ bonds)

Example 2: Describe the bonding of O_2 using the LE model.

a. Lewis Structure and Formal Charge:



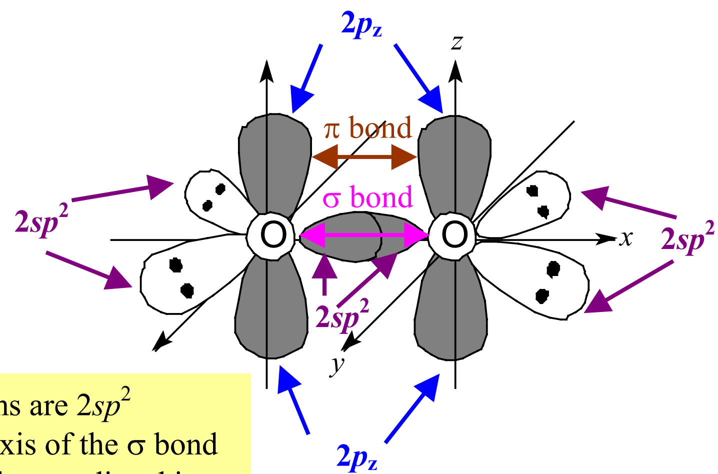
Minimizes Formal Charge
O = 6 – 4 – ½(4) = 0

b. VSEPR model:

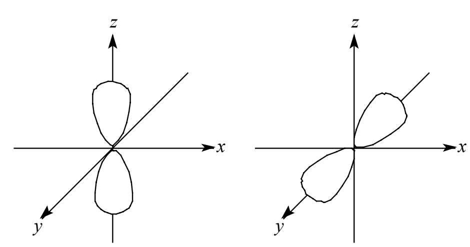
O_2 is **linear** because of 3 effective e^- pairs around oxygen with 2 lone pairs and 1 bonding pair. Due to the single bonding pair (σ and π bonds) between two nuclei, the **bond angle is 180°**.

All lone pairs and the σ bond around both oxygen atoms are $2sp^2$ orbitals. The $2p_z$ orbitals situate above and below the axis of the σ bond become the π bond. Together, they form a double bond as predicted in the Lewis structure.

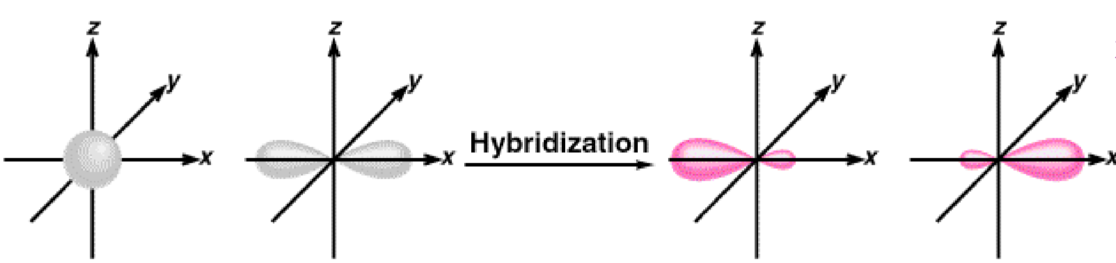
c. State the type hybrid orbitals



3. *sp* Hybridization: - characterized by **2 effective electron pairs** where one *s* and one *p* orbitals are mixed. Two sets of *p* orbitals remain unmixed and become two π bonds.
- orbital shape around the atom involved is linear.
- at least one bonding electron pair is a σ bond, two other bonding pairs are π bonds. (together they make a triple bond or two double bonds)
- the notable exception is beryllium compounds. Be has 2 valance electrons. Even with *sp* hybridization (due to the linear geometry), there is no electrons in the two unmixed *p* orbitals. Thus, no π bonds and no triple bond.
- bond angles are 180°.



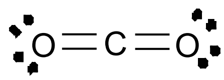
p_y and p_z orbitals for π bonds



2 Effective e^- Pairs (for lone pairs or σ bond)

Example 3: Describe the bonding of CO_2 using the LE model.

a. Lewis Structure and Formal Charge:

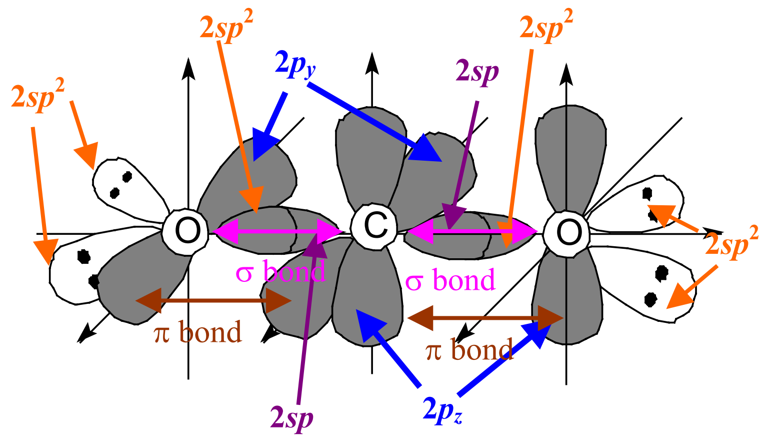


Minimize Formal Charges
C = 4 – 0 – ½(8) = 0
O = 6 – 4 – ½(4) = 0

b. VSEPR model:

CO_2 is **linear** because of 2 effective e^- pairs around the central carbon with no lone pairs and 2 bonding pair. Due to the two double bonds between the three nuclei, the **bond angle is 180°**.

c. State the type hybrid orbitals

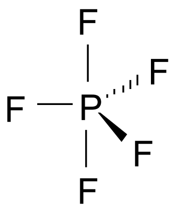


The 2*sp* orbital form the bonds on the left and right side of the carbon atom form the two σ bonds. All lone pairs and the σ bond around both oxygen atoms are $2sp^2$ orbitals. The $2p_z$ orbitals situate above and below the axis of the σ bond become the one of the two π bonds. The other π bond comes from the $2p_y$ orbital into and out of the page. Together, they form two double bonds as predicted in the Lewis structure.

