UNIT 4: CHEMICAL BONDING

Chapter 13: Electrons in Atoms

13.1: Models of Atom

As mentioned in Section 5.2: Structure of the Nuclear Atom, the evolution on the Atomic Theories is as follows:
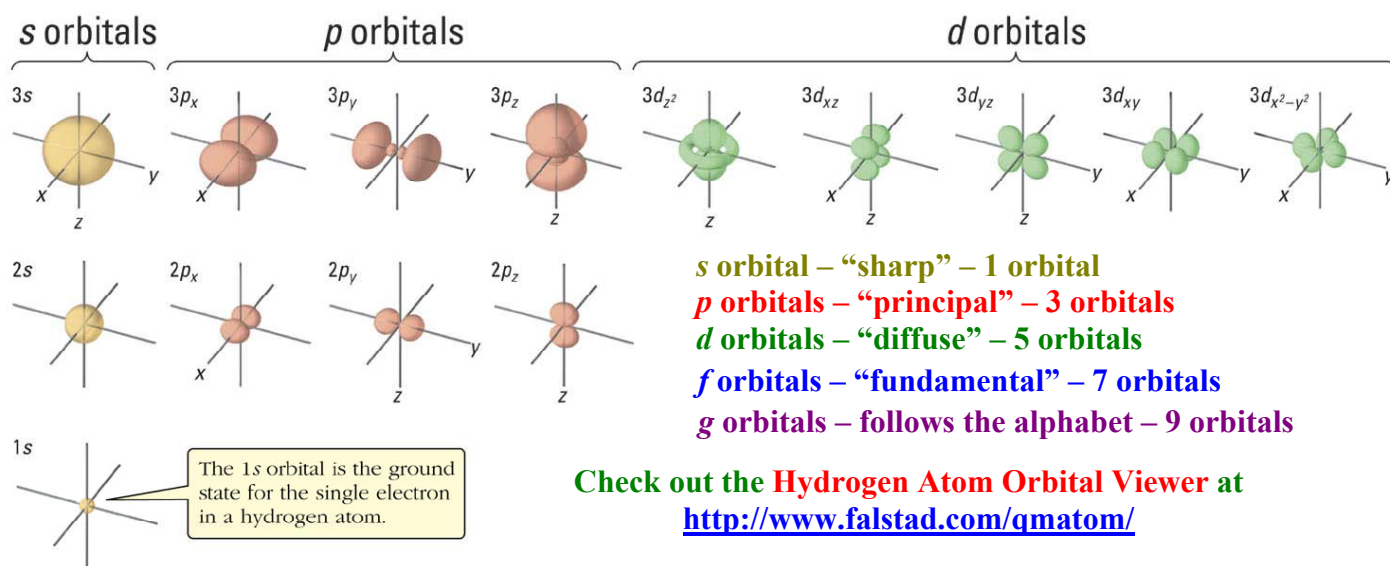
1. **Dalton's Atomic Model**: - John Dalton theorized that atoms are the smallest fundamental particle unique to different elements. They can never be created or destroyed.

2. **Thomson's Plum Pudding Model**: - negative subatomic particles called electrons are spread out around a "positive charged spherical cloud" much like plum pudding.

3. **Rutherford's Nuclear Model**: - the innermost part of the atom is called a nucleus, which consists of neutrons and protons. An equal number of electrons fly around the nucleus so an atom is neutral and mainly composed of empty space.

4. **Bohr's Energy Level Model**: - the electrons around the nucleus move about in a preset **orbits (energy level)** like planets around the sun. Each orbit can house different number of electrons. Electrons cannot exist between energy level. ***(Electrons are _quantized_ – can exist at one level at a time.)* Quantum refers to the amount of energy from one orbit to the next.** The number of electrons in each energy level is the same as the number of elements in each row of the Table of Elements. The higher the energy level, the unstable it is for the electrons because it has higher potential energy.

$n = \infty$

$n = 5$ $n = 6$ _____

$n = 4$ _____

$n = 3$ _____

$n = 2$ _____

$n = 1$ _____

5. **Quantum Mechanical Model**: - proposed by **Erwin Schrödinger (electrons have wave properties)** and **Werner Heisenberg (due to the speed of an electron, we can never locate its position and determine its speed at the same time)**, electrons in an atom moves around the nucleus in specific **orbitals (an region defined by the probability of where the electrons might be found).** *Note*: Orbitals do not have to be circular but it is three-dimensional in form and can come in different shape.

Quantum Atomic Orbitals: - are consisted of two parts: **the Principle Energy Level (n) and Type of Sublevel (s, p, d or f).**
- **each atomic orbitals can house _two electrons_ only**.

a. **Principal Energy Level (n)**: - natural number values {1, 2, 3, …} are used to describe the energy and size of the orbital.

b. **Type of Sublevel**: - indicate the shape of the atomic orbitals (s, p, d or f).

s orbital – "sharp" – 1 orbital
p orbitals – "principal" – 3 orbitals
d orbitals – "diffuse" – 5 orbitals
f orbitals – "fundamental" – 7 orbitals
g orbitals – follows the alphabet – 9 orbitals

Check out the **Hydrogen Atom Orbital Viewer** at
http://www.falstad.com/qmatom/

n	Sublevel	# of Orbitals	Total # of Orbitals	Total # of Electrons
1	1*s*	1	1	2
2	2*s*	1	4	8
	2*p*	3		
3	3*s*	1	9	18
	3*p*	3		
	3*d*	5		
4	4*s*	1	16	32
	4*p*	3		
	4*d*	5		
	4*f*	7		

> **Assignment**
> **13.1 pg. 366 #1 to 4**

13.2: Electron Arrangement in Atoms

Aufbau Principle: - "*Aufbau*" German for "building up"
- for each element, electrons are built up from the lowest energy orbital to the higher ones.
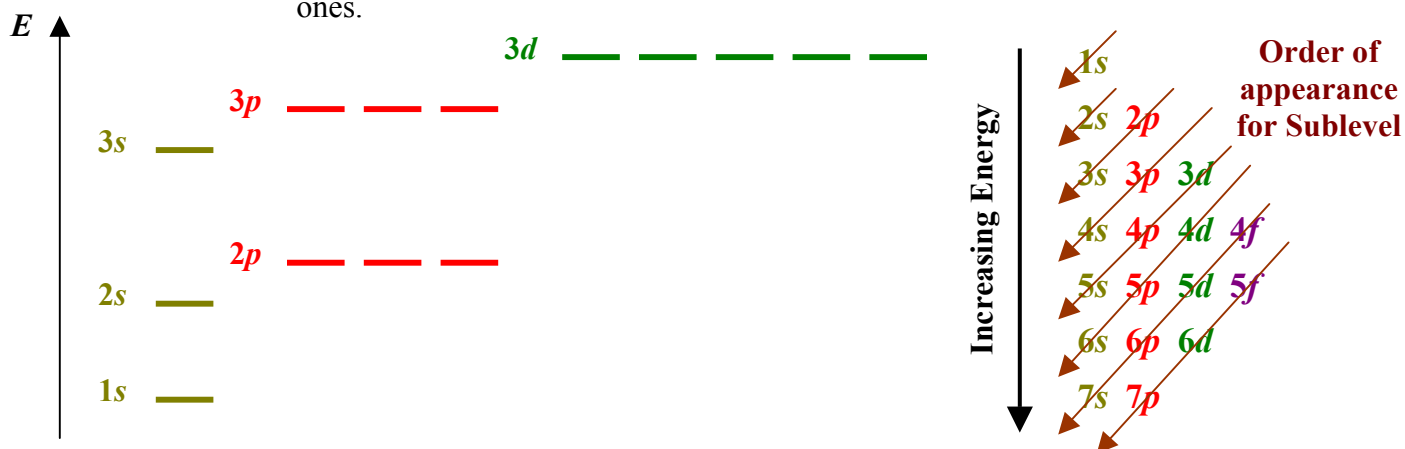
Electron Spin: - when electron spins clockwise, it creates a magnetic north pole in the upward direction. Conversely, when electron spins counter-clockwise, it creates a magnetic north pole in the downward direction.
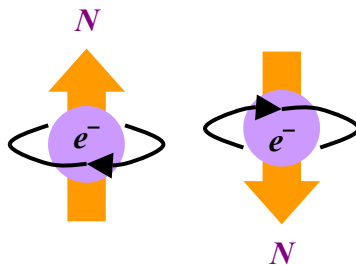
Pauli Exclusion Principle: - in a given atom, each atomic orbital can only have a maximum of two electrons with opposing spins.

Example 1: In the 1*s* orbital, the two electrons can be represented by

1*s* orbital

Hund's Rule: - for sublevels that can have more than 1 orbital (as in *p*, *d*, *f* …), the lowest energy can be achieved when the electrons are arranged so that there are a maximum number of unpaired electrons. These unpaired electrons are drawn "spinning up" (↑) in the orbital diagram.

Electron Configuration: - the arrangement of electrons in atomic sublevels.

Orbital Diagram: - a diagram that shows the arrangements of electrons in quantum sublevels.
Use the Electron Configuration Animation/Applet at
http://intro.chem.okstate.edu/WorkshopFolder/Electronconfnew.html to do the next two examples.
Note the exceptions for Cr and Cu.

Example 2: Draw the quantum orbital diagrams and state the electron configurations for the following atoms.

Atomic #	Atom	Electron Configuration	Orbital Diagram 1s 2s 2p
1	H	$1s^1$	
2	He	$1s^2$	
3	Li	$1s^2\,2s^1$	
4	Be	$1s^2\,2s^2$	
5	B	$1s^2\,2s^2\,2p^1$	
6	C	$1s^2\,2s^2\,2p^2$	
7	N	$1s^2\,2s^2\,2p^3$	
8	O	$1s^2\,2s^2\,2p^4$	
9	F	$1s^2\,2s^2\,2p^5$	
10	Ne	$1s^2\,2s^2\,2p^6$	

Example 3: Draw the quantum orbital diagrams and state the electron configurations for the following atoms.

Atomic #	Atom	Electron Configuration	Orbital Diagram 4s	3d	4p
19	K	[Ar] $4s^1$	[Ar] ↑	___ ___ ___ ___ ___	___ ___ ___
20	Ca	[Ar] $4s^2$	[Ar] ↑↓	___ ___ ___ ___ ___	___ ___ ___
21	Sc	[Ar] $4s^2 3d^1$	[Ar] ↑↓	↑ ___ ___ ___ ___	___ ___ ___
22	Ti	[Ar] $4s^2 3d^2$	[Ar] ↑↓	↑ ↑ ___ ___ ___	___ ___ ___
23	V	[Ar] $4s^2 3d^3$	[Ar] ↑↓	↑ ↑ ↑ ___ ___	___ ___ ___
24	***Cr**	[Ar] $4s^1 3d^5$	[Ar] ↑	↑ ↑ ↑ ↑ ↑	___ ___ ___
25	Mn	[Ar] $4s^2 3d^5$	[Ar] ↑↓	↑ ↑ ↑ ↑ ↑	___ ___ ___
26	Fe	[Ar] $4s^2 3d^6$	[Ar] ↑↓	↑↓ ↑ ↑ ↑ ↑	___ ___ ___
27	Co	[Ar] $4s^2 3d^7$	[Ar] ↑↓	↑↓ ↑↓ ↑ ↑ ↑	___ ___ ___
28	Ni	[Ar] $4s^2 3d^8$	[Ar] ↑↓	↑↓ ↑↓ ↑↓ ↑ ↑	___ ___ ___
29	***Cu**	[Ar] $4s^1 3d^{10}$	[Ar] ↑	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	___ ___ ___
30	Zn	[Ar] $4s^2 3d^{10}$	[Ar] ↑↓	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	___ ___ ___
31	Ga	[Ar] $4s^1 3d^{10} 4p^1$	[Ar] ↑↓	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑ ___ ___
32	Ge	[Ar] $4s^1 3d^{10} 4p^2$	[Ar] ↑↓	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑ ↑ ___
33	As	[Ar] $4s^1 3d^{10} 4p^3$	[Ar] ↑↓	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑ ↑ ↑
34	Se	[Ar] $4s^1 3d^{10} 4p^4$	[Ar] ↑↓	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑↓ ↑ ↑
35	Br	[Ar] $4s^1 3d^{10} 4p^5$	[Ar] ↑↓	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑↓ ↑↓ ↑
36	Kr	[Ar] $4s^1 3d^{10} 4p^6$	[Ar] ↑↓	↑↓ ↑↓ ↑↓ ↑↓ ↑↓	↑↓ ↑↓ ↑↓

***From Hund's Rule, Cr and Cu can achieved lowest energy if the $4s^2$ e^- was moved to the $3d^5$ or $3d^{10}$.**

Chapter 14: Chemical Periodicity

14.1: Classification of Elements

Different Groups and Periods in the Periodic Table of Elements

1. **Noble Gases**: - elements in the last column of the Table.
   - they are stable and generally non-reactive because their **outermost shell is completely filled** in the 1*s* (in the case of He) or the *p* orbitals (Ne, Ar, Kr, Xe and Rn).

