

Ch. BondingI. Bond Character

Bonds are usually combinations of ionic and covalent character.

The **electronegativity difference** is used to determine a bond's character.

## Electronegativity Difference

|                  |   |                     |   |                       |
|------------------|---|---------------------|---|-----------------------|
| <b>Covalent</b>  | < | <b>1.67</b>         | < | <b>Ionic</b>          |
| shared electrons |   | <b>50% ionic</b>    |   | transferred electrons |
| weaker bonds     |   | <b>50% covalent</b> |   | stronger bonds        |

Ex. 1) F—F bond in F<sub>2</sub>

4.0 4.0

$4.0 - 4.0 = 0 < 1.67$  **100% covalent**, no transfer of electrons

Ex. 2) Na—Cl in NaCl

0.9 3.0

$3.0 - 0.9 = 2.1 > 1.67$  **mainly ionic**  
(large difference in electronegativities)

Na—Cl is **polar**. There is a difference in charge.

$\delta(+)$   $\delta(-)$  Na wants to lose electrons, Cl wants to gain electrons.

Ex. 3) S—Cl in SCl<sub>6</sub>

2.5 3.0

$3.0 - 2.5 = 0.5 < 1.67$  **mainly covalent**

S and Cl both want to gain electrons, but Cl (higher electronegativity) wants electrons more than S. The bond is still **polar**, but not as much as NaCl.

**\*\* The farther apart the elements on the periodic table, the larger the electronegativity difference, the more ionic the bond, the more polar the bond and the stronger the bond.**

**Most Polar** (most ionic)

Na—Cl

(**farthest apart** on periodic table)

> S—Cl

**Least Polar** (least ionic)

F—F

(**closest together**)

Ex. 1) Which is more polar? Ga—P or Ga—F?

**Ga—F are farther apart, larger electronegativity difference, more polar**

A) For ionic bonds the energy can be calculated, using Coulomb's Law.

$$E = 2.31 \times 10^{-19} \text{ J} \cdot \text{nm} \frac{(Q_1 Q_2)}{r}$$

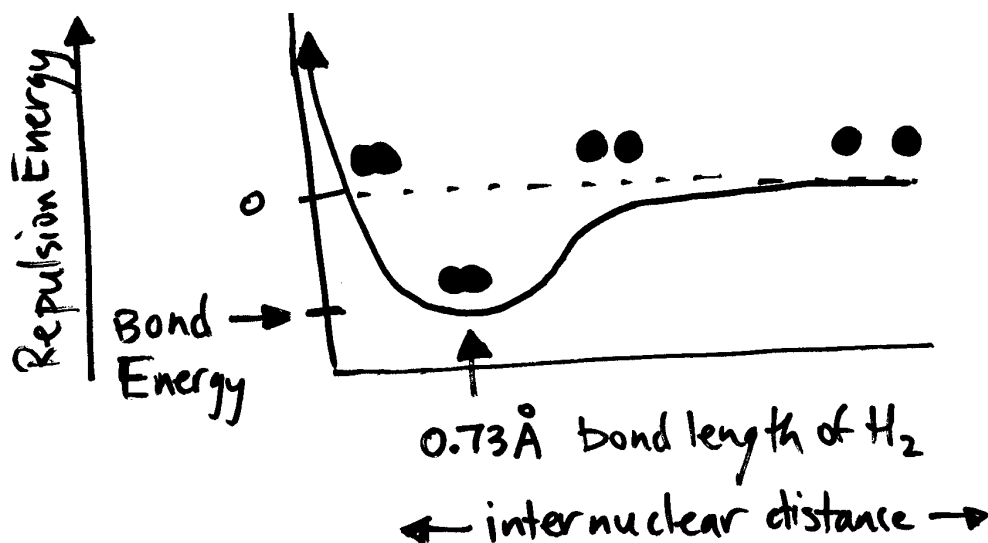
$Q_1, Q_2 = \text{the charges of the ions}$   
 $r = \text{the bond length}$

For NaCl:  $E = 2.31 \times 10^{-19} \text{ J} \cdot \text{nm} \frac{(+1)(-1)}{(0.276 \text{ nm})} = -8.37 \times 10^{-19} \text{ J}$

*the (-) shows that is an attractive force*

**\*\*The larger the charges, the stronger the bond, the greater the attraction.**

B) But covalent bonds share electrons, so the **Repulsion Energy** must be measured.



