Chem 111

Lecture 30

Announcement

- Class Next Wednesday
- Exam 3, Dec 6

Homework

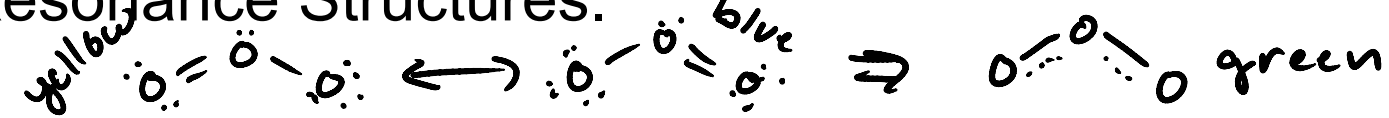
- Finish Reading Chapter 8
- Owl Homework

Recap

- Formal Charge.

$$FC = VE - (\text{non. be.} + \tfrac{1}{2}\,\text{bond } e^-)$$

- Resonance Structures.



- Exceptions to the octet.

→ odd # e-

⇒ incomp. octet ⇒ B, Be, Al

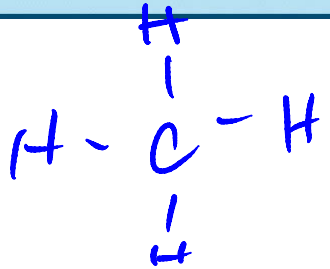
⇒ expanded octet ⇒ n > 3

~~N, O, F, C~~

VSEPR (valence shell electron pair repulsion)

Molecular Geometry – is the arrangement of atoms in space.

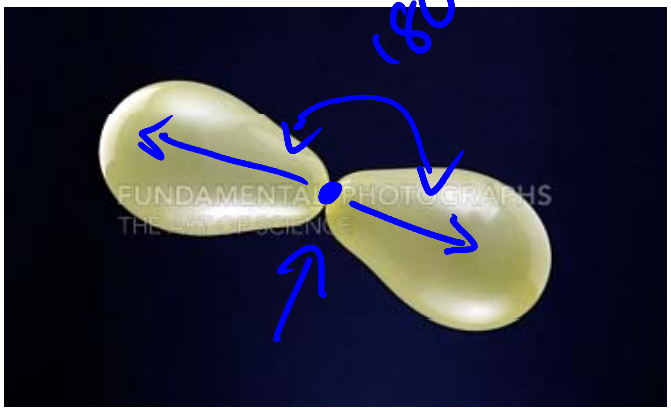
Number of electron regions	Arrangement
2	Linear
3	Trigonal planar
4	Tetrahedral
5	Trigonal bipyramidal
6	Octahedral

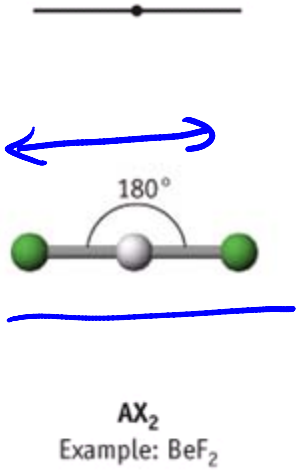


- Basic Tenants
  - 1. Regions of high electron density - bp(s) + lp(s) - take up positions as far apart as possible.
  - 2. Molecular shape is determined by the resulting atomic positions
  - 3. lone pairs take up more space than bond pairs

