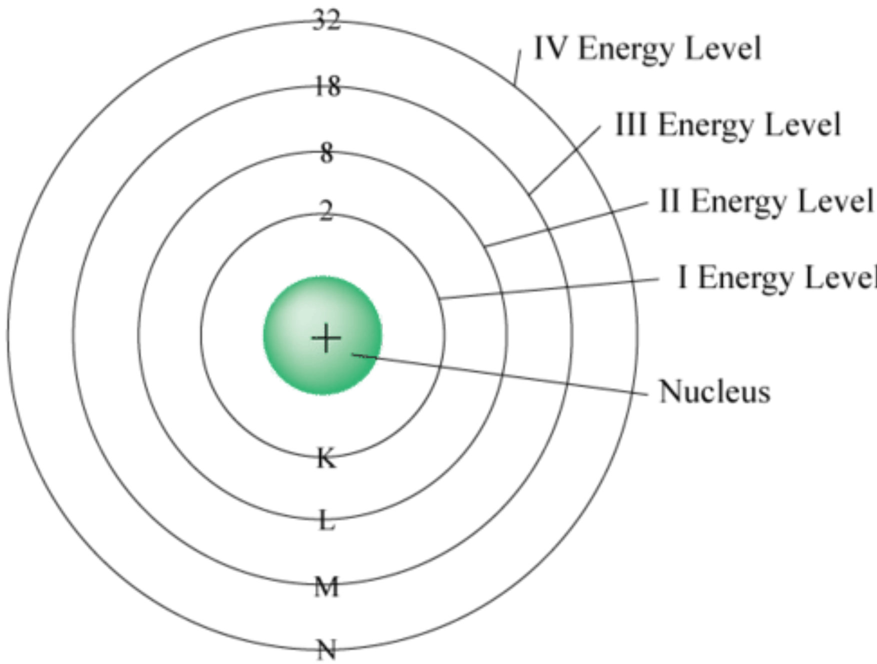
The effects of atomic charges

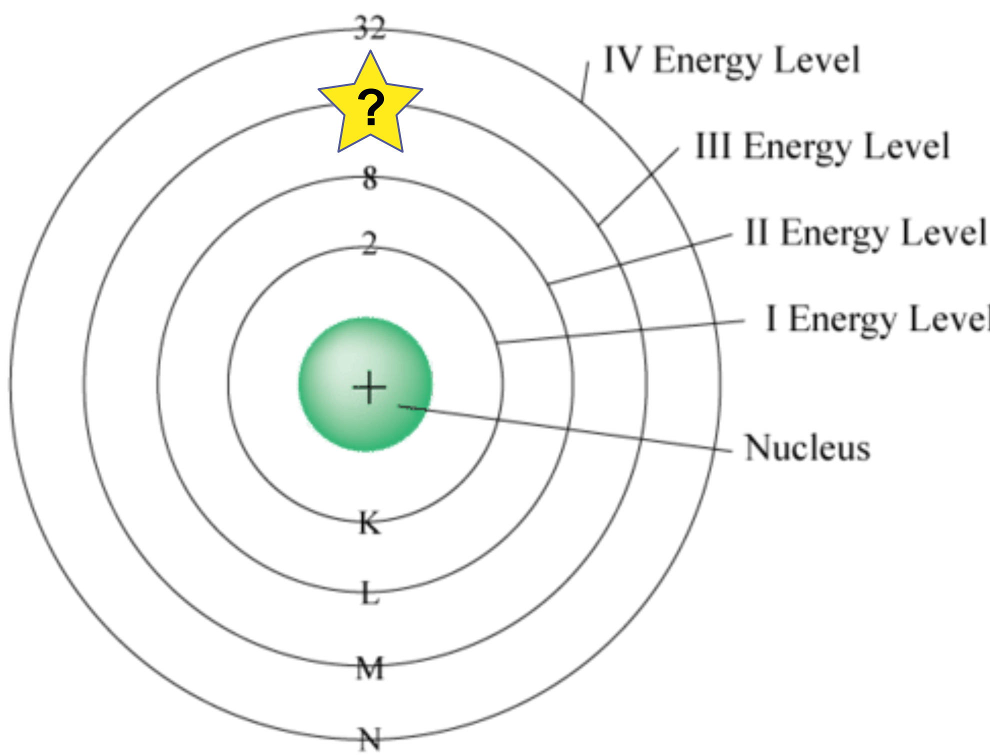
- **Protons in the nucleus attract electrons**
  - Electrons are located in the region of the atom knows as the electron cloud
    - Energy levels (also called electron shells) are fixed distances from the nucleus of an atom where electrons are most likely to be found.



  - The 1st shell or principal quantum number n = 1 is closest to the nucleus.
    - The 2nd energy level n = 2 follows n = 1. Then follows n = 3 etc.
  - Each level can theoretically hold a certain maximum number of electrons.
    - Maximum # of electrons in energy level n: X
    - Maximum # of electrons an energy level can hold: $X = 2n^2$

The effects of atomic charges

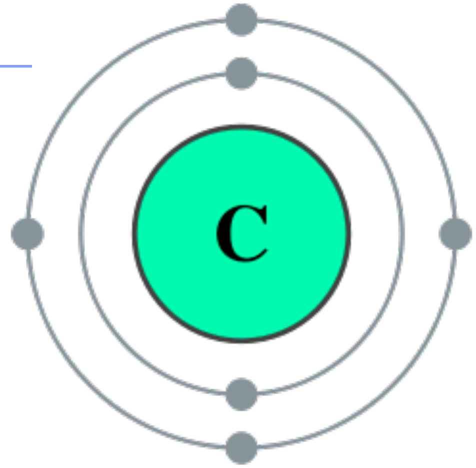
- **Maximum # of electrons an energy level can hold: $X = 2n^2$**
  - **EXERCISE: How many electrons can energy level 3 hold?**
    - **$X=2x^{32}=18$**
  - **Can this level hold 15 electrons?**
    - **Yes**
  - **What about 20?**
    - **No**



THE ELECTRON CLOUD

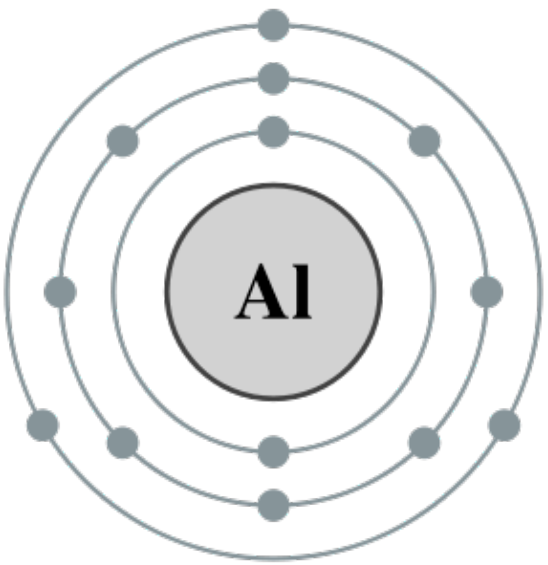
- Let's look at CARBON:
  - Atomic Number = 6 (6 p thus 6 e-).
    - The first 2 electrons fill shell n = 1.
    - The remaining 4 electrons fill shell n = 2.
      - Energy level 2 fills after 1 is full!

6: Carbon 2,4

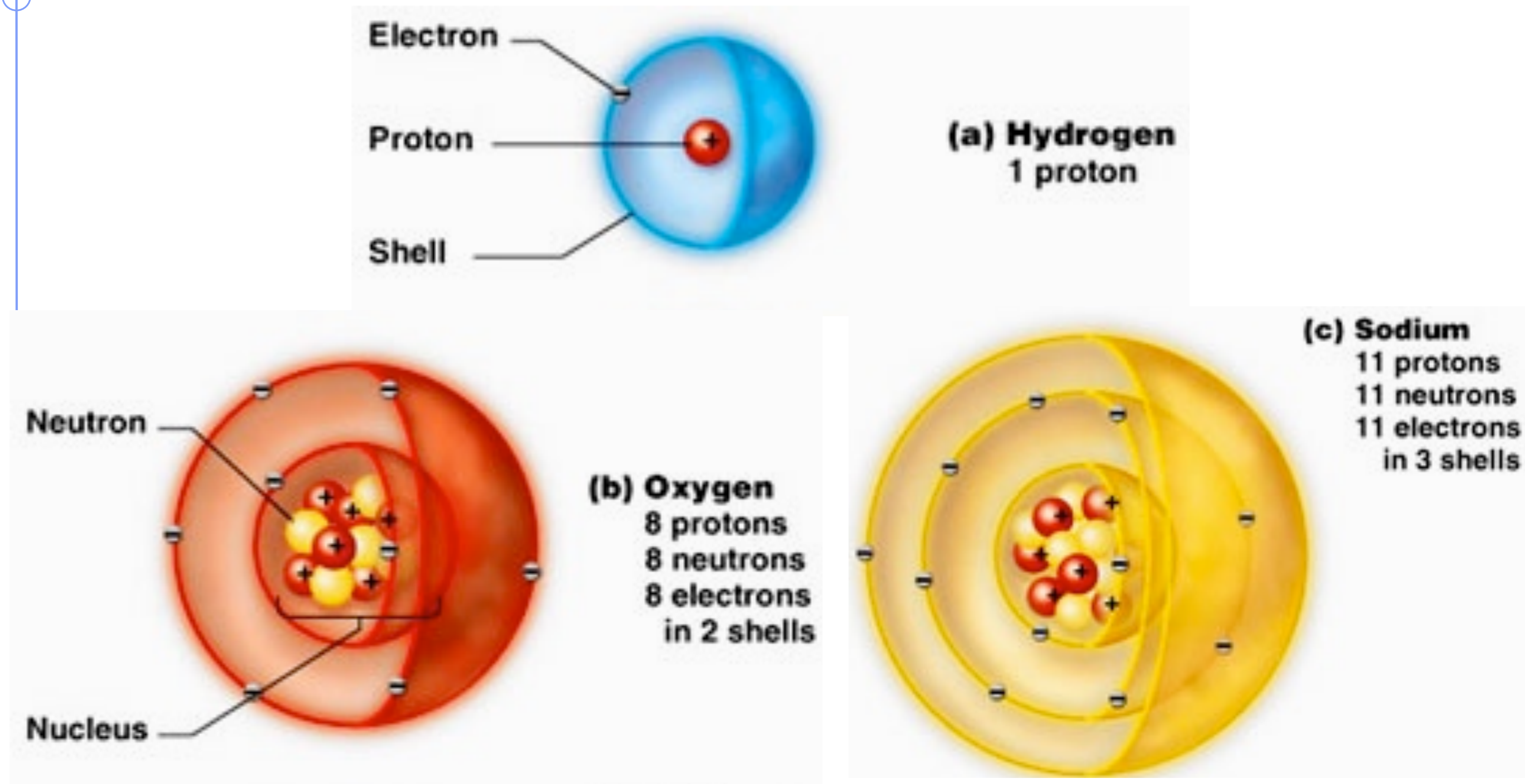


- Let's look at ALUMINUM:
  - Atomic Number = 13 (13 p thus 13 e-).
    - The first 2 electrons fill n = 1.
    - The next 8 electrons fill n = 2.
    - The last 3 electrons fill n = 3.
      - Energy level 3 fills after energy level 2 is full!

13: Aluminium 2,8,3



ATOMIC ENERGY LEVELS

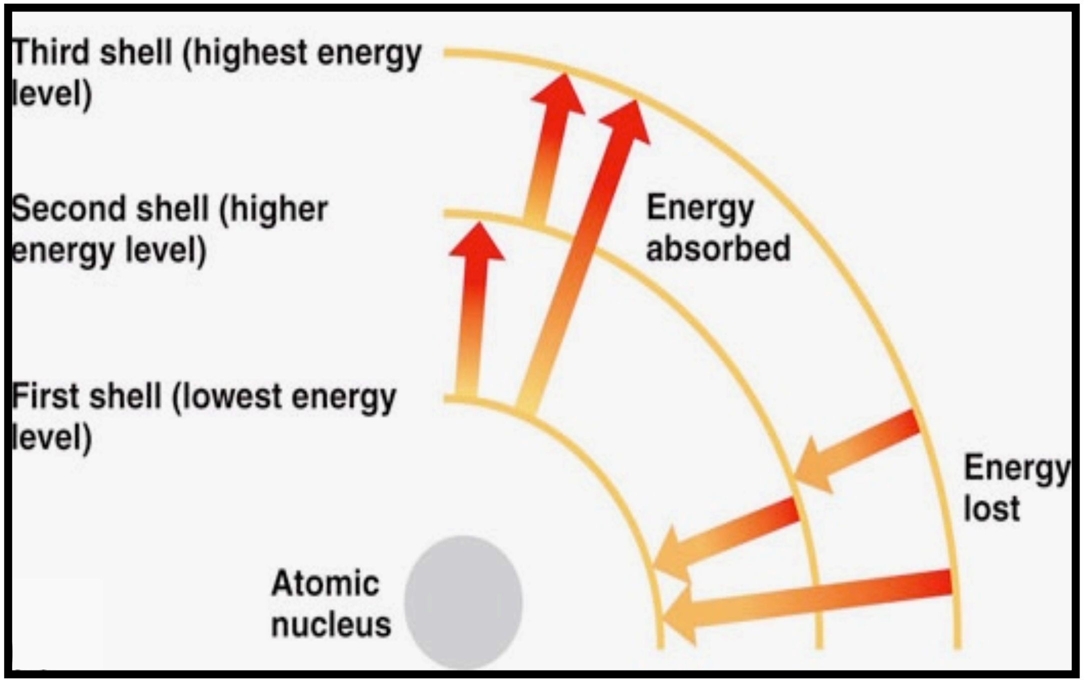


- **Remember that the principal energy levels are more like "clouds" than shells. We can never be sure exactly where an electron is located but we can know where the electron will most probably be found.**

AP

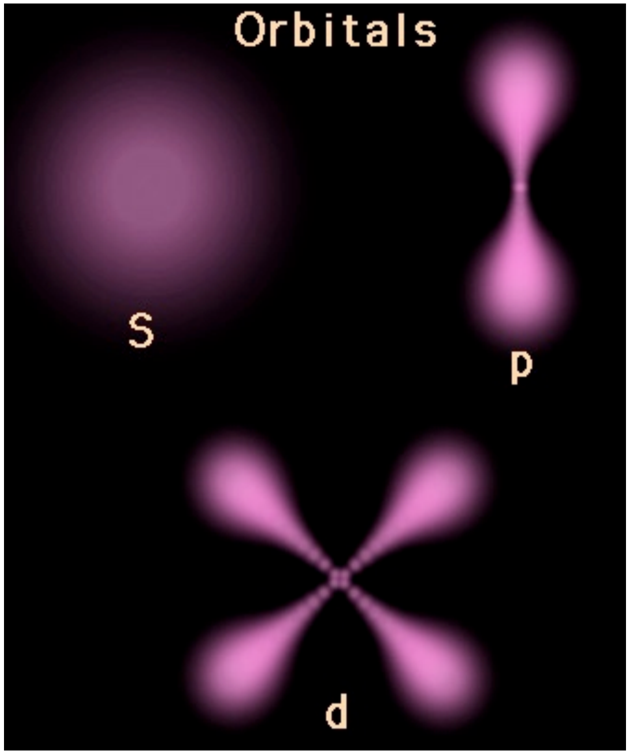
ATOMIC ENERGY LEVELS

- An electron sitting as close as possible to the nucleus has the lowest energy.
  - This atom is said to be in its lowest energy state or GROUND STATE.
- If a discrete quantity of additional energy were absorbed by the atom in some manner, the electron might be able to move into another orbit having a higher energy.
  - The atom would then be in an EXCITED STATE.
- When this atom returns to its ground state it releases energy.



