#52 Notes **Unit 7: Bonding**

Ch. Bonding

I. Bond Character

Bonds are usually combinations of ionic and covalent character.

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

		Electronegativity Difference		
Covalent	<	**1.67**	<	**Ionic**
shared electrons		**50% ionic**		transferred electrons
weaker bonds		**50% covalent**		stronger bonds

Ex. 1) F—F bond in F_2

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**

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

δ(+) δ(-) Na wants to lose electrons, Cl wants to gain electrons.

Ex. 3) S—Cl in SCl_6

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)				**Least Polar** (least ionic)
Na—Cl	>	S—Cl	>	F—F
(**farthest apart** on periodic table)				(closest together)

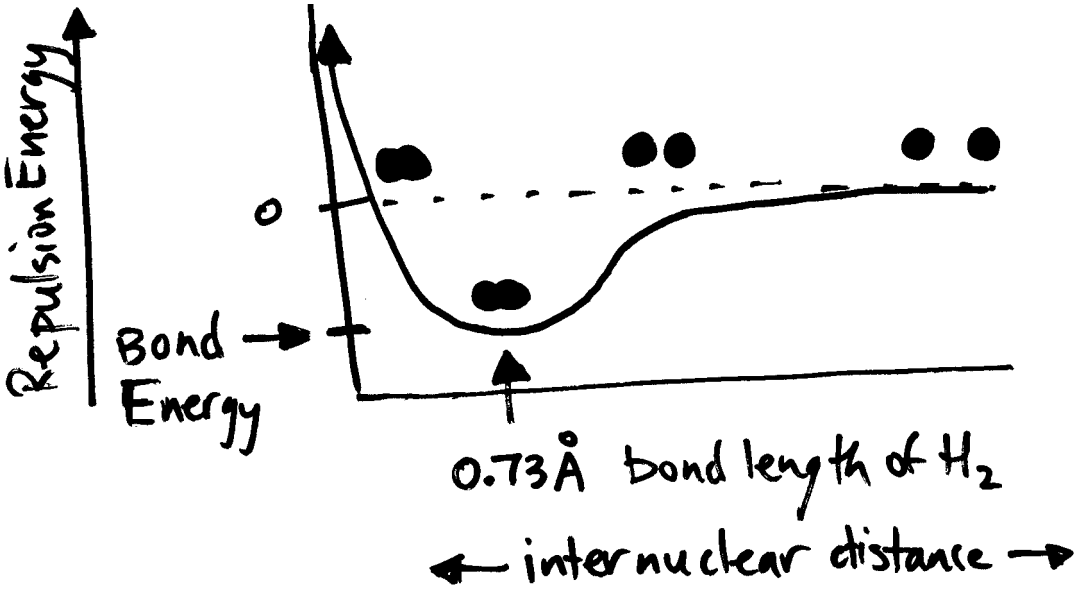
A) For ionic bonds the energy can be calculated, using Coulomb's Law.

$E = 2.31 \times 10^{-19}\ J \cdot nm \frac{(Q_1 Q_2)}{r}$ Q_1, Q_2 = the charges of the ions; r = the bond length

For NaCl: $E = 2.31 \times 10^{-19}\ J \cdot nm \frac{(+1)(-1)}{(0.276\ nm)} = \mathbf{-8.37 \times 10^{-19}\ J}$ *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 the 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 ΔH for the reaction.

$\Delta H_{reaction} = \Sigma E_{\text{bonds broken}} - \Sigma E_{\text{bonds formed}}$
reactants products

4 C—H	← cancels→	4 C—H
1 C=C		2 C—F
1 F—F		1 C—C

$\Delta H_{reaction}$ = [(1 C=C) (614 kJ) + (1 F—F) (154 kJ)] –
[(2 C—F) (485 kJ) + (1 C—C) (347 kJ)]
= 614 kJ + 154 kJ – 970 kJ – 347 kJ = **-549 kJ favorable**, since (-).

#53 Notes II. Lattice Energy (for ionic compounds)

-is the change in energy that takes place when separated gaseous ions are packed together into a solid. (energy is released, exothermic).

$M^{+}_{(g)} + X^{-}_{(g)} \rightarrow MX_{(s)}$

Lattice energy = $k \frac{(Q_1 Q_2)}{r}$ a modified version of Coulomb's Law

The **most exothermic lattice energy =the **most favorable** = the **largest attraction**

** The largest attraction will have a more concentrated charge or a larger charge difference.

Ex. 1a) Which has the most exothermic lattice energy?

NaCl or CsCl — **NaCl:** Na is a smaller ion, so its charge will be more concentrated, most favorable lattice energy.

Ex. 1b) $MgCl_2$ or NaCl — **$MgCl_2$**: Mg^{2+} Cl^{-1} has a larger charge difference (more concentrated) than Na^{+1} Cl^{-1}

The bond energies of ionic compounds can be calculated without Coulomb's Law, using the lattice energy with other energies.

Ex. 2) Find the bond energy of LiF.

$Li_{(s)} + ½ F_{2(g)} \rightarrow LiF_{(s)}$ Various energies will be provided.