Shapes

- Linear





AX_2
Example: BeF_2

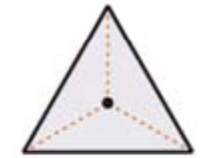
CO_2
BeF_2

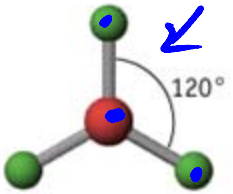
AX_2

BF_3

AY_3 BCl_3

- Trigonal Planar



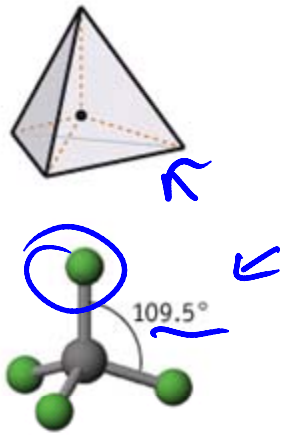


AX_3
Example: BF_3

Shapes

1 : 4

- Tetrahedral

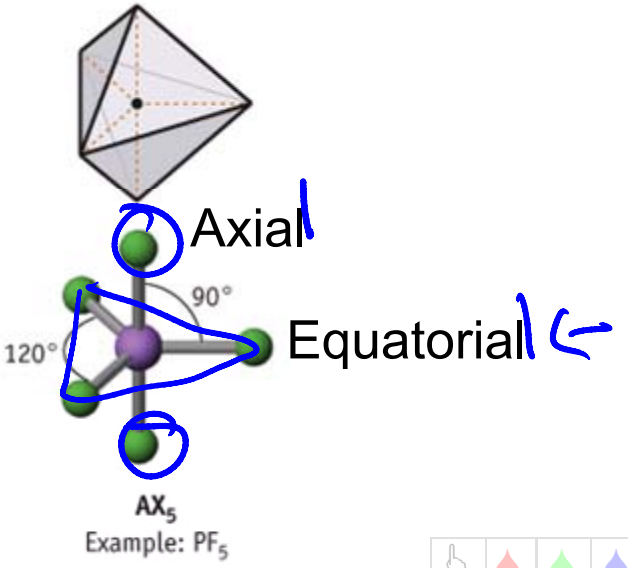


AX_4
Example: CF_4

Shapes

1 : 5

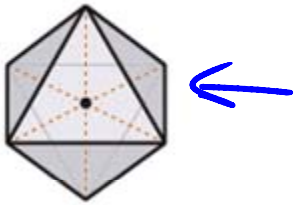
- Trigonal bipyramidal

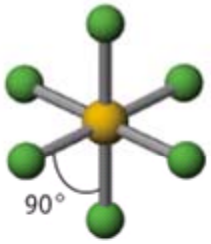


Shapes

1 : 6

- Octahedral





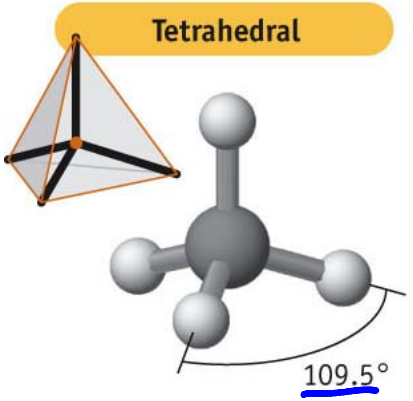
AX_6

Example: SF_6

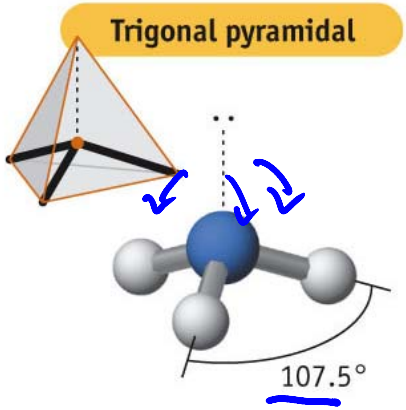
Lone Pair Geometry

- Lone pairs of electrons on the central atom occupy spatial positions.

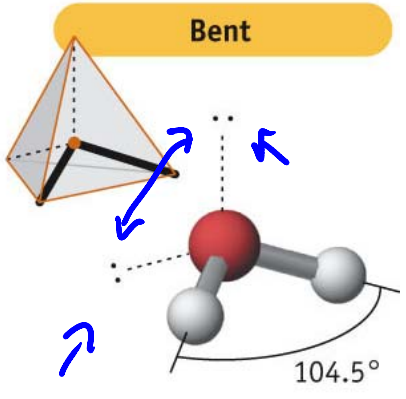
L.P.– L.P.> Lone Pair Bonding Pair > B.P. – B.P.



