<u>Bonding-General Concepts</u>

Chapter 8

<u>Chemical Bonds</u>

- Forces that hold groups of atoms together so they function as a unit
- Form to achieve a state of <u>lower energy</u> (more stable)

<u>Types of Bonds</u>

1. Ionic
2. Covalent

<u>Ionic Bonds</u>

- Formed between a <u>metal</u> and a <u>nonmetal</u>
- Results from the <u>transfer</u> of electrons
- Metal (low ionization energy) loses an electron to a nonmetal (high electron affinity)
- All monatomic ions achieve <u>octets</u>
- Can predict formulas for binary ionic compounds from the ion charges

Ex. Ca [Ar] $4s^2$ ➘
O [He] $2s^2,2p^4$ $Ca^{+2}O^{-2}$

Ex. Al [Ne] $3s^2,3p^1$ x2 = $6e^-$
O [He] $2s^2,2p^4$ x3 = $6e^-$ $Al_2^{+3}O_3^{-2}$

Ex. Ba [Xe] $6s^2$ x3 = $6e^-$
N [He] $2s^2,2p^3$ x2 = $6e^-$ $Ba_3^{+2}N_2^{-3}$

(As electrons are lost or gained, the size of the particle changes)

<u>Size of Ions</u>

<u>Positive</u> Ions

- Electrons are lost
- Fewer electrons = <u>less</u> repulsion
- Z_{eff} increases & the electrons are pulled in <u>more</u> tightly

∴ Positive ions are smaller than the atom they are formed from

<u>Negative</u> Ions

- Electrons are gained
- More electrons = <u>more</u> repulsion
- Z_{eff} decreases and the electrons are held <u>less</u> tightly

∴ Negative ions are larger than the atom they are formed from

<u>Isoelectronic Ions</u>

- Ions with the <u>same number</u> of electrons
- The greater the number of protons (<u>Z_{eff}</u>) the smaller the ion

Ex. $_{8}O^{-2} > {}_{9}F^{-1} > {}_{11}Na^{+1} > {}_{12}Mg^{+2} > {}_{13}Al^{+3}$

Energies Involved in Forming an Ionic Solid

- Ionic solids form from individual gaseous ions

  Ex. $Li_{(s)} + \frac{1}{2} F_{2\,(g)} \rightarrow LiF_{(s)}$

1. Sublimation of $Li_{(s)}$

   $Li_{(s)} \rightarrow Li_{(g)}$ ΔH=161kj/mol
2. Ionization of $Li_{(g)}$

   $Li_{(g)} \rightarrow Li^{+}_{(g)} + e^{-}$ ΔH=520 kj/mol
3. Dissociation of F_2

   $\frac{1}{2}F_2 \rightarrow F^{-}_{(g)}$ ΔH=154/2 kj/mol (77kj/mol)
4. Formation of $F^{-}_{(g)}$

   $F_{(g)} + e^{-} \rightarrow F^{-}_{(g)}$ ΔH=-328kj/mol
5. Formation of $LiF_{(s)}$

   $Li^{+}_{(g)} + F^{-}_{(g)} \rightarrow LiF_{(s)}$ ΔH=-1097kj/mol

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Overall: ΔH=-617kj/mol

Lower energy level (more stable)

Lattice Energy

- The energy change that occurs when separate gaseous ions are packed together to form an ionic solid
- It is directly proportional to the amount of the charge on the ions (larger charge = larger lattice energy)

  Ex. $Na^{+}\text{-}Cl^{-} < Mg^{+2}\text{-}Cl^{-} < Mg^{+2}\text{-}S^{-2}$
- It is inversely proportional to the size of the ions (as the distance between the charge centers increases, lattice energy decreases)

  Ex. NaCl > KCl because K^{+} is larger than Na^{+}

Covalent Bonds

- Formed between two nonmetallic atoms
- The atoms share one (or more) pairs of electrons
- The shared electrons reside primarily between the nuclei of the two bonded atoms
- Both nuclei are attracted to the shared electrons
- This results in a state of greater stability
- The distance between the bonded nuclei is called the Bond Length
- The attraction for the shared electrons is measured as "electronegativity"

Electronegativity

- The ability of an atom to attract electrons to itself
- Listed on p. 356 F~Cs = 0.7 F=4.0
- In general, the closer an element is to fluorine, the higher its electrongegativity
  - O=3.5 F=4.0 Cl=3.1
- the electronegativities of the bonded atoms determine how equally or unequally the pairs of electrons are shared.

