

---

**Unit#2**  
**AP Chem**  
**Topic#10**  
**Structure (Molecular)**

---

Teacher Edition

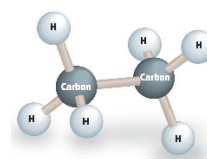
---

## Bonding Topic#10

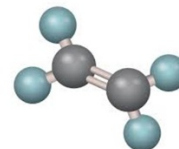
### Bonding

- atoms bond to achieve a lower energy state
- bonding relates to bp, mp, hardness, solubility, electrical and thermal conductivity
- **Intramolecular Bond** - hold atoms together to form compounds
- **Intermolecular Bond** - holds condensed states of matter together, i.e. liquids and solids
- **Bond Energy** - the energy needed to break a bond.
  - Bonds REQUIRE energy to break (BE - bond energy) and release energy when they form
- **Bond Length (BL)** - distance where PE (BE) is at a minimum (negative  $E$  value) between two bonded atoms.
- **Bond Order (BO)** - number of bonding pairs of electrons
  - BO 1 - single bond, one sigma bond ( $\sigma$ -bond)
  - BO 2 - double bond, one sigma bond ( $\sigma$ -bond) and one pi bond ( $\pi$ -bond)
  - BO 3 - triple bond, one sigma bond ( $\sigma$ -bond) and two pi bond ( $\pi$ -bond)

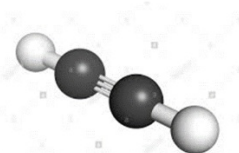
Bond	C-C	C=C	C $\equiv$ C
Bond Order	1	2	3
Bond Length(pm)	143	122	113
Bond Energy (kJ/mol)	347	614	839
- valence electrons (outer most  $s$  and  $p$  electrons) are used in bonding - Used with symbol in Lewis structures



ethane  
(C-C)



ethene  
(C=C)

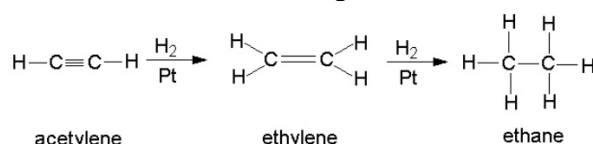


ethyne  
(C $\equiv$ C)  
(acetylene)

---

**Quick Organic****Bonding  
Topic#10**

---



catalyzed hydrogenation of ethyne (acetylene) to ethene to ethane

# of Carbons (n)	Alkane (C <sub>n</sub> H <sub>2n+2</sub> )	Alkene (C <sub>n</sub> H <sub>2n</sub> )	Alkyne (C <sub>n</sub> H <sub>2n-2</sub> )	Alcohol (C <sub>n</sub> H <sub>2n+1</sub> OH)	Carboxylic Acid
1	methane (CH <sub>4</sub> )	--	--	methanol (CH <sub>3</sub> OH)	methanoic acid (CHOOH)
2	ethane (C <sub>2</sub> H <sub>6</sub> )	ethene (C <sub>2</sub> H <sub>4</sub> )	ethyne (C <sub>2</sub> H <sub>2</sub> )	ethanol (C <sub>2</sub> H <sub>5</sub> OH)	ethanoic acid (CH <sub>3</sub> COOH)
3	propane (C <sub>3</sub> H <sub>8</sub> )	propene (C <sub>3</sub> H <sub>6</sub> )	propyne (C <sub>3</sub> H <sub>4</sub> )	propanol (C <sub>3</sub> H <sub>7</sub> OH)	propanoic acid (C <sub>2</sub> H <sub>5</sub> COOH)
4	butane (C <sub>4</sub> H <sub>10</sub> )	butene (C <sub>4</sub> H <sub>8</sub> )	butyne (C <sub>4</sub> H <sub>6</sub> )	butanol (C <sub>4</sub> H <sub>9</sub> OH)	butanoic acid (C <sub>3</sub> H <sub>7</sub> COOH)
5	pentane (C <sub>5</sub> H <sub>12</sub> )	pentene (C <sub>5</sub> H <sub>10</sub> )	pentyne (C <sub>5</sub> H <sub>8</sub> )	pentanol (C <sub>5</sub> H <sub>11</sub> OH)	pentanoic acid (C <sub>4</sub> H <sub>9</sub> COOH)
6	hexane (C <sub>6</sub> H <sub>14</sub> )	hexene (C <sub>6</sub> H <sub>12</sub> )	hexyne (C <sub>6</sub> H <sub>10</sub> )	hexanol (C <sub>6</sub> H <sub>13</sub> OH)	hexanoic acid (C <sub>5</sub> H <sub>11</sub> COOH)
7	heptane (C <sub>7</sub> H <sub>16</sub> )	heptene (C <sub>7</sub> H <sub>14</sub> )	heptyne (C <sub>7</sub> H <sub>12</sub> )	heptanol (C <sub>7</sub> H <sub>15</sub> OH)	heptanoic acid (C <sub>6</sub> H <sub>13</sub> COOH)
8	octane (C <sub>8</sub> H <sub>18</sub> )	octene (C <sub>8</sub> H <sub>16</sub> )	octyne (C <sub>8</sub> H <sub>14</sub> )	octanol (C <sub>8</sub> H <sub>17</sub> OH)	octanoic acid (C <sub>7</sub> H <sub>15</sub> COOH)
9	nonane (C <sub>9</sub> H <sub>20</sub> )	nonene (C <sub>9</sub> H <sub>18</sub> )	nonyne (C <sub>9</sub> H <sub>16</sub> )	nonanol (C <sub>9</sub> H <sub>19</sub> OH)	nonanoic acid (C <sub>8</sub> H <sub>17</sub> COOH)
10	decane (C <sub>10</sub> H <sub>22</sub> )	decene (C <sub>10</sub> H <sub>20</sub> )	decyne (C <sub>10</sub> H <sub>18</sub> )	decanol (C <sub>10</sub> H <sub>21</sub> OH)	decanoic acid (C <sub>9</sub> H <sub>19</sub> COOH)

**Common Names:**

ethyne (acetylene)

methanoic acid (formic acid)