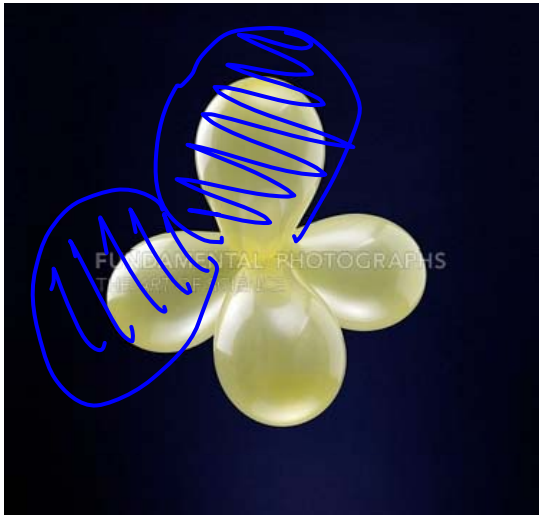
Methane, CH_4
4 bond pairs
no lone pairs



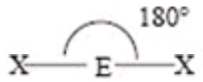
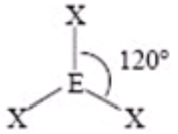
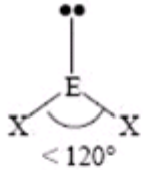
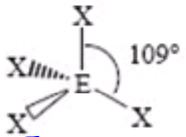
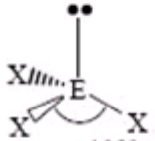
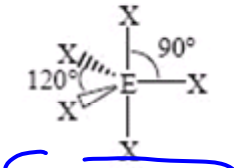
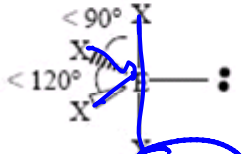
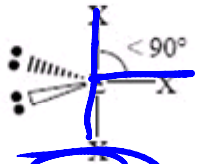
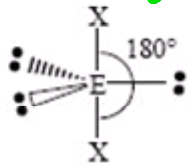
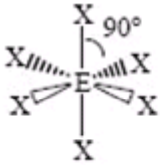
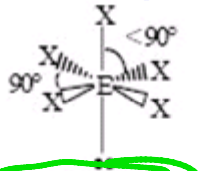
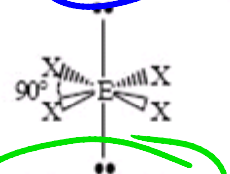
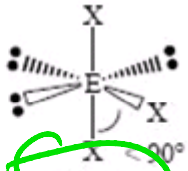
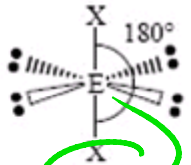
Ammonia, NH_3
3 bond pairs
1 lone pair

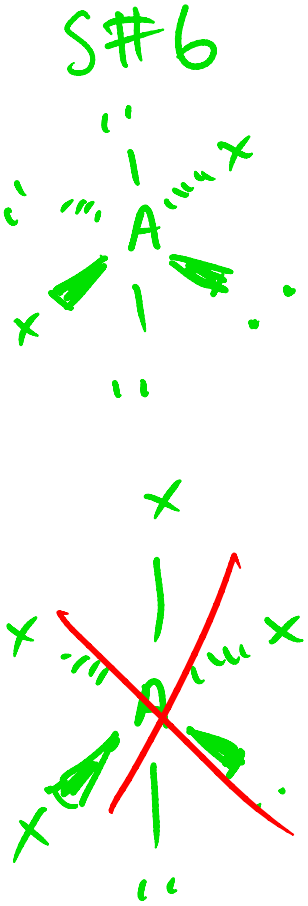


Water, H_2O
2 bond pairs
2 lone pairs



VSEPR

VSEPR Geometries					
Steric No.	Basic Geometry 0 lone pair	1 lone pair	2 lone pairs	3 lone pairs	4 lone pairs
2	 Linear				
3	 Trigonal Planar	 Bent or Angular			
4	 Tetrahedral	 Trigonal Pyramid	 Bent or Angular		
5	 Trigonal Bipyramid	 Sawhorse & Seesaw	 T-shape	 Linear	
6	 Octahedral	 Square Pyramid	 Square Planar	 T-shape	 Linear

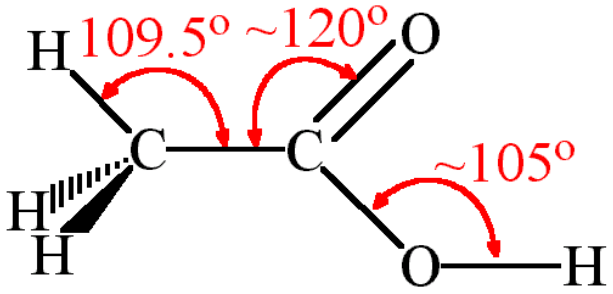


Molecular Geometry

1. Sketch the Lewis Structure.
2. Count the total number of electron pairs around the central atom (bonding and non-bonding) = steric number
3. Arrange electron pairs (bonding and non-bonding) on the central atom such that it minimizes electron pair replusion
4. Describe what shape you got.