On the left: the H atoms are too close together and the nuclei will repel each other.  
( High repulsion energy)

On the right: the H atoms are too far apart and there is no attraction between atoms.  
(Zero repulsion energy)

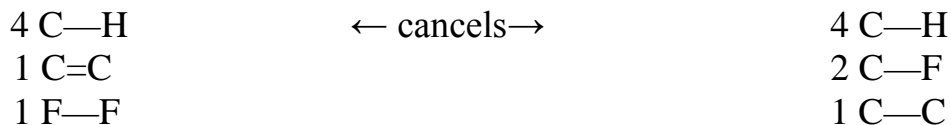
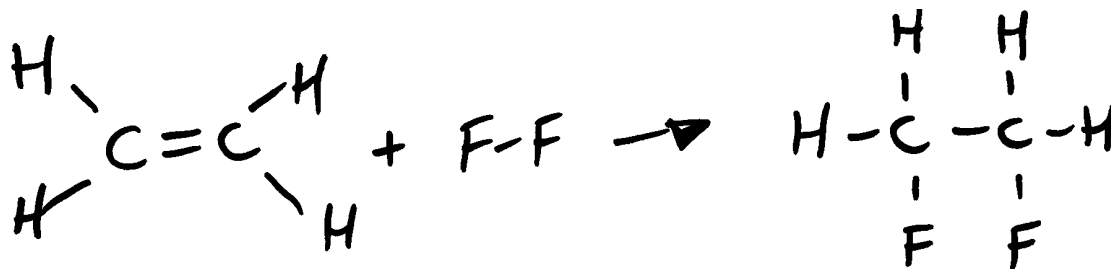
At the bond length of 0.73 Å: the H atoms are at the best distance, so that electrons are attracted to both nuclei and the electron repulsion is minimized. The atoms will bond.  
(**negative repulsion energy would equal positive attraction energy**)

These bond energies are measured and found on Bond Energy Table in textbook.

When reactions occur energy is gained (+) by atoms to break bonds and released (-) by atoms as new more stable bonds form. This calculates  $\Delta H$  for the reaction.

$$\Delta H_{\text{reaction}} = \sum E_{\text{bonds broken}} - \sum E_{\text{bonds formed}}$$

reactants                      products



$$\begin{aligned}
 \Delta H_{\text{reaction}} &= [(1 \text{ C}=\text{C}) (614 \text{ kJ}) + (1 \text{ F}-\text{F}) (154 \text{ kJ})] - \\
 &\quad [ (2 \text{ C}-\text{F}) (485 \text{ kJ}) + (1 \text{ C}-\text{C}) (347 \text{ kJ}) ] \\
 &= 614 \text{ kJ} + 154 \text{ kJ} - 970 \text{ kJ} - 347 \text{ kJ} = \mathbf{-549 \text{ kJ favorable}}, \text{ since } (-).
 \end{aligned}$$

## #61 Notes II. Localized Electron Model

A molecule is composed of atoms that are bound together by sharing pairs of electrons, using the atomic orbitals of the bound atoms.

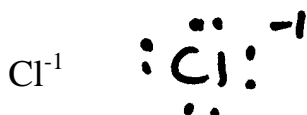
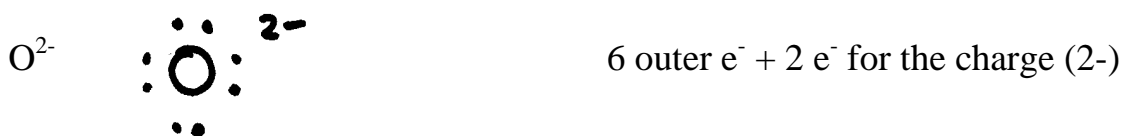
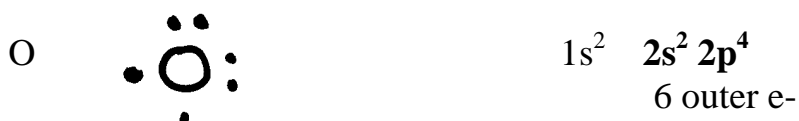
Bonding Pairs: pairs of  $e^-$  found in the space between atoms that form bonds

Lone Pairs: nonbonding pairs of  $e^-$  found elsewhere on an atom

### A) Lewis Structures

-show how the valence (outer shell) electrons are arranged around the atoms in a molecule.

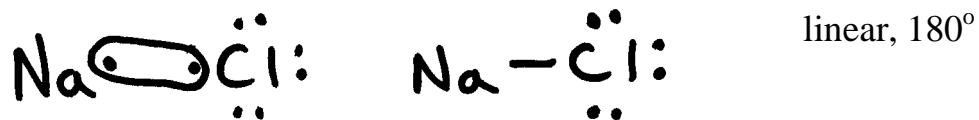
Octet Rule: atoms try to achieve a noble gas configuration of 8 electrons.



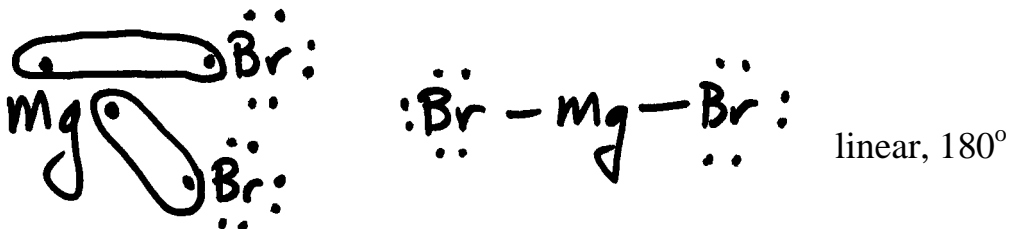
## B) VSEPR Model (Valence Shell Electron Pair Repulsion)

The structure around an atom is determined principally by minimizing electron pair repulsions.

