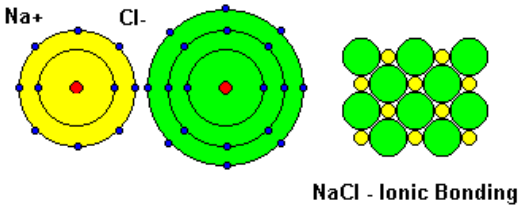
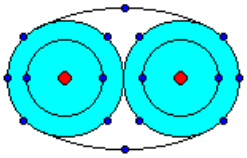
Ch 8 Bonding



NaCl - Ionic Bonding



Oxygen-
Covalent Bonding

Facts:

1) Ionic bonds - electrons are gained or lost (+/- charge)
2) Covalent bonds - electrons are shared, $\delta^{-/+}$ must be used to show how the electrons are "unequally" shared
3) Metallic bonds - electrons are mobile in a "Sea of electrons"

https://www.youtube.com/watch?v=pj0F-zv79rM

https://www.youtube.com/watch?v=D1mLBIjBdSg

Coulomb's Law - energy of interaction calculation between a pair of ions

$$E = (2.31 \times 10^{-19}\ J*nm)\left(\frac{Q_1Q_2}{r}\right)$$

Q = ion charge

r = nm distance between ion centers

E = energy (Joules)

If:

E = (-) atoms have a stable energy level when bonded, (attracted to each other)

E = (+) atoms have a repulsive energy (are not bonded)

Ex: Determine the Energy of attraction/repulsion for sodium and chlorine if 0.276 nm = distance between the nuclei.

Ionic Bonding

A) Atoms exchange electrons (lose and gain)

Groups 1A-3A= lose e-

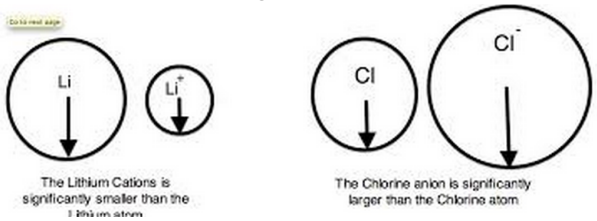
Groups 5A-7A = gain e-

B) Things to recall about ions

1) Size of ion vs its atom

Atom ---> anion (get larger)

Atom ---> cation (get smaller)



2) Isoelectronic ions - ions/atoms with same TOTAL e- number

EX: Arrange the following in order of decreasing size

Rb^{+} Se^{-2} Sr^{+2} Br^{-1}

3) Ion size varies

EX: Choose the largest ion in each group

Li+ Na+ K+ Rb+ Cs+

Ba^{+2} Cs+ I- Te^{-2}

4) Lattice energy - energy released when (g) ions form ionic solids

(-) exothermic value (favored)

(+) endothermic (unfavored)

Lattice Energy $= k\left(\frac{Q_1 * Q_2}{r}\right)$

SO: Which bond will have the greater favorability due to LE?

Ca and O or K and Br

Carbon in pencils vs diamonds

https://www.youtube.com/watch?v=fuinLNKkknI

COVALENT:

1) Electrons are shared
2) Recognized by non-metal : non-metal bond
3) Two types of covalent bonds:
    a) Non-polar covalent
    b) Polar covalent
4) Electronegativity difference dictates bond type

    Zero difference = NPC (0)

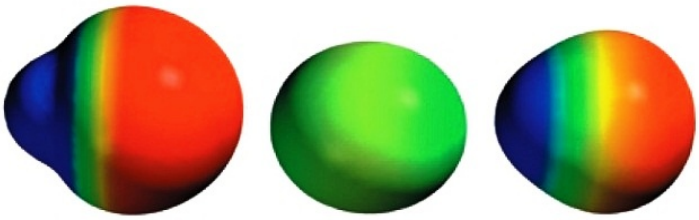
    Low difference = Low PC (~ 0.3)

    Intermediate difference = Definitely PC (up to ~1.7)

    High difference = Ionic (above ~1.7 and metal - non-metal bond)
5) Electrostatic potential maps show where high electron density is

    Red = electron rich

    Violet/blue = electron poor



LiH H_2 HF

Bond Polarities: Due to difference of electronegativity values

A) Higher the electronegativity difference = more polar

EX: Rank the following bonds in order of increasing polarity

H-H OH Cl-H S-H F-H

Dipole Moments:

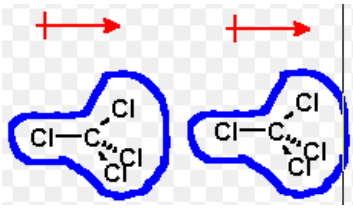
A) Molecule with PC bonds in which it is an overall POLAR molecule