** A double or triple bond is counted as one bonding pair when predicting geometry.

** Molecules with more than one “central atom” work the same way.

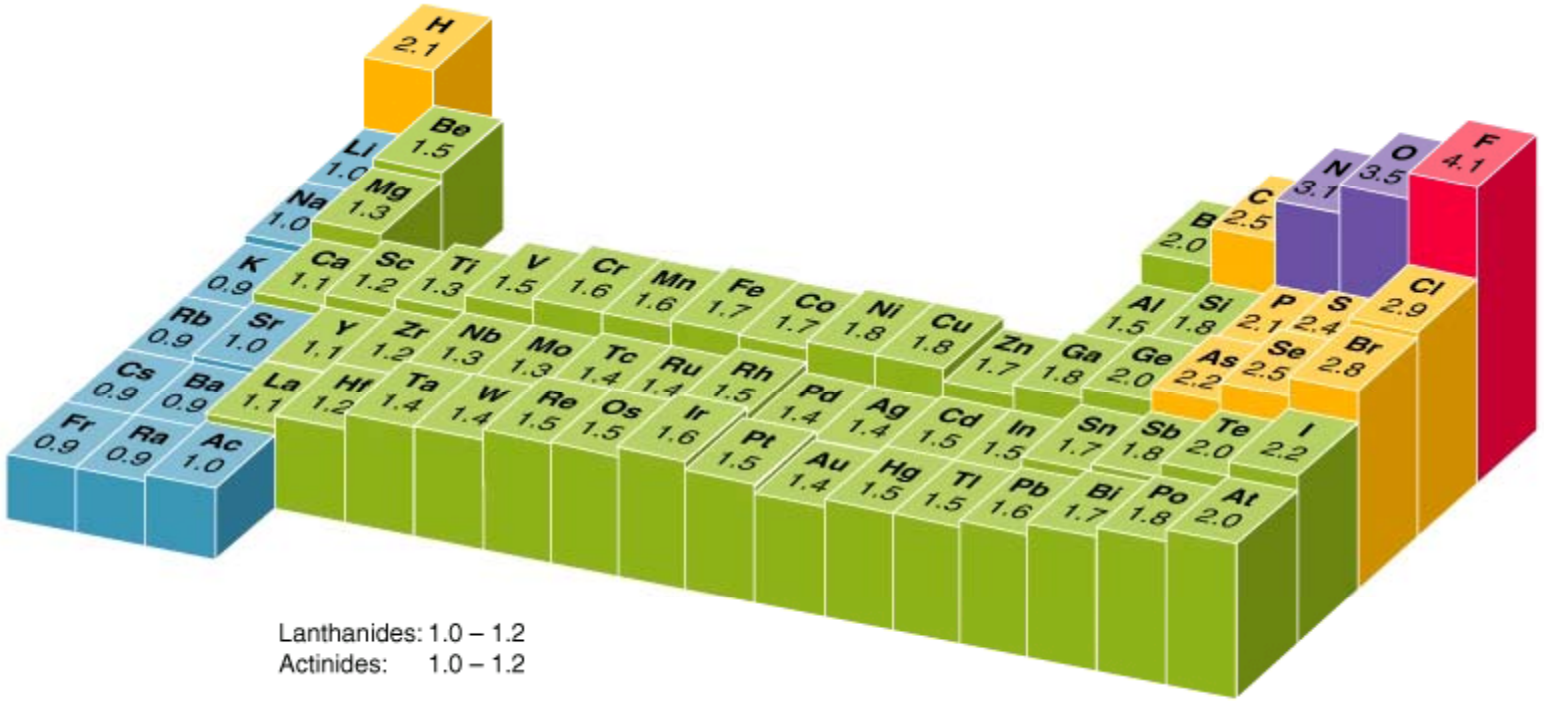


Let's Practice

Using VSEPR model, predict the molecular geometry of SF_4 and IF_5.