Li needs to be a gas: (enthalpy of sublimation)	$Li_{(s)} \rightarrow Li_{(g)}$		157 kJ/mol
Li needs to be a (+) ion: (loses e^-, ionization energy)	$Li_{(g)} \rightarrow Li^{+1}_{(g)} + e^-$		520 kJ/mol
F2 needs to be broken to F: (bond energy)	$F_{2(g)} \rightarrow 2\ F_{(g)}$	X 1/2	152 kJ/mol ÷ 2
F needs to be a (-) ion: (gains e^-, electron affinity)	$F_{(g)} + e^- \rightarrow F^{-1}_{(g)}$		-328 kJ/mol
The ions need to form a compound: (lattice energy)	$Li^{+1}_{(g)} + F^{-1}_{(g)} \rightarrow LiF_{(s)}$		-1036 kJ/mol
	$Li_{(s)} + ½ F_{2(g)} \rightarrow LiF_{(s)}$		**-611 kJ/mol**

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

A) Lewis Structures

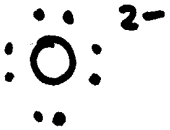
-show how the valence (outer shell) electrons are arranged around the atoms in a molecule.
Octet Rule: atoms try to achieve a noble gas configuration of 8 electrons.

Ex. 1) C 

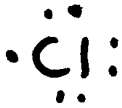
$1s^2$ $\mathbf{2s^2\ 2p^2}$
4 e^- in outer layer (valence e^-)

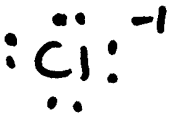
O 

$1s^2$ $\mathbf{2s^2\ 2p^4}$
6 outer e-

O^{2-} 

6 outer e^- + 2 e^- for the charge (2-)

Cl 

Cl^{-1} 

Na 

Na^{+1} 

Mg 

Mg^{2+} 

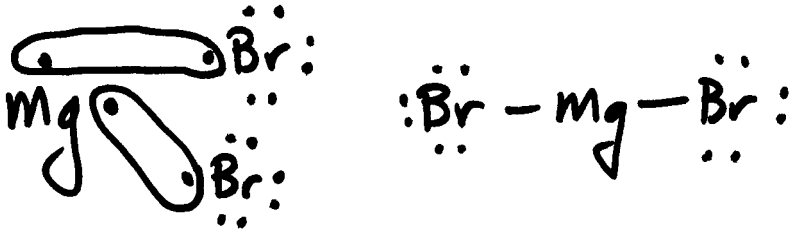
#54 Notes B) VSEPR Model (Valence Shell Electron Pair Repulsion)