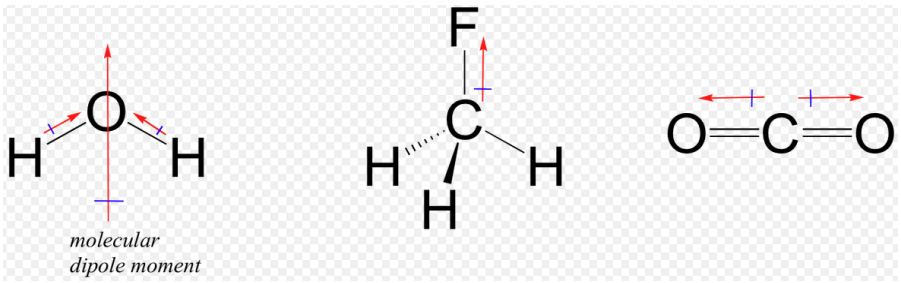
B) The partial + and partial - ends line up to form a "Dipole moment"

1) To be a polar molecule it must

a) Have PC bonds

b) NOT have symmetry





EX: For the following, show the direction of bond polarities and indicate if each as a dipole moment.

HCl

Cl_2

SO_3

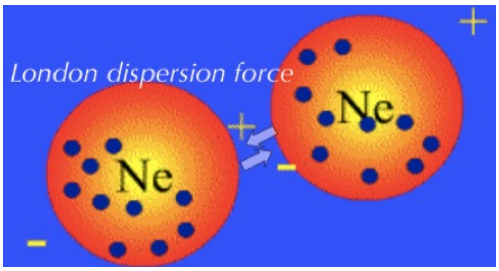
CH_4

H_2S

IMFs (Intermolecular forces) in general:

A) Dispersion (Van DerWaals) - Weak

- Due to the electron cloud attraction of 1 molecule to next

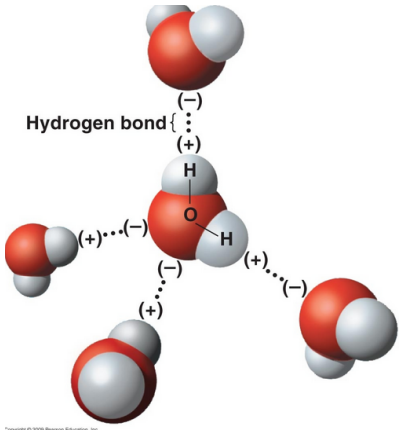


B) Dipole-Dipole - Intermediate strength

- Due to the alignment of 1 dipole molecule to the next dipole molecule

C) Hydrogen Bonding - very strong

- due to the H (δ+) to the (δ -) of an adjacent molecule
- Only found when H-NOF exists



Bond energy and enthalpy of bonds in reactions:

A) Bond breaking = (+) energy (endothermic)

Bond forming - (-) energy (exothermic)

B) All bond values have been found experimentally - see pg 374

C) In general, strength follows: - < = < ≡

D) To find an enthalpy of reaction value

$\Delta H = \sum n * D_{(\text{bonds broken})} - \sum n * D_{(\text{bonds formed})}$

$\sum$ = sum of

D = bond energy per mole

n = moles

Ex: Calculate the enthalpy of reaction for the following reaction:

$CH_{4(g)} + 2Cl_{2(g)} + 2F_{2(g)} \rightarrow CF_2Cl_{2(g)} + 2HF_{(g)} + 2HCl_{(g)}$

1) USE BOND ENERGIES TO ESTIMATE THE ΔH FOR THE FOLLOWING REACTION:

$$H_2O_2(aq) + CH_3OH(aq) \rightarrow H_2CO(aq) + 2H_20(l)$$

H - H: 432 kJ/mol	C - C: 347	C = C: 614
C - H: 413	H - O: 467	C = O: 745
C = N: 615	O - O: 146	O = O: 495
C - O: 358		

DOT STRUCTURES FOR ELEMENTS:

A) Show bonds in COVALENTLY bonded MOLECULES

B) **:** (lone pairs) -, = , ≡ (bonds)

C) Most atoms bond to get an octet
Some exceptions: H = 2 e-
B = 6 e-
3rd period and ↓ can have more than 8 valence
(can have an expanded octet due to the
d sublevel)
Ex: S can have 12 e-
P can have 10 e-

STEPS IN WRITING LEWIS STRUCTURES:

1) **Sum the valence electrons from all the atoms.** Do not worry about keeping track of which electrons come from which atoms. It is the total number of electrons that is important. If the particle is an ion, add electrons if the charge is negative and subtract electrons if the charge is positive.

2) Decide on a central atom.

3) Use a pair of electrons(dash) to form a bond between each pair of bound atoms.

4) Use any remaining pairs as lone pairs around each terminal atom (except H) so that each atom is surrounded by eight electrons.

5) If the central atom has fewer than eight electrons at this point (except H, Be, B), move one or more lone pairs on the terminal atoms into a position intermediate between the center and the terminal atom to form multiple bonds. Fluorine will never have a multiple bond. Do NOT form multiple bonds unless it is absolutely necessary.

6) If there are more electrons that need to be added, arrange them in pairs around the central atom making sure that they can have an expanded octet.

7) In an oxyacid, the hydrogen is always bounded to the oxygen atom.