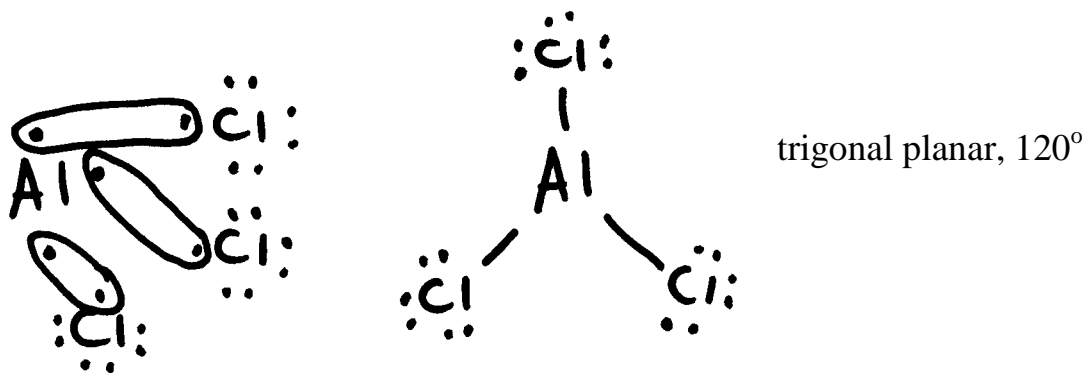
Ex. 1) NaCl



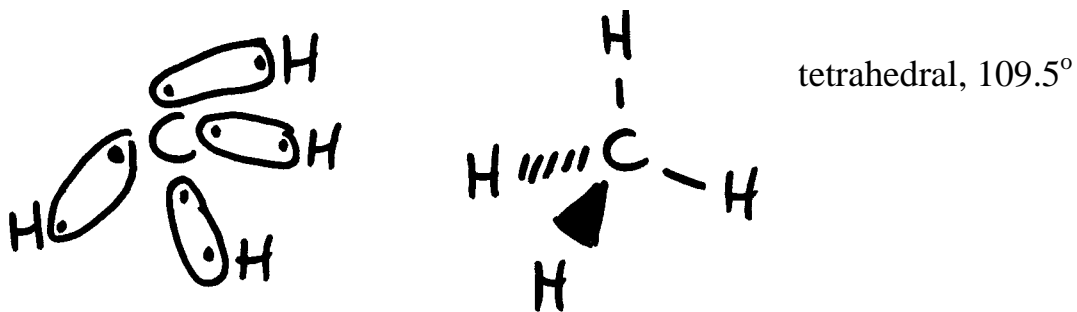
Ex. 2) MgBr<sub>2</sub>



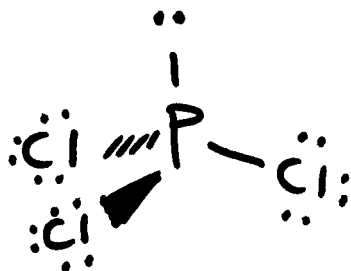
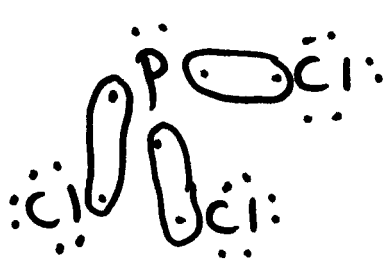
Ex. 3) AlCl<sub>3</sub>



Ex. 4) CH<sub>4</sub>

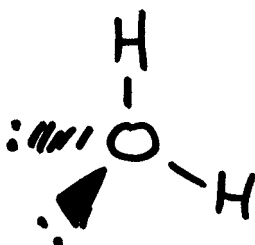


Ex. 5)  $\text{PCl}_3$



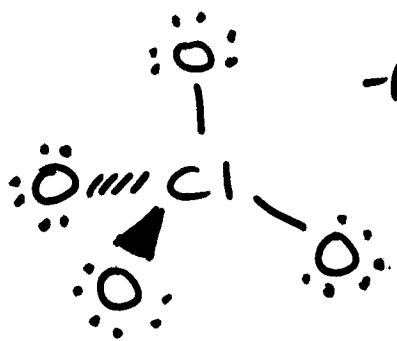
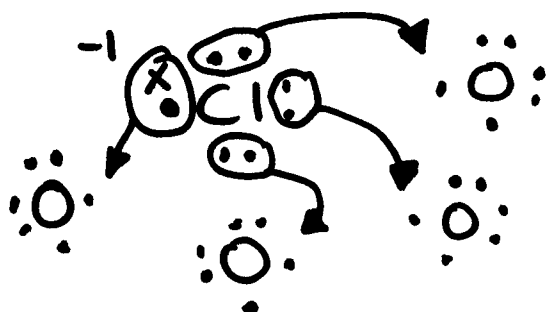
trigonal pyramidal,  $107^\circ$