- The greater the electronegativity difference the **<u>more unequal</u>** the sharing of electrons

NONPOLAR COVALENT BONDS

- A bond formed between two atoms of the **same non-metals**
- The electron pair is shared **equally**
- **NO** charges arise in the molecule
- the molecules formed are **nonpolar** molecules

    ex: H_2, P_4, S_8

POLAR COVALENT BONDS

- A bond between atoms of two **different nonmetals**
- Charges arise because the electrons are shared unequally the more electronegative element becomes negative
- The less electronegative element becomes positive
    - Ex:

Has electrons less of the time → $^{+}H - F^{-}$ ← has electrons most of the time

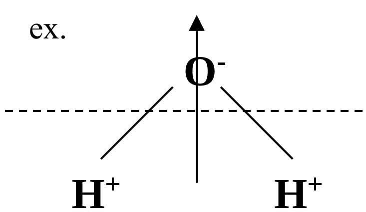
2.1 4.0

- the molecule formed could be a polar molecule or a nonpolar molecule

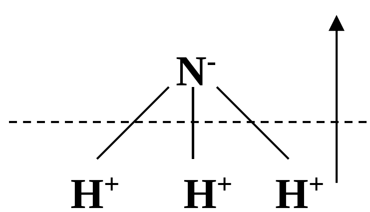
POLAR MOLECULE (a dipole)

- a molecule that has separate centers of positive and negative charge
- it has a "dipole moment"
- this is a measure of how polar the molecules is
- the larger the dipole moment, the more polar the molecule

ex.



Bent

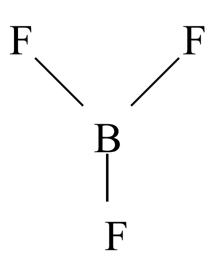


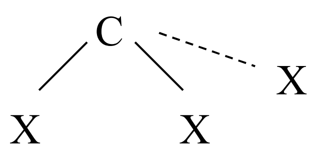
Pyramidal

NONPOLAR MOLECULE

CHARGE CENTERS CANCEL!!!

O = C = O





Which are polar? (Have a dipolar moment)

HCl SO_3 CH_4 H_2S

BOND ENERGY

- the energy that must be added to break a covalent bond
- also: the energy released when a bond is formed
- can be measured by experimentation
- can be used to calculate ΔH for a reaction

ex. $H_2 (g) + F_2 (g) \rightarrow 2HF (g)$ ΔH

$\Delta H = ?$

  - o bond energies are found in table 8.4 (p.367)

- multiple bonds are shorter and stronger than single bonds

	Bond Engery (Kj/mole)	Bond Length (Å)
C-C	347	1.54
C=C	615	1.37
C≡C	839	1.20

Ex. $2C_2H_2 + 5)2 \rightarrow 4\ CO_2 + 2H_2O$ $\Delta H =$

Think in terms of Structural Formulas!

Lewis Structures

- Shows how the valence electrons are arranged among the atoms in a molecule.
- The most important requirement for a stable compound is that the atoms achieve noble gas electron configurations.

Rules for Drawing Lewis Structures

1. Add up the total numbe of valence electrons for all of the atoms in the molecule.
2. Use the pair of electrons to form a bond between each pair of bonded atoms
3. Arrange the remaining electrons to satisfy the "duet" rule for hydrogen and the "octet" rule for other elements.

Ex: H_2	2 Valence electrons	H:H	(duet) -full first PEL (like He)
Ex: F_2	14 Valence electrons	F : F	(octets)

Octet Rule

- non-metals are most stable when surrounded by 8 electrons
(-always holds true for C, N, O, +F)

Ex: H_2O

Ex: CO_2

Ex: CN^{-1} (cyanide)

Bonding Pair

- 2 electrons shared between two atoms

Lone Pair

- 2 electrons localized on only 1 atom

Exceptions to the Octet Rule

- Boron- in some compounds less than 8e
  Ex. BF_3
- all B-F bonds are single bonds (exp. results)
- BF_3 reacts violently with other substances that already have a lone pair of electrons

Ex.

- Some atoms EXCEED the Octet Rule
  Ex. SF_6

- only atoms with **<u>3 or more occupied</u>** **<u>PEL's</u>** will exceed the octet rule
- (it is assumed that) that **d orbitals** are being used to accommodate the extra electrons.

PCl_5

- when it is necessary to exceed the octet rule, place any <u>extra</u> electrons **<u>on the central atom</u>** in the structure.

Ex: I_3^-

a) ClF_3

b) XeO_3

c) $RnCl_2$

d) ClO_3^-

e) ICl_4^-

<u>Resonance</u>

- when a molecule cannot be represented by a single Lewis structure
- The bonds in the molecule are of **<u>Intermediate</u>** strength (3/2, 4/3, etc)
- The "average" of the possible Lewis structures represents the molecule.

