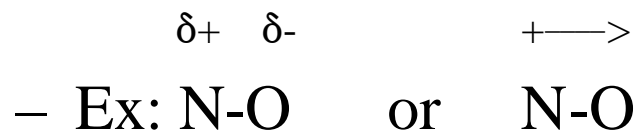


# Comments

- Final-review first two exams and quizzes-  
compilation will be posted
- Comments on second exam
- Lewis Structure page posted #117
- Born-Haber Cycles-you are responsible for the  
presentation as shown in page #167

## Electronegativity and bond polarity

- Electronegativity is a measure of the ability of an atom to attract bonding electrons
- Not surprisingly, it follows the same trends as the other electron attracting properties (ionization energy and electron affinity).
- Increases toward the upper right of the periodic table
- A heteronuclear bond will be polarized with the negative end toward the more electronegative element:



- Bond polarity introduces an ionic component to heteronuclear bonds, resulting in their being

# Exceptions to the Octet Rule

- The octet rule is violated very often.
  - Elements prior to Ne will never have more than 8 assigned electrons
  - Violations of the octet rule prior to Ne are of two types
    - Electron deficient-fewer than 8 total electrons- $\text{BH}_3$ ,  $\text{BF}_3$ . Much of the chemistry of electron deficient compounds can be explained by the “need” to obtain eight. They are generally electron acceptors in a variety of ways  $\text{BH}_4^-$ ,  $\text{BF}_4^-$
    - Odd electron compounds  $\cdot\text{NO}_2$  readily forms  $\text{NO}_2^-$  and dimerizes to make  $\text{N}_2\text{O}_4$   $\text{O}_2\text{N}-\text{N}_2\text{O}$
  - Electron rich compounds-nobel gas and interhalogens and so on:  
 $\text{XeF}_4$ ,  $\text{ClF}_3$ ,  $\text{SF}_6$

## VSEPR-Predicting shapes of polyatomic groups

- The shape of a polyatomic grouping can be predicted with considerable accuracy using a simple premise
  - The groups around the central atom (bonds and lone pairs) are all electron rich and repel each other
  - They will arrange in a geometry that minimizes the repulsions by maximizing the distances (and angles) between the groups
- If we describe the grouping as  $AB_z$ , where A is the central atom and there are z B groups (bonds and lone pairs) attached to it the geometries are

- For  $AB_z$

z	Geometry	angles
1	Linear	none
2	Linear	180°
3	Trigonal planar	120°
4	Tetrahedron	109.5°
5	Trigonal bipyramid or Square pyramid	90,120,180 90,120,180
6	octahedron	90,180

## Breaking down B

- B can be either a bond or lone pair. Thus, we can break the overall formula  $AB_z$  in into a more descriptive formula  $AX_mE_n$ , where X is a bond and E is a lone pair.
- Note that only molecules where a bond angle can exist will be discussed from this point on. This requires at least two groups attached to the central atom.
- Also, a complex molecule will have multiple centers.

For  $AX_mE_n$  (also see text – Table 7.4)

z	m	n	Example
2	2	0	$BeCl_2$
3	3	0	$BF_3$
3	2	1	$SO_2$
4	4	0	$CH_4$
4	3	1	$NH_3$
4	2	2	$H_2O$
5	5	0	$PF_5$
5	4	1	$SF_4$
5	3	2	$ClF_3$
5	2	3	$XeF_2$
6	6	0	$SF_6$
6	5	1	$BrF_5$
6	4	2	$XeF_4$
6	3	3	?

# Details-what are bonds and how do you get the shapes

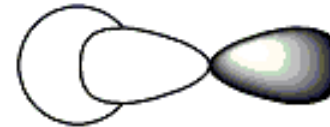
- VBT-bonds form from the overlap of atomic orbitals.
  - a bond is the result of an electron orbital that extends over more than one nucleus
  - two general types: $\sigma$ -symmetric about the internuclear axis