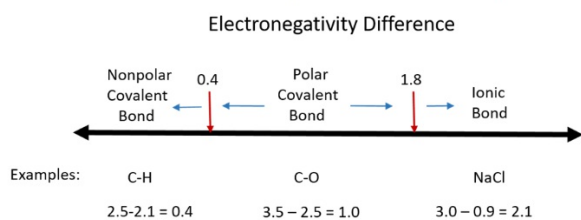
ethanoic acid (acetic acid)

## Bonding Topic#10

### Bonding

#### Orbital Theory

- bond orbital - the region where two electrons form a bond
  - energy is lower for the two electrons in a bond orbital where they are attracted to two nuclei.
- In an ionic bond, bond orbital is significantly displaced towards one nucleus.
- In a covalent bond, bond orbital is near center (nonpolar), or displaced towards one of the nuclei (one with a larger EN value).
- $EN_{diff}$  scale
  - $EN_{diff} < 0.4$  (nonpolar covalent, 5% ionic character),  $0.4 < 1.8$  (polar covalent, 5% to 50% ionic character) , and  $1.8 < 3.3$  (ionic, >50% ionic character)

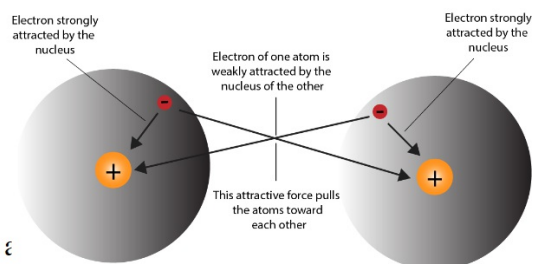


H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac	Unq	Unp	Unh	Uns	Uno	Une									
Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu				
Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr				

## Bonding Topic#10

### Covalent (Molecular) Bonding

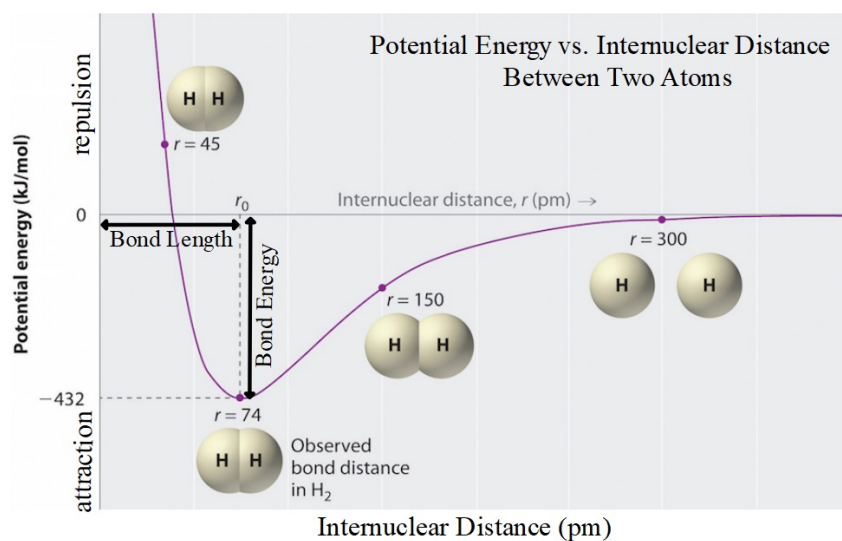
- sharing of electrons between the bonding atoms
  - Shared **equally** - nonpolar covalent bond (npc)
  - Shared **unequally** - polar bond (pc) (affected by a magnetic field)
- nonmetal to nonmetal bonding (H-O)
- formulas are in **true ratio** of atoms needed to make a molecule (molecular formula:  $C_6H_{12}O_6$ )
- may exist as a solid, liquid, or gas at room  $T$ , usually have a low melting point, and do not conduct electricity.
- Localized electron (LE) bonding model - sharing electrons using the atomic orbitals of the atoms involved in the bond (atoms have a small difference in EN values).
- Electron pairs are localized bonded electrons or unshared pairs around an atom
- sharing electrons to achieve octet (nonmetals)
  - single bond - 2 electrons in bonding region
  - double bond - 4 electrons in bonding region
  - triple bond - 6 electrons in bonding region
    - BE and BL are inversely proportionate
      - BL:  $C-C > C=C > C\equiv C$
      - BE:  $C-C < C=C < C\equiv C$



## Bonding Topic#10

### Covalent (Molecular) Bonding

- bond length is minimum PE (negative value) (remember it take energy to break a bonds and energy is released when a bond is formed)
- as the number of electrons in a bond increases, the bond energy increases too ( $C-C < C=C < C\equiv C$ )



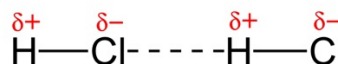
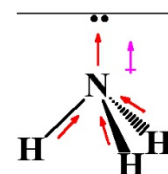
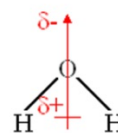
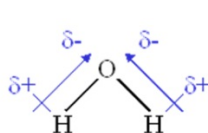


## Bond Polarity and Dipole Moments

### Polar Molecules

- the molecule has at least one polar bond and is asymmetrical in shape (usually linear, bent, or trigonal pyramidal).
- central atom usually has unshared pairs of electrons.
- many contain a highly EN element such as O, F, Cl, or N.
- Dipole moment - separation of charge in a molecule
- align themselves with an electric field
- Most notable: water (H<sub>2</sub>O) and ammonia (NH<sub>3</sub>)
- If octet rule is obeyed and all the surrounding bonds between the central atom and exterior atoms (symmetrical) are the same, molecule is nonpolar (CO<sub>2</sub>)

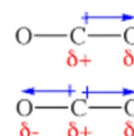
## Bonding Topic#10



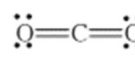
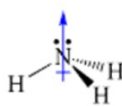
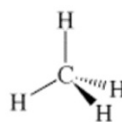
electronegativity: O = 3.5  
C = 2.5

Bond polarity = 3.5 - 2.5 = 1.0

Dipole moment = 1.0 - 1.0 = 0.0



*molecular dipole moment?*



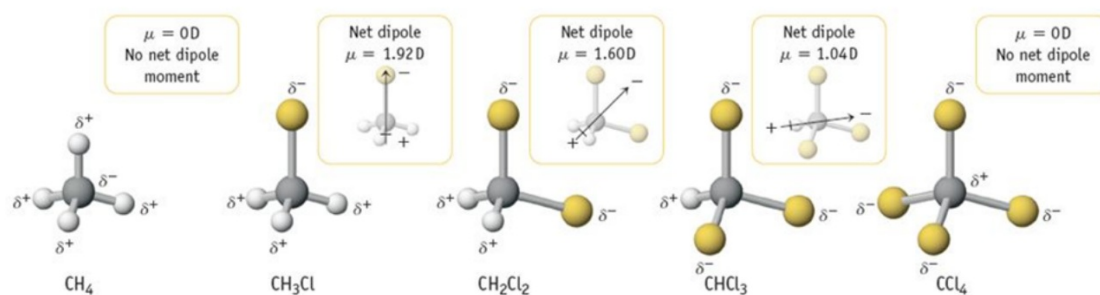


**Bonding  
Topic#10**

**Bond Polarity and Dipole Moments**

Example: Starting with methane ( $\text{CH}_4$ ) gradually substitute chlorine for hydrogen until carbon tetrachloride.  
What do you think happens to the boiling points of these compounds?