Ex. 6)  $\text{H}_2\text{O}$



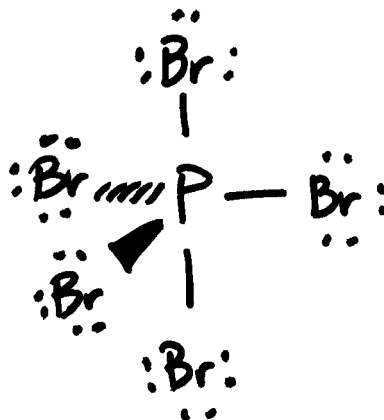
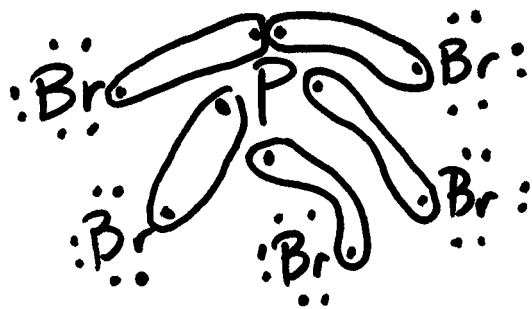
bent,  $104.5^\circ$

Ex. 7)  $\text{ClO}_4^-$

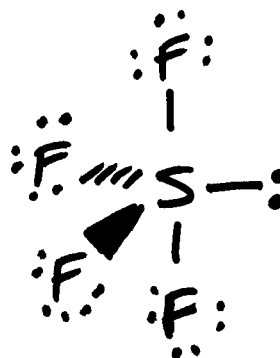


tetrahedral,  $109.5^\circ$

Oxygen will take two  $e^-$  to have a noble gas configuration, O is greedy!

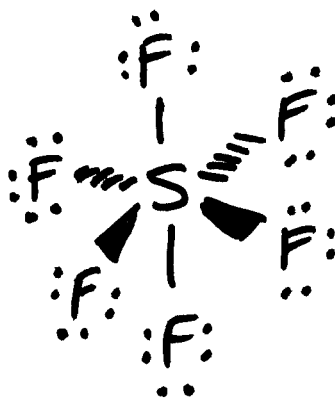
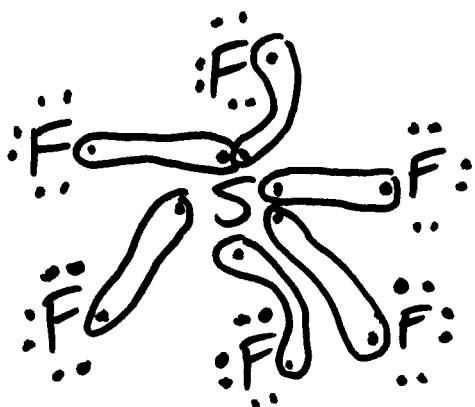


trigonal bipyramidal,  $90^\circ$  &  $120^\circ$



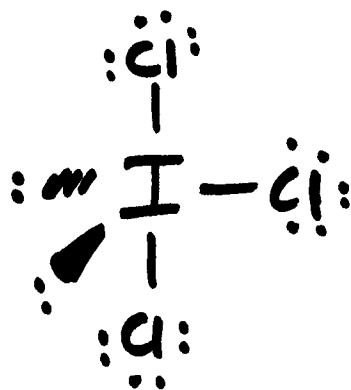
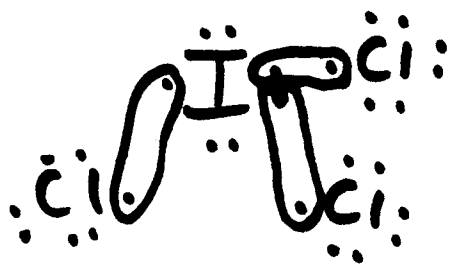
**\*\*e<sup>-</sup> must be around the middle**  
(irregular tetrahedron, bisphenoid)

seesaw,  $<90^\circ$  &  $<120^\circ$



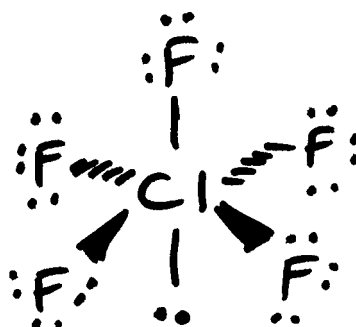
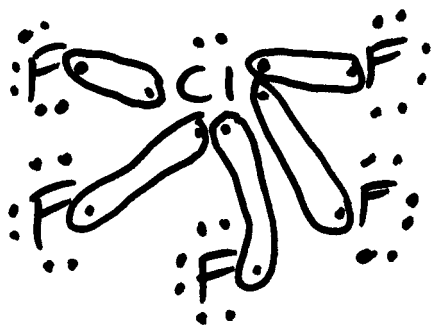
octahedral,  $90^\circ$

Ex. 11)  $\text{ICl}_3$



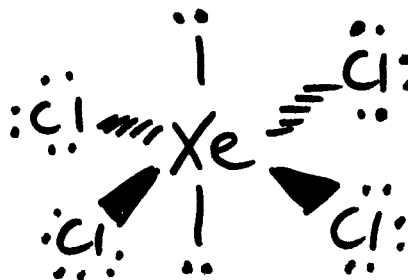
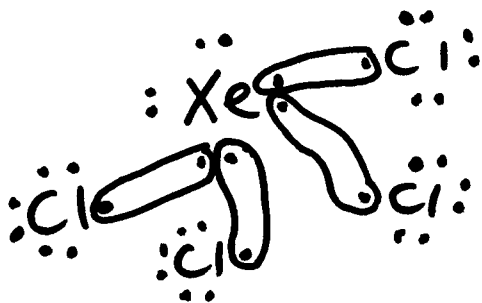
T-shaped,  $<90^\circ$   
( $e^-$  must be around middle)