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

Ex. 1) NaCl

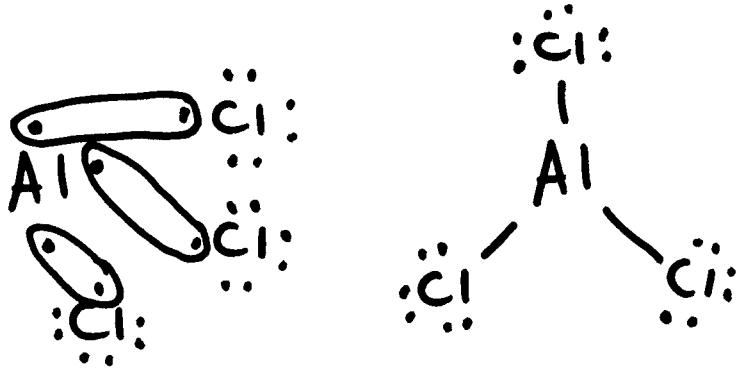
linear, 180°

Ex. 2) $MgBr_2$



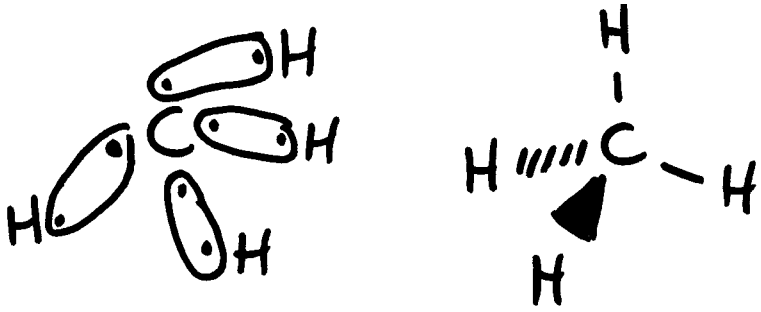
linear, 180°

Ex. 3) $AlCl_3$



trigonal planar, 120°

Ex. 4) CH_4



tetrahedral, 109.5°

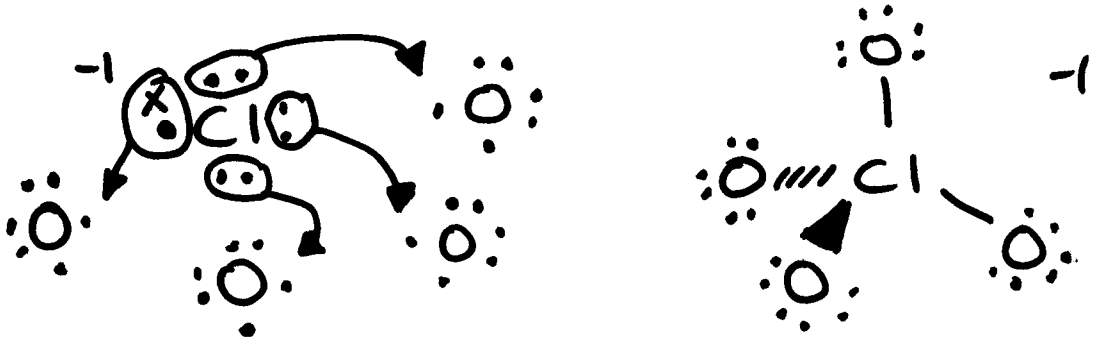
Ex. 5) PCl_3

trigonal pyramidal, 107°

Ex. 6) H_2O

bent, 104.5°

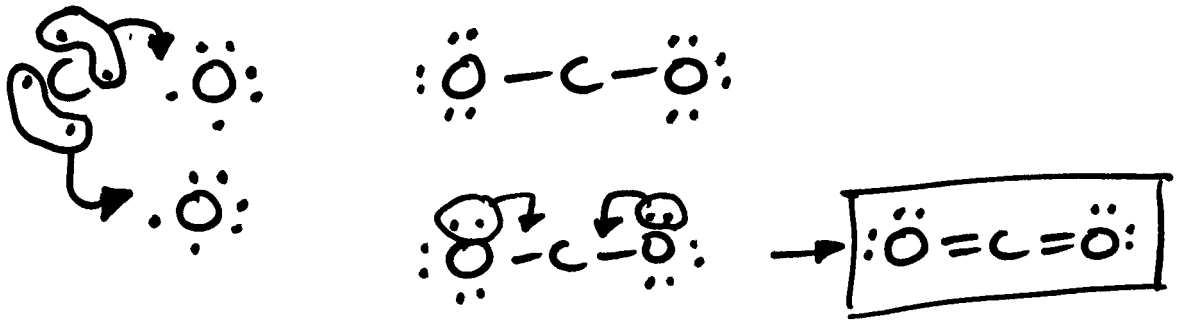
Ex. 7) ClO_4^-



tetrahedral, 109.5°

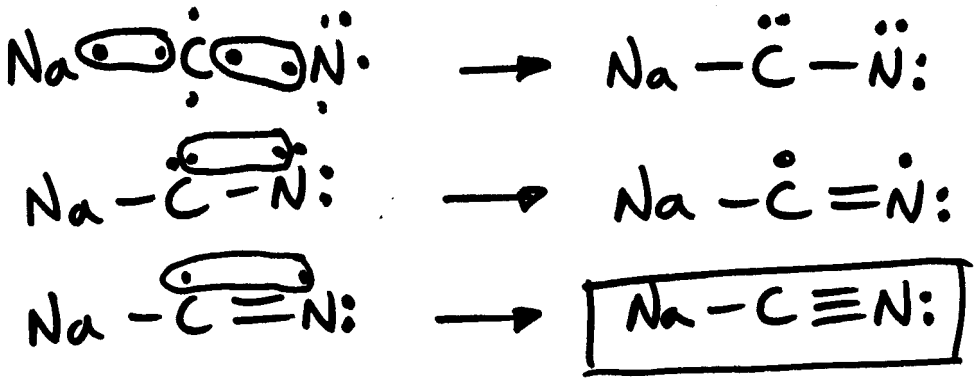
Oxygen will take two e^- to have a noble gas configuration, O is greedy!

Ex. 8) CO_2



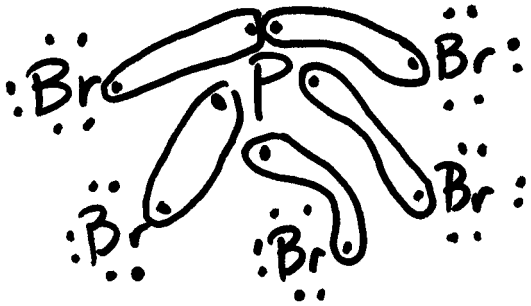
linear, 180°

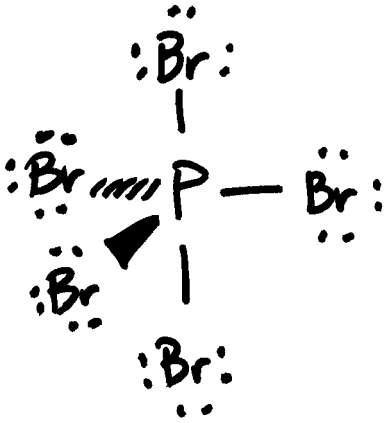
Ex. 9) NaCN



linear, 180^{o}

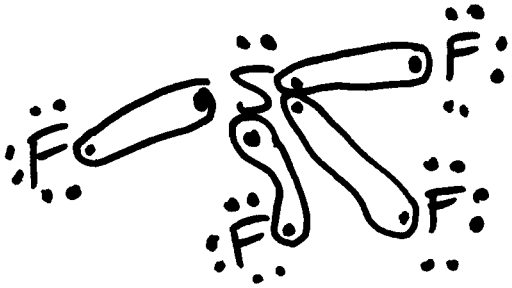
Ex. 10) PBr_5

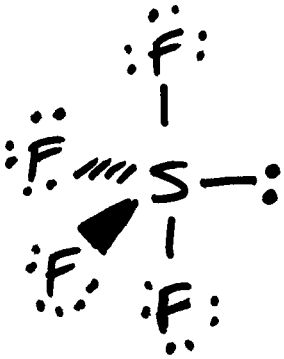




trigonal bipyramidal, 90^o & 120^o

Ex. 11) SF_4

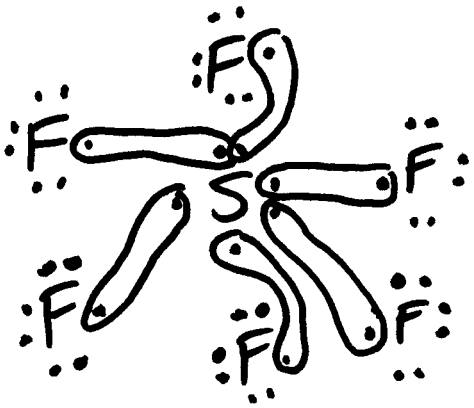


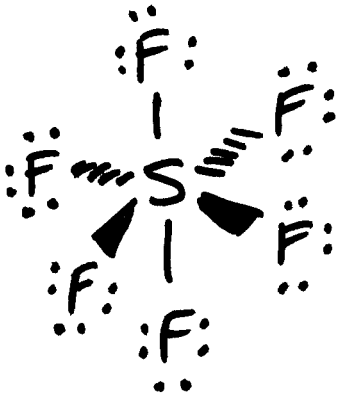


****e^- must be around the middle**

seesaw, $<90^o$ & $< 120^o$
(irregular tetrahedran, bisphenoid)