**$\text{CH}_4 \dots \text{CCl}_4$  Polar or Not?**



- Only  $\text{CH}_4$  and  $\text{CCl}_4$  are NOT polar. These are the only two molecules that are "symmetrical."

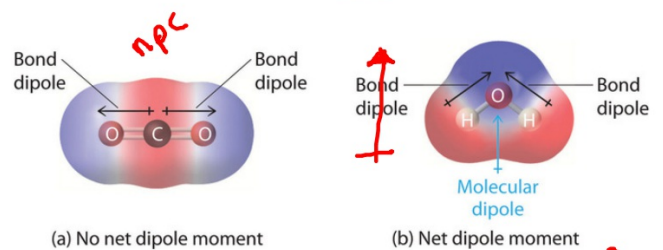
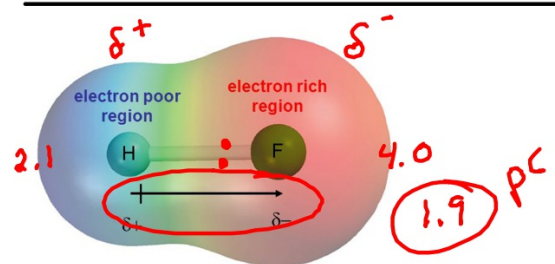
## Bonding Topic#10

### Bond Polarity and Dipole Moments

- Dipolar (dipole moment) molecules have a positive end and a negative end (polar covalent)
  - $EN_{diff}$  between 0.4 and 1.8
  - HF ( $EN_{diff} = 4.0 - 2.1 = 1.9$ )

TABLE 8.3 Bond Lengths, Electronegativity Differences, and Dipole Moments of the Hydrogen Halides

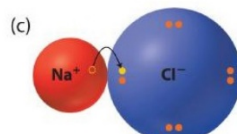
Compound	Bond Length (Å)	Electronegativity Difference	Dipole Moment (D)
HF	0.92	1.9	1.82
HCl	1.27	0.9	1.08
HBr	1.41	0.7	0.82
HI	1.61	0.4	0.44



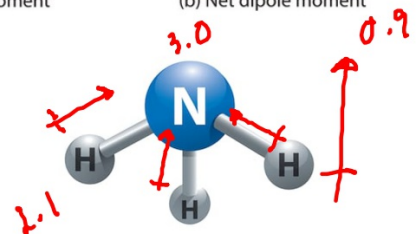
Bonding electrons shared equally between two atoms. No charges on atoms.



Bonding electrons shared unequally between two atoms. Partial charges on atoms.



Complete transfer of one or more valence electrons. Full charges on resulting ions.





Bonding  
Topic#10

Ion Sizes

- Cations < atoms
- Anions > atoms
- Decrease across a period
- Increase down a group

3. Arrange the ions  $\text{Se}^{2-}$ ,  $\text{Br}^-$ ,  $\text{Rb}^+$ , and  $\text{Sr}^{2+}$  in order of decreasing size.



isoelectric:  $\text{Se}^{2+}$   $\text{Br}^-$   $\boxed{\text{Kr}}$   $\text{Rb}^+$   $\text{Sr}^{2+}$

4. Choose the largest ion in each of the following groups.

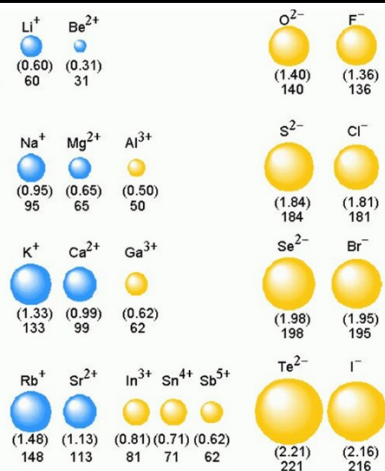
a.  $\text{Li}^+$ ,  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Rb}^+$ ,  $\boxed{\text{Cs}^+}$

b.  $\text{Ba}^{2+}$ ,  $\text{Cs}^+$ ,  $\text{I}^-$ ,  $\boxed{\text{Te}^{2-}}$

isoelectric series:



Table  
of Ion  
Sizes

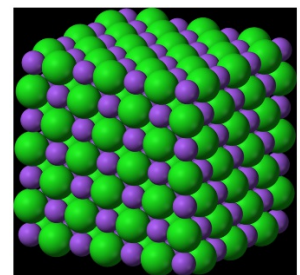
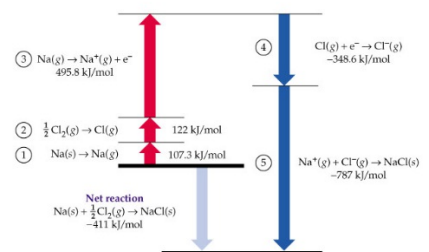


NaF vs. CsF  
Which ionic crystal has  
the highest mp?