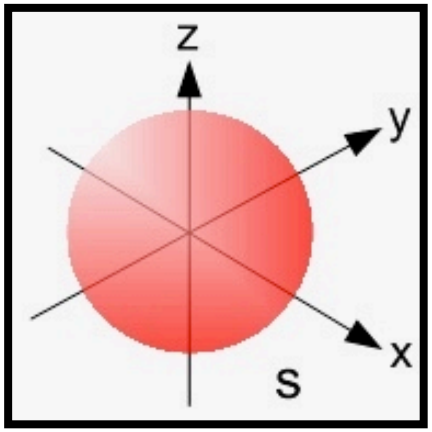
The Orbitals of the Electron Cloud

- Electrons within a shell do NOT follow the same path:
  - They occupy different sub-shells.
    - Within the ELECTRON CLOUD → Different ENERGY LEVELS or SHELLS
    - Within ENERGY LEVELS / SHELLS → Different SUB-SHELLS containing the electron's ORBITALS
      - Orbital = According to quantum mechanics, this is the regions were electrons are most probable to be found.
  - Each orbital can hold a maximum of two electrons.

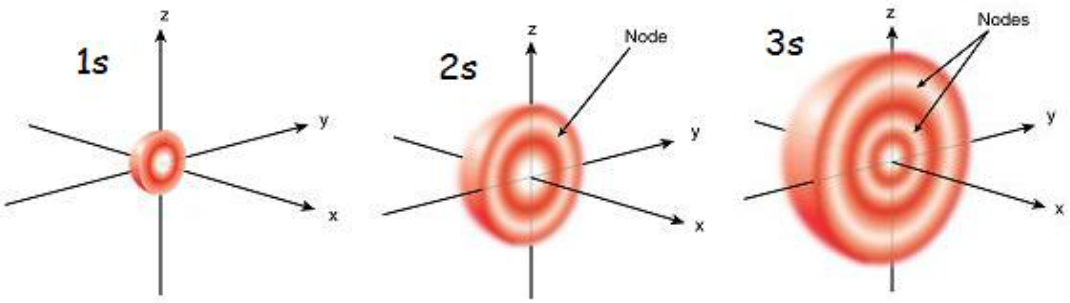


Electron Orbitals in Energy Level n = 1

- ORBITALS can hold only TWO electrons of opposite spins, electrons being repelled by nearby electrons, yet attracted to the protons in the nucleus

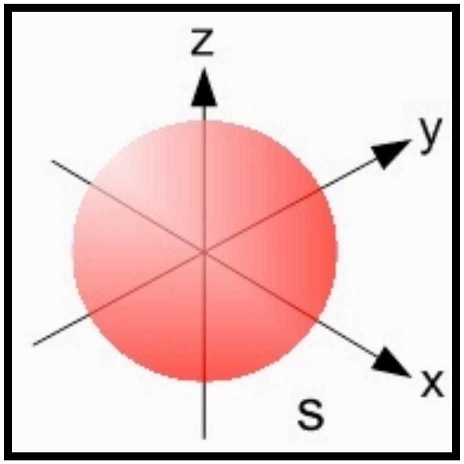


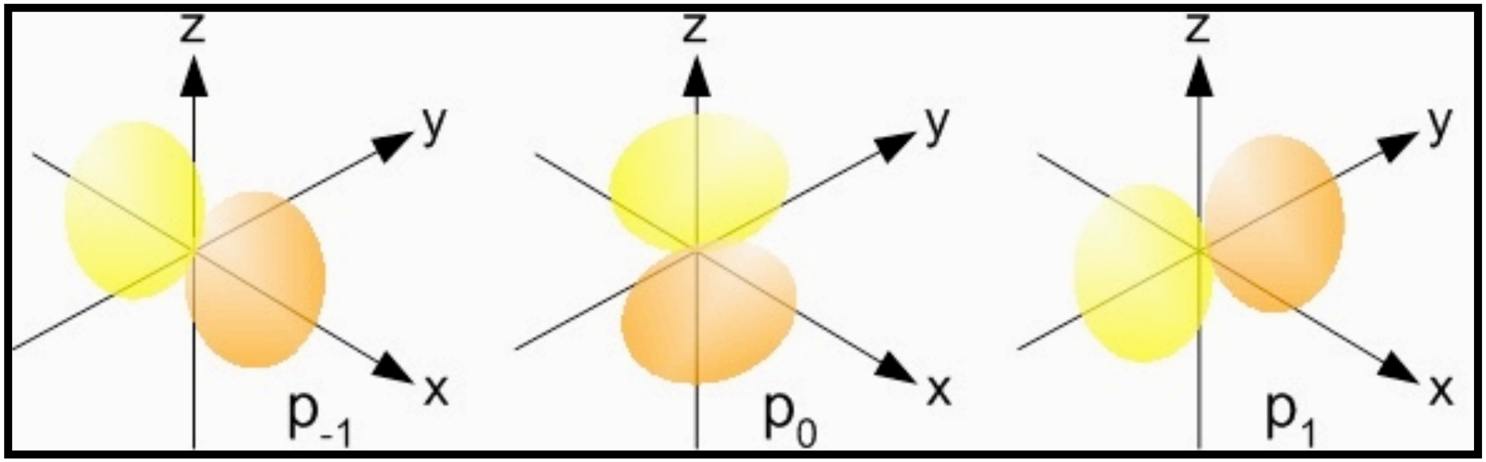
- Electron Orbitals: n = 1
  - In the 1st energy level, n = 1, there is only one sphere-shaped orbital: The 's' orbital.
    - An orbital exists if there are electrons in that region.
  - Additional s orbitals exist in certain atoms, each spherical region found further away from the nucleus.



Electron Orbitals in Energy Level n = 2

- **Electron Orbitals: n = 2**
  - In the 2nd energy level, n = 2, there is one sphere-shaped orbital (the 's' orbital) and three dumbbell-shaped orbitals (the 'p' orbital) that extend out of the nucleus at right angles, labeled the p_x, p_y, and p_z orbitals

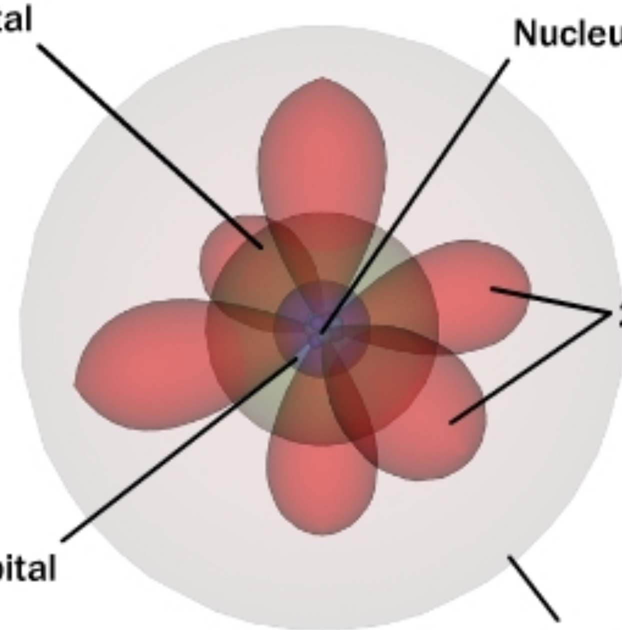




Electron Orbitals in Energy Level n = 2

The first energy level is made up of 1 spherical "s" orbital and can hold up to 2 electrons.

The second energy level is made up of 1 "s" orbital and up to 3 dumbbell shaped "p" orbitals and can hold up to 8 electrons.



- **Remember, as we move up in energy levels, the electrons are found further out from the nucleus.**
  - **For example, we find s and p orbitals in every energy level, they just get progressively larger in diameter as we move from lower to higher energy levels.**

Electron Orbitals in Energy Level n = 3 & up

- The larger energy levels have room for more electrons, which are held in additional orbitals such as the d orbitals and eventually the f orbitals.
  - The 3rd energy level, n = 3, can house up to one ‘s’ orbital, three ‘p’ orbitals, and five ‘d’ orbitals
  - The 4th energy levels, n=4, can house up to one ‘s’ orbital, three ‘p‘ orbitals, five ‘d‘ orbitals, and seven ‘f‘ orbitals.

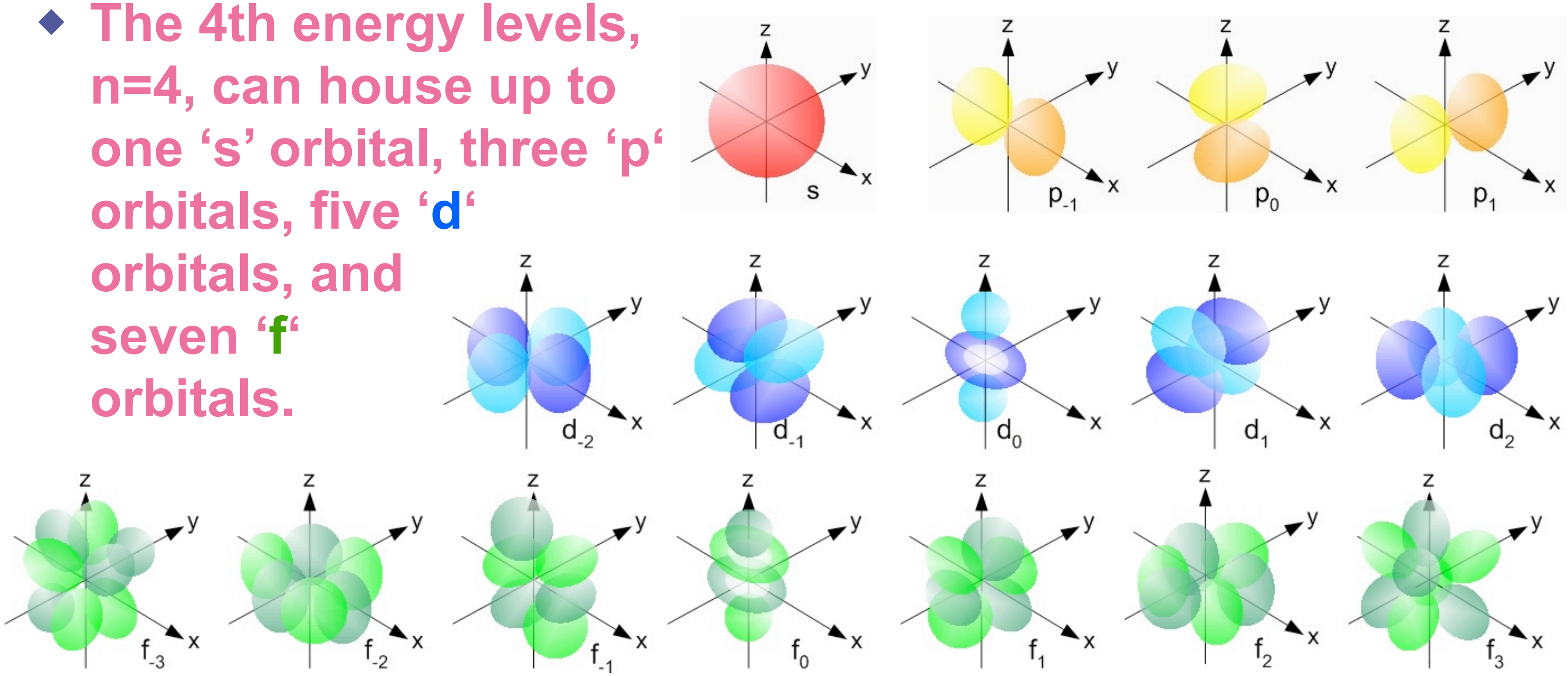
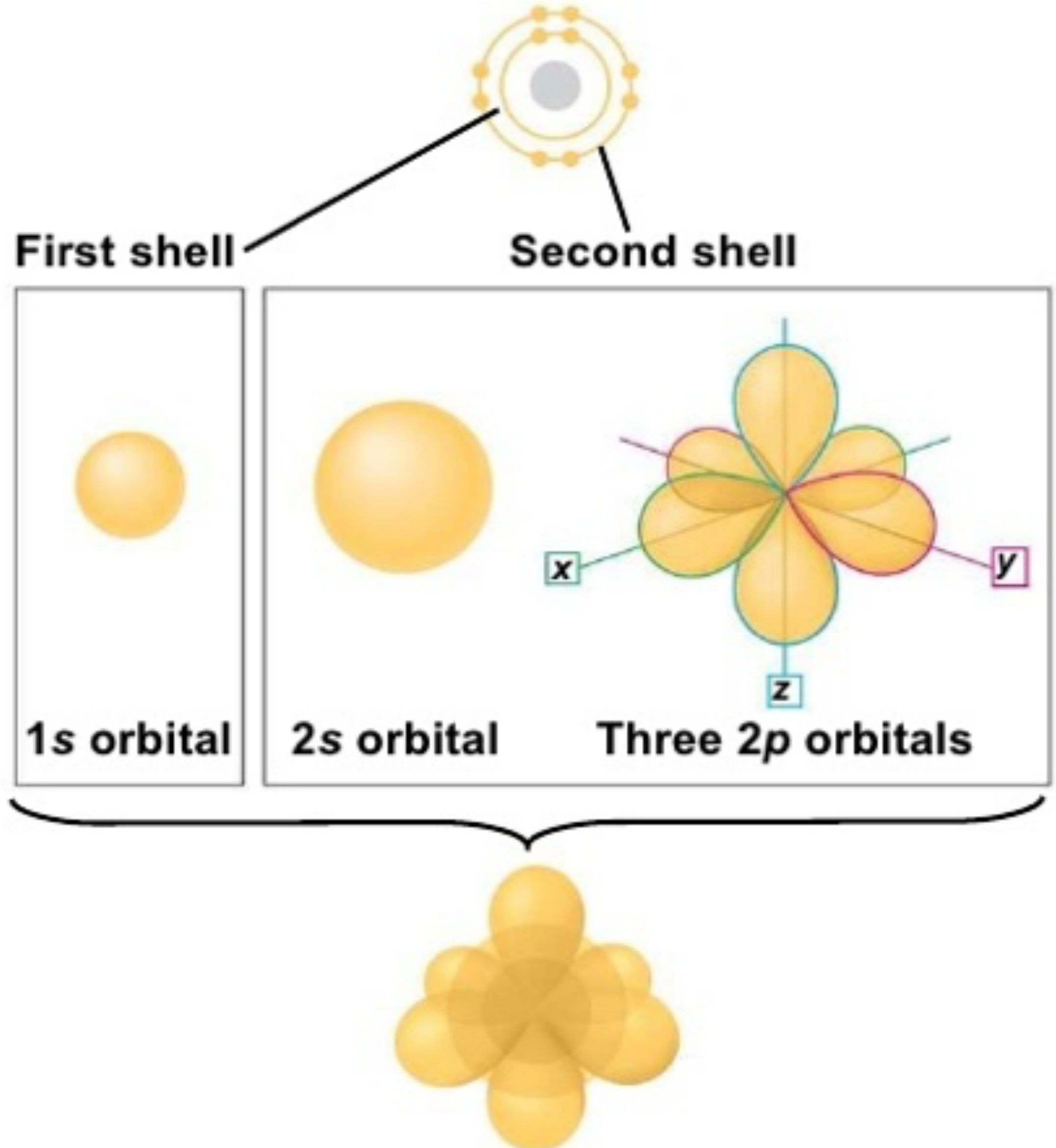