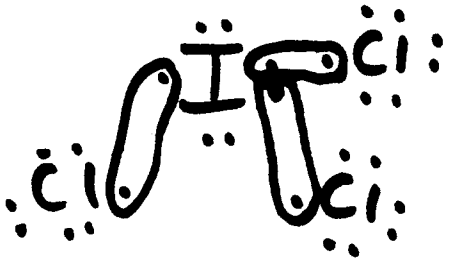
Ex. 12) SF_6

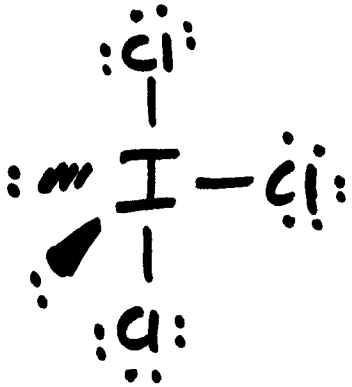




octahedral, 90^o

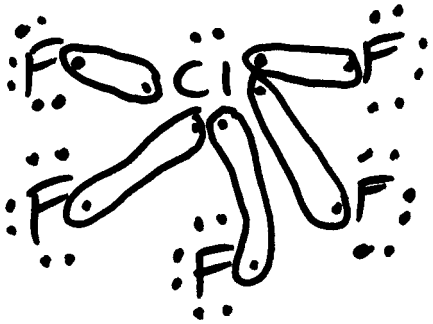
Ex. 13) ICl_3

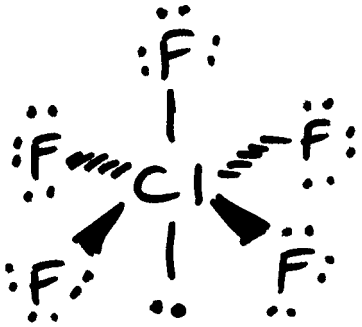




T-shaped, <90^o
(e^- must be around middle)

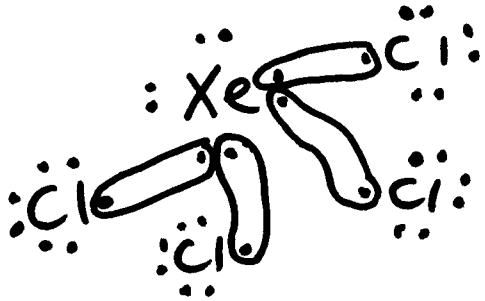
Ex. 14) ClF_5

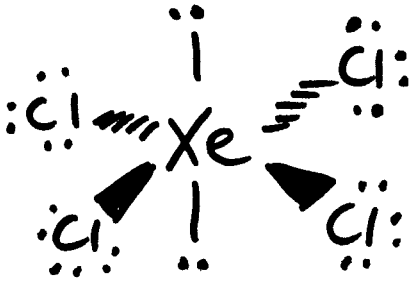




square pyramidal,
<90^o

Ex. 15) $XeCl_4$





square planar,
90^o

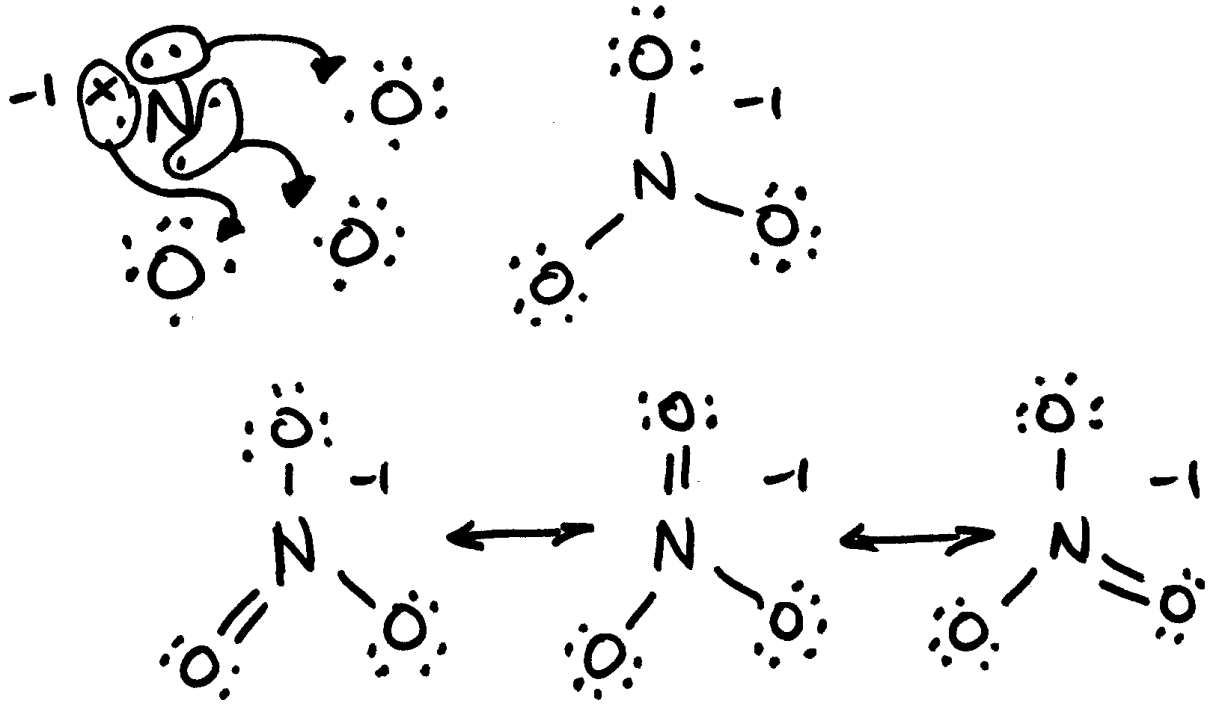
**** e- must be across from each other**