## Bonding Topic#10

### Binary Ionic Compounds

- electrostatic attraction between closely packed, oppositely charged ions.
- compound containing a metal (cation;  $\text{Na}^+$ ) and a nonmetal (anion;  $\text{Cl}^-$ )
  - cations (metal ions or ammonium,  $\text{NH}_4^+$ )
  - anions (nonmetal monatomic ions or polyatomic ions)
  - gain or lose electrons to form an octet (usually)
- formulas are in empirical form (simplest whole number ratios)
  - $\text{TiO}_2$  instead of  $\text{Ti}_2\text{O}_4$
  - formula unit
- good conductors of electricity in molten or dissolved state
- $EN_{\text{diff}} > 1.8$
- strong coulombic (electrostatic) attraction between cations and anions result is a solid crystal (crystal lattice) at room  $T$  with very high mp
  - **Lattice Energy** - the change in  $E$  that takes place when separated gaseous ions are placed together to form an ionic solid:  $\text{M}^+(\text{g}) + \text{X}^-(\text{g})$
  - Lattice energy is dependent on charge and size of ions;  $\text{MgO} > \text{NaF}$
- **Operational definition** of an ionic compounds is any compound that conducts an electric current when melted is ionic.

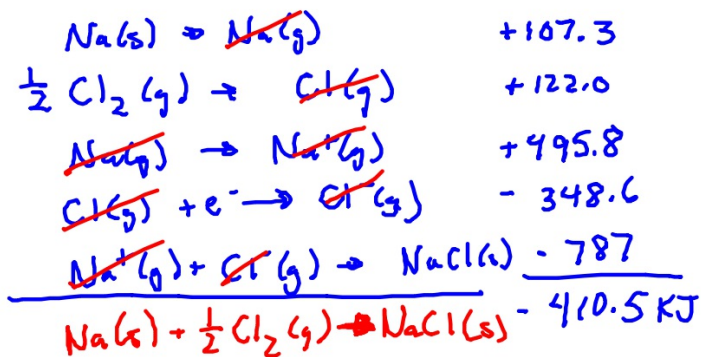
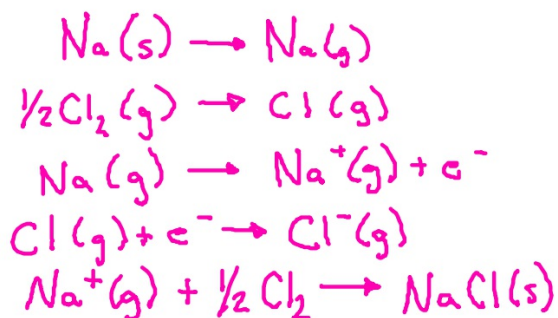
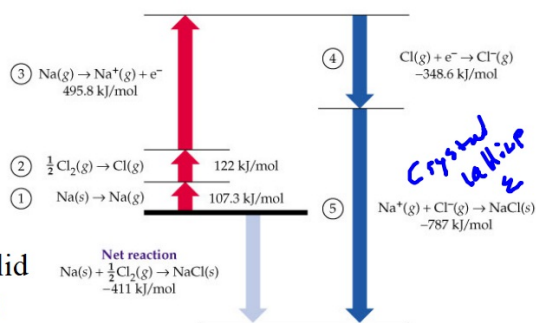


**Bonding  
Topic#10**

**Lattice Energy**

1. Sublimation of sodium:  $\text{Na}(s) \rightarrow \text{Na}(g)$
2. Dissociation of chlorine molecules:  $\frac{1}{2} \text{Cl}_2(g) \rightarrow \text{Cl}(g)$
3. Ionization of sodium:  $\text{Na}(g) \rightarrow \text{Na}^+ + e^-$
4. Electron affinity of chlorine:  $\text{Cl}(g) + e^- \rightarrow \text{Cl}^-(g)$
5. Formation of solid NaCl:  $\text{Na}^+(g) + \text{Cl}^-(g) \rightarrow \text{NaCl}(s)$

5. Calculate net energy change for the productio of NaCl(s) from solid sodium and gaseous chlorine.  
(Ans: -411 kJ)

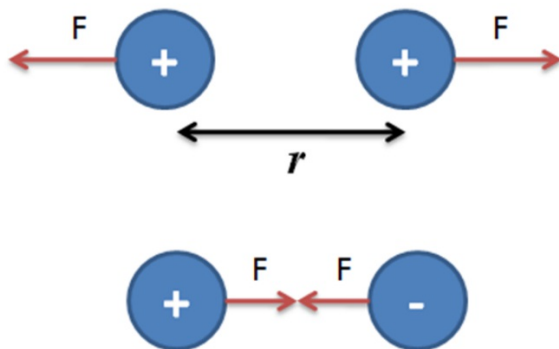


Bonding  
Topic#10

Lattice Energy  
Coulomb's Law

- Force is a function of charge ( $q$ ) and distance ( $d$ ) between two charged particles
  - a negative value indicates an ATTRACTIVE force
  - a positive value indicates a REPULSIVE force

$$F = \frac{kq_1q_2}{r^2} \quad F = k \frac{q_1 q_2}{d^2}$$



NaF vs. CsF  
 $q_1 \times q_2 = -1$      $q_1 \times q_2 = -1$   
 $BL_{NaF} < BL_{CsF}$

Compare the general lattice energies of MgO vs. NaF.

MgO vs. NaF  
 $z_1 \times z_2 = -4$      $z_1 \times z_2 = -1$   
 $BL_{MgO} \gg BL_{NaF}$

$mp_{MgO} > mp_{NaF}$

SWIMS

## Bonding Topic#10

### Bond Energies and Chemical Reactions

- Remember that BE increase with the number of bonds (localised electrons) between two atoms.
  - $C \equiv C > C = C > C - C$
- Each bonded pairs of atoms has a BE found in a table of BEs. **Note:** this is an average of bonds energies.
  - i.e. the C-H bond will have different BEs in  $CH_4$  than in  $CH_3Br$ , so the value in the table is an average of the most common C-H bonds found in compounds.