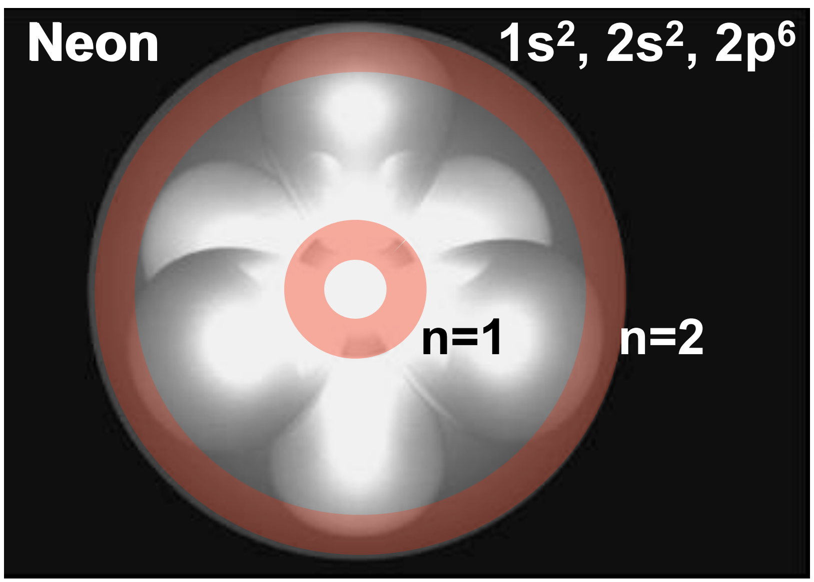
Fig. 2-10-4

Neon, with two filled shells (10 electrons)

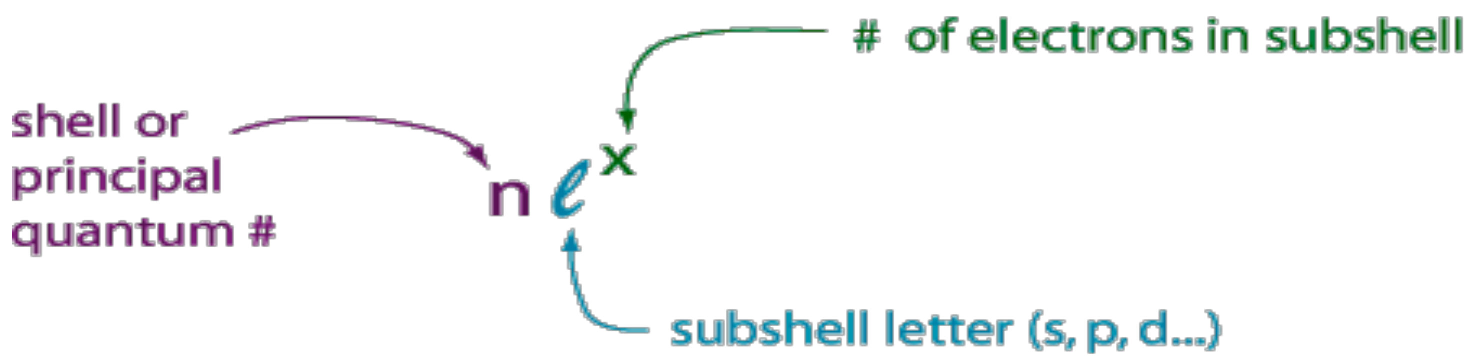
(a) Electron-distribution diagram

(b) Separate electron orbitals

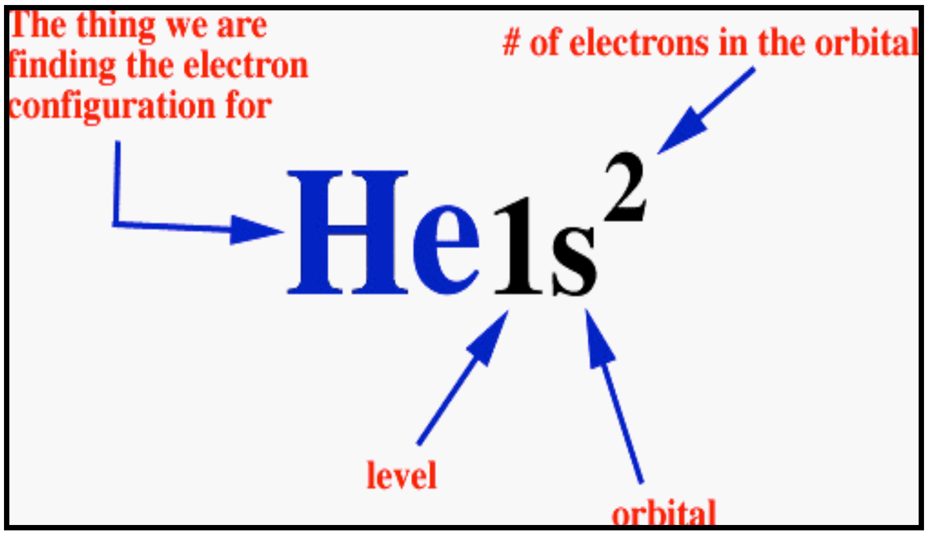




Electron Configuration Notation



EXAMPLE: Helium (He) → Atomic Number 2 → 2 protons & 2 electrons



EXAMPLE: What is the Electron Configuration of Lead (Pb)?

Pb = Atomic # 82. With 82 p, a neutral Pb has 82 e-

$1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^6$, $4s^2$, $3d^{10}$, $4p^6$, $5s^2$, $4d^{10}$, $5p^6$, $6s^2$, $4f^{14}$, $5d^{10}$, $6p^2$

What orbitals are occupied by the outermost electrons?

The outermost electrons ALWAYS occupy the outermost S and P orbitals

Sample Electron Configurations

- Notice how the electrons located in the outermost energy shell, what we call the valence electrons, are those occupying the s or the s and one, or more, p orbitals always

Which atoms have their outermost shell S and P electrons maximally filled?

S $1s^2, 2s^2, 2p^6, 3s^2, 3p^4$

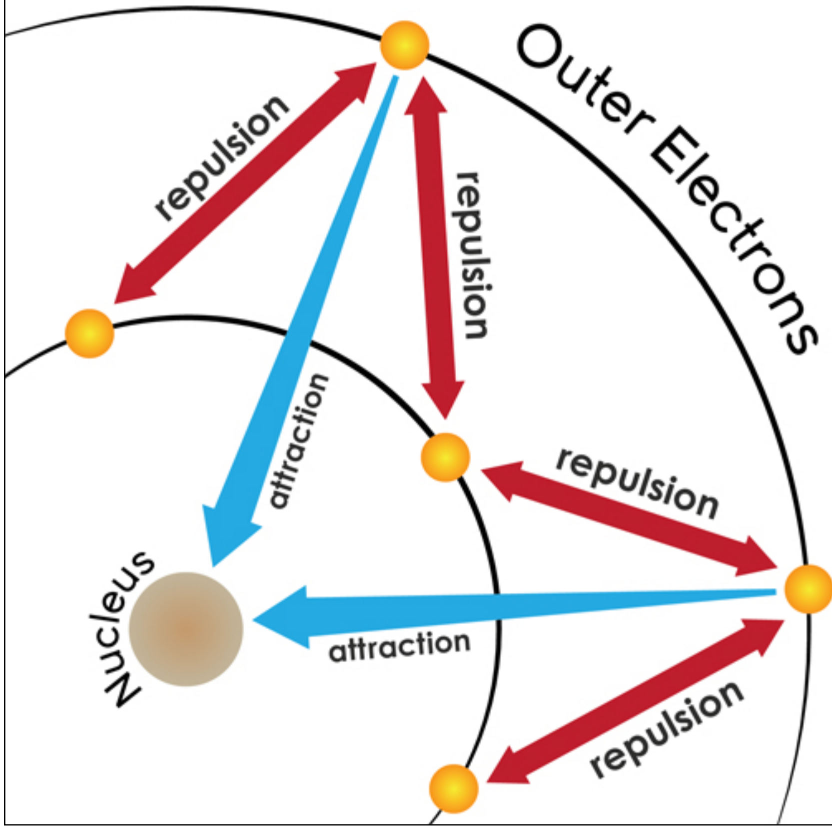
Rn $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 4s^2, 3d^{10}, 4p^6, 5s^2, 4d^{10}, 5p^6, 6s^2, 4f^{14}, 5d^{10}, 6p^6$

Ac $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 4s^2, 3d^{10}, 4p^6, 5s^2, 4d^{10}, 5p^6, 6s^2, 4f^{14}, 5d^{10}, 6p^6, 7s^2, 6d^1$

Hf $1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 4s^2, 3d^{10}, 4p^6, 5s^2, 4d^{10}, 5p^6, 6s^2, 4f^{14}, 5d^2$

Electron Orbitals & Valence Electrons

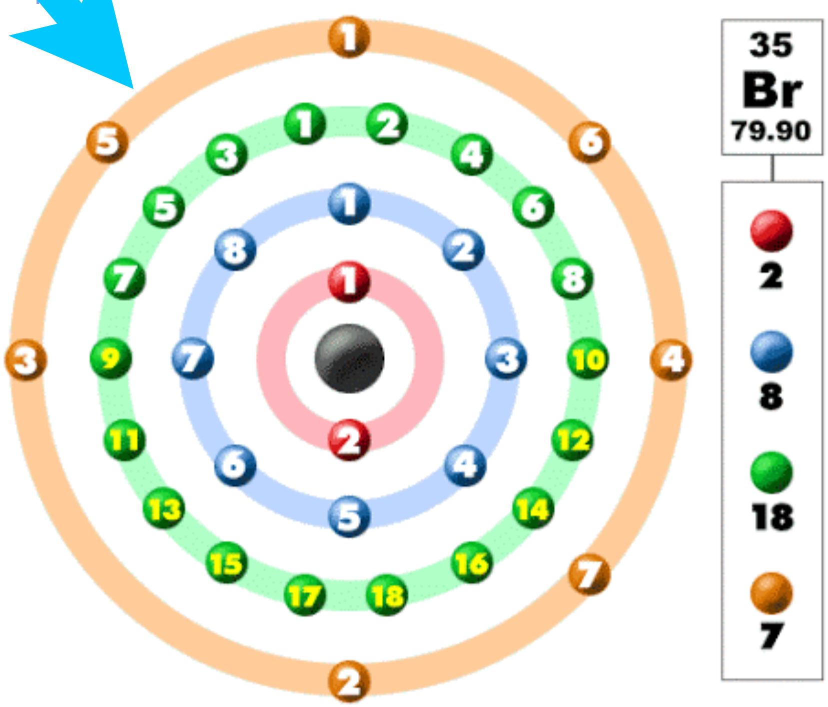
- Electrons are attracted to the protons in the nucleus, but still remain in their energy shells because of the electrostatic repulsions between the electrons in successive shells.

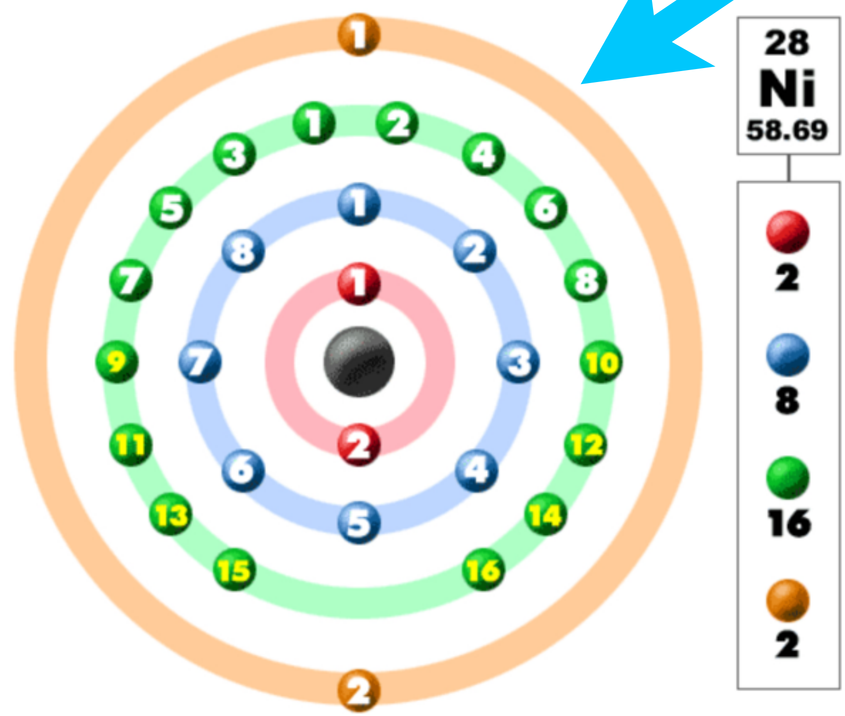


- Due to this electron-electron repulsion, electrons farthest from the nucleus, outermost shell electrons, are pushed father away and are thus held less tightly.
  - The outer electrons are SHIELDED by the inner energy level electrons from the attractive forces asserted by the positive protons in the nucleus.

Electron Orbitals & Valence Electrons

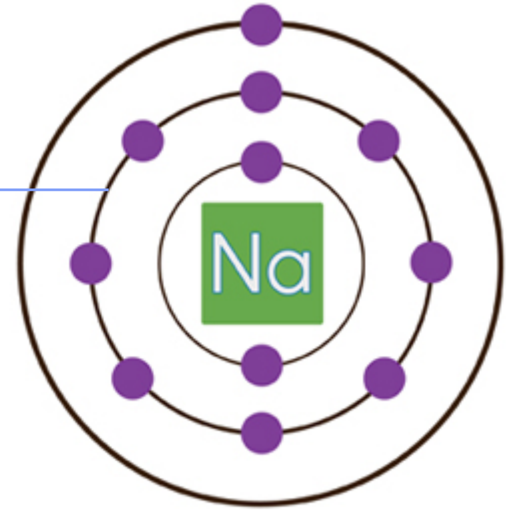
- The VALENCE SHELL is the outermost energy level of an atom.
  - The electrons that fill it, the VALENCE ELECTRONS, determine the chemical properties of the elements.