linear, 180^o

IV. Resonance

-is when more than one Lewis structure is possible.

NO_3^-

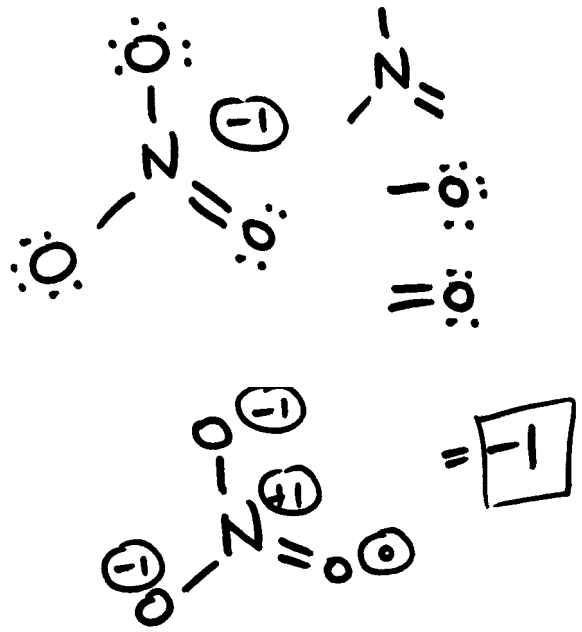


trigonal planar, 120^o

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.

#56 Notes V. Formal Charge

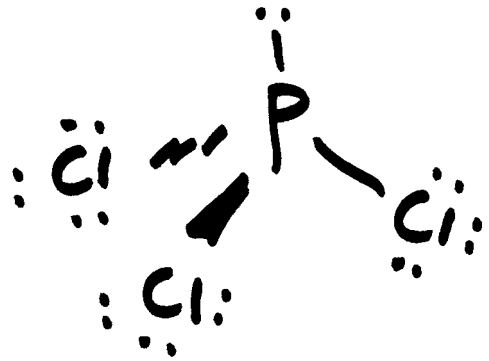
Formal Charge = # valence electrons on lone atom (outer e^- from the periodic table)
- # valence electrons on the atom in the compound (all lone electrons plus one electron per bond)



N: F.C.= 5 e^- - 4 e^- = **+1**
(5e^- from periodic table – 4 e^- { 1 e- per bond})

single bond O: F.C. = 6e^- - 7e^- = **-1**
(6e^- per. table – {1 e^- from bond + 6 lone e^-})

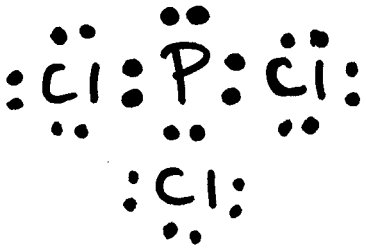
double bond O: F.C. = 6e^- - 6e^- = **0**
(6e^- per. table – {2 e^- from bonds + 4 lone e^-})



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

P F.C. = 5 e^- - 5e^- = 0
(5e^- per. table – {3 e^- from bonds + 2 lone e^-})

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



VI. Polarity

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

** unsymmetrical (**<u>un</u>balanced**) = {(+) and (-) ends to the molecule} = **polar**

symmetrical (balanced**, it will not have (+)/(-) ends, the ends are the same) = **<u>non</u>polar**

[2 prefixes not together (un & non)]

(see notes #54-55 for structures)

Ex. 1) NaCl polar
Ex. 2) $MgBr_2$ nonpolar
Ex. 3) $AlCl_3$ nonpolar
Ex. 4) CH_4 nonpolar
Ex. 5) PCl_3 polar
Ex. 6) H_2O polar
Ex. 7) ClO_4^- nonpolar
Ex. 8) CO_2 nonpolar
Ex. 9) NaCN polar
Ex. 10) PBr_5 nonpolar
Ex. 11) SF_4 polar
Ex. 12) SF_6 nonpolar
Ex. 13) IBr_3 polar
Ex. 14) ClF_5 polar
Ex. 15) $XeCl_4$ nonpolar

#57 Notes Ch. Bonding Orbitals

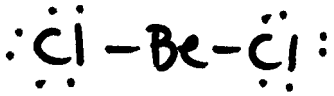
I. Hybridization (a mixture of orbitals)

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

Compound	# of bonds	orbitals used	hybrid
Ex. 1) H_2	**1**	**s**	**none**

H—H H ↑_ The electron from the other H can go into this
1s orbital to make the bond.