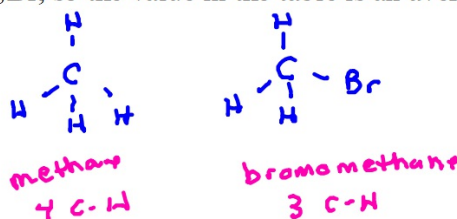


Table 3-3 | Average Bond Energies (kJ/mol)

Single Bonds				Multiple Bonds			
H—H	432	N—H	391	I—I	149	C=C	614
H—F	565	N—N	160	I—Cl	208	C≡C	839
H—Cl	427	N—F	272	I—Br	175	O—O	495
H—Br	363	N—Cl	200	S—H	347	C=O*	745
H—I	295	N—Br	243	S—F	327	C≡O	1072
C—H	413	N—O	201	S—Cl	253	N=O	607
C—C	347	O—H	467	S—Br	218	N—N	418
C—N	305	O—O	146	S—S	266	N≡N	941
C—O	358	O—F	190	C≡N	891	C=N	615
C—F	485	O—Cl	203	C=N	891	C=N	615
C—Cl	339	O—I	234	Si—Si	340		
C—Br	276	F—F	154	Si—H	393		
C—I	240	F—Cl	253	Si—C	360		
C—S	259	F—Br	237	Si—O	452		
		Cl—Cl	239				
		Cl—Br	218				
		Br—Br	193				

\*C=O (in  $CO_2$ ) = 799

Bond	Length (pm)	Energy (kJ/mol)
C—C	154	346
C=C	134	612
C≡C	120	835
C—N	147	305
C=N	132	615
C≡N	116	887
C—O	143	358
C=O	120	799
C=O	113	1072
N—N	145	180
N=N	125	418
N≡N	110	942



---

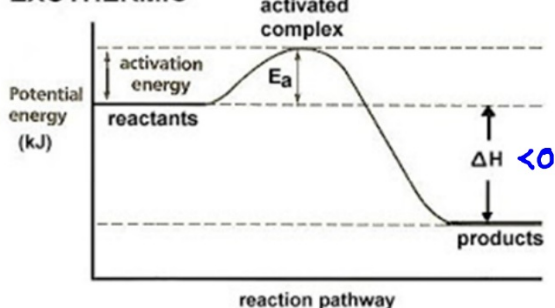
**Bonding**  
**Topic#10**

---

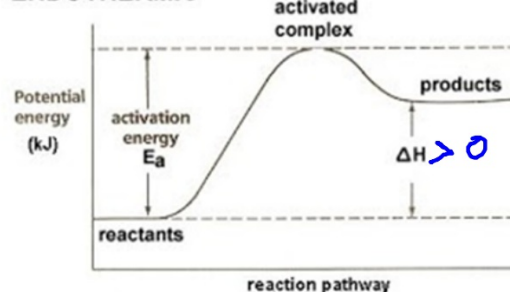
**Change Enthalpy of Reaction ( $\Delta H_{rxn}$ )**

- Enthalpy - a quantity related to the total heat of a system.
  - $H = E + PV$
  - Change in Enthalpy:  $\Delta H = \Delta E + \Delta PV$ 
    - A measure of the change in the total heat of the system.
      - $-\Delta H$  is exothermic ( $\Delta H < 0$ ; a decrease of the heat energy in the system)
      - $+\Delta H$  is endothermic ( $\Delta H > 0$ ; an increase of the heat energy in the system)
- Enthalpy is a state function. A state function refers to a property of the system that depends only on its *present state*. A change in enthalpy ( $\Delta H$ ) does not depend on the pathway between two states.

**EXOTHERMIC**



**ENDOTHERMIC**



## Bonding Topic#10

### Bond Energies and Chemical Reactions

- Remember that BE increase with the number of bonds (localised electrons) between two atoms.
  - $C \equiv C > C=C > C-C$
- Each bonded pairs of atoms has a BE found in a table of BEs. Note: This is an average of bonds.
  - i.e. the C-H bond will have a different BEs in  $CH_4$  than in  $CH_3Br$ , so the value in the table is an average of the most common C-H bonds found in compounds.

- Using BE to calculate the  $\Delta H_{rxn}$

$$\Delta H_{rxn} = \sum BE_{\text{reactants}} - \sum BE_{\text{products}}$$

6. Using the bond energies listed in the table to the right, calculate  $\Delta H_{rxn}$  for the reaction of methane with chlorine and fluorine to give Freon-12 ( $CF_2Cl_2$ ).

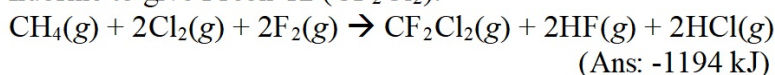
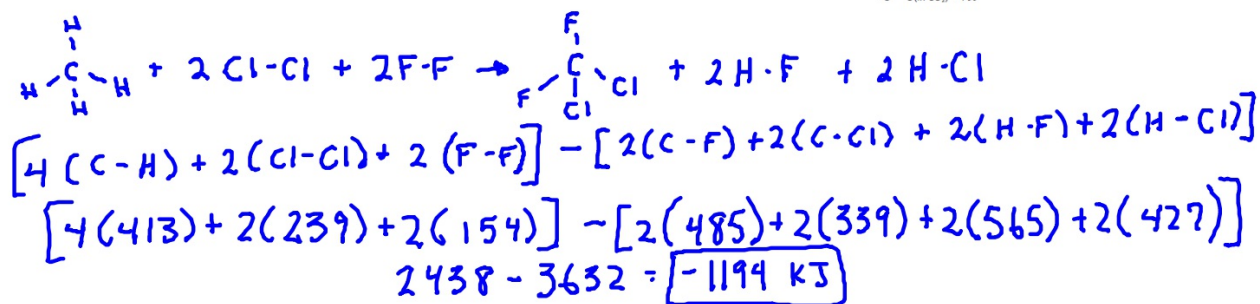


Table 3-3 | Average Bond Energies (kJ/mol)

Single Bonds		Multiple Bonds					
H-H	432	N-H	391	I-I	149	C=C	614
H-F	565	N-N	160	I-Cl	208	C≡C	839
H-Cl	427	N-F	272	I-Br	175	O=O	495
H-Br	363	N-Cl	200	S-H	347	O=O*	745
H-I	295	N-Br	243	S-F	327	C=O	1072
C-H	413	N-O	201	S-Cl	253	N=O	607
C-C	347	O-H	467	S-Br	218	N=N	418
C-N	305	O-F	190	S-S	266	C=N	891
C-O	358	O-Cl	203	Si-Si	340	C=N	615
C-F	485	O-I	234	Si-H	393		
C-Cl	339	F-F	154	Si-C	360		
C-Br	276	F-Cl	253	Si-O	452		
C-I	240	F-Br	237				
C-S	259	Cl-Cl	239				
		Cl-Br	218				
		Br-Br	193				