Two s orbitals



Two p orbitals



s + p

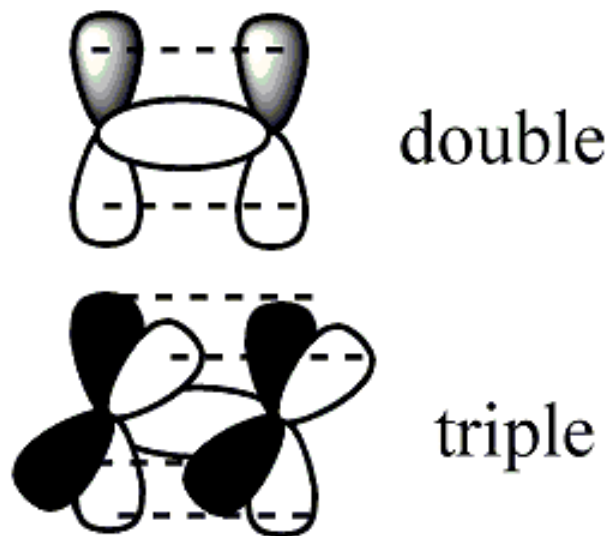
- $\pi$ -normally from the side on overlap of p orbitals-node along the internuclear axis





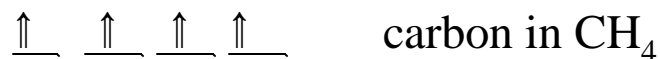
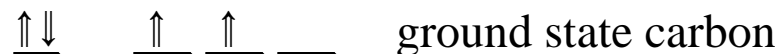
## More on bonding orbitals

- All single bonds are of type  $\sigma$
- Multiple bonds consist of a  $\sigma$  plus the number of  $\pi$  bonds needed for the total bond order:
  - double =  $\sigma$  + one  $\pi$
  - triple =  $\sigma$  + two  $\pi$



# Hybridization

- $\text{CH}_4$  is known to be a tetrahedral molecule with 4 single bonds from the C to the Hs all the same. This would seem to require 4 equivalent orbitals on the carbon at  $109.5^\circ$  each having one unpaired electron. Carbon's valence orbitals consist of the 2s and the three 2p, which certainly don't meet the criteria.

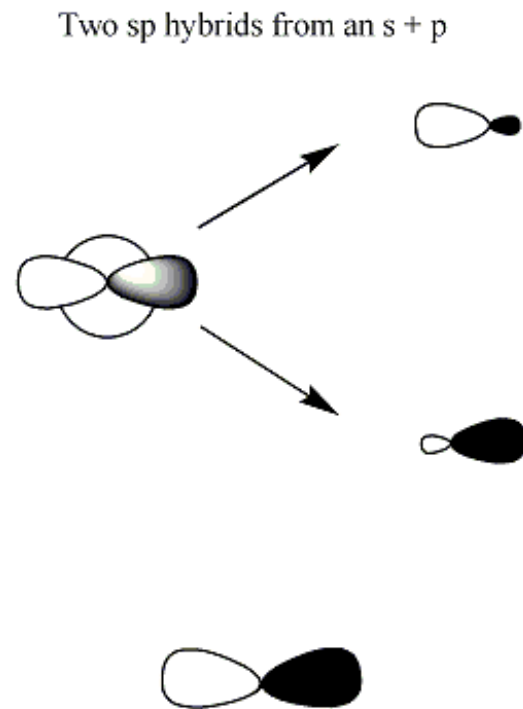


The process is described as having two steps. The promotion of a 2s electron to the 2p orbital and a mixing of the s and ps to generate the four equivalent orbitals

The Hs all have the config  $\uparrow$

# Hybridization

- The explanation involves the combination of the valence atomic orbitals on an atom to produce a new set-this is called hybridization.
  - an s plus a p orbital produces a new orbital (and shape)



# Hybridization Types

- Hybridization is an approach to explaining structures which do not fit the available valence orbitals
  - hybrids are used in the  $\sigma$  component and for lone pairs of electrons, so the number of hybrids equals the number of such groups. Unhybridized p orbitals are used in  $\pi$  bonds
    - $sp^3$  – a total of four  $\sigma$  bonds and lone pairs – no  $\pi$  bonds
    - $sp^2$  – a total of three  $\sigma$  bonds and lone pairs – one  $\pi$  bond is possible
    - $sp$  – a total of two  $\sigma$  bonds and lone pairs – two  $\pi$  bonds are possible
  - invoking hybridization usually requires information about the species, in particular bond angles. Geometries are based on atom positions. Thus,  $CH_4$  is tetrahedral,  $NH_3$  (3 bonds and one lone pair) is pyramidal and  $H_2O$  (2 bonds and two lone pairs) is bent.