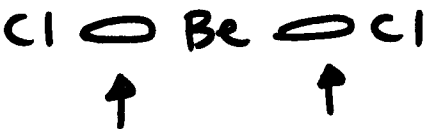
Ex. 2) $BeCl_2$	**2**	**s, p**	**sp**



Be ↑↓ __ __ __
2s 2p

Be ↑_ ↑_ __ __
2s 2p

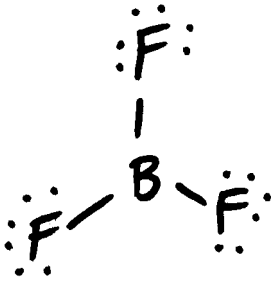
Now that the electrons are separated, the 2 Cl's can each move in one electron to make a bond.



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

sp sp

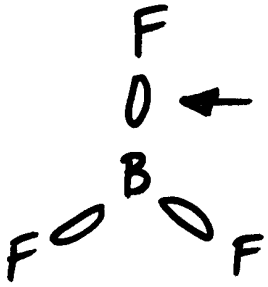
Ex. 3) BF_3	**3**	**s, p, p**	**sp^2**



B ↑↓ ↑_ __ __
2s 2p

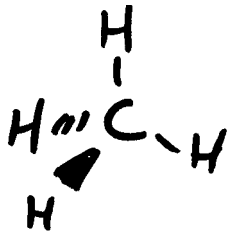
B ↑_ ↑_ ↑_ __
2s 2p

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).

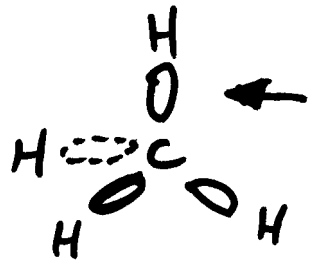
Ex. 4) CH_4 **4** **s, p, p, p** **sp^3**



C ↑↓ ↑ ↑ —
2s 2p

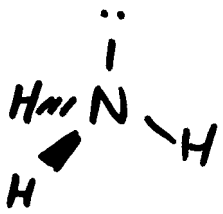
C ↑ ↑ ↑ ↑
2s 2p

Now each H can move in one electron to bond.



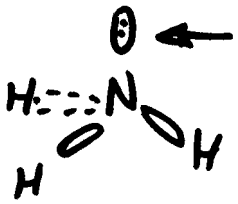
sp^3 4 equivalent orbitals (1/4 s, 3/4 p).

Ex. 5) NH_3 **3 + 1 lone pair** **s, p, p, p** **sp^3**



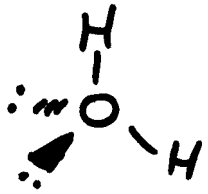
N ↑↓ ↑ ↑ ↑
2s 2p

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



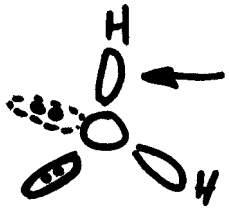
sp^3 4 equivalent orbitals (1/4 s, 3/4 p).

Ex. 6) H_2O **2 + 2 lone pairs** **s, p, p, p** **sp^3**



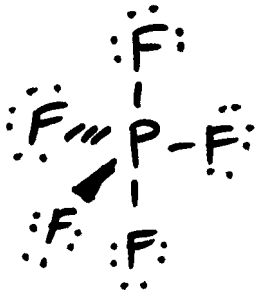
O ↑↓ ↑↓ ↑ ↑
2s 2p

Each H can move in one electron to bond.



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

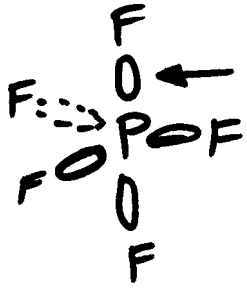
Ex. 7) PF_5 5 s, p, p, p, d dsp^3



P ↑↓ ↑ ↑ ↑ — — — — —
3s 3p 3d

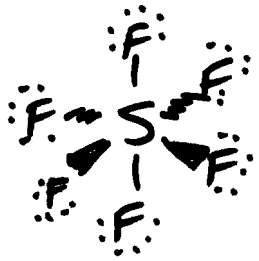
P ↑ ↑ ↑ ↑ ↑ — — — —
3s 3p 3d

Now each F can move in an electron to bond.



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

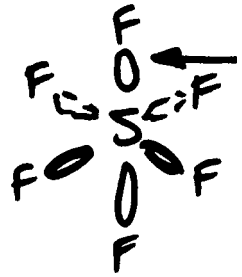
Ex. 8) SF_6 6 s, p, p, p, d, d d^2sp^3



S ↑↓ ↑↓ ↑ ↑ — — — — —
3s 3p 3d

S ↑ ↑ ↑ ↑ ↑ ↑ — — —
3s 3p 3d

Now each F can move in one electron to bond.