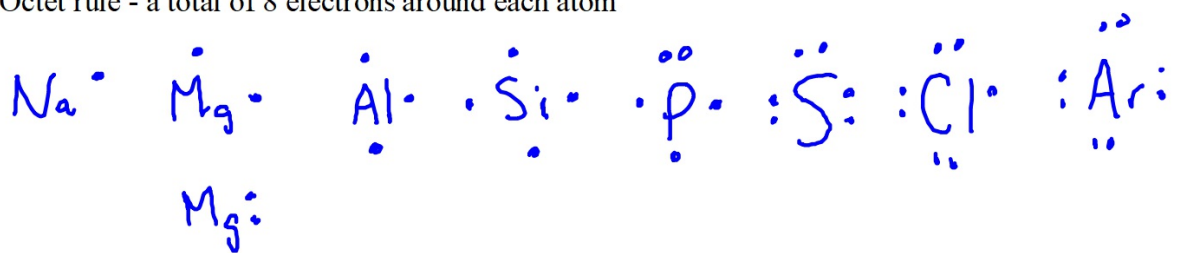
\*C=O (in  $CO_2$ ) = 799



**Bonding**  
**Topic#10**

**Localized Electron (LE) Bonding Model**

- A molecule is composed of atoms that are bound together by sharing pairs of electrons, using the atomic orbitals of the bound atoms.
- Pairs of electrons localized on an atom are called **lone pairs**.
- Pairs found in the space between bonded atoms are called **bonding pairs**.
- Has three parts:
  1. Description of the valence electron arrangement in the molecule using Lewis structures.
  2. Prediction of the geometry of the molecule using the valence shell electron-pair repulsion (VSEPR) model.
  3. Description of the type of atomic orbitals used by the atoms to share electrons or hold lone pairs.
- **Lewis structures** show how the valence electrons are arranged among the atoms in a molecule.
  - Atoms share electrons to achieve a noble gas electron configuration.
    - Use the electron dot for each element based on their number of valence electrons.
    - Duet rule - hydrogen - two electrons
    - Octet rule - a total of 8 electrons around each atom



**Bonding  
Topic#10**

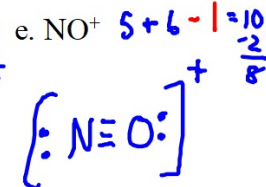
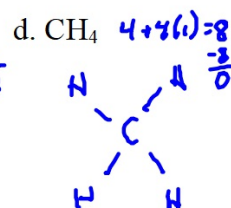
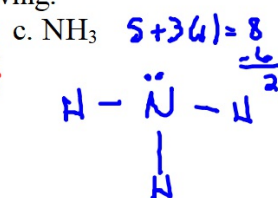
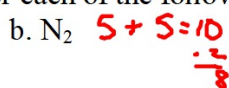
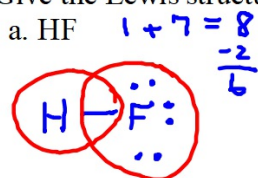
**Lewis Structures**



- Lewis Structure Strategy
  - Sum the valence electrons from all atoms
  - Draw a skeleton of the structure.
    - Use the atom that can form the most bonds as the center atom (usually the LEAST electronegative atom in the group such as C, N, O, etc).
  - Use a pair of electrons to form a single bond between the center atom and the exterior atoms (usually the more electronegative atoms such as O, F, Cl, etc.)
  - Satisfy the octet for the exterior atoms by drawing in pairs of electrons around the atom's symbol.
  - Any remaining electrons go around the center atom.
    - If no electrons are left after satisfying the exterior atoms' octets and the center atom does not have an octet, then double or triple bonds are needed. Usually, one electron from each atom is used to create the double/triple bond, but sometimes one atom donates all of the electrons needed for the double/triple bond.
  - Lone pairs around the center atom group together.
  - Polyatomic ions need brackets and the charge written outside the brackets in the upper right.

**Topic#10 Structure (Molecular) SW#2 - Lewis Structures**

1. Give the Lewis structure for each of the following.



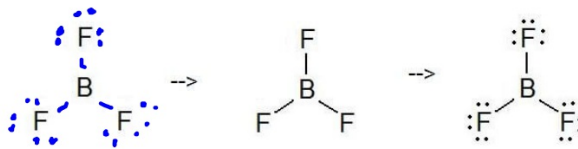
**Bonding**  
**Topic#10**

**Lewis Structures**

- Exceptions to the octet rule
- p-block nonmetals with a principal quantum number of  $n = 3 - 6$  can ACCEPT more the 8 electrons around them. This is due to them having the ability to use the *d* orbitals in the same energy level.
  - i.e. sulfur is in the 3*p* and can use the 3*d* to expand its octet.
- On the other hand, boron can only have 6 electrons around it. Three bonds with its valence electrons gives 6 electrons around it.

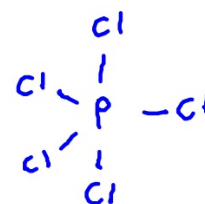
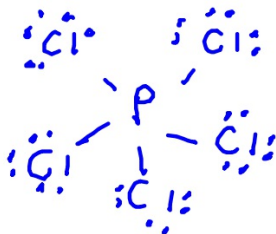
▪ i.e.  $\text{BF}_3$

$$\begin{array}{r} 21 \\ + 3 \\ \hline 24 \\ - 6 \\ \hline 18 \end{array}$$



2. Write the Lewis structure for  $\text{PCl}_5$ .

$$\begin{array}{r} 5 + 5(7) = 40 \\ - 10 \\ \hline 30 \\ - 30 \\ \hline 0 \end{array}$$