2. **Representative Elements**: - elements in the *A* groups where the ***s* or *p* orbitals are partially filled**.

3. **Transition Metals**: - elements in the *B* groups characterized by the ***d* orbitals**.

4. **Inner Transition Metals**: - elements in the ***f* orbitals** in the Lanthanide and Actinide Series.

Electron Configurations in the Periodic Table of Elements

Core Electrons: - inner electrons that have completed a row in the Periodic Table of Elements.

Valance Electrons: - electrons in the outermost principal energy level of an atom.
                         - elements in the same group or family contains the same valence electron configuration.

> ### Assignment
> **14.1 pg. 396 #1 to 5**

14.2: Periodic Trends

There are many different trends regarding the physical and chemical properties of the elements in the Periodic Table. However, we will limit to four atomic properties. They are atomic size, ionization energy, ionic size, and electronegativity.

Shielding Effect: - the outer electrons are pushed away because of the repulsion between them and the core electrons. The net result is that the protons in the nucleus cannot hold on to these outer electrons as tightly as they would for the core electrons.
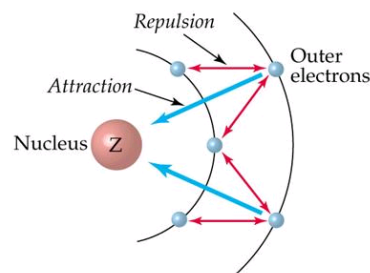
Effective Nuclear Charge (Z_{eff}): - the net nuclear charge actually experienced by an electron (the difference between the number of protons, Z, and the number of "shielded" core electrons).
       - **the higher it is for Z_{eff}, the less shielding effect the outer electrons will experience (The nucleus will have more pull on the outermost electrons).**

$$Z_{eff} = \text{Atomic Number } (Z) - \text{"Shield" Core Electrons}$$

Example 1: Calculate the effective nuclear charge of Na and Ar (first and last elements of period 3).

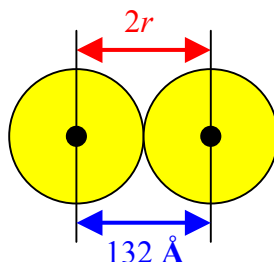|	

For Na: $(1s^2\, 2s^2\, 2p^6\, 3s^1) = 11$ electrons
 $Z_{eff} = 11 - 10\ (1s^2\, 2s^2\, 2p^6)$
           $Z_{eff} = 1$ for Na
	For Ar: $(1s^2\, 2s^2\, 2p^6\, 3s^2\, 3p^6) = 18$ electrons
	 $Z_{eff} = 18 - 10\ (1s^2\, 2s^2\, 2p^6)$
	           $Z_{eff} = 8$ for Ar

Therefore, there is less shielding for Ar and the nucleus for Ar can hold on to its valence electrons a lot better than Na.

Atomic Radius: - the size of an atom as measured by the distances between atoms in chemical compound.
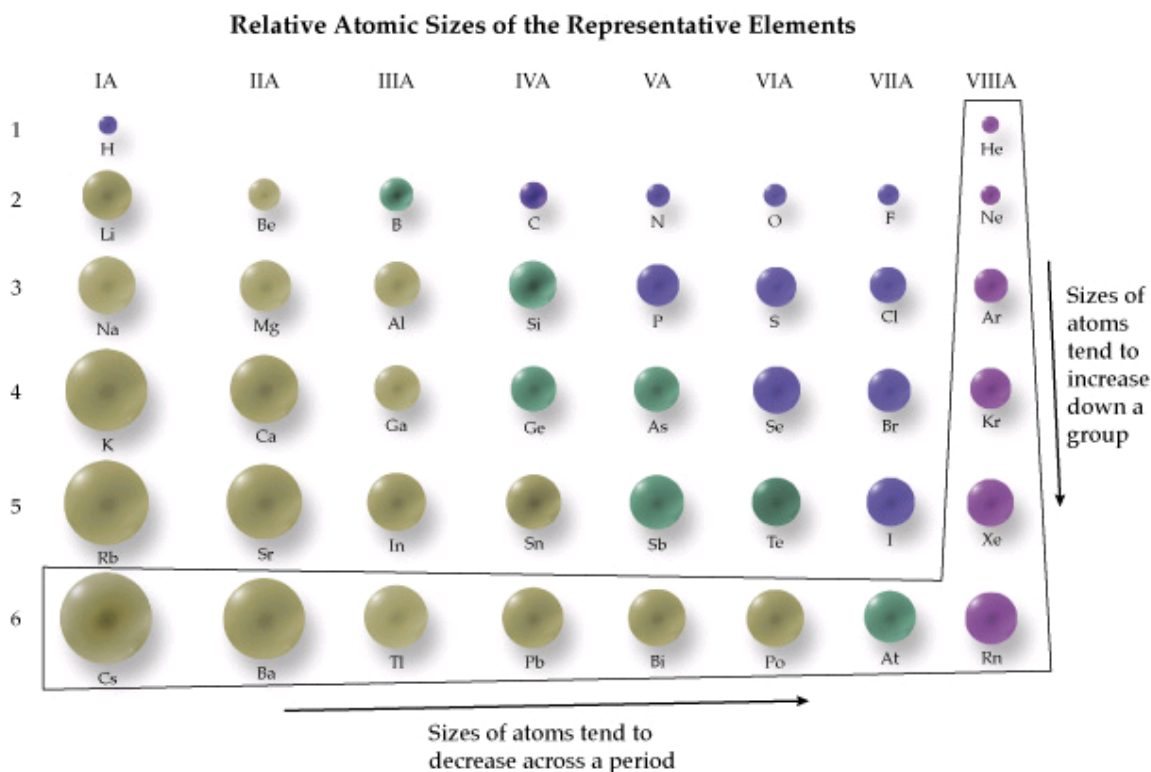

Cl_2 Molecule
$2r = 132$ Å

Cl Atom
$r = 66$ Å

$1\ \text{Å} = 1 \times 10^{-10}\ \text{m}$
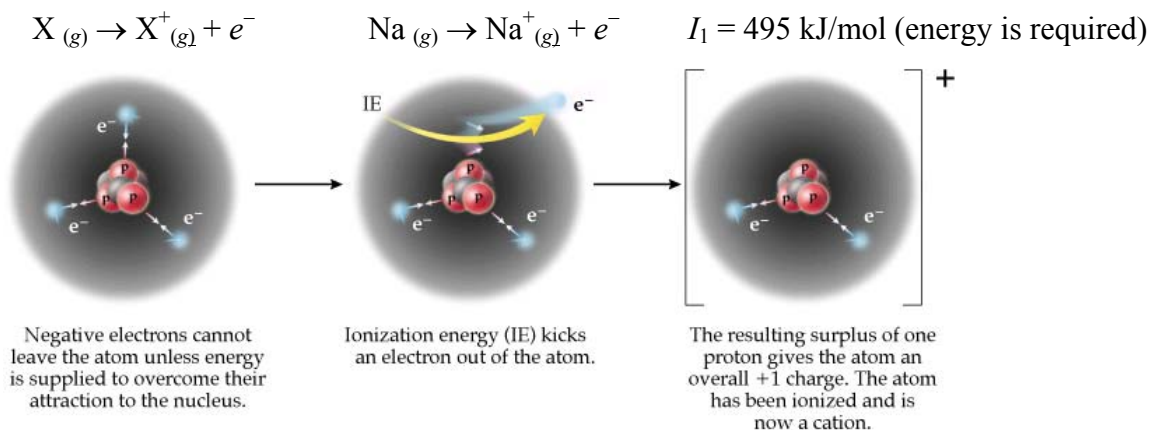
Several Notes on Trends in Atomic Radii

1. In general, <u>**Atomic Radii DECREASE as one move to the RIGHT of a period**</u>. This is because the increases in protons in the same row increase the effective nuclear charge (the protons in the nucleus have more pull on the outer electrons, decreasing shielding), thus drawing these outer electrons closer to the nucleus, decreasing in sizes as the result.

2. <u>**Atomic Radii INCRESES Down a Group**</u>. This is due to the fact there are more orbitals as the number of row increases. The outer electrons are, of course, further away from the nucleus

Relative Atomic Sizes of the Representative Elements

Sizes of atoms tend to
decrease across a period

Sizes of atoms tend to increase down a group

Ionization Energy: - the energy needed to completely remove an electron from a gaseous atom or gaseous ion (plasma).

First Ionization Energy: - the ionization energy required to remove the highest-energy electron from the atom.

$$X_{(g)} \rightarrow X^+_{(g)} + e^- \qquad Na_{(g)} \rightarrow Na^+_{(g)} + e^- \qquad I_1 = 495 \text{ kJ/mol (energy is required)}$$

Negative electrons cannot leave the atom unless energy is supplied to overcome their attraction to the nucleus.

Ionization energy (IE) kicks an electron out of the atom.

The resulting surplus of one proton gives the atom an overall +1 charge. The atom has been ionized and is now a cation.

Second Ionization Energy: - the ionization energy required to remove the second highest-energy electron from the ion.

$$X^+_{(g)} \rightarrow X^{2+}_{(g)} + e^- \qquad Na^+_{(g)} \rightarrow Na^{2+}_{(g)} + e^- \qquad I_2 = 4560 \text{ kJ/mol}$$
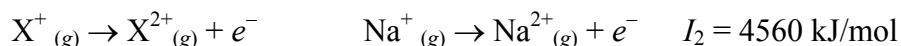
Successive Ionization Energies (kJ/mol) for Elements in Row 3 of the Periodic Table

Elements	I_1	I_2	I_3	I_4	I_5	I_6	I_7
Na	495	4560					
Mg	735	1445	7730		Core Electrons		
Al	580	1815	2740	11600			
Si	780	1575	3220	4350	16100		
P	1060	1890	2905	4950	6270	21200	
S	1005	2260	3375	4565	6950	8490	27000
Cl	1255	2295	3850	5160	6560	9360	11000
Ar	1527	2665	3945	5770	7230	8780	12000

First Ionization Energies generally INCREASE within a Period.

Successive Ionization Energies INCREASES within each element. ($I_1 < I_2 < I_3 < \ldots$)

**Several Notes on Trends in Ionization Energies**

1. There is an **Increase in Successive Ionization Energies** because each successive electron has to jump from a lower level. Besides, these successive electrons are bind more tightly with the nucleus because they are closer to the protons.

2. **Ionization Energies Decrease Down a Group**. This is due to the fact as the atom has more orbitals. It is increasing in size. It is easier (takes less energy) to take away a valence electron because the protons are having a more difficult time to "hold on" to the electron.

3. In general, **Ionization Energies Increase as one move from Left to the Right of a Period**. This is because the increases in protons in the same row increase the effective nuclear charge (the protons in the nucleus have more pull on the outer electrons, decreasing shielding), thus requiring more energy to ionize them.


Ionization Energy Compared to Atomic Number
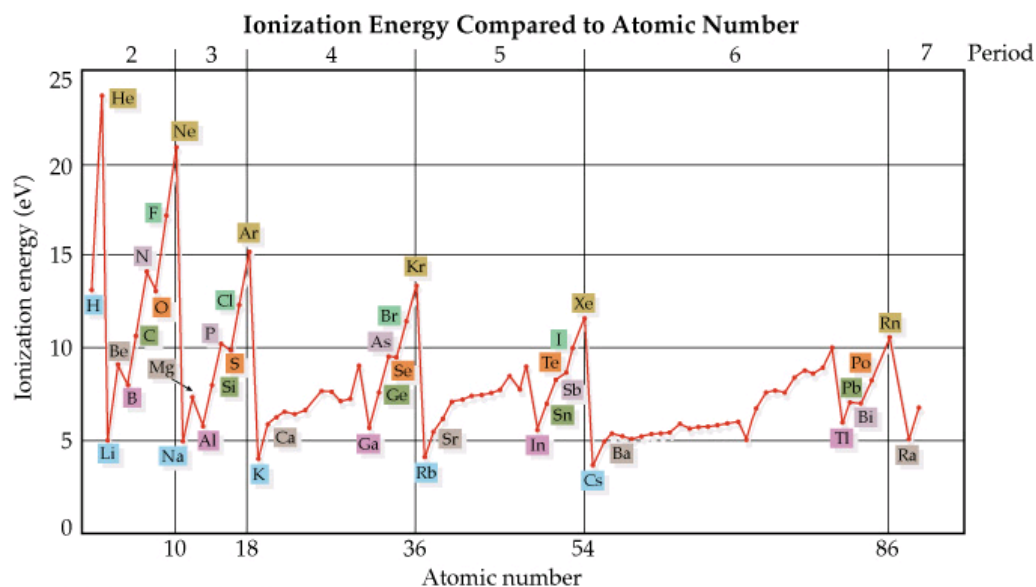
Ions Sizes: - the size of cations and anions.