4. dsp^3 Hybridization: - characterized by **5 effective electron pairs** where one *s*, three *p* and one *d* orbitals are mixed.
- possible orbital shapes around the atom involved are trigono bipyramid, see-saw, T-shape, and linear.
- all bonding electron pairs are σ bonds.
- bond angles can be 120° and 90°, or 180°.

Example 4: Describe the bonding of PF_5 using the LE model.

a. Lewis Structure and Formal Charge:

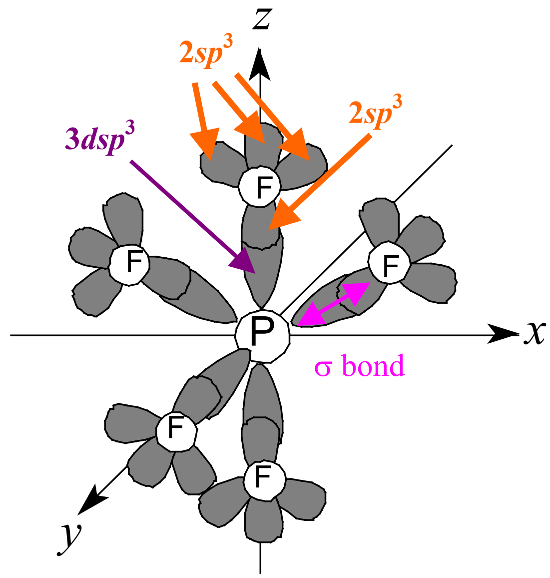


Minimize Formal Charges
P = 5 – 0 – ½(10) = 0
F = 7 – 6 – ½(2) = 0

b. VSEPR model:

PF_5 is **trigono bipyramid** because of 5 effective e^- pairs around the central phosphorus atom with no lone pairs and 5 bonding pair. Due to these five bonding pairs, the **bond angles are 120° and 90°**.

c. State the type hybrid orbitals

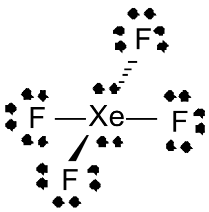


All e^- pairs around the phosphorus atom have $3dsp^3$ orbitals, and all five fluorine atoms have $2sp^3$ orbitals. There are a total of 5 sigma bonds. Each composes of an overlapping between these $3dsp^3$ and $2sp^3$ orbitals.

5. d^2sp^3 Hybridization: - characterized by **6 effective electron pairs** where one *s* and two *p* orbitals are mixed.
- possible orbital shapes around the atom involved are octahedral, square pyramid and square planar.
- all bonding electron pairs are σ bonds.
- bond angles are 90°.

Example 5: Describe the bonding of XeF_4 using the LE model.

a. Lewis Structure and Formal Charge:

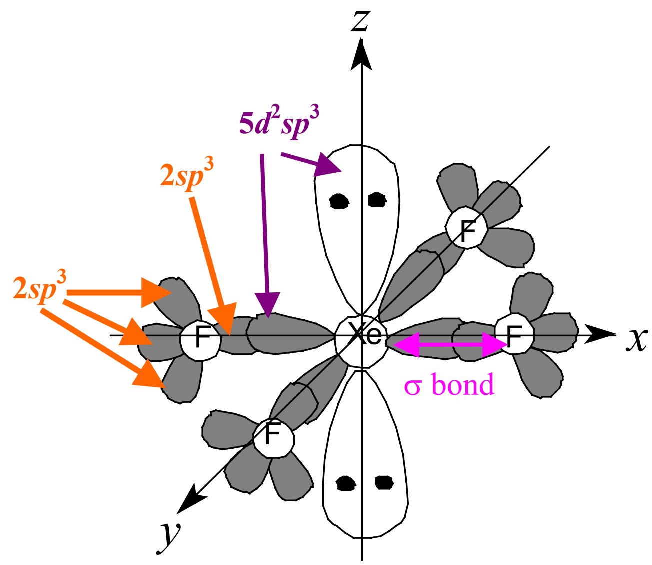


Minimize Formal Charges
Xe = 8 – 4 – ½(8) = 0
F = 7 – 6 – ½(2) = 0

b. VSEPR model:

XeF_5 is **<u>square planar</u>** because of 6 effective e^- pairs around the central xenon atom with two lone pairs and 4 bonding pair. Due to these four bonding pairs bonding pairs, the **<u>bond angles are 90°</u>**.

c. State the type hybrid orbitals



All e^- pairs around the xenon atom have $5d^2sp^3$ orbitals, and all four fluorine atoms have $2sp^3$ orbitals. There are a total of 4 σ bonds and 2 lone pairs. Each sigma bond composes of an overlapping between these $5d^2sp^3$ and $2sp^3$ orbitals.

<u>Assignment</u>
9.1 pg.441 – 442 #11 to 14, 19 to 23