Ex. 12)  $\text{ClF}_5$



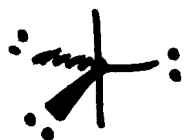
square pyramidal,  
 $<90^\circ$

Ex. 13)  $\text{XeCl}_4$



square planar,  
 $90^\circ$

\*\*  $e^-$  must be across from each other



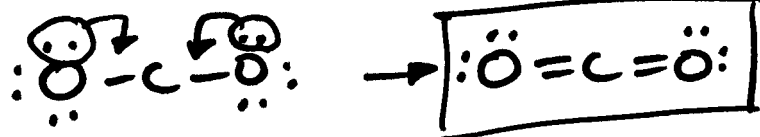
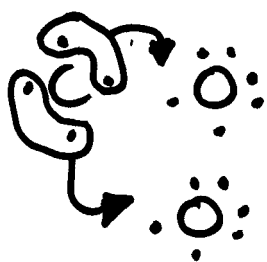
linear,  $180^\circ$

Ex. 14) NaCN



linear,  $180^\circ$

Ex. 15) CO<sub>2</sub>



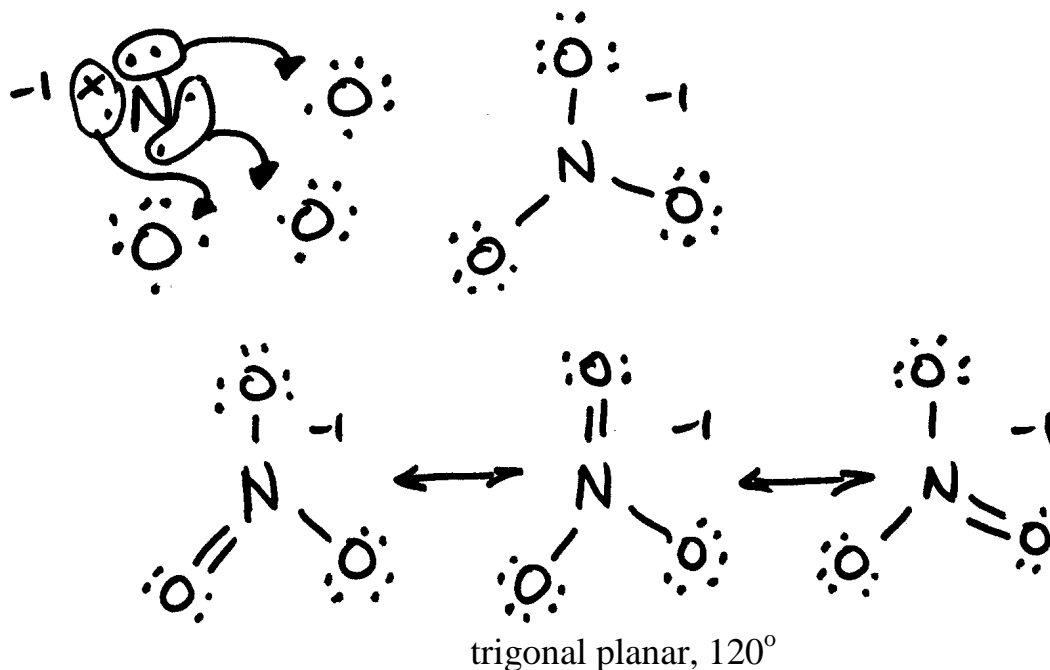
linear,  $180^\circ$



### #63 Notes III. Resonance

-is when more than one Lewis structure is possible.