Several Notes on Trends in Ion Size

1. **Metal Cations are generally Smaller than Non-Metal Anions WITHIN the Same Group**. Metal cations tend to lose electrons to achieve the same number of valence electrons as the previous noble gas. Thereby, losing an energy level in the process. **Metal Cations are always Smaller than the Parent Neutral Atoms. Non-Metal Anions are always Larger than the Parent Neutral Atoms.**

2. In general, **Ion Sizes Decrease as one move from LEFT to RIGHT of a period WITHIN the METAL GROUPS and WITHIN the NON-METAL GROUPS**. This is because the increases in protons in the same row increase the effective nuclear charge (the protons in the nucleus have more pull on the outer electrons, decreasing shielding), thus drawing these outer electrons closer to the nucleus, decreasing in sizes as the result.

3. **Ionic Radii INCRESES Down a Group**. This is due to the fact there are more orbitals as the number of row increases. The outer electrons are, of course, further away from the nucleus
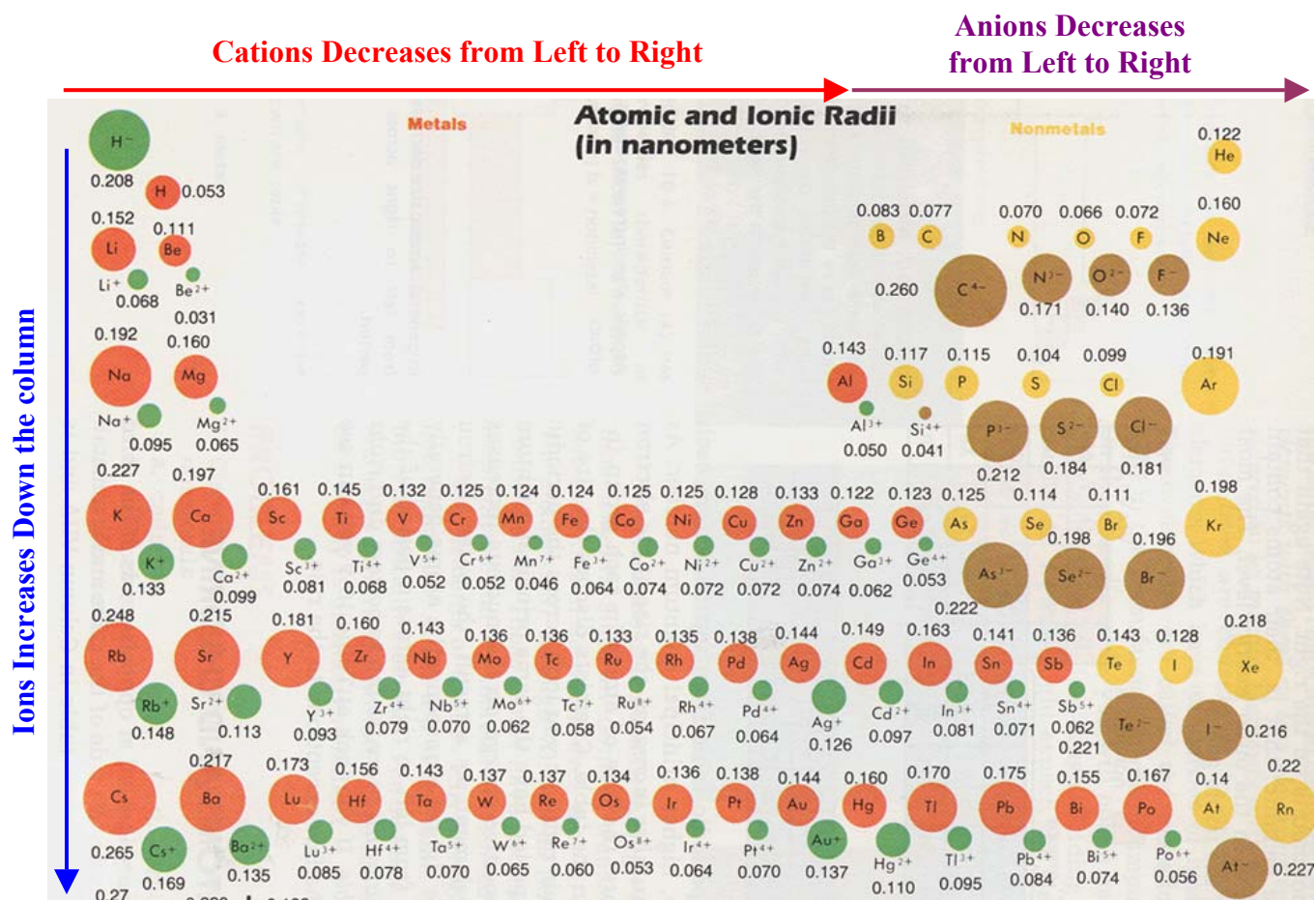
Example 2: Order the following ions from the smallest to the largest.

a. Te^{2-}, S^{2-}, Se^{2-}, O^{2-}

b. Na^+, Mg^{2+}, P^{3-}, S^{2-}, Cl^-
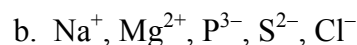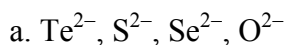
These anions are within the same **Group (column)**. As we move down the column, ion size increases. Therefore,
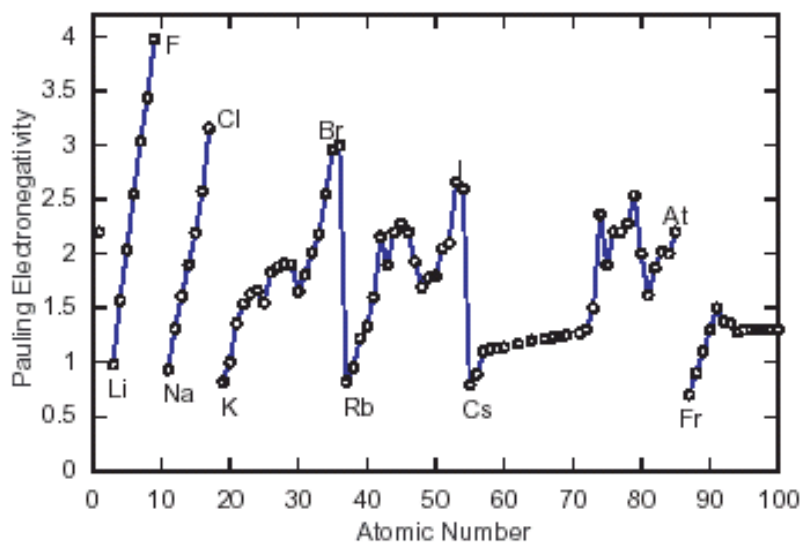
$$O^{2-} < S^{2-} < Se^{2-} < Te^{2-}$$

These ions are within the same **Period (row)**. As we move to the right, ion size **decreases within each of the metal and non-metal groups**. Therefore,

$$Mg^{2+} < Na^+ < Cl^- < S^{2-} < P^{3-}$$

Electronegativity: - first determined by **Linus Pauling**, it is a measure of the **capability of an atom within a molecule to attract shared electrons around itself**.
- the better the atom is able to attract electrons, the higher the electronegativity value.
- electronegativity of noble gases is 0 as their outer orbitals are filled and do not attract electrons.

Several Notes on Trends in Electronegativity

1. In general, **Electronegativities INCREASE as one move to the right of a period (up to and including halogens)**. This is because non-metals tend to form anions to fill the valence orbitals, and therefore, they can better attract electrons. Metals, which have high ionization energies, like to give away electrons to form cations. Hence, they do not like to attract electrons and a lower electronegativity is the result.

2. **Electronegativities DECRESE Down a Group**. This is due to the fact there are more orbitals as the number of row increases. The outer electrons are, of course, further away from the nucleus. Hence, it is more difficult for the protons of the nucleus to attract electrons into the valence orbitals.

> **Assignment**
> **14.2 pg. 406 #6 to 9**
> **Chapter 14 Review: pg. 409−410 #10 to 32**

Chapter 15: Ionic Bonding and Ionic Compounds

15.1: Electron Configuration in Ionic Bonding

Valance Electrons: - electrons that are in the outermost *s* and *p* orbitals of an atom or an ion.

Lewis Structure: - sometimes refer to as **Lewis Dot Diagram** or **Electron Dot Diagram**.
                           - only show electrons of valence electron for all atoms involve in a molecule.

Lewis Structure for Atoms in the First Three Rows of the Periodic Table of Elements

H•   He :

Li•   •Be•   •B•   •C•   •N•   •O•   :F•   :Ne:

Na•   •Mg•   •Al•   •Si•   •P•   •S•   :Cl•   :Ar:
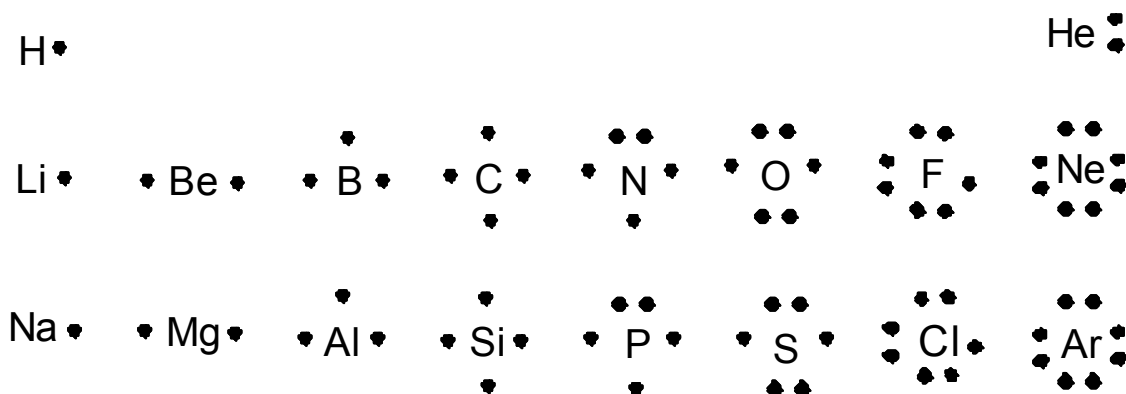
Duet Rule: - two electrons will form a stable shell around atoms in the first period (H and He).

Octet Rule: - eight electrons are required to form a stable shell around atoms in the second and third periods.
              - in general, small noble gases like Ne and Ar do not form compounds because they have
                already attain eight valence electrons.

Electron Configurations of Ions: - for **metals, which like to lose electrons to form cations**, they have the
                                        same electron configurations as the **noble gas of the previous row**.
                                     - for **non-metals, which like to gain electrons to form anions**, they
                                       have the same electron configurations as the **noble gas at the end of
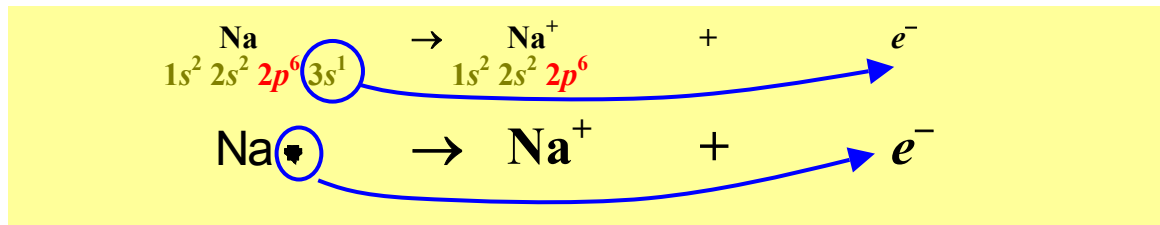   the same row**.