Ex. SO_2

-exp. Shows that both S-O bonds are of the same strength & length (1.50
-exp shows a bond < of 120°

- the actual structure of SO_2 is considered to be the "average" of both structures

NO_2^-

- Lewis structures are limited to only representing single, double or triple bonds

Ex. SO_3

-exp shows 3 equal bonds (~1.3)
-exp shows 120° bond <

SO:

-the number of resonance structures needed is determined by the number of sites in which the multiple bond can be placed

Ex. NO_3^-

(From Regents Chemistry)
Benzene
-all C-C bonds
Are 1.5 length
And strength

Molecular Structure: The VSEPR Model
-a system, or model that is used to predict the geometry of a molecule from its number of pairs of electrons.

- important because structure determines properties
- the structure around a given atom is determined by minimizing electron pair repulsion
- the bonding and lone pairs of electrons on an atom will be positioned as far apart as possible
- an atom can have from 2→6 pairs of electrons (normally) that repel each other

- one pair, like H:H, doesn't experience repulsion because no other electrons are present

<u>2 pairs of electrons</u>:

Y:X:Y $\angle = 180°$, linear ___________

<u>3 pairs of electrons</u>:

$\angle = 120°$, trigonal planar (triangle in one plane)

<u>4 pairs of electrons</u>:

$\angle = 109.5°$, tetrahedral (tetrahedron)

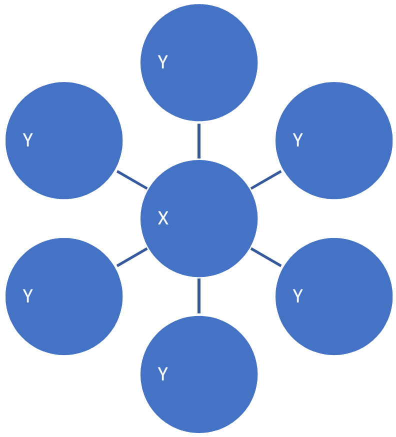
<u>5 pairs of electrons</u>:

$\angle = 90°$ between axial & equatorial positions

$\angle = 120°$ between equatorial positions

Trigonal bipyramidal

6 Pairs of electrons



Angle = 90 degrees between any two neighboring positions.

Octahedral

For Example:

1. 2pairs of electrons

$BeCl_2$

$2+2(7) = 16$

```
 ..   ..   ..
: Cl : Be : Cl :
 ..        ..
```

2 pairs of e- on Be

2. 3 Pairs of Electrons

BF_3

$3 + 3(7) = 24_e$

3. 4 pairs of electrons

CH4

4 +4(1) = 8e

To Determine the Molecules Shape:

1. Draw Lewis structure to determine pairs of electrons on central atom.
2. Decide on proper (positions) for electron pairs.
3. Name molecular structure from positions of the atoms in their molecule.

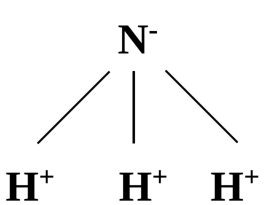
But – What if some pairs are lone pairs?

-repulsion determines position of electron pairs

- position of atoms determines structure

NH3

5 +3(1) = 8e -4e pairs = tetrahedral orientation



- Because there is no atom at the lone pair site the shape is now pyramidal (trigonal pyramid).
- The bond angle is 107
  - the lone pair of electrons is localized on the N atom.

  -because they never move off the N they exert a greater repulsion on the bonded pairs.

  - this decreases the bond angle as the bonded pairs are pushed closer together.

H_2O H : O : H

2 + 6 = 8e

-4 pairs of e- = tetrahedral orientation (2 bonded 2 lone)

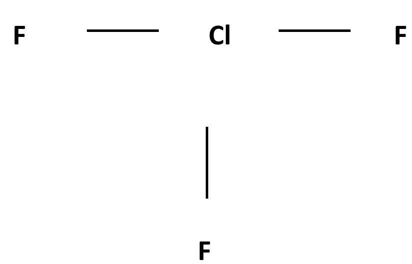
Angle = 104.5 (lone pairs exerting greater repulsion)
Bent (or v-shaped) ∠109 H_2Se (bent)
(build a model of this one)

4. 5 pairs of electrons PCl_5 5+5(7) = 40 e^- ∠=90°, 120°

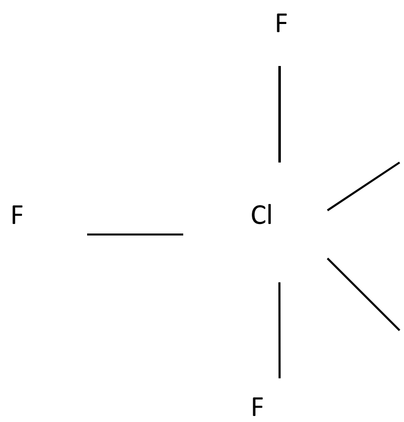
Lone Pairs: SF_4 6+4(7) = 34e^- 4 bonded + 1 lone pair = 5 pair of e^- so it has trigonal bipyramidal orientation.