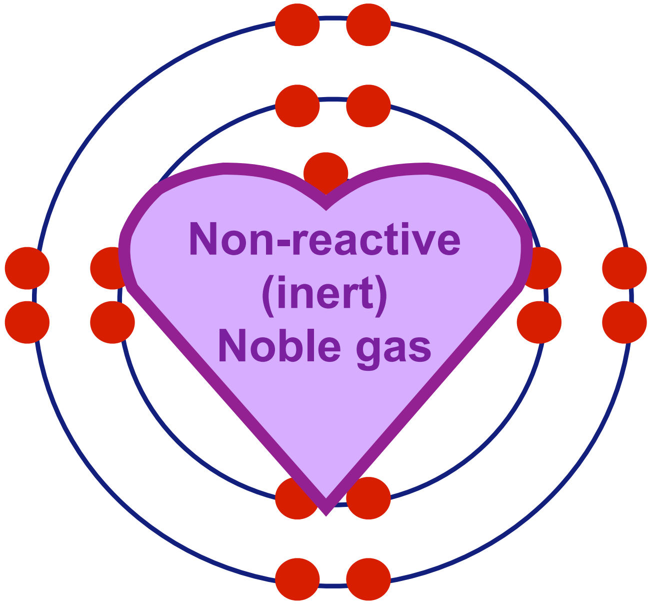




Bonding properties

- **Effect of electrons**
  - Being neutral (# e- = #p) does ***not*** mean the atom is most stable.
    - Atoms want the orbitals in their outermost energy shell (the **Valence Shell**) to be filled to be stable
    - Chemical behavior thus depends on the # of electron in the Valence Shell
      - For H, He, Li, Be etc..., this means having 2 electrons in their outer shell
      - For most atoms, though, this means having 8 electrons in the outer shell
        - Atoms will react with each other try to become more stable - to get a full valence shell
  - Electrons determine chemical behavior of atom *(how atoms behave around other atoms)*



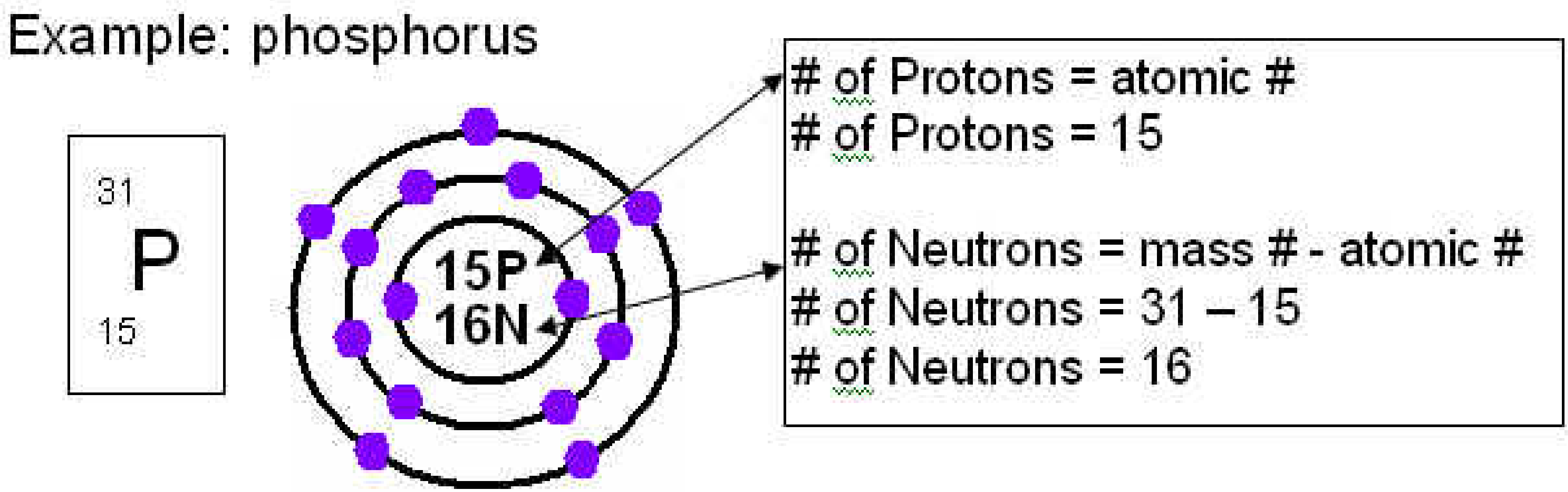


How do these atoms behave?

BOHR-RUTHERFORD DIAGRAM

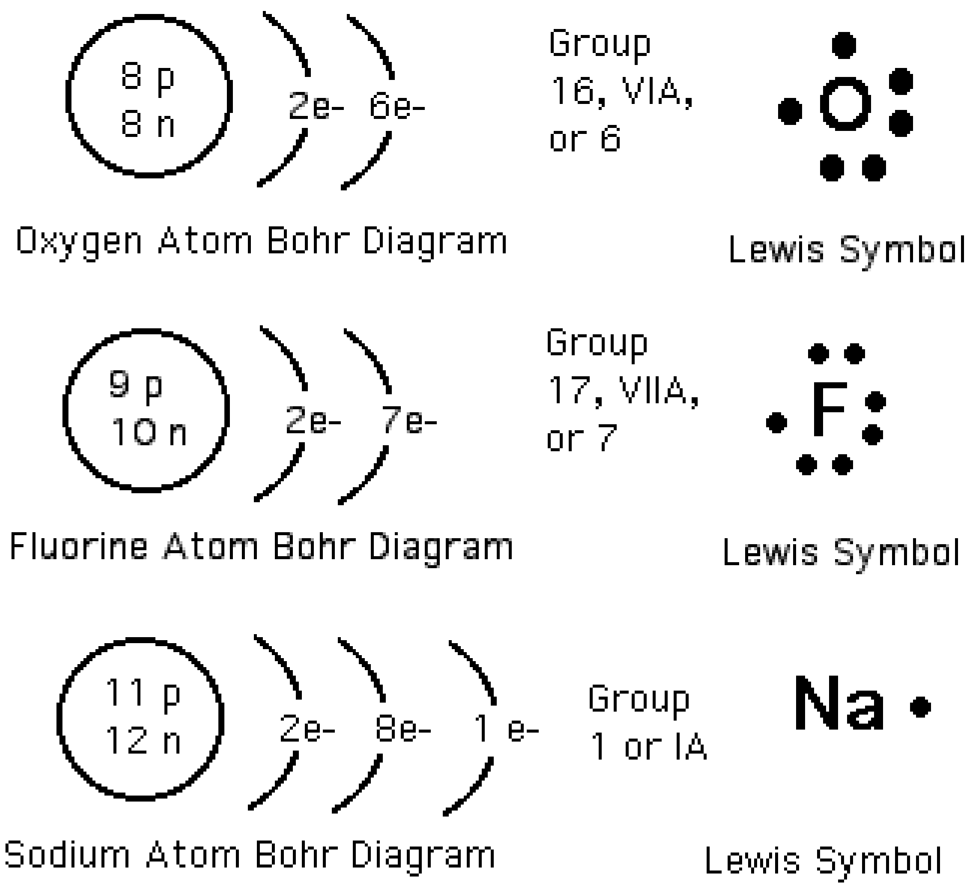
- A **BOHR-RUTHERFORD OR BOHR DIAGRAM** is a way to visually represent the Electron Shells and the Electron Configuration of an atom.

1. **Draw the nucleus as a solid circle.**
2. **Put the # of protons (Atomic #) in the nucleus with the # of neutrons (Mass # – Atomic #) under it.**
3. **Place the # of electrons as dots on concentric circles around the nucleus representing the Electron Shells.**



ELECTRON (LEWIS) - DOT STRUCTURES

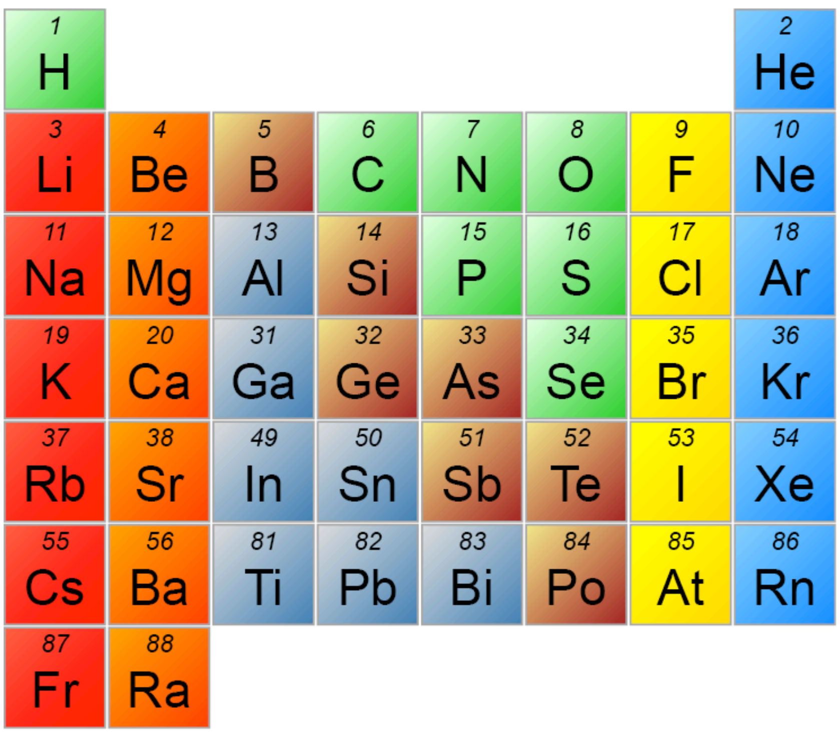
- **Simplified Bohr diagrams which only consider electrons in outer energy levels are called <u>Lewis Symbols or Lewis Dot Structure</u>.**



A Lewis Symbol consists of the element's symbol surrounded by "dots" to represent the number of electrons in the outer energy level as represented by a Bohr Diagram.

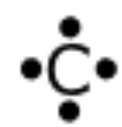
ELECTRON (LEWIS) - DOT STRUCTURES

- **Valence electrons are represented as dots placed on sides, top, bottom of the symbol for the element.**
  - **1, 2, 3 or 4 valence electrons are arranged around the element as a single dot on each side.**
    - **When there are more than 4 valence electrons, the dots are paired (no more than 2 per side).**

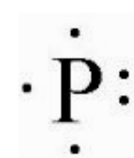


- **Write the electron-dot structure of Hydrogen?**
    - **Symbol: H, Group 1A, so 1 valence e-**

- **Carbon?**
    - **Symbol: C, Group 4A, so 4 valence e-**

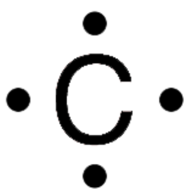


- **Phosphorous?**
    - **Symbol: P, Group 5A, so 5 valence e-**

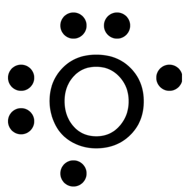


VALENCE & VALENCE ELECTRONS

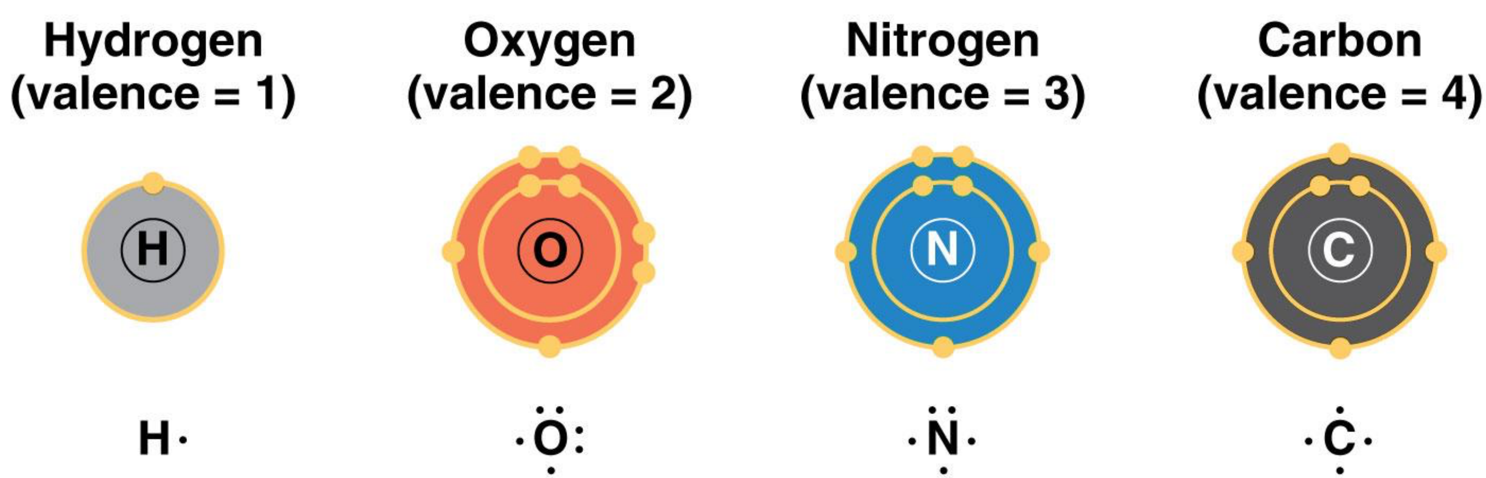
- **The number of unpaired of electrons is called the atoms VALENCE.**
  - This valence number is the number of covalent bonds that that atom is capable of forming.



    - EXAMPLE: Carbon, which has 6 electrons, has 4 valence electrons and a valence of 4 - it has 4 unpaired electrons.
      - The fact that C can form so many bonds explains why it forms the backbone of the organic molecules of life.

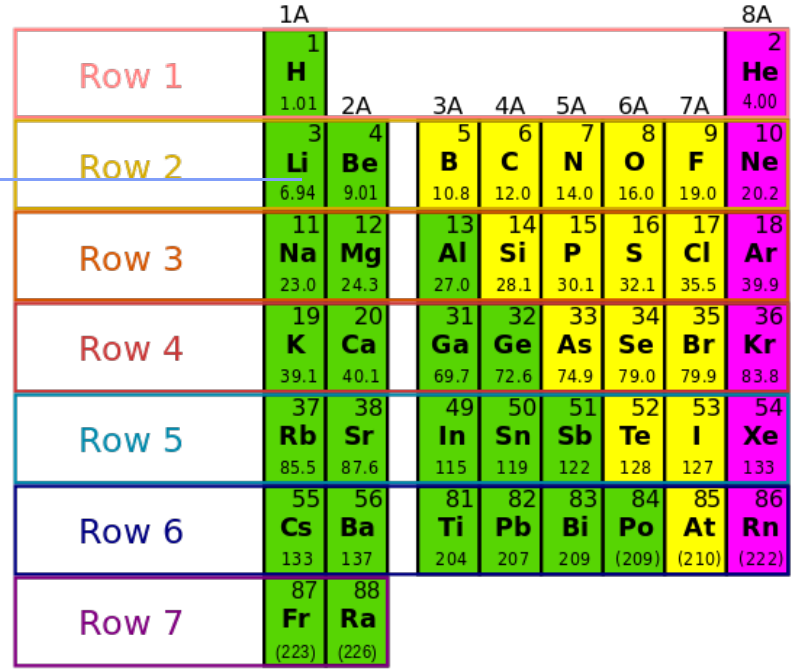


    - EXAMPLE: Oxygen which has 8 electrons, has 6 valence electrons and has a valence of 2 - it has 2 unpaired electrons.