Alkali Cations: - cations that were the result as alkali metals (Group 1 or IA) losing one valence electron.
                 - they are Li^+, Na^+, K^+, Rb^+, Cs^+ and Fr^+

Alkaline Cations: - cations that were the result as alkaline earths (Group 2 or IIA) losing two valence
                    electrons.
                  - they are Be^{2+}, Mg^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+} and Ra^{2+}

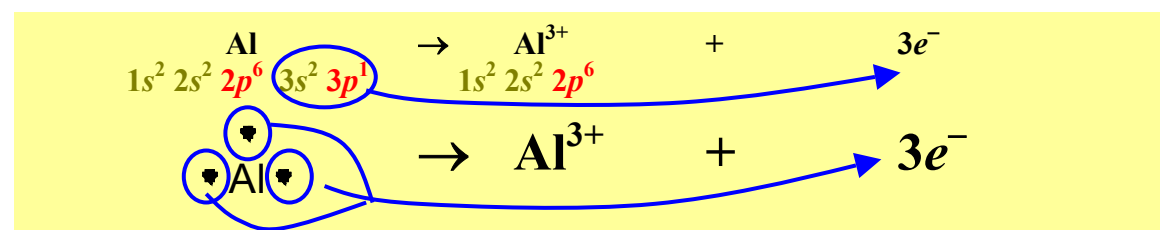**Halide Ions**: - anions that were the result as halogen (Group 17 or VIIA) gaining one valence electron to
                satisfy the octet rule.
              - they are F^-, Cl^-, Br^-, I^- and At^-

Example 1: Write the electron configuration and an ionic equation showing the gaining or losing of electrons when each of the following atoms becomes their most popular ions. Draw the Lewis dot diagram for each atom and ion involved.
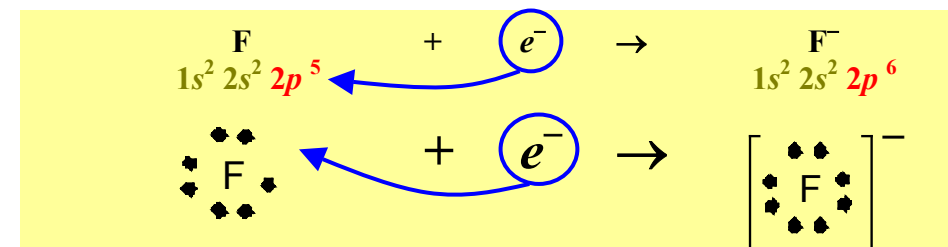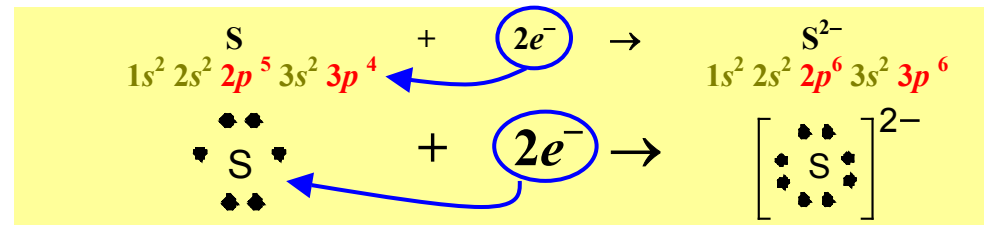
a. sodium atom to sodium ion

$$\text{Na} \rightarrow \text{Na}^+ + e^-$$
$$1s^2\,2s^2\,2p^6\,3s^1 \qquad 1s^2\,2s^2\,2p^6$$

$$\text{Na}\cdot \rightarrow \text{Na}^+ + e^-$$

b. aluminium atom to aluminium ion

$$\text{Al} \rightarrow \text{Al}^{3+} + 3e^-$$
$$1s^2\,2s^2\,2p^6\,3s^2\,3p^1 \qquad 1s^2\,2s^2\,2p^6$$

$$\cdot\overset{\cdot}{\text{Al}}\cdot \rightarrow \text{Al}^{3+} + 3e^-$$

c. fluorine atom to fluoride

$$\text{F} + e^- \rightarrow \text{F}^-$$
$$1s^2\,2s^2\,2p^5 \qquad\qquad 1s^2\,2s^2\,2p^6$$

$$\cdot\overset{\cdot\cdot}{\underset{\cdot\cdot}{\text{F}}}\cdot + e^- \rightarrow \left[\cdot\overset{\cdot\cdot}{\underset{\cdot\cdot}{\text{F}}}\cdot\right]^-$$

d. sulfur atom to sulfide

$$\text{S} + 2e^- \rightarrow \text{S}^{2-}$$
$$1s^2\,2s^2\,2p^5\,3s^2\,3p^4 \qquad 1s^2\,2s^2\,2p^6\,3s^2\,3p^6$$

$$\cdot\overset{\cdot\cdot}{\underset{\cdot\cdot}{\text{S}}}\cdot + 2e^- \rightarrow \left[\cdot\overset{\cdot\cdot}{\underset{\cdot\cdot}{\text{S}}}\cdot\right]^{2-}$$

15.2: Ionic Bonds

Ionic Bonds: - the attraction force between metal and non-metal due to the transfer of electron(s) from a
                metal element to non-metal element.
           - the resulting attraction between the cation(s) and anion(s) is the ionic bond within an ionic
               compound.

Example 2: For each ionic compound, draw the Lewis dot diagram for each atom and ion involved.

a. Mg and F
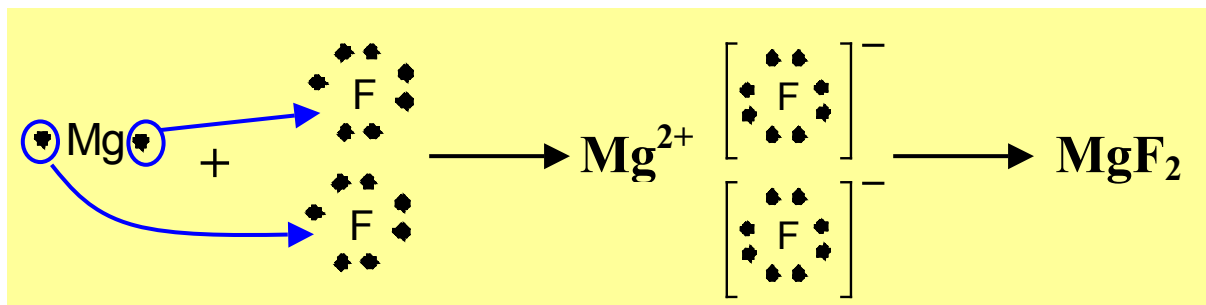
b. Al and S
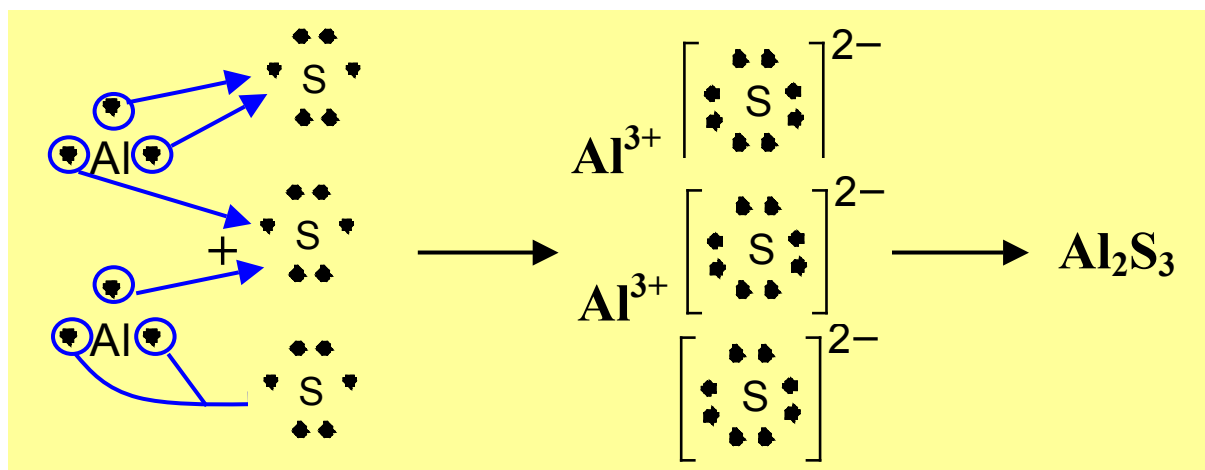
Properties of Ionic Compounds

1. **Ionic Compounds have a definite Crystalline Structure and are Poor Conductors of Electricity and Heat in their Solid Form.** Conduction of electricity and heat requires ions to move freely within the solid. The lattice (crystalline) structure of the solid ionic compounds do not allow ions to move freely.
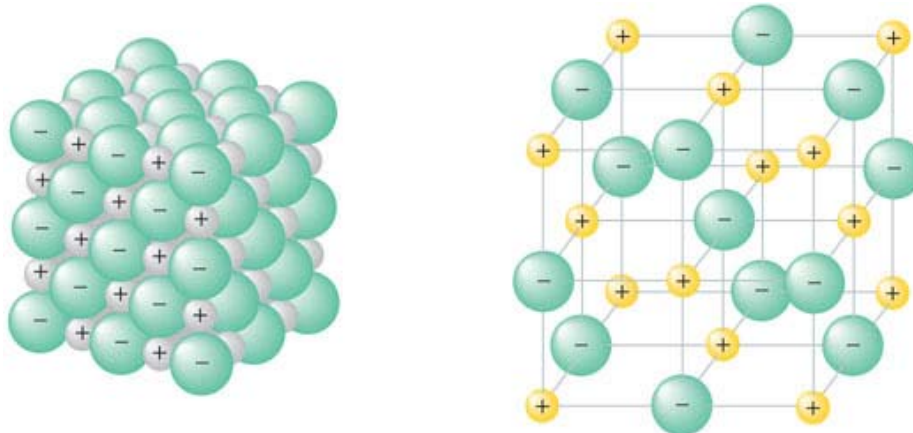
Crystalline Structure of NaCl (+ is Na$^+$ and − is Cl$^-$)

2. **Ionic solids are generally High Melting Points (typically 300°C to 1000°C).** Since a strong force can only shatter the crystal but not bend it as in metals, **the energy needed to completely break up the crystalline structure (lattice energy)** is very large and it is the same energy needed to melt the ionic compounds.

3. **Ionic solids are Hard and Brittle.** The crystalline structure of all ionic compounds holds the ions in definite positions. When the compound encountered a strong force, the close proximity of the ions stay close together. This causes the crystal to **shatter**, not bent like metal solid would.

4. **Ionic solids can be Melted to form Liquids that are Electrical Conductors.** Ionic solids melt when the ions gain enough energy to break the crystalline structure. They are move freely and can carry electrical charge through the liquid. This explains why a molten ionic substance conducts electricity, but a solid ionic material doesn't. The ions move through the liquid can carry charge from one place to another.

5. **Soluble ionic solids dissolve to form solutions that are Electrical Conductors. (Not all ionic substances are soluble in water.)** Soluble ionic compounds form **electrolytes (ions in aqueous from)** that allow the conduction of electricity.

Assignment
15.1 pg. 418 #1 to 6
15.2 pg. 421 #7 and 8; pg. 425 #9 to 13
Chapter 15 Review: pg. 432 #20 to 35, 44 to 49, 52, 54 and 55

Chapter 16: Covalent Bonding

16.1: The Nature of Covalent Bonding

Covalent Bond: - an attraction force between two non-metal elements where the sharing of valence
electrons is taken place so each atom can achieve the stable duet (for hydrogen) or octet
(second and third row elements) condition.

H• + •H → (H(•)H) — **2 valence e^- around each H atom (duet rule)**

:Cl• + •Cl: → (:Cl(:)Cl:) — **8 valence e^- around each Cl atom (octet rule)**
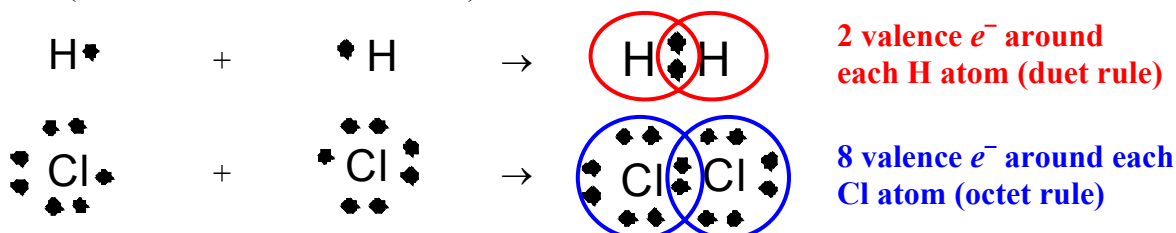
Single Covalent Bond: - covalent bond where there are only **two valence electrons** being shared between
two atoms (also refer to as **bonding electrons**).