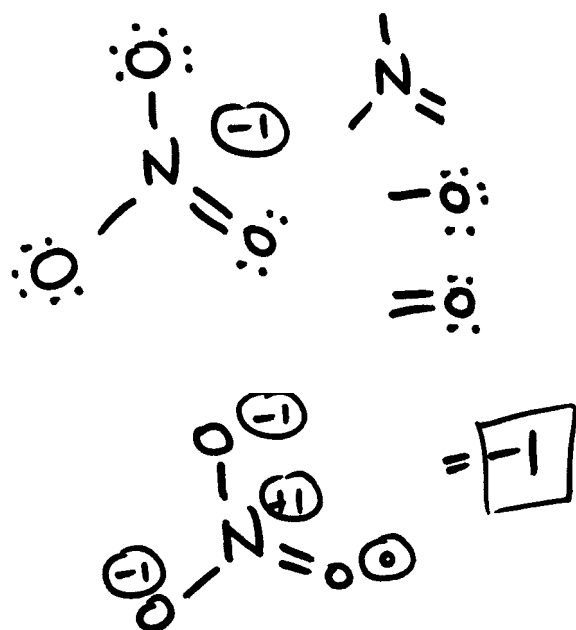
$\text{NO}_3^-$

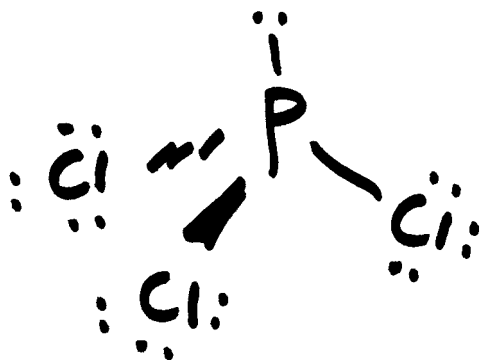


The electrons in the bonds are delocalized, making this more stable than all single bonds.  
\*\*Each N—O bond is  $2/3$  single and  $1/3$  double in character.

### IV. Formal Charge

Formal Charge = # valence electrons on lone atom (outer  $e^-$  from the periodic table)  
- # valence electrons on the atom in the compound ( all lone electrons plus one electron per bond)

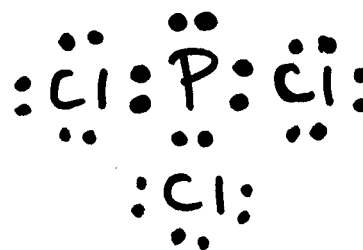




←Don't count the stick, it only shows position of the electrons on P. (only 2 e<sup>-</sup> total)

$$\begin{aligned} \text{P} \quad \text{F.C.} &= 5 \text{ e}^- - 5 \text{ e}^- = 0 \\ & (5 \text{ e}^- \text{ per. table} - \{3 \text{ e}^- \text{ from bonds} + 2 \text{ lone e}^-\}) \end{aligned}$$

**Official Lewis Dot Diagrams** only show electrons  
(no bonds):



## V. Polarity

*Polar means (+)/(-) ends on the molecule. The ends are different!*

\*\* unsymmetrical (**unbalanced**) = {(+) and (-) ends to the molecule} = **polar**

\*\*symmetrical (**balanced**, it will not have (+)/(-) ends, the ends are the same) = **nonpolar**  
[ 2 prefixes not together ( un & non) ]

(see notes #61-62 for structures)

|                                      |          |
|--------------------------------------|----------|
| Ex. 1) NaCl                          | polar    |
| Ex. 2) MgBr <sub>2</sub>             | nonpolar |
| Ex. 3) AlCl <sub>3</sub>             | nonpolar |
| Ex. 4) CH <sub>4</sub>               | nonpolar |
| Ex. 5) PCl <sub>3</sub>              | polar    |
| Ex. 6) H <sub>2</sub> O              | polar    |
| Ex. 7) ClO <sub>4</sub> <sup>-</sup> | nonpolar |
| Ex. 8) CO <sub>2</sub>               | nonpolar |
| Ex. 9) NaCN                          | polar    |
| Ex. 10) PBr <sub>5</sub>             | nonpolar |
| Ex. 11) SF <sub>4</sub>              | polar    |
| Ex. 12) SF <sub>6</sub>              | nonpolar |
| Ex. 13) IBr <sub>3</sub>             | polar    |
| Ex. 14) ClF <sub>5</sub>             | polar    |
| Ex. 15) XeCl <sub>4</sub>            | nonpolar |

#64 Notes Ch. Bonding Orbitals

I. Hybridization (a mixture of orbitals)

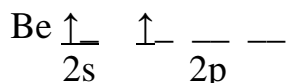
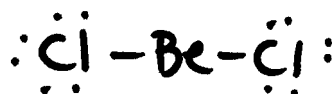
-is a modification to the localized electron model to account for the observation that atoms will continue and modify orbitals when bonding.

| <u>Compound</u> | <u># of bonds</u> | <u>orbitals used</u> | <u>hybrid</u> |
|-----------------|-------------------|----------------------|---------------|
|-----------------|-------------------|----------------------|---------------|

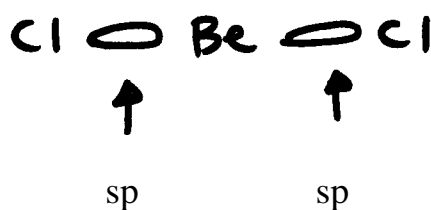
|                             |          |          |             |
|-----------------------------|----------|----------|-------------|
| <b>Ex. 1) H<sub>2</sub></b> | <b>1</b> | <b>s</b> | <b>none</b> |
|-----------------------------|----------|----------|-------------|

H—H      H  $\uparrow$     The electron from the other H can go into this  
                  1s    orbital to make the bond.

|                                |          |             |           |
|--------------------------------|----------|-------------|-----------|
| <b>Ex. 2) BeCl<sub>2</sub></b> | <b>2</b> | <b>s, p</b> | <b>sp</b> |
|--------------------------------|----------|-------------|-----------|

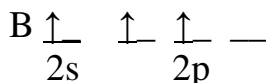
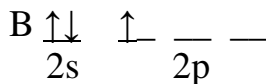
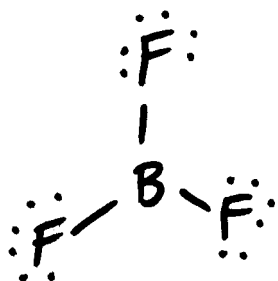


Now that the electrons are separated, the 2 Cl's can each move in one electron to make a bond.