Bonding properties

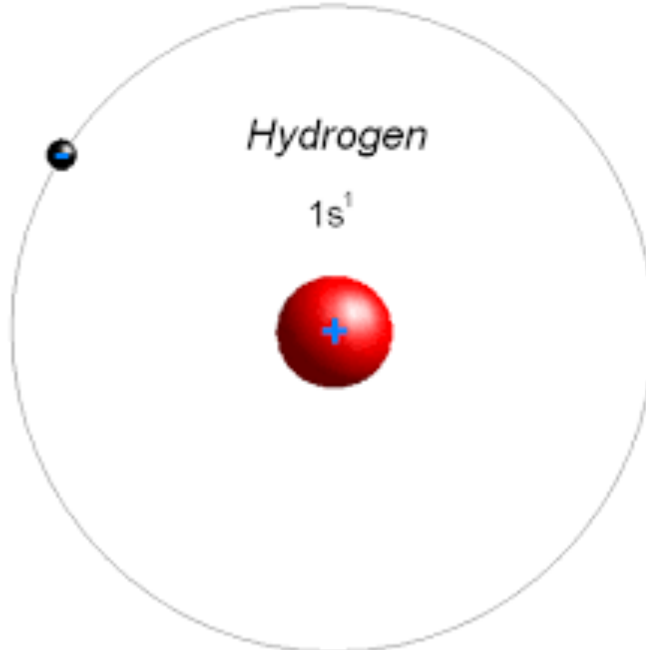
- **OCTET (& Duet) RULE:**
  - **The noble (inert) gases (group 8A) already have a stable octet of 8 valence electrons due to their *filled outermost S orbital and three filled outermost P orbitals.***
  - **Atoms of the other elements (including Groups 1A to 7A) form ions, compounds, or molecules together in an effort to be more stable, to have their outermost valence electron shell filled with the maximum amount of electrons.**
    - **For most this means having a total of 8 electrons in the valence shell *(for some it means having a total of 2 electrons in the valence shell)***

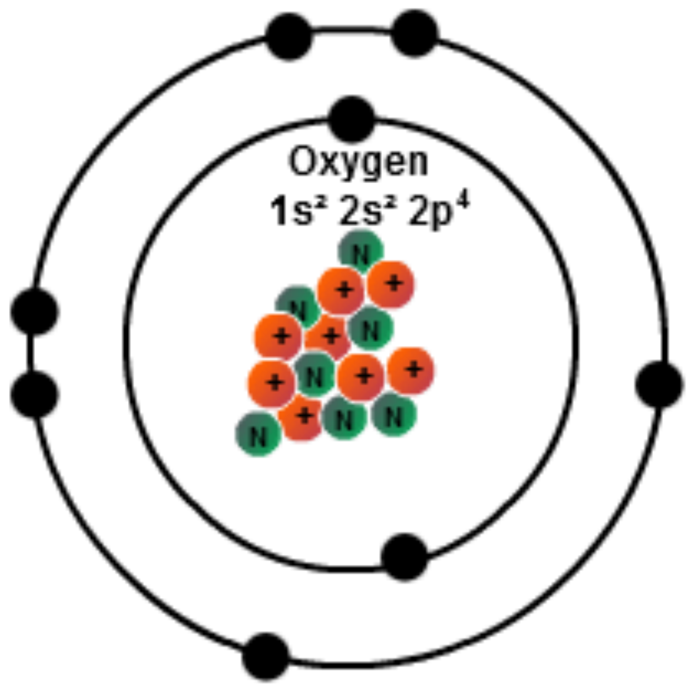


Group	Total Valence e-
All of 1A	1e-
All of 2A	2e-
All of 3A	3e-
All of 4A	4e-
All of 5A	5e-
All of 6A	6e-
All of 7A	7e-
All of 8A	8e-

Bonding properties

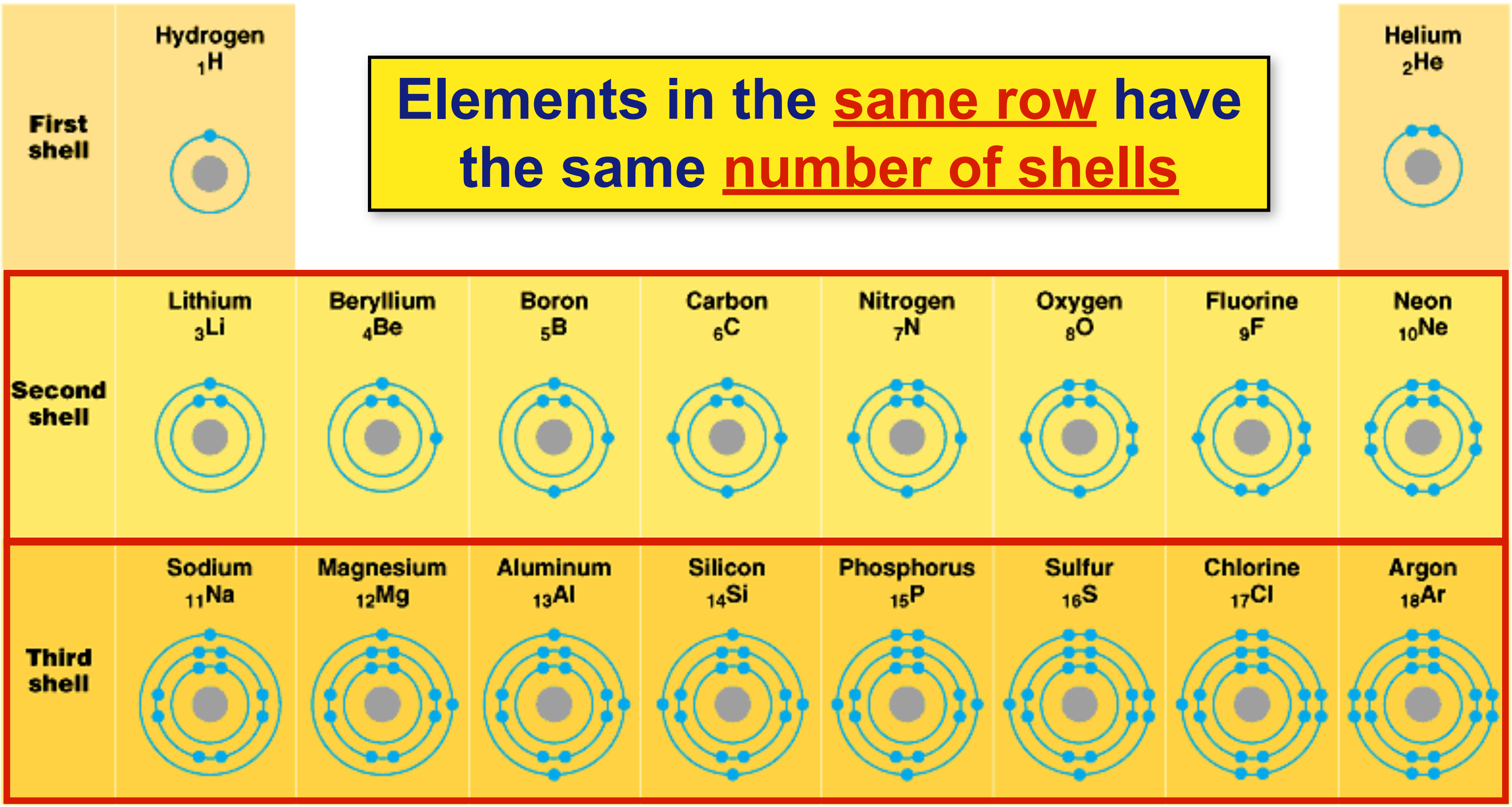
- Ex: Hydrogen (H) and Helium (He) have 1 and 2 electrons, respectively, so their electrons only occupy the 1S orbital (the 1st energy shell cannot house any any P orbitals).
  - All orbitals can hold a maximum of 2 electrons.
    - H & He are stable with a duet of only 2 valence electrons and are said to follow the Duet rather than Octet Rule.
- Ex: Oxygen (O) has 8 total electrons, 6 of which are valence electrons.
    - O is stable with an octet of 8 valence electrons and is said to follow the Octet Rule.





Elements & their valence shells

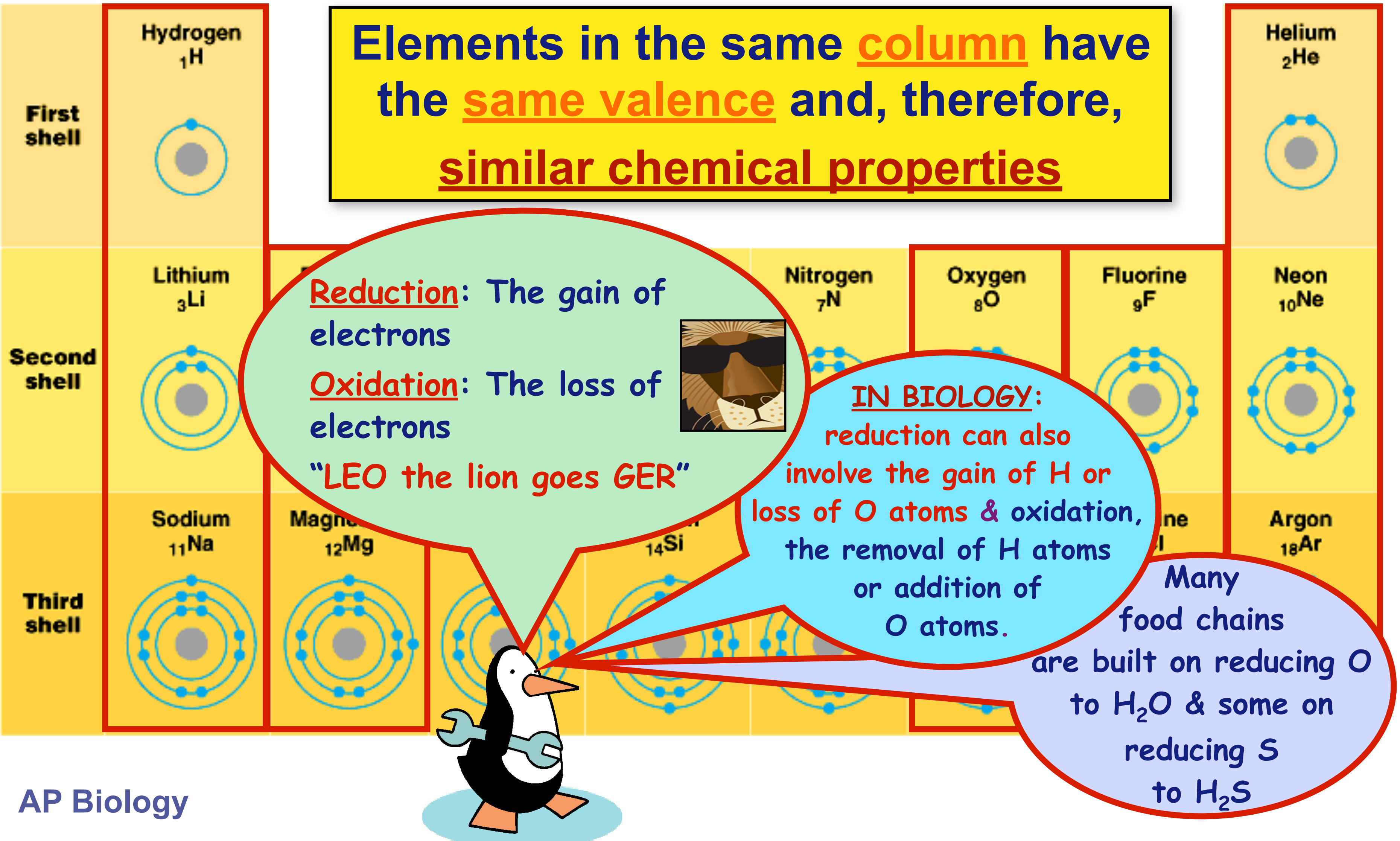
Elements in the <u>same row</u> have the same <u>number of shells</u>



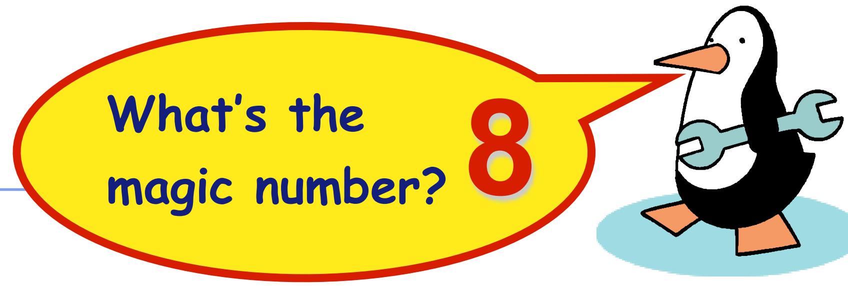
Moving from left to right, each element has a sequential addition of protons *(each new proton attracting another electron)*.

Elements & their valence shells

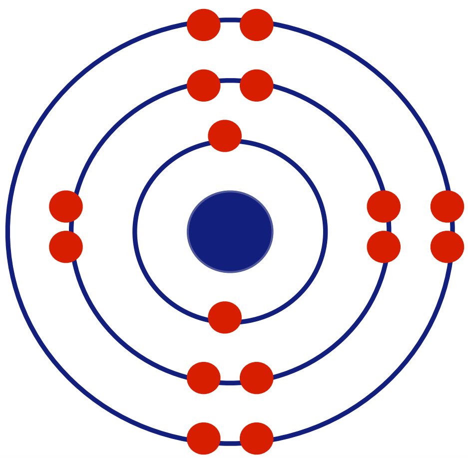
Elements in the same column have the same valence and, therefore, similar chemical properties



Bonding properties

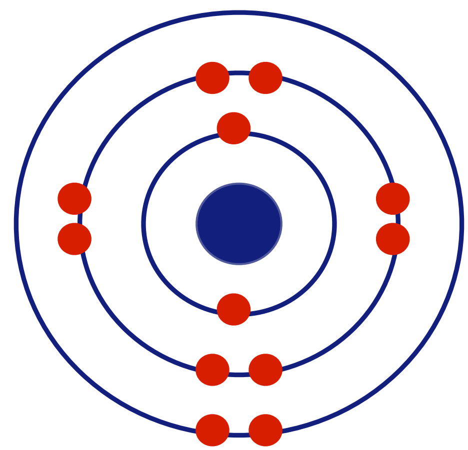


- ## Effect of electrons
  - The chemical behavior of an atom depends on number of electrons in its valence shell. To be stable, the orbitals in the outermost energy level/shell must be full. Remember the **OCTET (& DUET) Rules** - *atoms, with certain exceptions like Hydrogen & Helium, want 8 valence electrons to be stable.*



How does this atom behave?

With 6 valence e-'s, this atom, being a nonmetal, will either covalently bond or steal 2 additional electrons from another atom in order to complete its valence shell (the third Electron Shell)



How does this atom behave?

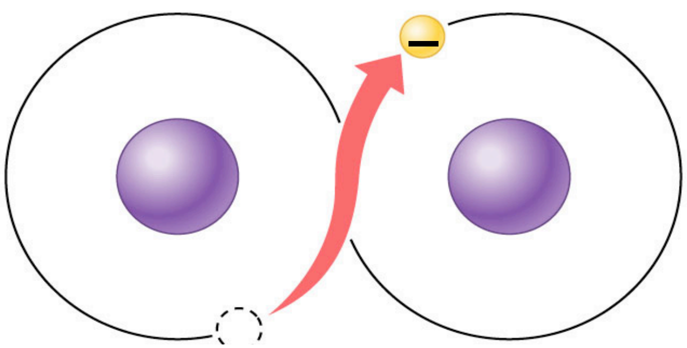
With 2 valence e-'s, and being a metal, this atom will lose both valence e-'s becoming a positively charged ion (cation) with a 2+ charge that now has a full valence shell (The second Electron Shell)

Chemical reactivity

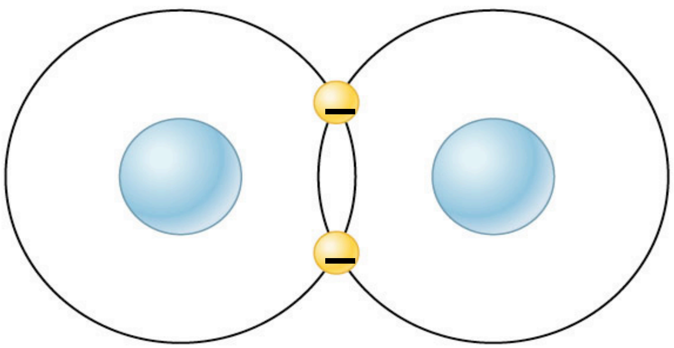
- To become more stable, atoms tend to...
  - complete a partially filled valence shell <u>or</u>
  - empty a partially filled valence shell

This tendency drives chemical reactions…

and creates chemical bonds (each bond forms between 2 atoms)