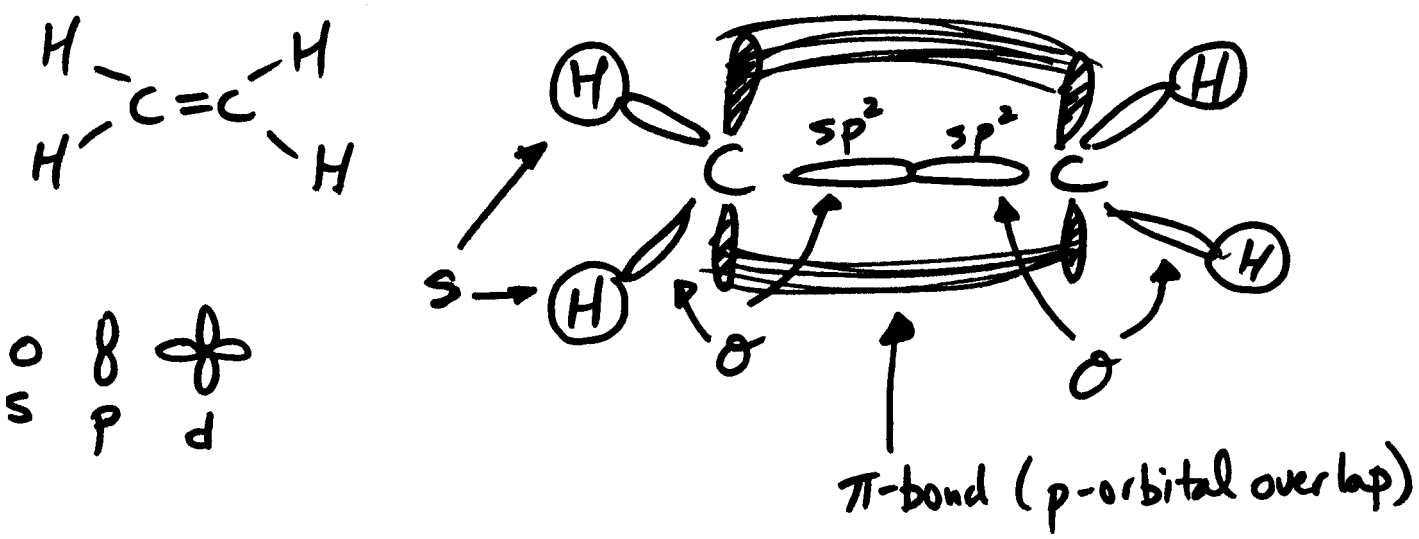


d^2sp^3 6 equivalent orbitals (1/6 s, 3/6 p, 2/6 d).
=1/6 s, 1/2 p, 1/3 d

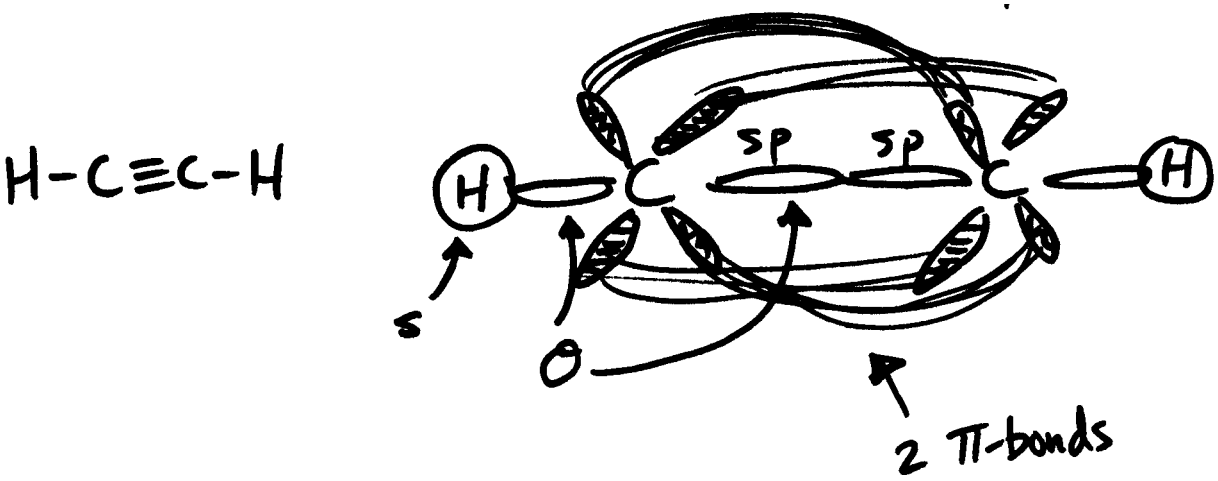
On fingers do: SF_4 (4 bonds and 1 e^- pair = 5 positions/orbitals needed), so **dsp^3**,

XeF_4 (4 bonds and 2 e^- pairs = 6 positions/orbitals needed), so **d^2sp^3**

#58 Notes II. Multiple Bonds and Hybridization



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



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

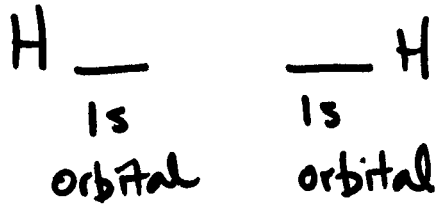
**They become successively stronger, less flexible, and more reactive.

III. Molecular Orbital Theory
-is a way of determining whether a compound will have single, double or triple bonds.

A) Homonuclear Diatomic Molecules

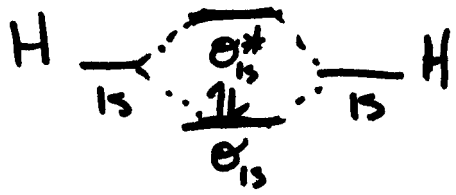
1) Simple Molecules with s-orbitals only. (H_2, He_2)

Ex. 1) H_2



The 2 "old" orbitals will make 2 "new" orbitals. (1 bonding and 1 anti-bonding)

Each H has 1 e^- in the 1s orbital, so H_2 has 2 e^- total.