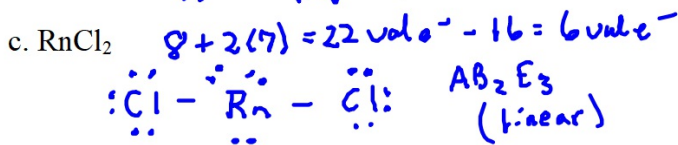
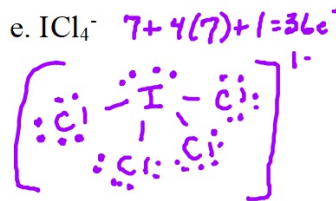
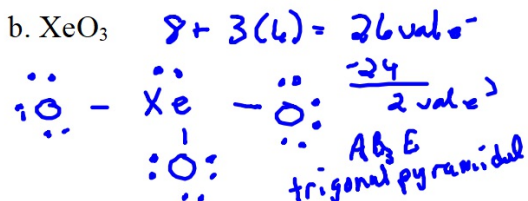
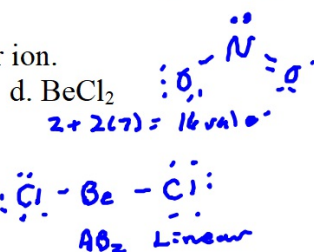
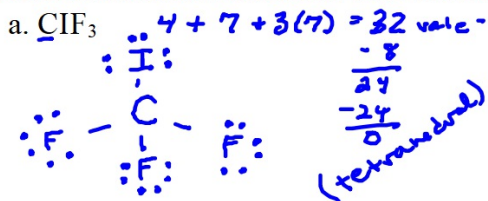


no known  
 $\text{NCl}_5$

## Lewis Structures

- What if all the atoms can have more than 8 electrons around it?
- Then the rule is the extra electrons go around the center atom.
- In other words, satisfy the octet for the exterior atoms then place any extra around the center atom.

3. Write the Lewis structure for each molecule or ion.



$\text{AB}_2\text{E}_2$  - bent / see saw

$\text{AB}_2\text{E}_3$  - linear

$\text{AB}_4\text{E}_2$  - square planar

A - center atom

B - exterior atoms

E - electron pair(s)

$\text{AB}$  - linear ( $\text{HCl}$ )

$\text{AB}_2$  - linear ( $\text{CO}_2$ )

$\text{AB}_2\text{E}$  - bent ( $\text{NO}_2$ )

$\text{AB}_2\text{E}_2$  - bent ( $\text{H}_2\text{O}$ )

$\text{AB}_3$  - trigonal planar ( $\text{SO}_3$ )

$\text{AB}_3\text{E}$  - trigonal pyramidal ( $\text{NH}_3$ )

$\text{AB}_4$  - tetrahedral ( $\text{CH}_4$ )

$\text{AB}_5$  - trigonal bipyramidal ( $\text{PCl}_5$ )

$\text{AB}_6$  - octahedral ( $\text{SF}_6$ )

---

**Bonding**  
**Topic#10**

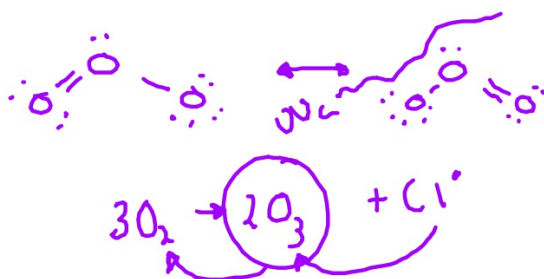
---

**Lewis Structures**

- Sometimes after all of the electrons have been used, the center atom does not have an octet.
- After creating a double/triple bond, you notice all of the exterior atoms are the same atom.
- Here we are forced to acknowledge the double/triple bond can actually be made between ANY of the exterior atoms, thus a number of valid Lewis structures exist.
- In actuality, the bond between the center and the exterior atoms is not made up of single bonds and one double bond, but a hybrid bond that has a BL and BE in between a single and double bond.
- To show this, one must draw a number of other Lewis structures to show this.
- These are called **resonance structures** and the true Lewis structure is an average of these structures.

**Resonance Structures**

Examples: Ozone ( $O_3$ ) and carbonate ion ( $CO_3^{2-}$ )



---

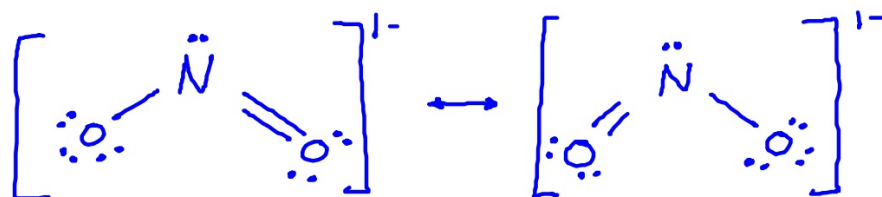
Lewis Structures

**Bonding**  
**Topic#10**

---

4. Describe the electron arrangement in the nitrite anion ( $\text{NO}_2^-$ ) using localized electron model.

$$\text{Valence electrons: } 5 + 2(6) + 1 = \underline{18}$$



2 resonance structures for the nitrite ion ( $\text{NO}_2^-$ )



**Bonding**  
**Topic#10**

**Formal Charge**

- Used to determine the best Lewis structure for a molecule.
  - For odd number molecules such as NO (nitric oxide).
  - For deciding the correct Lewis structure among several valid structures such as  $\text{SO}_4^{2-}$ .
- Process of determining the formal charge on each atom in the structure.
  - Calculate the number of valence electrons on the free atom,  $\text{VE}_{\text{free}}$ .
  - Calculate the number of valence electrons that belong to the atom in the molecule,  $\text{VE}_{\text{molecule}}$ .
    - Lone pair electrons belong entirely to the atom in question
    - Shared electrons are *divided equally* between the two sharing atom.
    - Calculation for assigned valence electrons for an atom in the molecule:

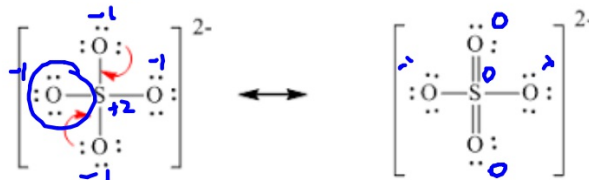
$$\text{VE}_{\text{molecule}} = (\text{number of lone pairs}) + 1/2 (\text{number of shared electrons})$$

$$\text{FC} = \text{VE}_{\text{free}} - \text{VE}_{\text{molecule}} = \text{VE}_{\text{free}} - (\text{number of lone pairs} + 1/2(\text{shared electrons}))$$

- The structure is the best representation when atoms in a molecule have a formal charge as close to **zero** as possible, and any **negative formal charges** are expected to reside on the most **electronegative** atoms.
- Sum of formal charges **MUST** equal the charge on the ion or zero for a molecule!
- Let us look at  $\text{SO}_4^{2-}$ . Using formal charges, determine the best Lewis structure for  $\text{SO}_4^{2-}$ .