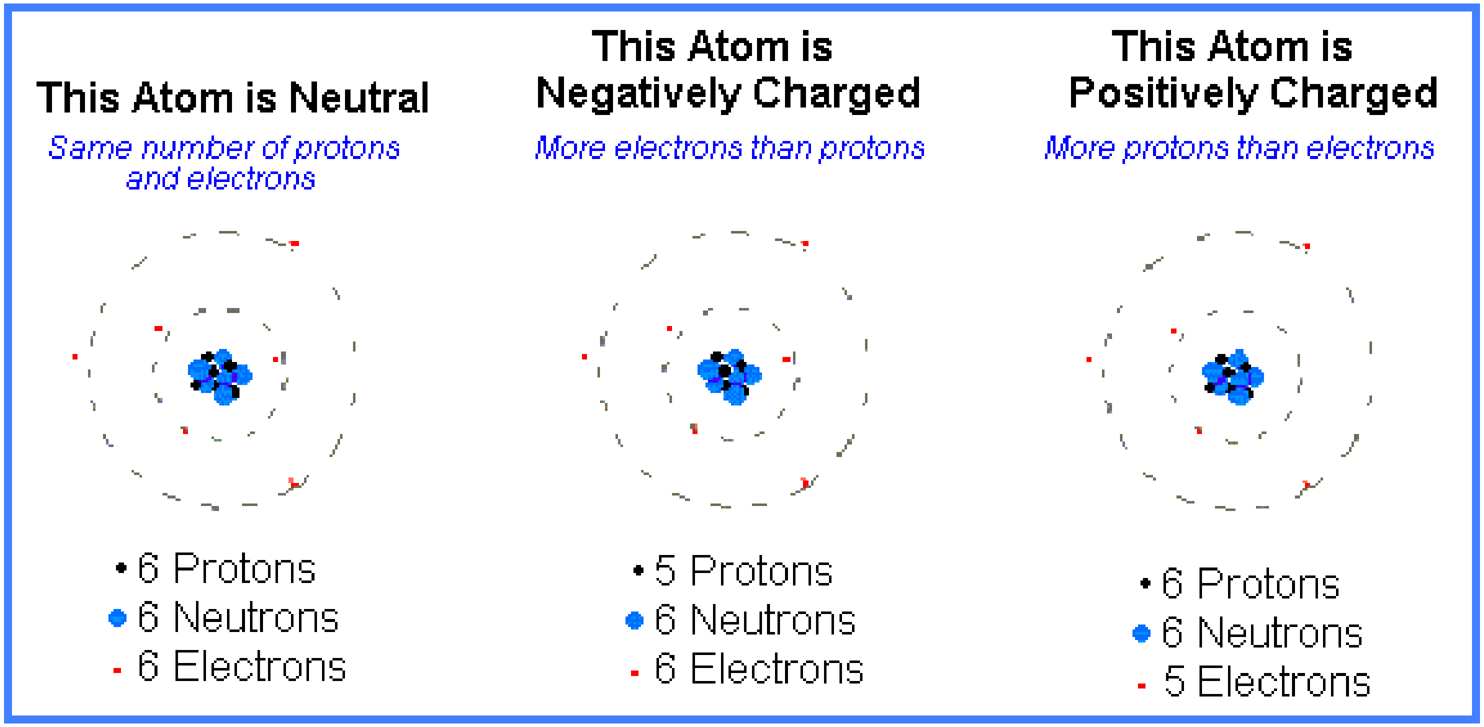


<u>Ionic bonds</u> form when one atom steals electrons from another atom. Both now become oppositely charged ions, which are now <u>attracted</u> each other.



<u>Covalent bonds</u> form when two atoms <u>share</u> electrons in order for each to complete their valence shells.

Ions are charged atoms or molecules



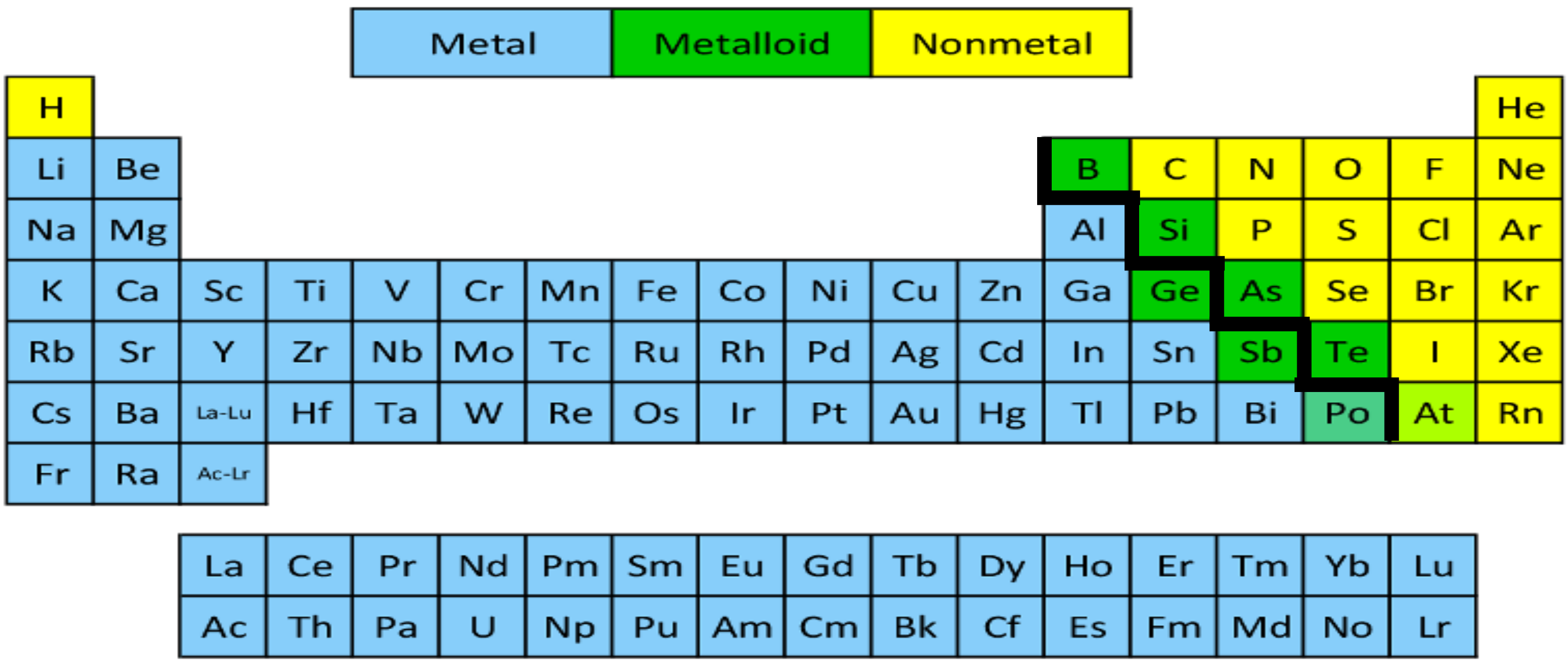
All charges in a neutral atom add up to <u>ZERO</u>! (#p = #e-)

Ions form when an atom gains or loses electrons. (#p ≠ #e-)

<u>Cations</u> = positively charged ions
<u>Anions</u> = negatively charged ions

The Periodic Table of Elements

1. Except for hydrogen (H) on the top left, elements on the left-hand side of the zigzag line, which runs from Boron (B) to astatine (At), are metals. (Blue).
2. All elements to the right of the zigzag line and Hydrogen (H) on the top left are nonmetals. (Yellow).
3. Seven of the nine elements that touch the zigzag line are semimetals. (Green)



The Periodic Table of Elements

EXERCISE: **Are the following elements metals, nonmetals, or semimetals (metalloids) ?**

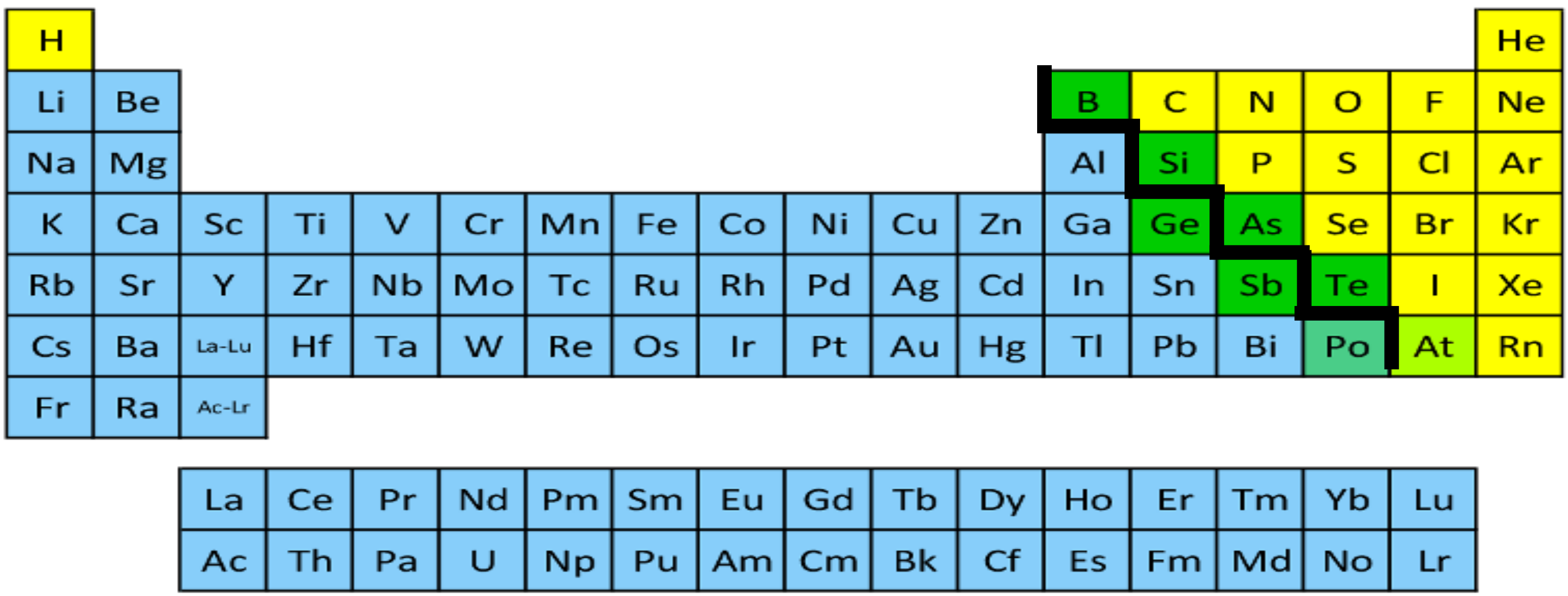
Ca (Calcium) ?

H (Hydrogen) ?

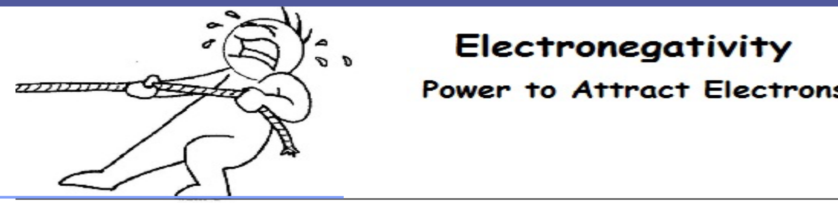
Si (Silicone) ?

Fe (Iron) ?

O (Oxygen) ?



Electronegativity



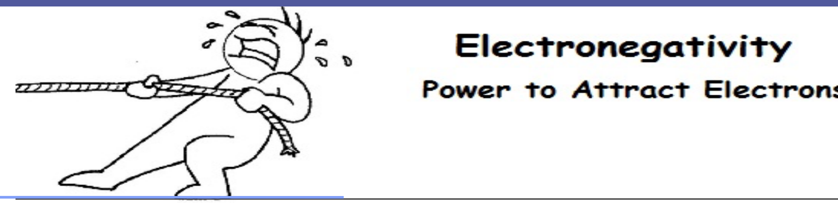
- Electronegativity is a measure of the tendency of an atom to attract a bonding pair of electrons *(a measure of "how strong a nucleus pulls on electrons")*
  - *Electronegativity ranges in value from 0.7 to 4.0*
    - Generally, metals tend to be the LEAST electronegative while nonmetals tend to be the MOST electronegative
      - Atoms may lose or gain electrons in order to ensure their

Electronegativity values of the elements (Pauling scale)

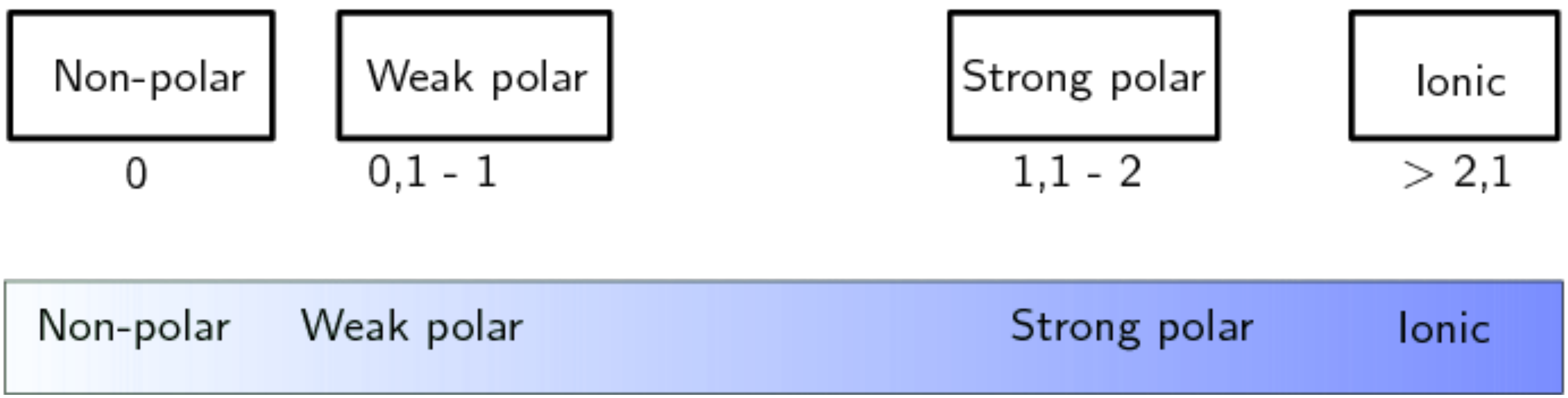
H 2.1																	He
[illegible]	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	Ne
Na 0.9	Mg 1.2											Al 1.5	[illegible] 1.8	[illegible]	[illegible] 2.5	Cl 3.0	Ar
[illegible] 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu [illegible]	[illegible]	[illegible] 1.6	[illegible] 1.8	[illegible] 2.0	Se 2.4	Br 2.8	Kr 3.0
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc [illegible]	Ru [illegible]	[illegible]	[illegible] 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	Xe 2.6
Cs 0.7	Ba 0.9	La 1.1	Hf [illegible]	Ta [illegible]	[illegible] 1.7	[illegible] 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Ti 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2	Rn 2.4
Fr 0.7	[illegible]	[illegible] 1.1															

Ce 1.1	Pr 1.1	Nd 1.1	Pm 1.1	Sm 1.1	Eu 1.1	Gd 1.1	Tb 1.1	Dy 1.1	Ho 1.1	Er 1.1	Tm 1.1	Yb 1.1	Lu 1.2
Th 1.3	Pa 1.5	U 1.7	Np 1.3	Pu 1.3	Am 1.3	Cm 1.3	Bk 1.3	Cf 1.3	Es 1.3	Fm 1.3	Md 1.3	No 1.3	Lr

Electronegativity



- **When two atoms near each other, the difference in their Electronegativity will determine what kind of bond results.**
  - **Large differences lead to one atom stealing valence electrons from another, leading to ion formation and, thus, ionic bonding**
  - **Small difference lead to two atoms sharing the electron more equally as part of a non-polar covalent bond**
  - **Medium differences lead to two atoms sharing electrons more unequally as part of a polar covalent bond**



Positive Ions

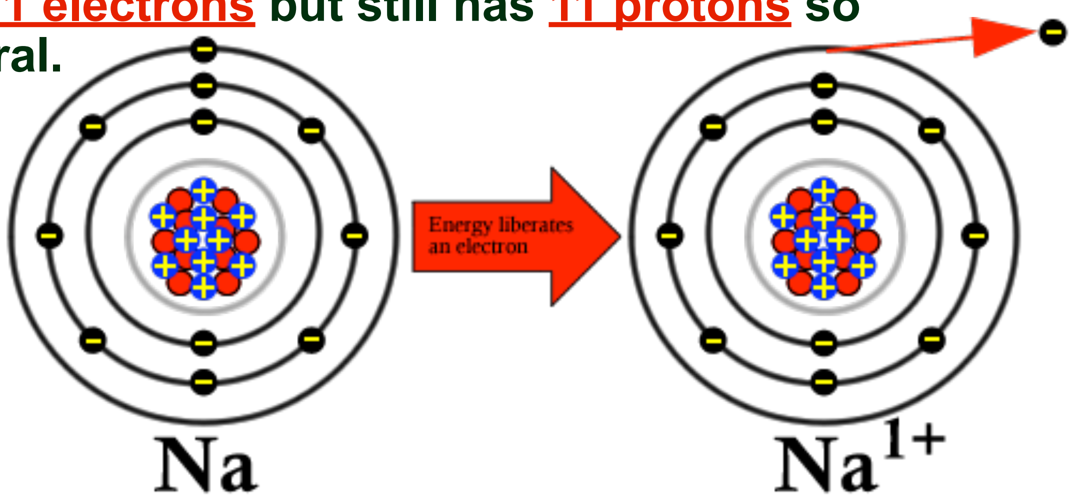
- Recall that the <u># of valence electrons</u> in groups 1A to 8A is <u>equal to the group number.</u>
- <u>Metals</u>
  - <u>Low Electronegativity</u> (= how strongly an atom's nucleus pulls on electrons)
    - <u>LOSE</u> their valence electrons to much more electronegative nonmetal atoms and attain a noble gas electron configuration, forming <u>CATIONS</u> *(positively charged atoms or ions)*

<u>Example</u>: Sodium (<u>Na</u>) is in Group 1A so it has 1 valence e- instead of 8. It looses its valence e- to a much more electronegative atom (a nonmetal) and becomes a <u>positive ion</u>.