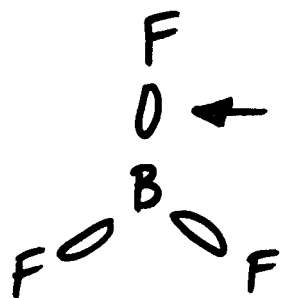


Two equivalent orbitals (1/2 s, 1/2 p).

|                              |          |                |                       |
|------------------------------|----------|----------------|-----------------------|
| <b>Ex. 3) BF<sub>3</sub></b> | <b>3</b> | <b>s, p, p</b> | <b>sp<sup>2</sup></b> |
|------------------------------|----------|----------------|-----------------------|



Now the electrons are separated and each F can move in one electron to make a bond.

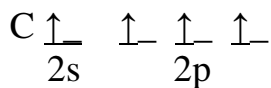
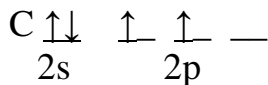
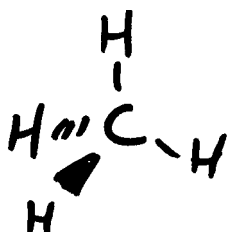


$sp^2$  Three equivalent orbitals (1/3 s, 2/3 p).

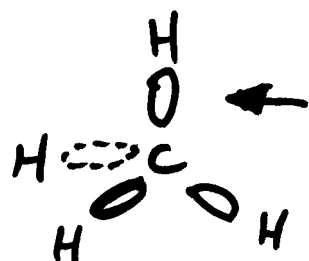
Ex. 4)  $CH_4$

4 s, p, p, p

$sp^3$



Now each H can move in one electron to bond.

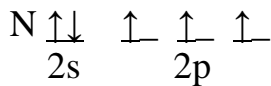
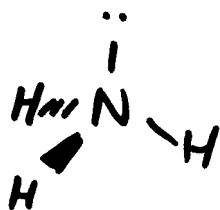


$sp^3$  4 equivalent orbitals (1/4 s, 3/4 p).

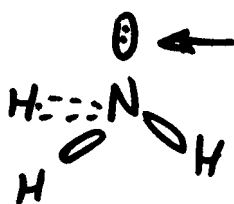
Ex. 5)  $NH_3$

3 + 1 lone pair s, p, p, p

$sp^3$



Each H can move in one electron (2  $e^-$  in the 2s are the lone pair of electrons) to bond.

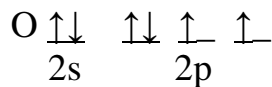
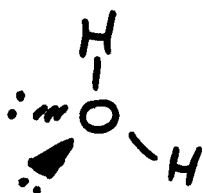


$sp^3$  4 equivalent orbitals (1/4 s, 3/4 p).

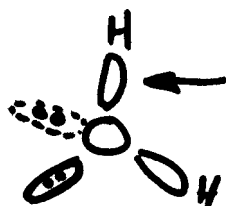
Ex. 6) H<sub>2</sub>O

2 + 2 lone pairs s, p, p, p

sp<sup>3</sup>



Each H can move in one electron to bond.



sp<sup>3</sup>

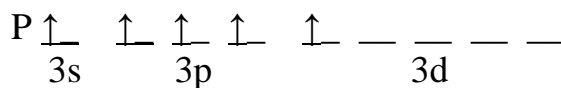
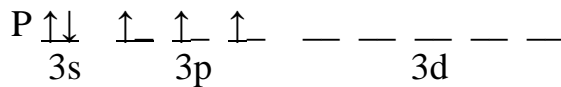
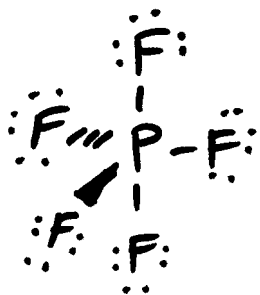
4 equivalent orbitals (1/4 s, 3/4 p).

Ex. 7) PF<sub>5</sub>

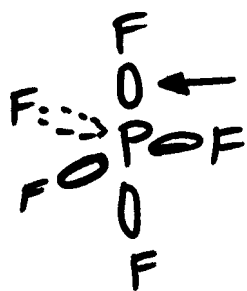
5

s, p, p, p, d

dsp<sup>3</sup>



Now each F can move in an electron to bond.



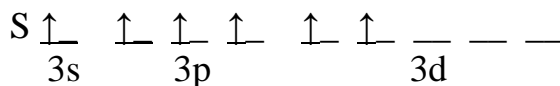
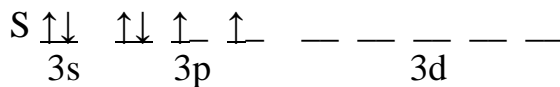
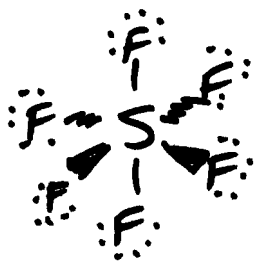
dsp<sup>3</sup>

5 equivalent orbitals (1/5 s, 3/5 p, 1/5 d).