Electronegativity

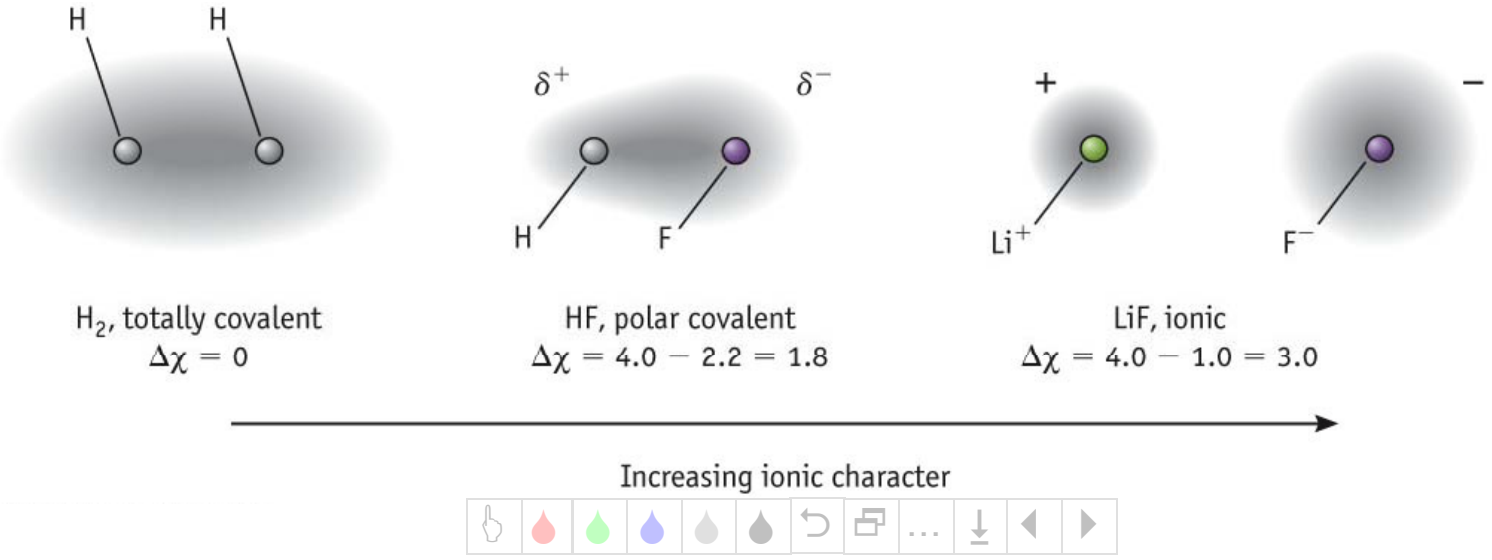
- The power of an atom to attract electrons when it is part of a compound
- Mulliken - $\chi_m = 1/2\ (I + E_a)$



Bond Polarity

- **Bond Polarity –** is the separation of charge leading to a molecule to have a dipole moment