<u>Na</u> now has <u>10 instead of 11 electrons</u> but still has <u>11 protons</u> so the atom is no longer neutral.

It carries an electrical charge, or <u>ionic charge</u>, of <u>1+</u>.

<u>Ionic charge</u> is written in the <u>upper right-hand corner of the element's symbol</u>



Has 1 valence e- in the 3s orbital

Now, has 8 valence e-'s in the 2s & all three 2p orbitals

Positive Ions

Electron configuration of neutral Na: Na $1s^2, 2s^2, 2p^6, 3s^1$

With only 1 electron in its outer most valence shell (Energy Level n=3), Na is unstable. To be stable, sodium obeys the Octet Rule and wants all s and p orbitals filled in it's outermost, valence shell.

Na can either gain 7 extra e-'s or just loose 1. Because it is low in electronegativity, it will loose the 1 valence e- easily to another more electronegative atom (a nonmetal). This deletes the third Electron Shell entirely, leaving sodium with a new electron configuration that is similar to that of the stable Noble Gas Neon with 8 valence e-'s in its valence shell:

Na $1s^2, 2s^2, 2p^6,$ ~~$3s^1$~~ → Na $1s^2, 2s^2, 2p^6$

Ne $1s^2, 2s^2, 2p^6$

Positive Ions

Na $1s^2, 2s^2, 2p^6, \cancel{3s^1}$ → Na $1s^2, 2s^2, 2p^6$

Note that the number of protons did NOT change, but the number of electrons did.

Total p = 11
Total e- in neutral Na = 11
New Total e- after loosing 1 valence e- = 11 - 1 = 10

Net Charge on new Na Atom: **(+11) + (-10) = +1**

The neutral sodium atom now has a charge imbalance and is no longer neutral, but has become an ion, or a cation to be more specific.

The symbol for the ion of sodium is Na^{1+} or Na^{+}

Negative Ions

- NON-Metals
  - High Electronegativity
    - GAIN one or more valence electron(s) from much less electronegative metal atoms in order to attain a noble gas forming negatively charged ions or ANIONS.
      (negatively charged atoms or ions)

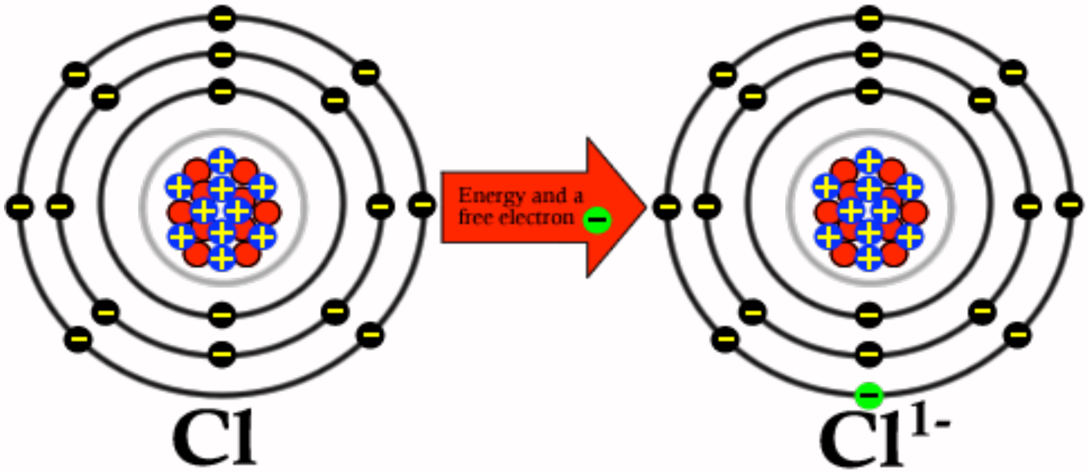
- EXAMPLE: Cl = Belongs to Group 7A so has 7 valence electrons

When it gains an extra outer e^-, it will achieve noble gas arrangement like Argon (Ar) of Group 8A becoming a negatively charged Cl^-

Cl now has 18 instead of 17 electrons but still has 17 protons so the atom is no longer neutral.

It carries an electrical charge, or ionic charge, of 1-.

Ionic charge is written in the upper right-hand corner of the element's symbol



Has 7 valence e-'s in the 3s & three 3p orbitals

Now, has 8 valence e-'s in the 3s & three 3p orbitals

Negative Ions

Electron configuration of neutral Cl: Cl $1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^5$

Cl is unstable because it has only 7 e- in its outermost valence shell, Energy Level n=3. To be stable, chlorine obeys the Octet Rule and wants all s and p orbitals filled in it's outermost, valence shell.

Cl can either gain 1 extra e- or loose 7 e-'s to obtain a fully filled valence shell. It will gain the 1 valence e-, stealing the electron from a much less electronegative atom (a metal), leaving chlorine with a new electron configuration that is similar to that of the stable Noble Gas Atgon with 8 valence e-'s in its valence shell:

Cl $1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^5$ → Cl $1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^6$

Ar $1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^6$

Negative Ions

Cl $1s^2, 2s^2, 2p^6, 3s^2, 3p^5$ → Cl $1s^2, 2s^2, 2p^6, 3s^2, 3p^6$

Note that the number of protons did NOT change but the number of electrons did.

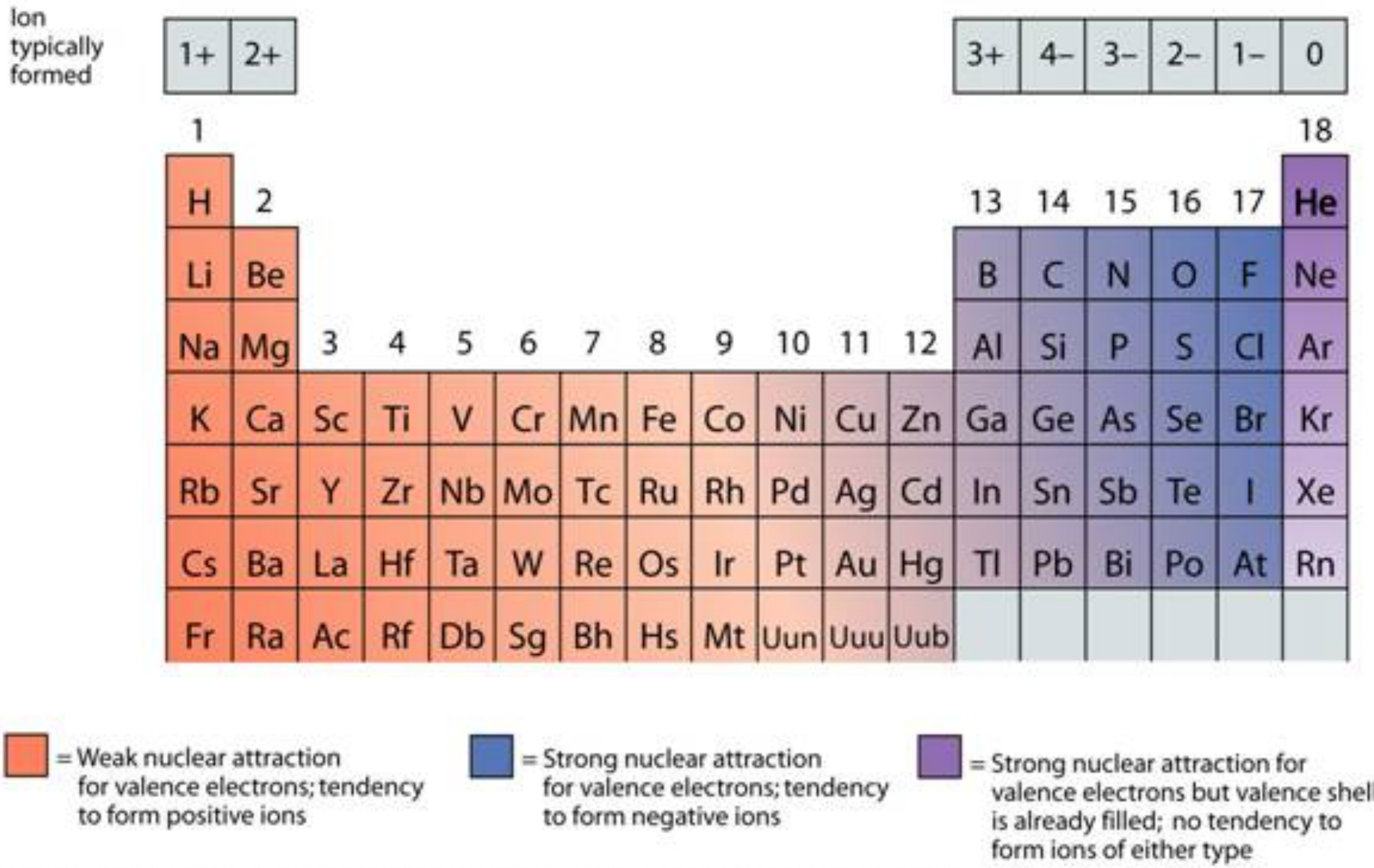
Total p = 17
Total e- in neutral Cl = 17
New Total e- after gaining 1 valence e- = 17 + 1 = 18

Net Charge on new Cl Atom: (+17) + (-18) = -1

The neutral chlorine atom now has a charge imbalance and is no longer neutral but has become an ion or a anion to be more specific.

The symbol for the ion of chlorine is Cl^{1-} or Cl^{-}

The Formation of Ions



Common Ionic States of Elements

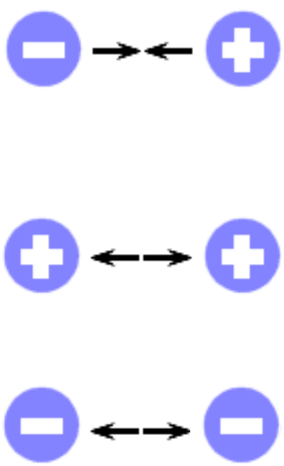
Legend: 1 (Atomic number) — H^+ (Common ionic state) — HYDROGEN (Element name)

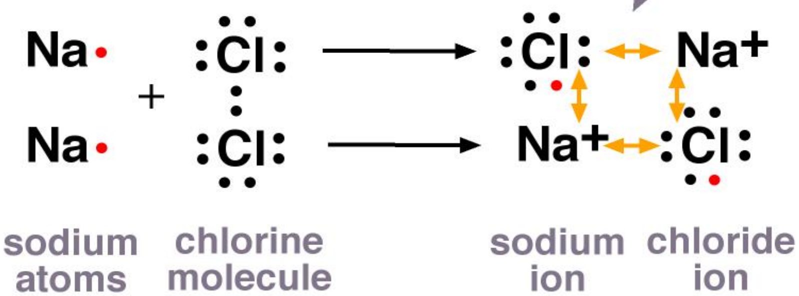
+1	+2											+3		-3	-2	-1	
1 H^+ HYDROGEN																	2 He HELIUM
3 Li^+ LITHIUM	4 Be^{2+} BERYLLIUM											5 B BORON	6 C CARBON	7 N^{3-} NITROGEN	8 O^{2-} OXYGEN	9 F^- FLUORINE	10 Ne NEON
11 Na^+ SODIUM	12 Mg^{2+} MAGNESIUM											13 Al^{3+} ALUMINIUM	14 Si SILICON	15 P^{3-} PHOSPHORUS	16 S^{2-} SULFUR	17 Cl^- CHLORINE	18 Ar ARGON
19 K^+ POTASSIUM	20 Ca^{2+} CALCIUM	21 Sc^{3+} SCANDIUM	22 Ti^{3+} / Ti^{4+} TITANIUM	23 V^{3+} / V^{5+} VANADIUM	24 Cr^{2+} / Cr^{3+} CHROMIUM	25 Mn^{2+} / Mn^{4+} MANGANESE	26 Fe^{2+} / Fe^{3+} IRON	27 Co^{2+} / Co^{3+} COBALT	28 Ni^{2+} / Ni^{3+} NICKEL	29 Cu^+ / Cu^{2+} COPPER	30 Zn^{2+} ZINC	31 Ga^{3+} GALLIUM	32 Ge^{4+} GERMANIUM	33 As^{3-} ARSENIC	34 Se^{2-} SELENIUM	35 Br^- BROMINE	36 Kr KRYPTON
37 Rb^+ RUBIDIUM	38 Sr^{2+} STRONTIUM	39 Y^{3+} YTTRIUM	40 Zr^{4+} ZIRCONIUM	41 Nb^{3+} / Nb^{5+} NIOBIUM	42 Mo^{6+} MOLYBDENUM	43 Tc^{7+} TECHNETIUM	44 Ru^{3+} / Ru^{4+} RUTHENIUM	45 Rh^{3+} RHODIUM	46 Pd^{2+} / Pd^{4+} PALLADIUM	47 Ag^+ SILVER	48 Cd^{2+} CADMIUM	49 In^{3+} INDIUM	50 Sn^{2+} / Sn^{4+} TIN	51 Sb^{3+} / Sb^{5+} ANTIMONY	52 Te^{2-} TELLURIUM	53 I^- IODINE	54 Xe XENON
55 Cs^+ CESIUM	56 Ba^{2+} BARIUM	71 Lu^{3+} LUTETIUM	72 Hf^{4+} HAFNIUM	73 Ta^{5+} TANTALUM	74 W^{6+} TUNGSTEN	75 Re^{7+} RHENIUM	76 Os^{4+} OSMIUM	77 Ir^{4+} IRIDIUM	78 Pt^{2+} / Pt^{4+} PLATINUM	79 Au^+ / Au^{3+} GOLD	80 Hg_2^{2+} / Hg^{2+} MERCURY	81 Tl^+ / Tl^{3+} THALLIUM	82 Pb^{2+} / Pb^{4+} LEAD	83 Bi^{3+} / Bi^{5+} BISMUTH	84 Po^{2+} / Po^{4+} POLONIUM	85 At^- ASTATINE	86 Rn RADON
87 Fr^+ FRANCIUM	88 Ra^{2+} RADIUM	103 Lr^{3+} LAWRENCIUM															