- lone electron pair will be found in an equatorial position
- equatorial position ∠ of 120° is less repulsion than axial position of 90°
- With 5e^- pairs, lone pairs will always be found in equatorial positions
- ∠ = 90°, 120° Shape is seesaw (looks like a folded square)

ClF_3
7+3(7) = 28e-



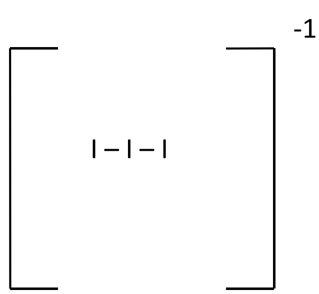
5 pairs of electrons so trigonal bipyramidal orientation.



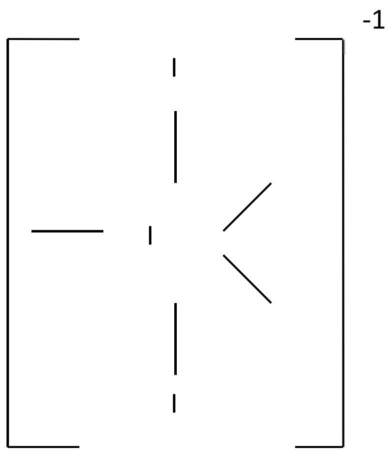
- lone pairs occupy equatorial positions
- angle = 90
- T-shaped

I_3^{-1}

3(7) +1=22 e-



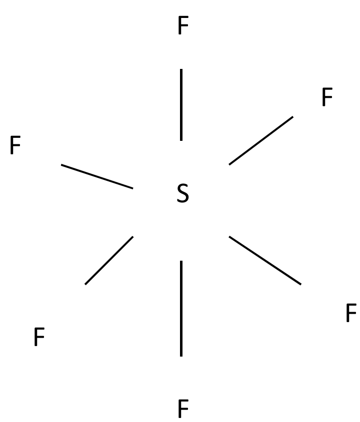
5 e- pairs so triagonal bipyramidal orientation



- lone pairs occupy equatorial positions
- angle = 180°
- linear

6 pairs of electrons

SF_6
$6 + 6(7) = 48e-$

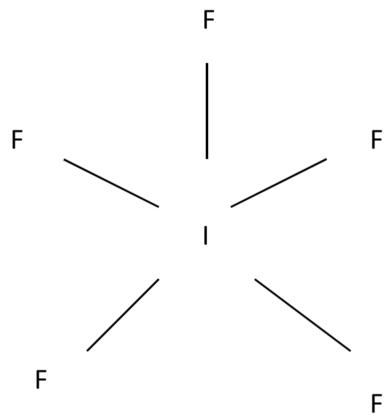


Angle = 90°

Octahedral

(Lone Pairs)

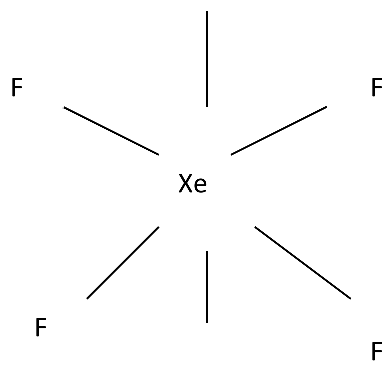
IF_5
$7 + 5(7) = 42e-$



6e- pairs so octahedral orientation

(5 bonding, 1 lone)

Square pyramidal



Angle = 90

Square Planar

Square planar

<u>What about Double or Triple Bonds?</u>

- All shared pairs in a double or triple bond are in the space between the 2 bonded nuclei.
- A double or triple bond is counted as 1 shared pair in the VSEPR model.

Ex. SO_2 6 + 2(6) 3 e^- pairs so it is Trigonal planar orientation with a 120° angle
V-shaped

- VSEPR has been presented here for molecules that have a central atom
- It is a fairly simple system
- When applied to molecules that do not have a central atom, the model still works very well

Ex. CH_3OH (all are tetrahedral angles, even the O-H bond