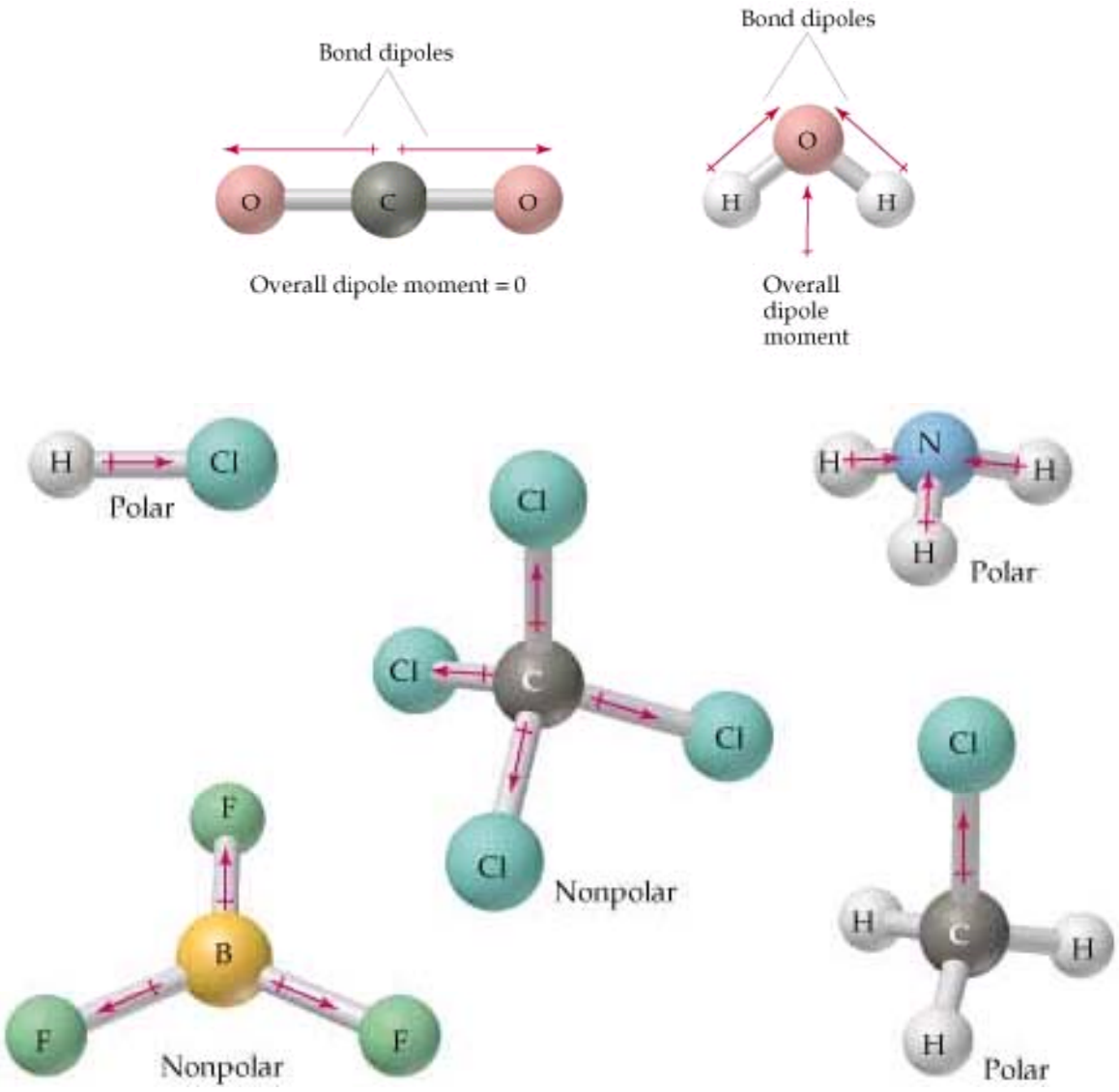
- We can use the difference in electronegativity between two atoms to gauge the polarity of the bond.



Polar Molecules

- Align themselves in an electrical field, including other ions.
- Negative ends attracted positive ends and visa-versa
- A **Dipole** is established when two electrical charges of equal magnitude but opposite sign are separated by distance.
- The size of a dipole is measured by its dipole moment, μ – measured in debyes(D).

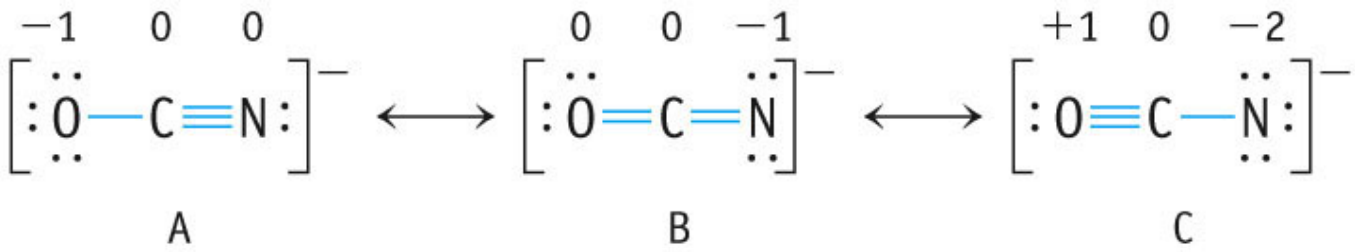
Identifying Polar Molecules



Electroneutrality

Formal charges

Resonance structures



Bond Order

Bond order - is the number of bonding electron pairs shared by two atoms.