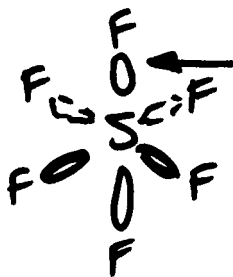
Ex. 8) SF<sub>6</sub>

6

s, p, p, p, d, d      d<sup>2</sup>sp<sup>3</sup>



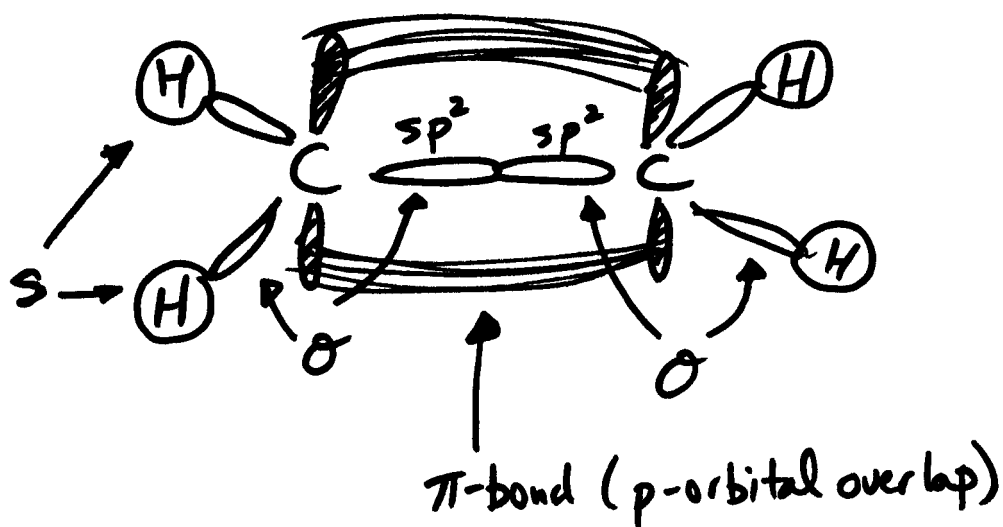
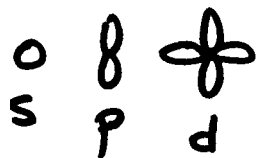
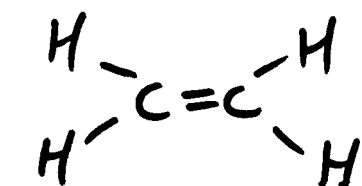
Now each F can move in one electron to bond.



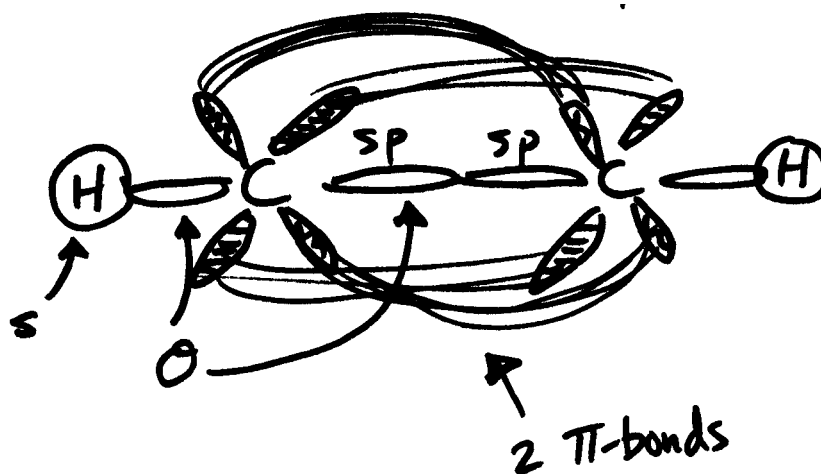
d<sup>2</sup>sp<sup>3</sup>

6 equivalent orbitals (1/6 s, 3/6 p, 2/6 d).  
 = 1/6 s, 1/2 p, 1/3 d

On fingers do: SF<sub>4</sub> (4 bonds and 1 e<sup>-</sup> pair = 5 positions/orbitals needed), so **dsp<sup>3</sup>**,  
 XeF<sub>4</sub> (4 bonds and 2 e<sup>-</sup> pairs = 6 positions/orbitals needed), so **d<sup>2</sup>sp<sup>3</sup>**



Double Bond = 1  $\sigma$  (sigma) bond & 1  $\pi$  (pi) bond {stronger than single bond}  
 1 hotdog ( $\sigma$ ) + 1 bun (2 parts of  $\pi$  bond)



Triple Bond = 1  $\sigma$  (sigma) bond & 2  $\pi$  (pi) bonds {stronger than double bond}  
 1 hotdog ( $\sigma$ ) + 2 buns ( $\pi$ )

\*\*They become successively stronger, less flexible, and more reactive.

**\*End of Notes\*** (Assignment #66 is a Review Assignment. There are no notes for this assignment.)