Unshared Electron Pairs (Lone Pairs): - pairs of electrons **not** involving in the **actual covalent bonds**.

**Unshared e^- pairs
(Lone Pairs)** ⟷ :Cl(:)Cl: ⟷ **Unshared e^- pairs
(Lone Pairs)**
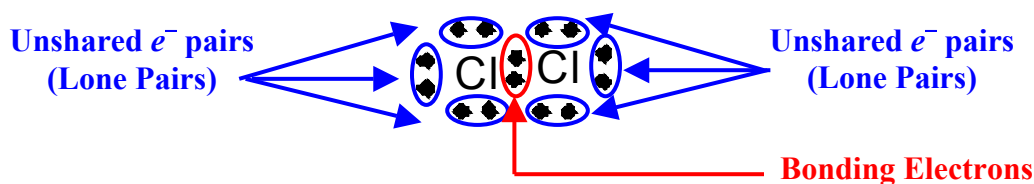
Bonding Electrons

Structural Formula: - a Lewis dot diagram of a molecule where the bonding electrons are replaced by a
short line.

:Cl—Cl:
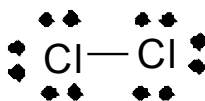
Double Covalent Bond: - covalent bond where there are only **four valence electrons** being shared
between two atoms.
- denotes by a double line in the structural formula.

•Ö• + •Ö• → :O::O: → :O::O: → :O=O:

**only 7 e^- around
each O atom**   **2 unshared e^- become
another bonding pair**   **double bond results and
$8e^-$ around each O atom**
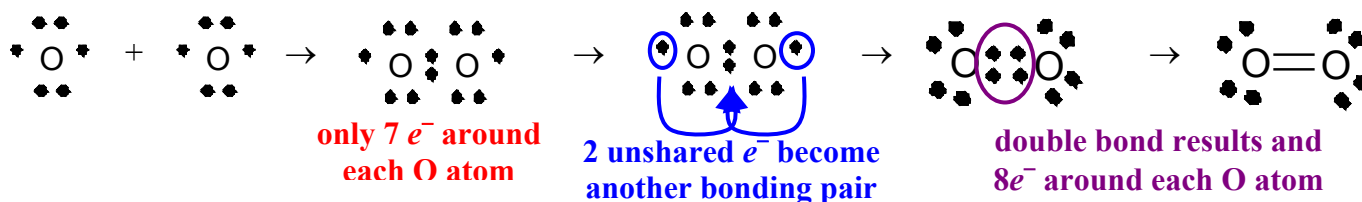
Triple Covalent Bond: - covalent bond where there are only **six valence electrons** being shared between
two atoms.
- denotes by a triple line in the structural formula.

:N• + •N: → :N:N: → :N:::N: → :N≡N:

**only 6 e^- around
each N atom**   **4 unshared e^- become
2 other bonding pairs**   **triple bond results and
$8e^-$ around each N atom**
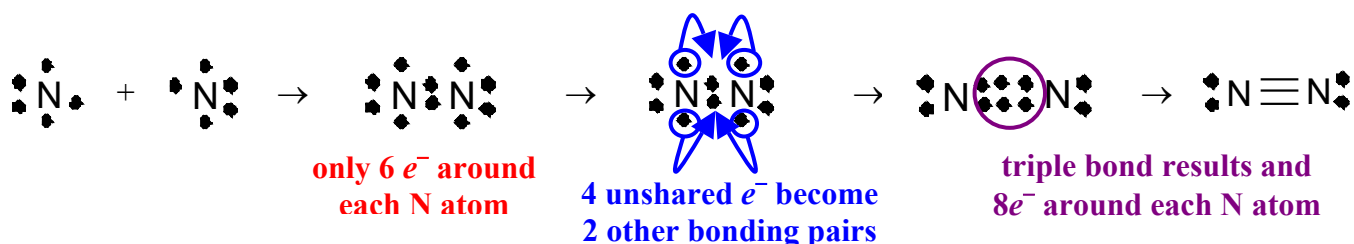
Coordinate Covalent Bond: - where an atom contributes an unshared electron pair (lone pair) to form double or triple bonds to achieve a stable octet around both atoms.
       - sometimes refer to as **multiple bond**.

Procedure to draw Lewis Dot Diagram for Covalent Molecules

1. **Add up all the valence electrons available from all atoms and extra charges from complex ions (ex: charge of 1– means one more electron; charge of 1+ means one less electron).**

2. **Decide on the central atom. Usually, it is the atom with the most available bonding sites (carbon and silicon has the most bonding sites – 4 valence e^-) or it is element with the least number of atoms. Place a pair of electrons to form a single bond between each atom.**

3. **Arrange any remaining electrons around all atoms such that the octet rule is followed for the second and third periods atoms and duet rule is satisfied for the first period atoms. This may sometimes mean setting up multiple bonds (moving lone pairs to the central atom so that it satisfies the octet rule).**

4. **Final Lewis structure of Polyatomic Ion must include a big square bracket and the indication of net charge.**

Example 1: Draw the Lewis structure for the following molecules and polyatomic ions.

a. H_2O

$2e^-$ (2 H atoms)
$+ \ 6e^-$ (1 O atom)
$8e^-$ Total
$- \ 4e^-$ (2 single bonds)
$4e^-$ Left
$- \ 4e^-$ (O needs $4e^-$ to achieve octet)
$0e^-$

H   O   H

H – O – H
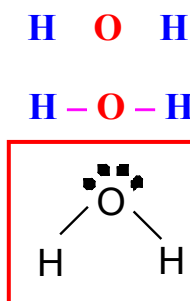
Reason for why the H_2O structure is bent will be explained in section 16.2

b. CO_2

$4e^-$ (1 C atom)
$+ \ 12e^-$ (2 O atoms)
$16e^-$ Total
$- \ \ 4e^-$ (2 single bonds)
$12e^-$ Left
$- \ 12e^-$ (each O need $6e^-$ to achieve octet)
$0e^-$

O   C   O

O – C – O
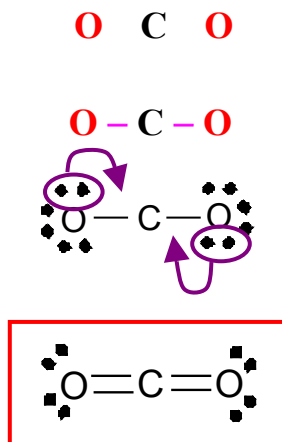
There are only have 4 e^- around C. Oxygen atoms need to contribute unshared e^- pairs (2 lone pairs) to form two double bonds.

c. NH_4^+

$5e^-$ (1 N atom)
$+$ $4e^-$ (4 H atoms)
$-$ $1e^-$ (+1 charge of NH_4^+ ion)
    $8e^-$ Total
$-$ $8e^-$ (4 single bonds)
    $0e^-$

d. CN^-

$5e^-$ (1 N atom)
$+$ $4e^-$ (1 C atom)
$+$ $1e^-$ (−1 charge of CN^- ion)
    $10e^-$ Total
$-$ $2e^-$ (1 single bond)
    $8e^-$ Left
$-$ $6e^-$ (N need $6e^-$ to achieve octet)
    $2e^-$ (the rest will go to the C atom)

$[C \quad N]^-$
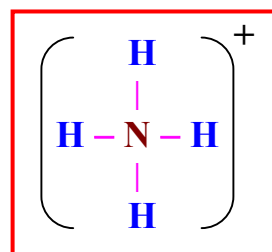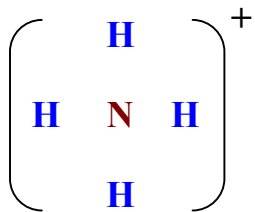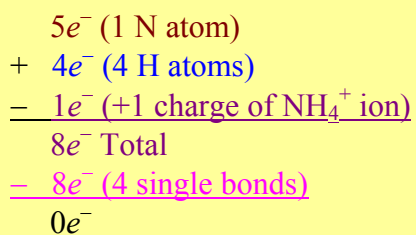
$[C - N]^-$
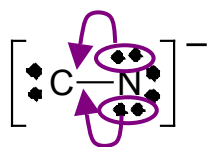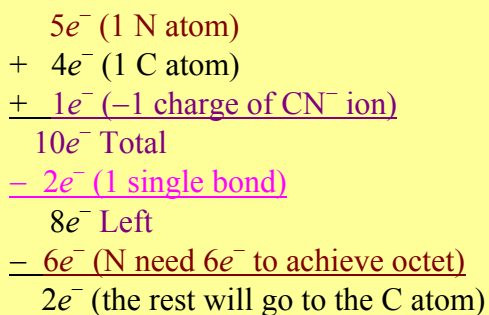
There are only have 4 e^- around C. Nitrogen atoms need to contribute unshared e^- pairs (2 lone pairs) to form a triple bond.
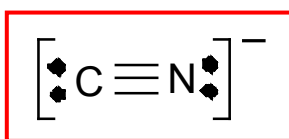
Bond Energy: - the energy needed to break the covalent bond.
                    - commonly known as **bond dissociation energy**.

Bond Length: - the distance between centres of the two atoms involved in the covalent bond.

Note: **In general, bond energy increases and bond length decreases with multiple bonds.**

Bond and Bond Type	Bond Length (pm)	Bond Energy (kJ/mol)
C – C (single bond)	154	247
C = C (double bond)	134	614
C ≡ C (triple bond)	120	839

Resonance: - occurs when more than one Lewis structure exists for a molecule.

Resonance Structure: - different variations of a resonance molecule can be drawn using a double headed
                        arrow, ↔, between the diagrams.

Example 2: Draw the Lewis structure for nitrate.

Nitrate = NO_3^-

$5e^-$ (1 N atom)
$+ 18e^-$ (3 O atoms)
$+ \underline{\quad 1e^-}$ (−1 charge of NO_3^- ion)
$24e^-$ Total
$\underline{- \quad 6e^-}$ (3 single bond)
$18e^-$ Left
$\underline{-18e^-}$ (each O atom need $6e^-$ to achieve octet)
$0e^-$
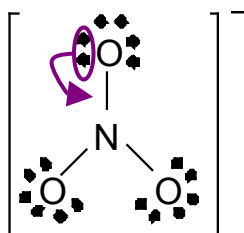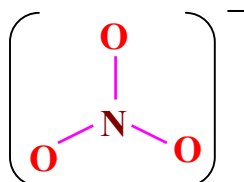
There are only have $6e^-$ around N. One oxygen atom needs to contribute unshared e^- pair (1 lone pair) to form a double bond.

There will be three resonance structures as the double bond can "rotate" around the central N atom.
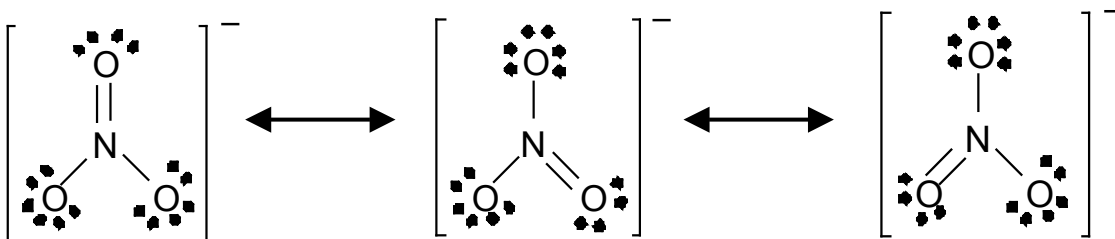
Exceptions to the Octet Rule

1. **In the second row, due to the 2s and the 2p orbitals, C, N, O, and F should always follow the octet rule. Overall, the second period elements will never exceed the octet rule.**

2. **Boron (B) follows the $6e^-$ rule.**

3. **In the third period, heavier atoms towards the right of the Table often satisfy the octet rule. This being said, there are times that they can use the empty 3d orbitals to exceed the 8 electrons limit. (Examples: P can have $10e^-$ rule; S and Cl can have $10e^-$ or $12e^-$ rule)**

4. **Elements in higher row can definitely exceed the octet rule. This sometimes applies to larger noble gases as well. (Examples: Br, I, Xe, Rn can have $10e^-$ or $12e^-$)**

Example 3: Draw the Lewis structure for the following molecules.