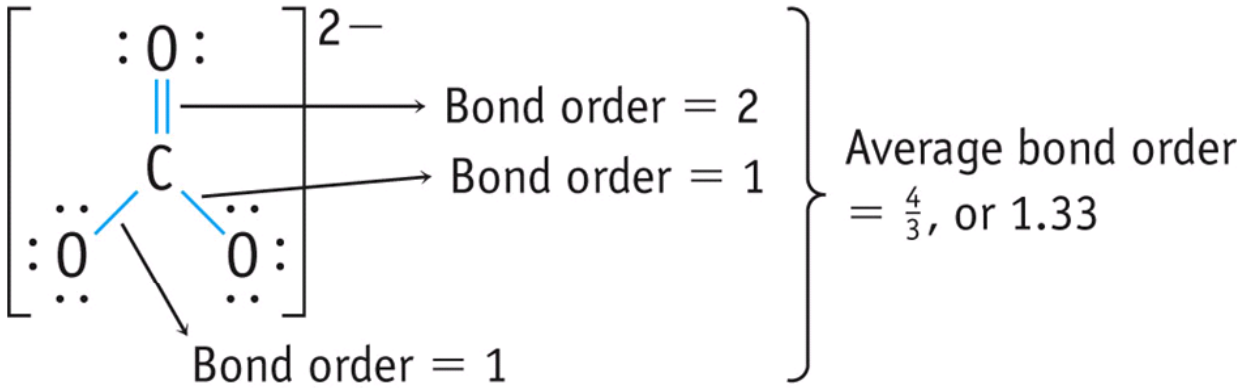
Tentative way (using Lewis structures)-

Bond order = 1 → single bond

Bond order = 2 → double bond

Bond order = 3 → triple bond

$$Bond\ Order = \frac{number\ of\ shared\ pairs\ in\ all\ X-Y\ bonds}{number\ of\ X-Y\ links\ involved\ in\ resonance}$$



Bond Length

Single Bond > Double Bond >Triple Bond

Bond length is related to the atoms involved in the bond.

TABLE 8.8 Some Average Single- and Multiple-Bond Lengths in Picometers (pm)*

Single Bond Lengths

	Group 1A	4A	5A	6A	7A	4A	5A	6A	7A	7A	7A
	H	C	N	O	F	Si	P	S	Cl	Br	I
H	74	110	98	94	92	145	138	132	127	142	161
C		154	147	143	141	194	187	181	176	191	210
N			140	136	134	187	180	174	169	184	203
O				132	130	183	176	170	165	180	199
F					128	181	174	168	163	178	197
Si						234	227	221	216	231	250
P							220	214	209	224	243
S								208	203	218	237
Cl									200	213	232
Br										228	247
I											266

Bond Dissociation Enthalpy

$H_3C\text{-}CH_3\ (g) \rightarrow H_3C^{\cdot}\ (g) + H_3C^{\cdot}\ (g)$ $\quad \Delta_r H = +386$ kJ/mol

$H_2C{=}CH_2\ (g) \rightarrow H_2C{:}\ (g) + H_2C{:}\ (g)$ $\quad \Delta_r H = +682$ kJ/mol

$HC{\equiv}CH\ (g) \rightarrow H\dot{C}{:}\ (g) + H\dot{C}{:}\ (g)$ $\quad \Delta_r H = +962$ kJ/mol

Single Bond < Double Bond <Triple Bond

TABLE 8.9 Some Average Bond Dissociation Enthalpies (kJ/mol)*

Single Bonds

	H	C	N	O	F	Si	P	S	Cl	Br	I
H	436	413	391	463	565	328	322	347	432	366	299
C		346	305	358	485	—	—	272	339	285	213
N			163	201	283	—	—	—	192	—	—
O				146	—	452	335	—	218	201	201
F					155	565	490	284	253	249	278
Si						222	—	293	381	310	234
P							201	—	326	—	184
S								226	255	—	—
Cl									242	216	208
Br										193	175
I											151

Multiple Bonds

N═N	418	C═C	610
N≡N	945	C≡C	835
C═N	615	C═O	745
C≡N	887	C≡O	1046
O═O (in O_2)	498		

Bond Dissociation Enthaply

$\Delta_r H = \Sigma\Delta H(\text{bonds broken}) - \Sigma\Delta H(\text{bonds formed})$

$CH_3CHCH_2\ (g) + H_2(g) \rightarrow CH_3CH_2CH_3\ (g)$