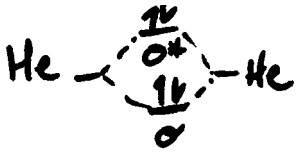


Bond Order = $\frac{\text{\# bonding } e^- \text{ - \# anti-bonding } e^-}{2} = \frac{2-0}{2}$ = **1 favorable (single bond)**

Any Bond Order > 0 is favorable (0 is non-bonding).

Ex. 2) He_2

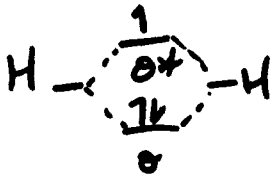
Each He has 2 e^- in the 1s, so He_2 has a total of 4 e^-.



B.O. = $\frac{2-2}{2}$ = **0 unfavorable, no bonding**

Ex. 3) H_2^-

Each H has 1e^- in the 1s, so H_2 has 2 e^-. The (-) tells us to add 1 e^-, so 3 e^- total .

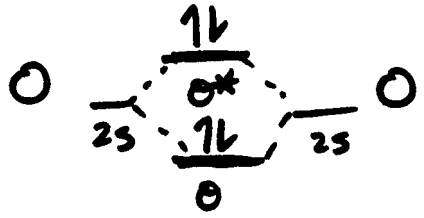


B.O. = $\frac{2-1}{2}$ = **1/2 favorable**

2) Molecules with p-orbitals.

Ex. 1) O_2

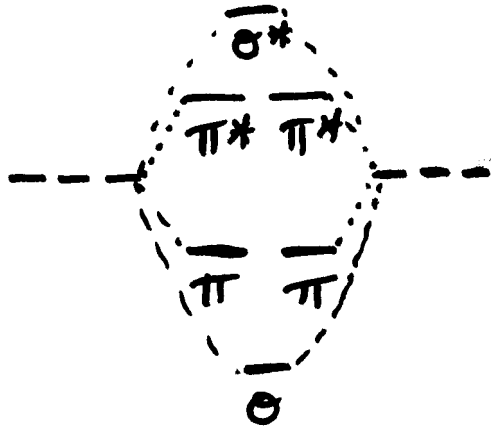
Each O has 2 e^- in the s orbital and 4 e^- in the p orbital.
So O_2 has 4e^- in the s orbital and 8 e^- in the p orbital.



B.O. = $\frac{2-2}{2}$ = **0** **Non bonding**

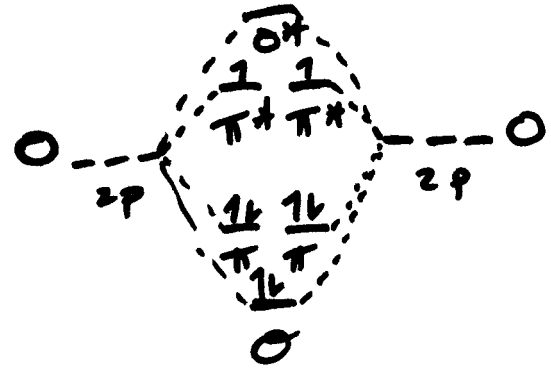
Since the s-orbitals will always be full and the bond order will be zero, it can be ignored.

For the p-orbitals: each O has 3 p-orbitals, making a total of 6 p-orbitals. These will make 6 new orbitals.



Remember: Triple Bond has **1 σ & 2 π**

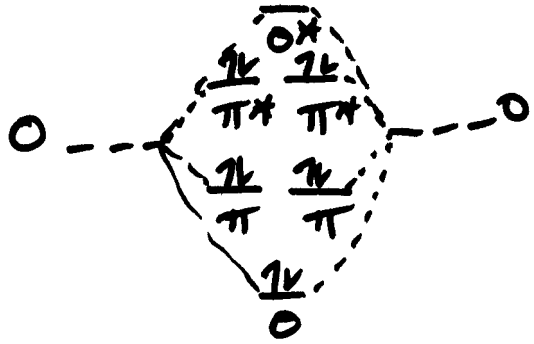
Each O has 4 e^- in the p, so 8 e^- total.



B.O. = $\frac{6-2}{2}$ = **2 favorable (double bond)**

Ex. 2) O_2^{2-}

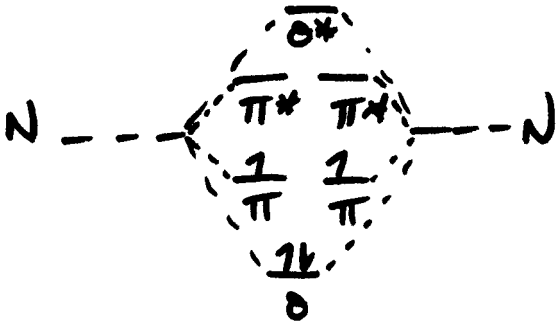
Each O has 4 e^- in the p, so O_2 has 8 e^- in the p, but the (2-) is 2 extra electrons = 10 e^-



B.O. = $\frac{6-4}{2}$ = **1 favorable**

Ex. 3) N_2^{2+}

Each N has 3e^- in the p, so N_2 has 6e^- in the p, but the (2+) is 2 fewer electrons = 4 e^-



B.O. = $\frac{4-0}{2}$ = **2 favorable**

End of Notes (Assignments #59-60 are Review Assignments. There are no notes for these assignments.)