a. BCl_3 b. PF_5 c. SCl_6
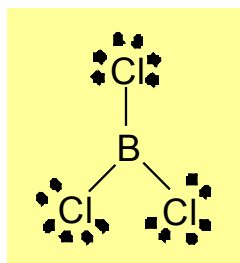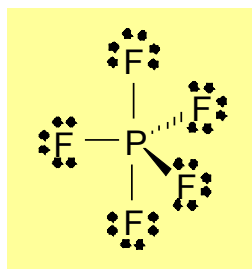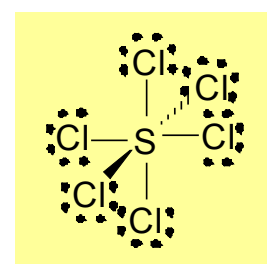
$6e^-$ around B   **$10e^-$ around P**   **$12e^-$ around S**

16.2: Bonding Theories
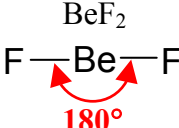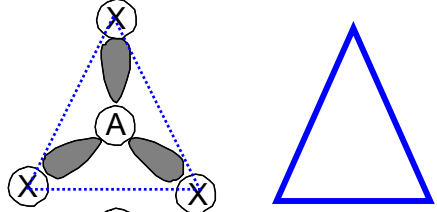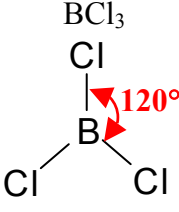
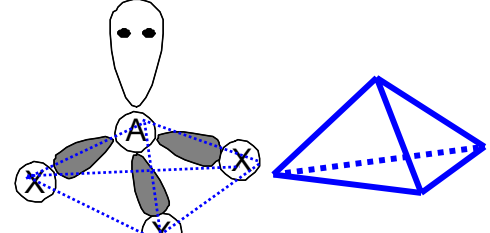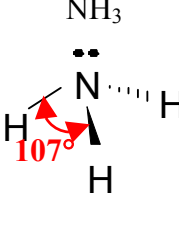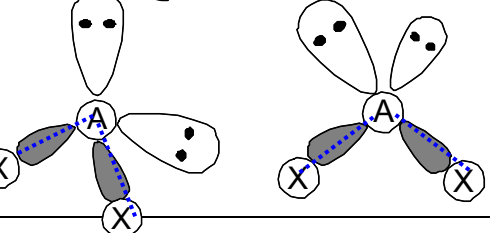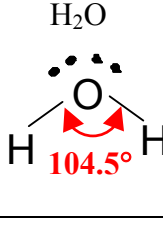**Valence Shell Electron-Pair Repulsion (VSEPR) Model**:
- *the best structure for a molecule is one that minimizes electrons lone pairs repulsion*.
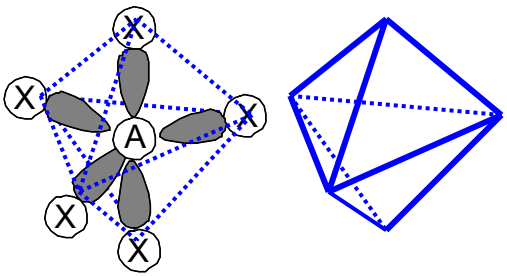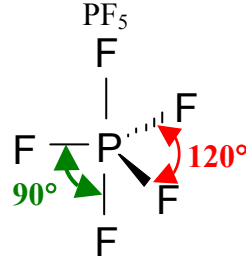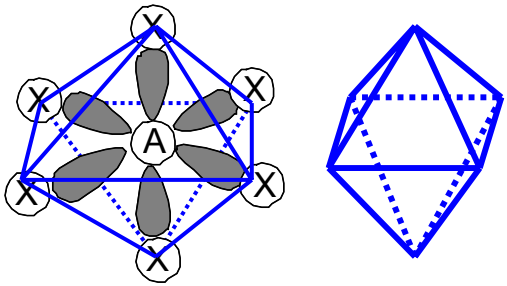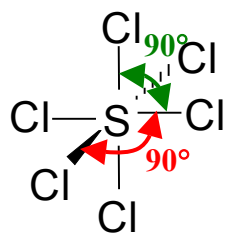- most often used to predict molecular structures involving non-metals.
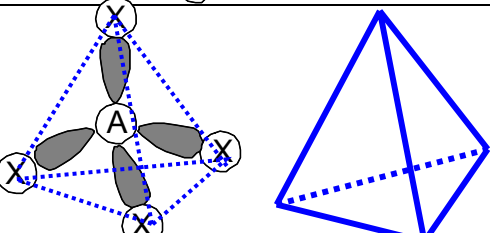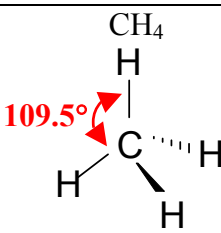
Example: For molecules with a total of 4 e^- pairs, the bond angles decreases from 109.5° as more lone pairs added. (Repulsion of Lone Pair(s) with bond electrons pushed the angle down.)

Effective Electron Pairs:- sometimes refer to as **substituents**
- the number of lone pairs on the central atom of a molecule and the number of connections between the central atom with the outer atom(s). Each set of Multiple Bond (like double and triple bonds) count as one connection or one effective electron pair.

### Summary of Geometrical Shape of Single Bond Molecules

Around Central Atom		Molecular Structures	Geometrical Shape	Example and Bond Angles
Total # of Eff. e^- Pairs	**# of Lone Pairs**			
2	0		Linear	BeF_2 F—Be—F **180°**
3	0		Trigonal planar	BCl_3 Cl **120°** B Cl Cl
4	0		Tetrahedral	CH_4 H **109.5°** C····H H H
4	1		Trigonal pyramid	NH_3 N····H H **107°** H
4	2		V-Shape (Bent)	H_2O O H H **104.5°**

| Around Central Atom | | Molecular Structures | Geometrical Shape | Example and Bond Angles |
Total # of Eff. e^- Pairs	# of Lone Pairs			
5	0		Trigonal bipyramid	PF_5
6	0		Octahedral	SCl_6

Using VSEPR Model with Multiple Bonds Molecule.

1. **Look at multiple bonds as single bonds (only to determine molecule geometry).**
2. **Using the number of bonds and line pairs around the central atom, determine the geometry of the molecule from the charts above.**

Example 1: From Example 2 of Section 16.1, determine the geometrical shape of NO_3^-. What is the possible bond angle in this complex ion?
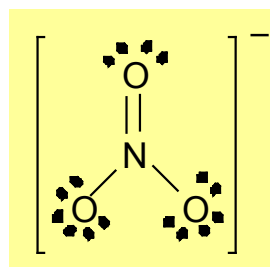
Since there are 3 bonds around nitrogen (we look at the double bond as a single bond when deciding on molecular geometry), and there are no lone pairs around the central atom, the NO_3^- ion is in the shape of trigonal planar with bond angles at 120°.
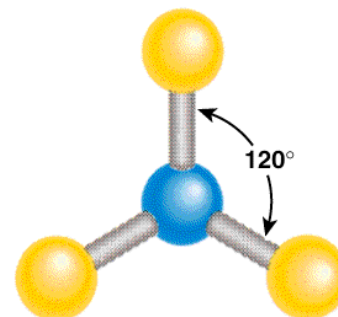
Assignment
16.1 pg. 440 #1 and 2; pg. 446 #3, 4; pg. 447 #5, 6; pg. 451 #7 to 11
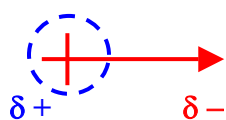**16.2 pg. 459 #14**

16.3: Polar Bonds and Molecules

1. **Intramolecular Forces**: - attraction forces between atoms **WITHIN** a molecule.
   - **Ionic Bonding is the intramolecular force of an ionic compound** (metal and non-metal).
   - **Covalent Bonding is the intramolecular force of a molecular compound** (non-metal and non-metal)
   - **the strengths of the intramolecular forces explain the amount of energy involved in a chemical change.**

   Bond Polarity: - the distribution of electrons within a molecule based on the electronegativities of the individual atoms.

   a. **Polar Covalent Bonds**: - the bonds in a covalent compound that exhibit an uneven bond polarity.

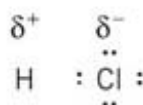   **Polar Molecule**: - when the entire molecule has a net resultant polarity.

   Dipole Moment: - the arrow which indicates the **two poles** (**partial negative, $\delta -$** and **partial positive, $\delta +$**) of a molecule or an individual bond. (δ - Small case Greek letter "delta").
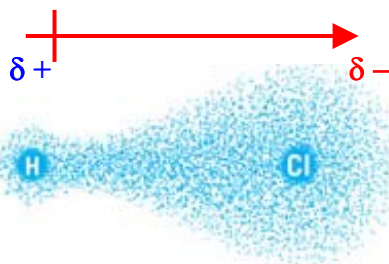   - is a vector that has magnitude (difference in electronegativities) and a direction (based on the geometry of the molecule as dictated by VSERP).
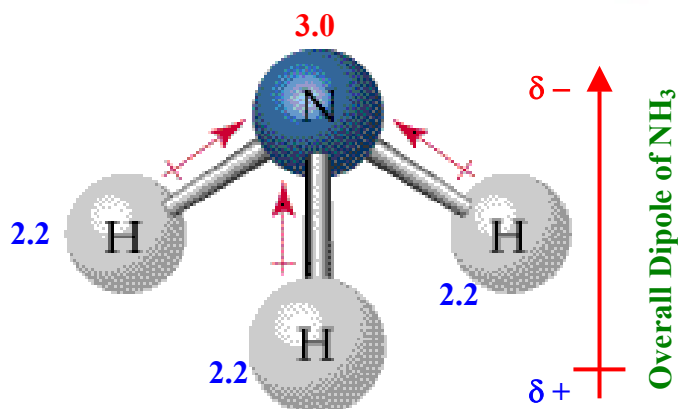

Trigonal pyramid geometry with all N–H bond polarities pointing upward causes an overall dipole for NH_3, making it a polar molecule
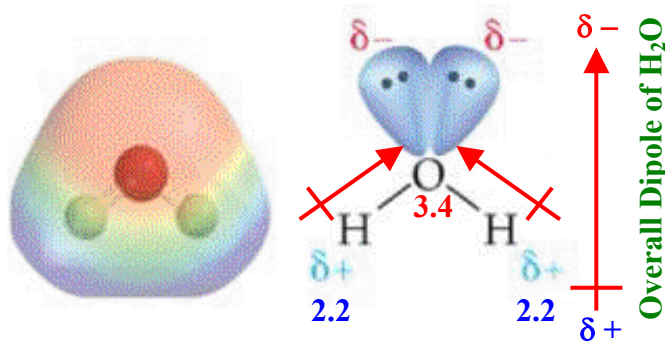
**V-shape or Bent geometry with both O–H bond polarities pointing upward causes an overall dipole for H_2O, making it a polar molecule**

   b. **Non-polar Covalent Bonds**: - when the bond in a covalent compound has an evenly distributed bond polarity.
   - occurs when two atoms of the same electronegativity are sharing electrons.