$$\begin{aligned} \text{FC} &= \underline{6} - (6 + \frac{1}{2}(2)) \\ \text{:}\ddot{\text{O}}\text{:} &= 6 - 7 = \underline{-1} \end{aligned}$$

$$\begin{aligned} \text{FC} &= 6 - (0 + \frac{1}{2}(8)) \\ &= 6 - 4 = \underline{+2} \end{aligned}$$



Two Lewis structure for  $\text{SO}_4^{2-}$  molecule

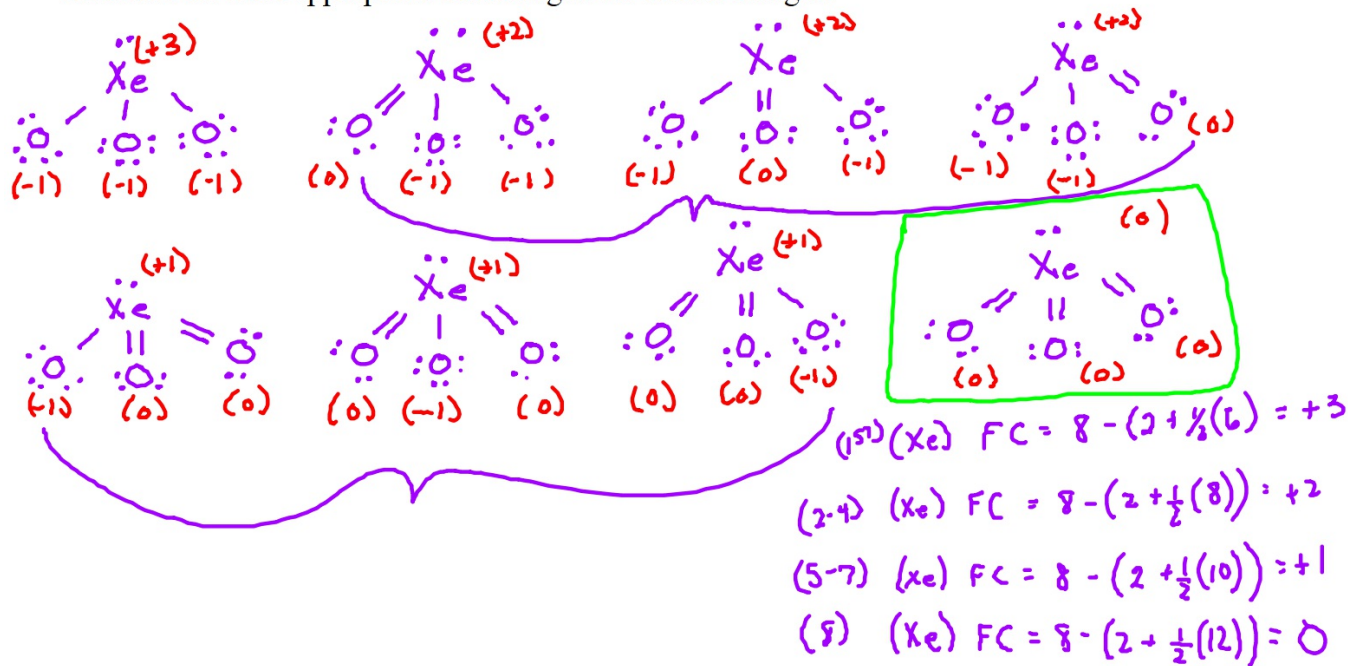
$$(\text{O}) : \text{FC} = 6 - (4 + \frac{1}{2}(2)) = 0$$

$$(\text{S}) : \text{FC} = 6 - (0 + \frac{1}{2}(8)) = 0$$

Formal Charge

Bonding  
Topic#10

5. Give possible Lewis structures for XeO<sub>3</sub>, an explosive compound of xenon. Which Lewis structure or structures are most appropriate according to the formal charges?



---

**Bonding**  
**Topic#10**

---

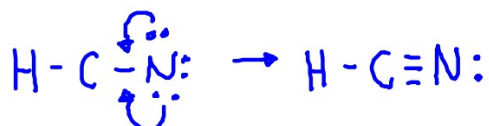
**Review - Lewis Structures**

**Drawing Lewis Structures Review**

- H and F are terminal/exterior atoms in a compound (ALWAYS)
- Element with lowest EN value is central atom (can bond the most)
- Add up all the valence electrons for all of the elements in the compound.
- Place low EN atom in middle with others arranged around the central atom.
- Form one single bond ( $\sigma$ -bond) between the central and exterior atoms.
- Subtract these bonded electrons from your total valence electrons.
- Satisfy octet of exterior atoms. Except H.
- Extra electrons go around central atom as unshared pairs.
- Form double bonds ( $\pi$ -bonds, a double has one  $\pi$ -bond and one  $\sigma$ -bond, and a triple has two  $\pi$ -bonds and one  $\sigma$ -bond) between exterior atoms and central atom to satisfy the octet of the central atom.
- Check for resonance (all the exterior atoms are the same element, but one has a double bond, usually oxygen is involved).



$1 + 4 + 5 = 10$  valence electrons



**Bonding  
Topic#10**

**Hybridization**

$sp \rightarrow 2$   
 $sp^2 \rightarrow 3$   
 $sp^3 \rightarrow 4$

**Molecular Shape, Bonding Region and Hybridization**

- Bonding region - a bond or unshared pair
- Hybridization - a hybrid orbital made up of an *s* and *p* orbital or a *s*, *p*, and *d* orbital
  - $sp$  - two BR,  $sp^2$  - three BR,  $sp^3$  - 4 BR,  $sp^3d$  - 5 BR, and  $sp^3d^2$  - 6BR
- VSEPR - valence shell electron pair repulsion theory
  - unshared electrons influence the geometry of a molecule
  - Around central atom

$H-C \equiv N: sp$

Shape	Bonding Regions	Hybridization	Bond Angle	Example
linear	2 $O=C=O$	$sp$	180	HCN
bent	3 or 4	$sp^2/sp^3$	104.5-109.5	SO <sub>2</sub> /H <sub>2</sub> O
trigonal planar	3	$sp^2$	120	SO <sub>3</sub>
trigonal pyramidal	4	$sp^3$	107.5	NH <sub>3</sub>
tetrahedral	4	$sp^3$	109.5	CH <sub>4</sub>
trigonal bipyramidal	5	$sp^3d$		
octahedral	6	$sp^3d^2$		