Let's practice some Lewis Dot structures:

H_2O

CO_2

CN^-

HF

N_2

NH_3

CH_4

NO+

BF_3

More practice - little harder

SF_6

I_3^-

ClF_3

XeO_3

$RnCl_2$

$BeCl_2$

ICl_4^-

RESONANCE:

A) Having more than 1 valid Lewis dot structure
B) Show resonance contributors with a <---->
C) The correct structure is the AVERAGE of each of the contributors

EX: NO_3^{-1}

FORMAL CHARGE:

Formal Charge Concept:

- doesn't imply the presence of actual ionic charges in a molecule
- a device for electron bookkeeping
- Count how many e- are "owned" by an atom in the bonded structure
  * each atom 'owns' 1/2 of the e- in the bond they are engaged in
  * if they own the same number in the molecule as they did as the atom, they will have no formal charge
  * if an atom has lone pairs, it "owns" both of the e-
- formal charges often give clues about chemical activity
- ***Best molecular structure*** **=** lowest FC total, or at least giving the (-) FC to the most electronegative atom and the (+) FC to the least electronegative atom

FC = (# val. e- of neutral atom) - (# e- "owned" by atom in bonded structure)

Ex: Calculate the FC in all possible structures of SO_4^{-2} (3), then decide which structure is the most accurate?

EX: Draw all possible resonance structures for XeO3 (8), then decide which is the best structure based on the FCs found.

VSEPR Theory and Molecular Shapes

1) Draw Lewis dot structure, count bonded and unbonded clouds around central atom only.

2) Shape will be determined by placement of clouds on central atom as far apart as possible from one another (e- repulsion) - using all 360^0

3) Electron lone pair clouds need more room and are stronger than bonded clouds - they will have an effect on the bond angle

BOND ATOMS	LONE PR.	ELEC. GR. ARR.	MOLEC. SHAPE	BOND ANGLE	MOLEC.** POLARITY
2	0	LINEAR	LINEAR	180	
3	0	TRIGONAL PLANAR	TRIGONAL PLANAR	120	
2	1	"	V-SHAPED (bent)	<120 (117)	
4	0	TETRAHEDRAL	TETRAHEDRAL	109.5	
3	1	"	TRIG PYRAMIDAL	<109.5 (107.3)	
2	2	"	V-SHAPED (bent)	<<109.5 (104.5)	
5	0	TRIGONAL BIPYRAMIDAL	TRIGONAL BIPYRAMIDAL	90 120	
4	1	"	SEESAW	<90,<120	
3	2	"	T-SHAPED	<90	
2	3	"	LINEAR	<90	
6	0	OCTAHEDRAL	OCTAHEDRAL	90	
5	1	"	SQ. PYRAMIDAL	<90	
4	2	"	SQUARE PLANAR	90	

** DENOTES THAT POLAR BONDS ARE PRESENT

** DENOTES ALL BONDING ATOMS ARE THE SAME

Draw the dot structures for the following and give their molecular shape:

a) PCl_5

b) $COCl_2$

c) ICl_2^{-1}

d) XeF_4

e) BCl_3

More VSEPR:

Ex: Methanol (CH_3OH) - multiple centers

Ex: PH_3 - exception to angle expected (Compare to NH_3)

Some Lewis dot and VSEPR review:

1) Draw the dot structure of CCl_2F_2
2) Draw the dot structure of O_3 and determine the O-O bond order.
3) Draw all the resonance forms of NCO^{-1} and determine which is the most important.
4) Draw the dot structure of H_2SO_3. Can a better structure be drawn with respect to formal charge?
5) Draw the dot structure of the following giving the molecular shape, all the possible bond angles: BCl_2F, XeF_2, C_2H_2, CH_3^{-1}, BrF_4^{+1}

Draw the dot structures for the following giving
a) electron group arrangement
b) molecular shape (geometry)
c) bond angle(s)
d) molecular polarity (whether or not it has a dipole moment)

1) $CHCl_3$

2) H_2SO_4

3) KrF_2

4) ICl_3

5) HCN

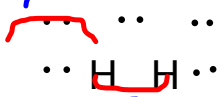
6) PCl_3

7) BrF_5

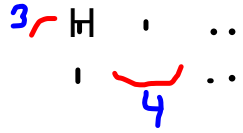
8) SO_3

Give approximate values for the indicated bond angles:

9) H---O---N = O



10) H---C---C = O



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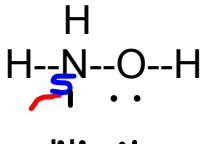
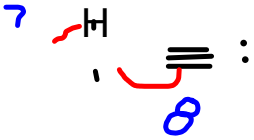


12)



Ch 9.6 PES

A) High energy photons are directed at a n element sample

B) Electrons are ejected and their KE measured

Energy of electron = energy of photons - KE of e-

or $E_{electron} = h\nu - KE$

C) Data is displayed in a graph

i) area of each peak is proportional to the # of e- with that particular Energy

ii) The higher the energy level (like n = 7) the larger the amount of Energy produced

iii) Remember the order of sublevels

1s 2s 2p 3s 3p 4s 3d 4p...