Non-polar Molecule: - when the entire molecule has a net resultant of zero polarity.
- occurs when all dipole moments of all bonds cancel one another (in directions and magnitudes).
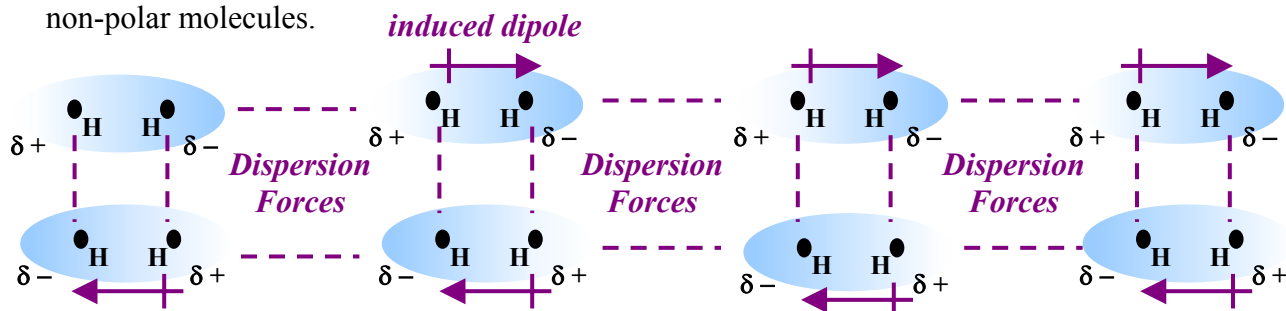
Nonpolar   : C̈l : C̈l :   Pairs of electrons in bond shared equally

BF₃ is Non-polar   **4.0**   **Trigonal planar geometry with equal dipoles of B–F bonds cancels out all bond polarities**

CCl₄ is Non-polar   **3.2**   **Tetrahedral geometry with equal dipoles of C–Cl bonds cancels out all bond polarities**
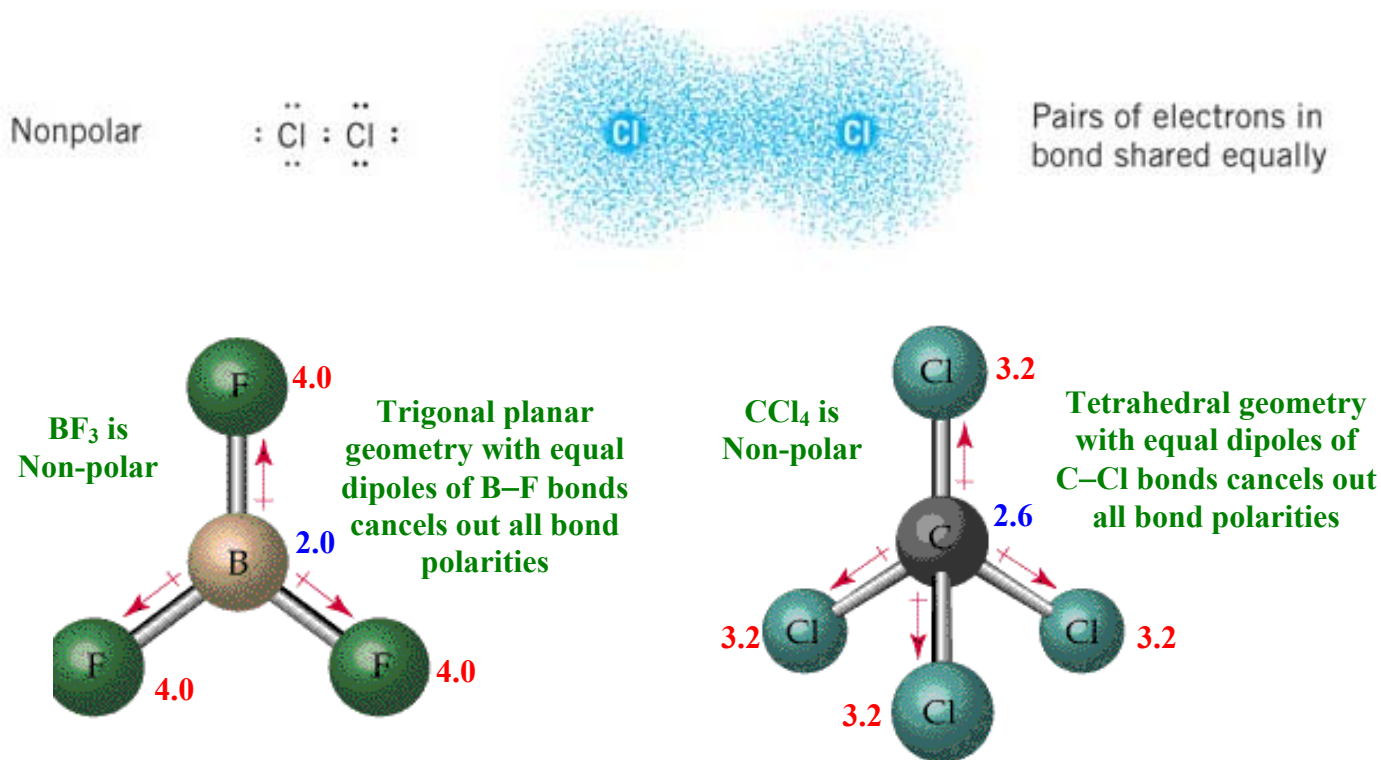
2. Intermolecular Forces: - attraction forces between molecules in a compound
- **the strengths of the intermolecular forces <u>explain</u> the <u>physical properties</u> of compounds (solubility, boiling and freezing points).**

a.   van der Waals Forces: - named after Johannes van der Waals who studied real gases and interaction between molecules.
- there are two kinds of van der Waals forces.
- they are **Dispersion Forces** and **Dipole-Dipole Interactions**.

i. <u>Dispersion Forces</u>: - also known as **<u>London Dispersion Forces</u>** (named after Fritz London who first proposed how this force works).

- on average, the non-polar molecules do not have any permanent dipoles like polar molecules

H   H   H₂

+
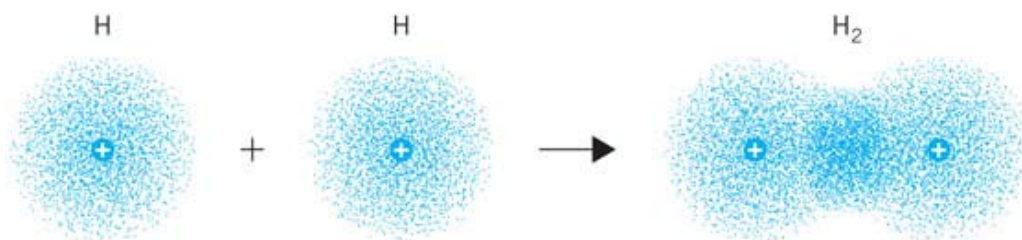
- the "*dispersion*" is the **temporary dipole** that forms within the molecules even in non-polar molecules due the constant motions of electrons. In one instance, they can move to one side of the molecule making it temporary polar. In another instance, electrons will move and the direction of this temporary dipole will switch.

"*Electrons sloshing*"
causes Temporary dipoles

H   H   H   H

δ +   δ −   δ −   δ +
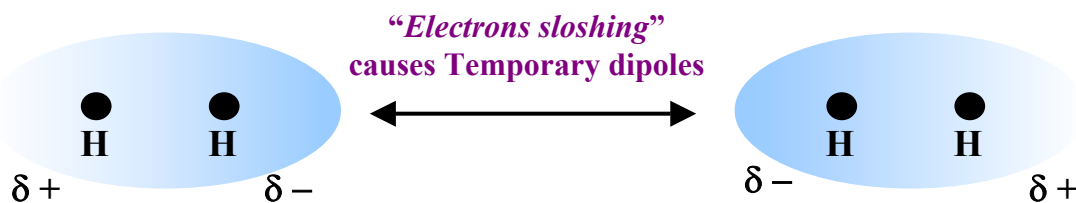
- **This constant "sloshing around" of electrons causes non-polar molecules to have these temporary dipoles**. These temporary "*induced*" dipoles are what cause the attractions between non-polar molecules.

induced dipole

δ + H H δ −   δ + H H δ −   δ + H H δ −   δ + H H δ −

Dispersion   *Dispersion*   *Dispersion*
Forces   *Forces*   *Forces*

δ − H H δ +   δ − H H δ +   δ − H H δ +   δ − H H δ +

- even monoatomic element like Helium has London Forces. **(Check out animation at http://www.super-tech.ro/teoretic.html)**

- in general, *the higher the molar mass or the more electrons there are in a molecule, the stronger the London Dispersion Force* **(attraction between molecules – intermolecular force).** *This causes an increase in melting and boiling points of the chemical*.

- *Note:* **All molecules have electrons. Hence, ALL molecules have London Dispersion Force.**


# of e^- or molar mass in atom or molecule ↑, London Dispersion Force ↑, Melting and Boiling Point ↑

Example 1: Explain the boiling points and the melting points of the noble gases.

| Noble Gases	# of e^-	Molar Mass (g/mol)	Melting Point	Boiling Point
He	2	4.00	−272°C (1 K)	−269°C (4 K)
Ne	10	20.18	−249°C (24 K)	−246°C (27 K)
Ar	18	39.95	−189°C (84 K)	−186°C (87 K)
Kr	36	83.80	−157°C (116 K)	−153°C (120 K)
Xe	54	131.29	−112°C (161 K)	−108°C (165 K)
Rn	86	222.00	−71°C (202 K)	−62°C (211 K)

All atoms of noble gases are monoatomic non-polar. The only intermolecular force that governs the melting and boiling points is the London Dispersion Force. As the number of electrons in the noble gases increase, London dispersion force makes the attraction between the atoms greater. This in turn has an effect of increasing the boiling and melting point of the noble gas as one goes down the column.

ii. **Dipole-Dipole Interactions**: - also known as simply **Dipole Interactions**.
- intermolecular forces resulted from polar molecules.
- dipole interaction is **much stronger than Dispersion Force**.
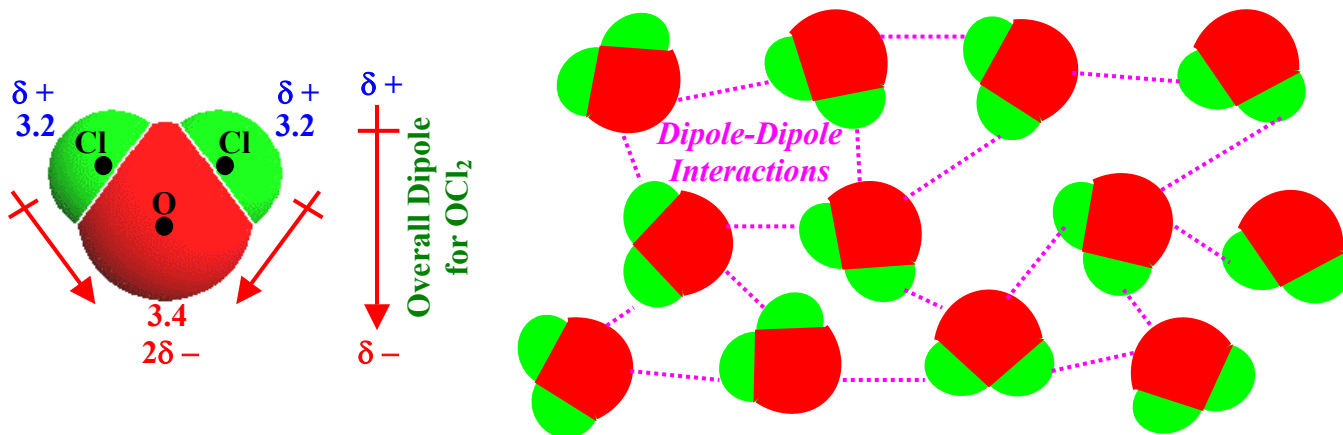
Example 2: Order the boiling points from the least to greatest for the following compounds with similar molar mass. PH_3 (34.00 g/mol), CH_3F (34.04 g/mol), and SiH_4 (32.13 g/mol)

Since PH_3, CH_3F and SiH_4 have similar molar mass, any differences in boiling points cannot be due to London Dispersion forces. Since dipole-dipole interactions exist in polar molecules, we have to examine the molecular geometry and structure of each compound.
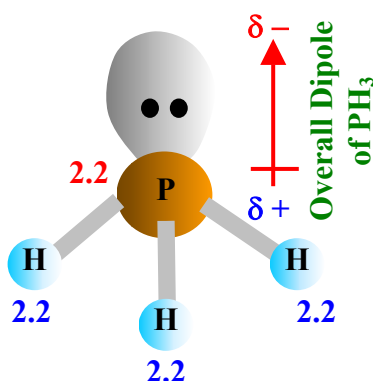
PH_3 has a trigonal pyramid geometry (VSEPR) and is Polar. Even though the P−H bonds have no polarity (electronegativities of P and H are the same), the lone pair on one end of the P atom.
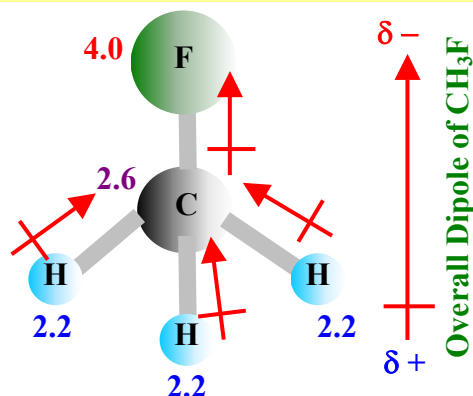
CH_3F has a tetrahedral geometry and is very polar. The C−F bond along with the C−H bonds have strong polarity. The overall dipole moment for the molecule has electrons around the F atom.
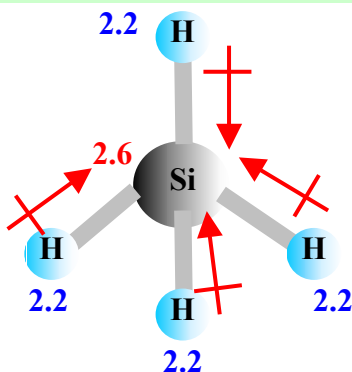

SiH_4 has a tetrahedral geometry with equal dipoles of Si−H bonds cancels out all bond polarities. Hence, SiH_4 is Non-Polar.

Since non-polar molecule have no dipole interactions, SiH_4 should have the lowest boiling point. PH_3 is less polar than CH_3F due to the difference in electronegativities between P−H bond and C−F with C−H bonds. Therefore, CH_3F must have the highest boiling point.
                Boiling Point: **$SiH_4 < PH_3 < CH_3F$**

b. **Hydrogen Bonds**: - are intermolecular bonds that involve **hydrogen atom with very electronegative atom that also consists of lone pairs**.
- these **include O−H, N−H, and H−X (halogen atoms) bonds**.
- the resulting molecule is always polar. Therefore, **all hydrogen bonding molecules also have dipole interactions**.
- hydrogen bond is the **STRONGEST** of the intermolecular bonds.
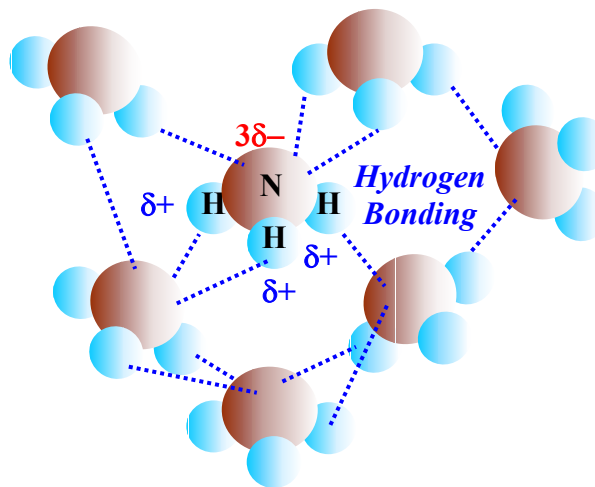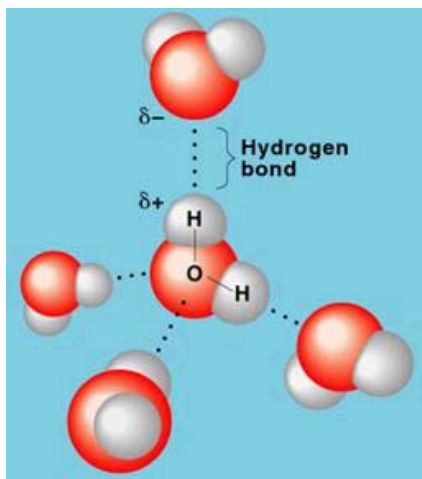
**(Check out the Hydrogen Bond Animation at
http://www.northland.cc.mn.us/biology/Biology1111/animations/hydrogenbonds.html)**

Example 3: Account for the differences in the boiling points of the compounds listed below.

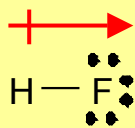| Molecule	Molar Mass (g/mol)	London Dispersion Forces	Dipole Interactions	Hydrogen Bonds	Boiling Point
OF_2	54.00	✔	✔	✘	−145°C (128 K)
Ne	20.18	✔	✘	✘	−246°C (27 K)
HF	20.01	✔	✔	✔	19°C (292 K)
H_2O	18.02	✔	✔	✔	100°C (373 K)
NH_3	17.04	✔	✔	✔	−33°C (240 K)
CH_4	16.05	✔	✘	✘	−161°C (112 K)

Again, we need to draw the structural formulas of these molecules and compare their polarities.
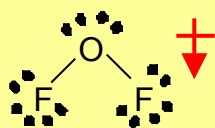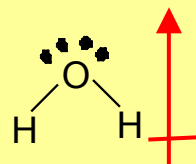

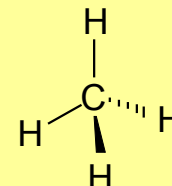OF_2 is polar with dipole interactions | Ne is non-polar with dispersion forces only | HF is polar with hydrogen bonds | H_2O is polar with hydrogen bonds | NH_3 is polar with hydrogen bonds | CH_4 is non-polar with dispersion forces only
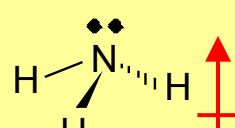
Notice that the hydrogen bond molecules (HF, H_2O and NH_3) have boiling points much higher than molecule with just dipole interactions (OF_2) and the ones with only London Dispersion Forces (Ne and CH_4).

Example 4: Given the graph below on the boiling points of hydrogen compounds with different group series, explain the following using the concepts of chemical bonding.

Boiling Point of Hydrogen Compounds
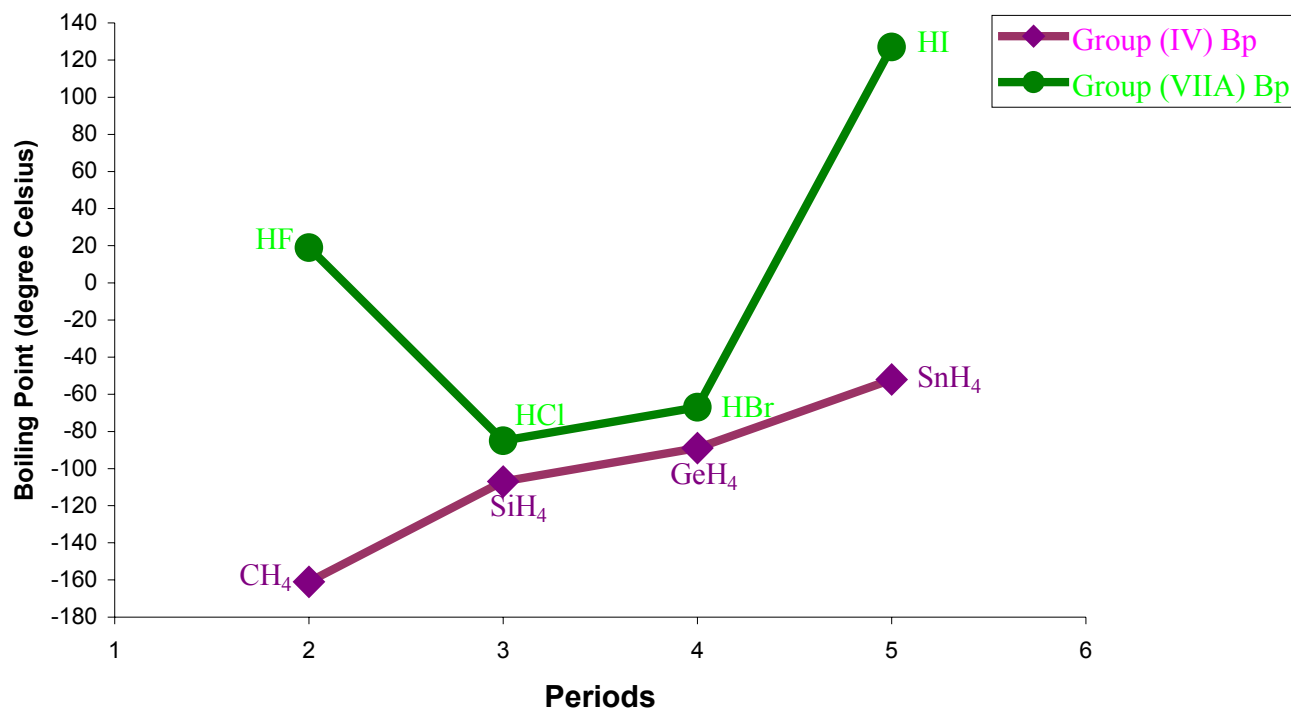
a.   The hydrogen compounds in the Group (VIIA) series have higher boiling points than hydrogen compounds in the Group (IVA) series.

b.   HF has a higher boiling point than HCl and HBr in the Group (VIIA) series while CH_4 has a lowest boiling point in its own Group (IVA) series.

a. <u>**All hydrogen compounds in the Group (VIIA) series are polar and have hydrogen bonds**</u>**. On the other hand, <u>all hydrogen compounds in the Group (IVA) series are non-polar and only have London dispersion forces</u>. Since <u>hydrogen bonds are stronger intermolecular forces</u> than London dispersion forces, the hydrogen compounds in the Group (VIIA) series have generally higher boiling points than the counterparts in the Group (IVA) series.**

b. <u>**HF has a stronger hydrogen bond than HCl and HBr**</u>**. The difference between the electronegativities in HF is 2.2–4.0 while for HCl and HBr are 2.2–3.2 and 2.2–3.0 respectively. <u>This huge difference in electronegativities in HF is what causes its boiling point to *buckle the trend*</u>. After HF, the rest of the hydrogen compounds in the Group (VIIA) series follow the effect of London dispersion forces, the higher the molar mass, the stronger the dispersion forces, and the increase in boiling points is the result.**
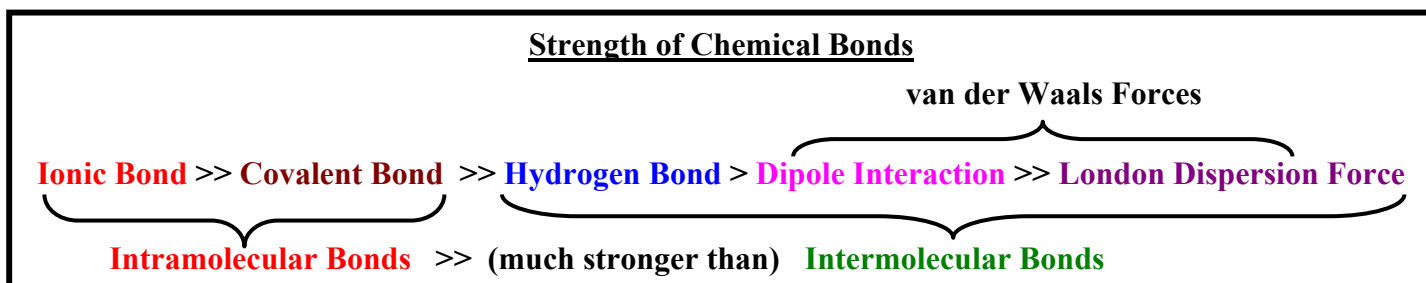
<u>**CH_4 in the Group (IVA) series do not buckle the trend because the entire series are non-polar**</u>**. The only intermolecular force at work is the London dispersion force. Hence, CH_4 has a lower boiling point than SiH_4 and HF has a higher boiling point than HCl and HBr.**

Properties of Covalent (Molecular) Compounds

1. **Covalent Compounds tend to have much Lower Boiling and Melting Points than ionic compounds.** This is because solid covalent compounds' **crystalline structures** are made up of mostly **weak intermolecular forces**. Their boiling points are lower than ionic compounds because there are **no ion interactions in liquid state, only intermolecular forces**.

2. **Solid Covalent Compounds are Soft.** Again, covalent compounds' **weak crystalline structure** makes them soft.

3. **Covalent Compounds tend to be More Flammable than ionic compound.** This is due to the some non-metals like carbon and sulfur, which **combine readily with oxygen in combustion reactions**.

4. **Most Covalent Compounds are Insoluble in Water.** Because **water is very polar** and has lots of hydrogen bonds, it can only dissolve covalent compounds that are polar as well "***Like Dissolves Like***". Since **most covalent compounds are fairly non-polar**, they do not dissolve in polar water well.

5. **Soluble Covalent Compounds do NOT Conduct Electricity in Water.** This is simply due to the fact that covalent compounds **do not dissociate into ions or electrolytes** like soluble ionic compounds do.

Summary of Chemical Bonding

1. **Intramolecular bonds such as covalent and ionic bonds deal with bond strength between atoms within an atom. They explain amount of energy in a chemical change.**

2. **Intermolecular Bonds involve in a compound explain its physical properties such as solubility ("*like dissolves like*" – section 17.3, boiling and melting points – energy involved in physical phase change).**

3. **van der Waals Forces consist of London Dispersion forces (apply to all molecules) and Dipole Interactions (apply to polar molecules).**

4. **Hydrogen Bonding is the *strongest* of all intermolecular bonds.**

Strength of Chemical Bonds

van der Waals Forces

Ionic Bond >> **Covalent Bond** >> **Hydrogen Bond** > **Dipole Interaction** >> **London Dispersion Force**

Intramolecular Bonds >> (much stronger than) **Intermolecular Bonds**

Assignment

16.3 pg. 466 #21 to 24, 26
Chapter 16 Review: pg. 470–471 #27 to 33, 37, 38, 41, 43, 48, 51, 52, 54, 56 to 58

Assignment

Unit 4 Review: pg. 389 #1 to 3, 5 to 13, 18; pg. 411 #1 to 4, 7 to 16; pg. 435 #1 to 10; pg. 471 #61 to 63; pg. 473 #1 to 12, 14 to 17