57 La^{3+} LANTHANUM	58 Ce^{3+} CERIUM	59 Pr^{3+} PRASEODYMIUM	60 Nd^{3+} NEODYMIUM	61 Pm^{3+} PROMETHIUM	62 Sm^{2+} / Sm^{3+} SAMARIUM	63 Eu^{2+} / Eu^{3+} EUROPIUM	64 Gd^{3+} GADOLINIUM	65 Tb^{3+} TERBIUM	66 Dy^{3+} DYSPROSIUM	67 Ho^{3+} HOLMIUM	68 Er^{3+} ERBIUM	69 Tm^{3+} THULIUM	70 Yb^{3+} YTTERBIUM
89 Ac^{3+} ACTINIUM	90 Th^{4+} THORIUM	91 Pa^{4+} / Pa^{5+} PROTACTINIUM	92 U^{4+} / U^{6+} URANIUM	93 Np^{5+} NEPTUNIUM	94 Pu^{4+} / Pu^{4+} PLUTONIUM	95 Am^{3+} / Am^{4+} AMERICIUM	96 Cm^{3+} CURIUM	97 Bk^{3+} BERKELIUM	98 Cf^{3+} CALIFORNIUM	99 Es^{3+} EINSTEINIUM	100 Fm^{3+} FERMIUM	101 Md^{2+} / Md^{3+} MENDELEVIUM	102 No^{2+} / No^{3+} NOBELIUM

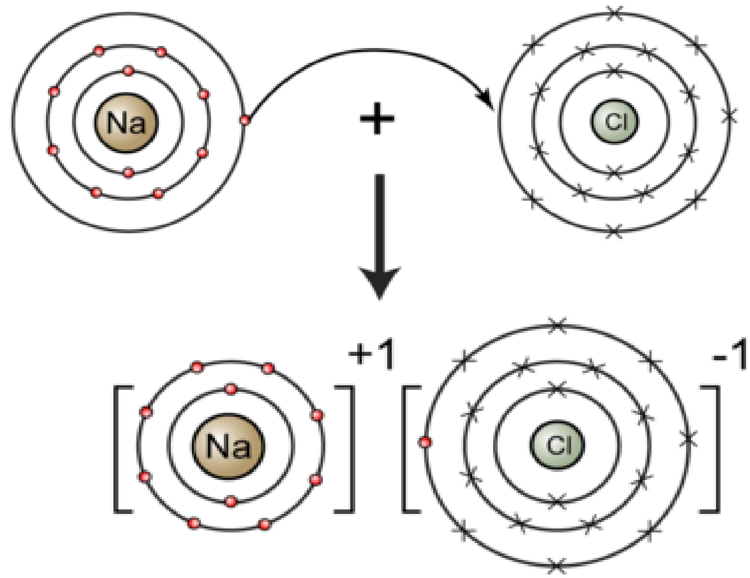
Opposites Attract

Oppositely charged particles will attract each other.





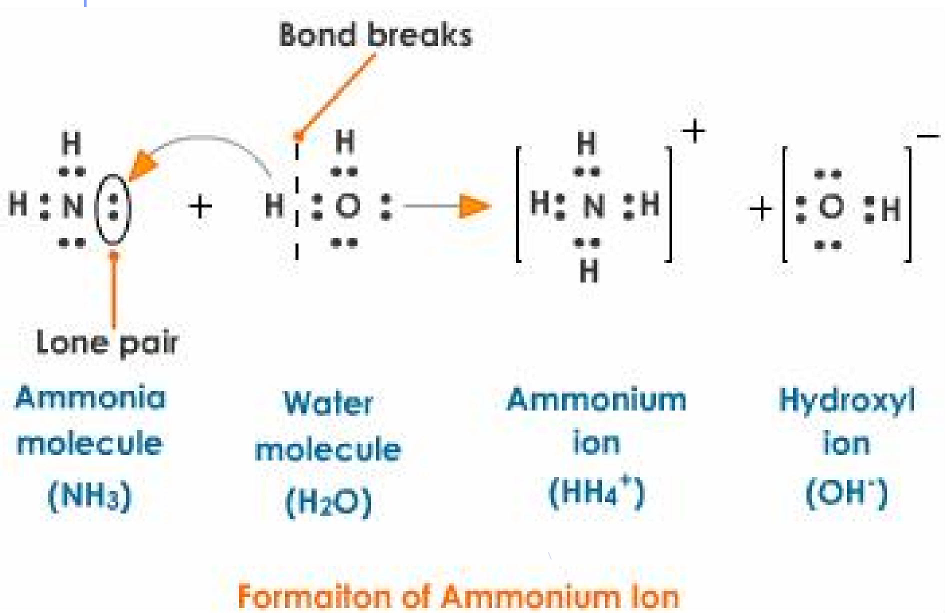
the electron lost by a sodium atom is gained by a chlorine atom to produce a sodium ion and a chloride ion



Oppositely charged ions attract each other, that attraction called an ionic bond.

Ions can be molecules - charged molecules

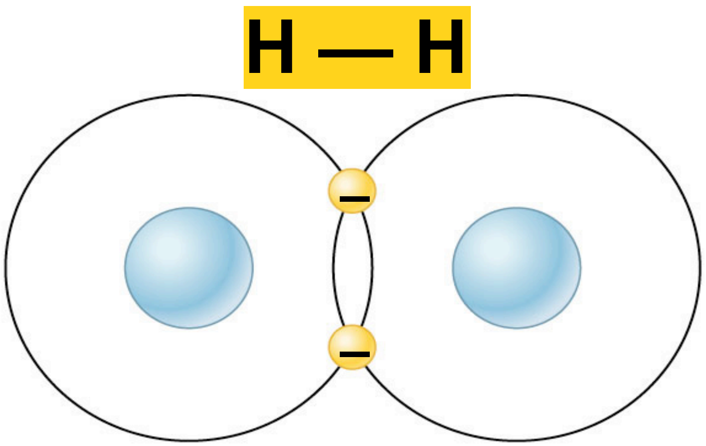
Polyatomic ions are <u>covalently bonded molecules that carry a charge</u> due to an imbalance in the total number of protons versus electrons in the molecule.



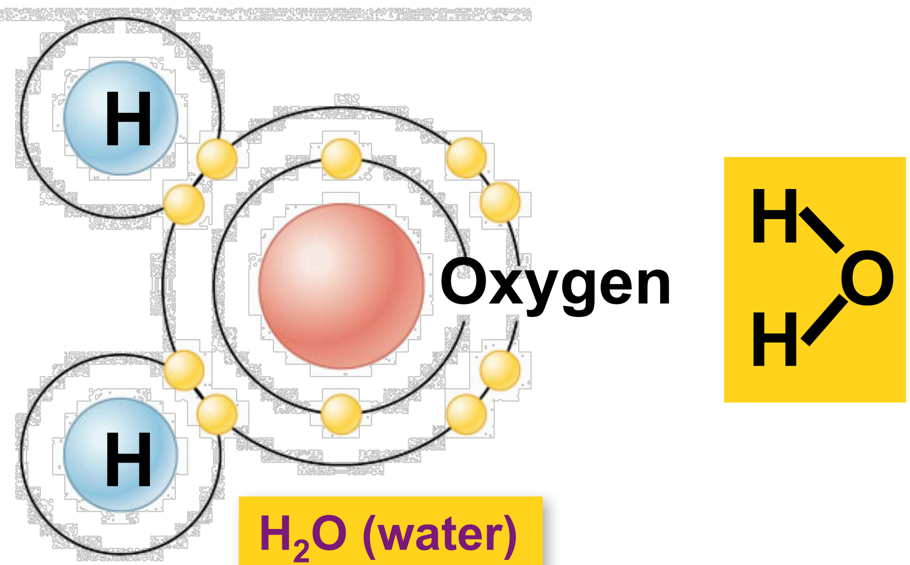
Common Polyatomic Ions			
$C_2H_3O_2^-$	acetate	OH^-	hydroxide
NH_4^+	ammonium	ClO^-	hypochlorite
CO_3^{2-}	carbonate	NO_3^-	nitrate
ClO_3^-	chlorate	NO_2^-	nitrite
ClO_2^-	chlorite	$C_2O_4^{2-}$	oxalate
CrO_4^{2-}	chromate	ClO_4^-	perchlorate
CN^-	cyanide	MnO_4^-	permanganate
$Cr_2O_7^{2-}$	dichromate	PO_4^{3-}	phosphate
HCO_3^-	bicarbonate	SO_4^{2-}	sulfate
HSO_4^-	bisulfate	SO_3^{2-}	sulfite
HSO_3^-	bisulfite		

Covalent bonds

- Ionic bonds form between a metal atom and a nonmetal atom (atoms very different in Electronegativity).
  - But what happens when the two atoms are closer in electronegativity as is the case when two nonmetals meet?
- Why are covalent bonds strong bonds?
  - two atoms share a pair of electrons
  - both atoms' positively charged nuclei pull & hold onto the electrons
  - Since they are strong bonds, they are very stable
- Molecules are groups of atoms joined via covalent bonds



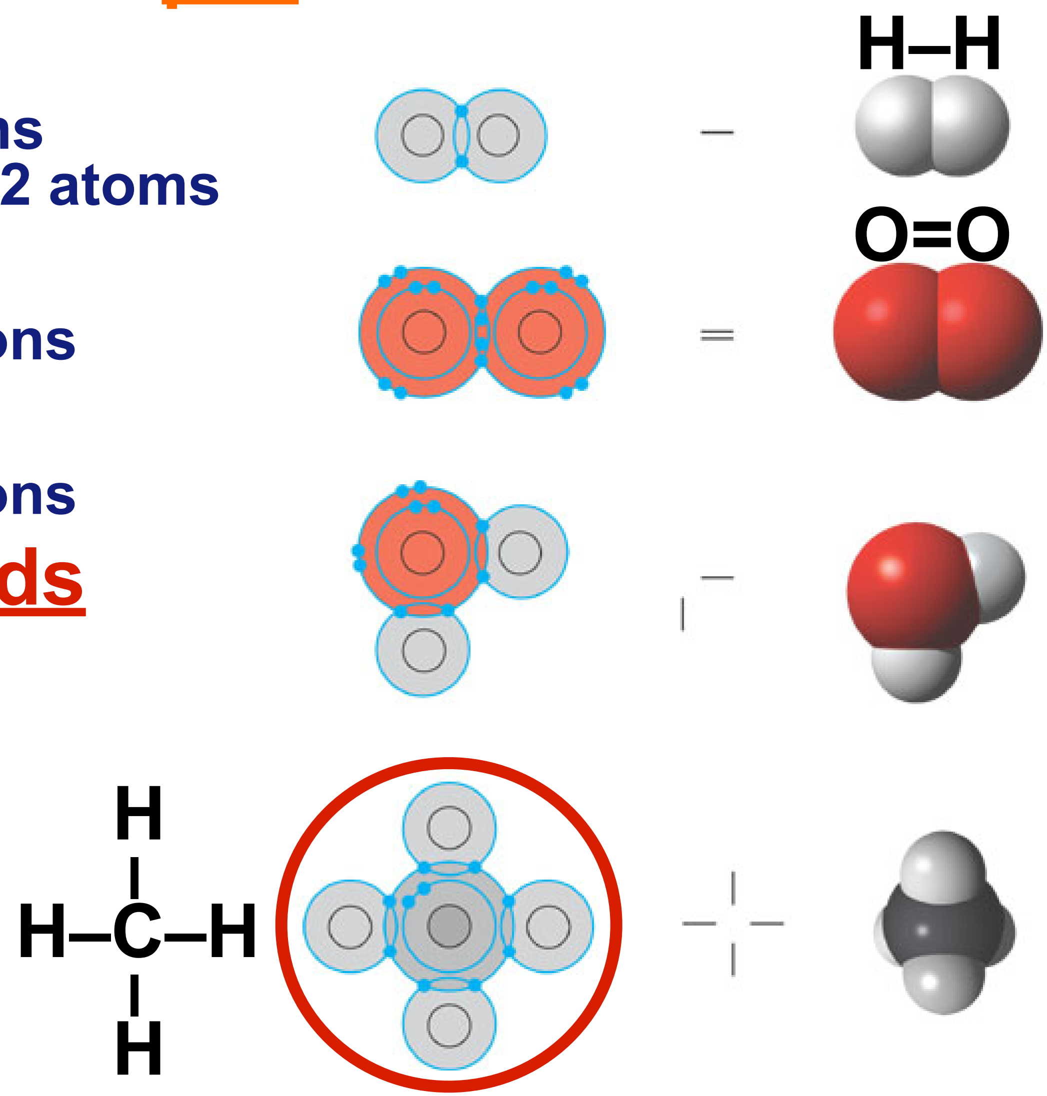
H_2 (hydrogen gas)

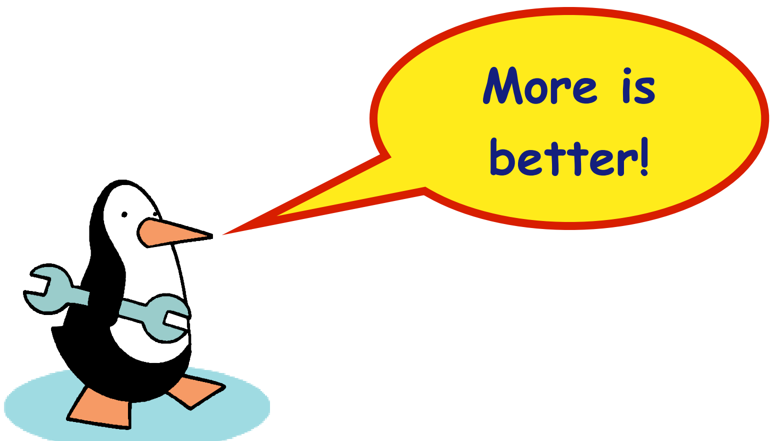


H_2O (water)

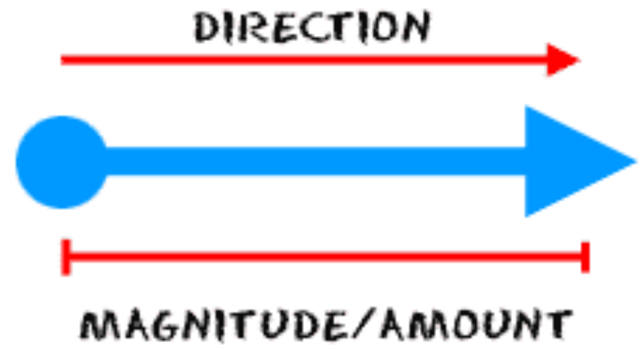
Multiple covalent bonds

- 2 atoms can share >1 pair of electrons
  - single bonds
    - 1 pair of electrons shared between 2 atoms
  - double bonds
    - 2 pairs of electrons
  - triple bonds
    - 3 pairs of electrons
- Very strong bonds

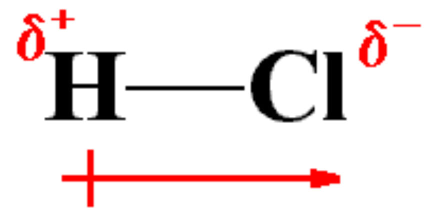




Vectors - Chemical Dipole Moments

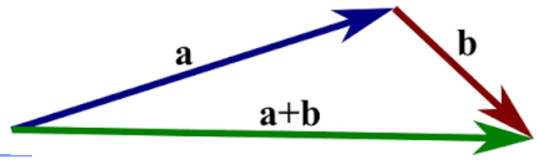


- Covalent bonds involve the nuclei of two atoms exerting forces of attraction on the valence electrons being "shared."
  - These forces (in chemistry referred to as dipole moments) have a certain directions & magnitudes that can be symbolized by vectors.
    - The vector's arrow head points in the direction of the force of attraction, towards the nucleus, which is electronegative.
    - The length of the vector indicates the strength of the force, the pull by the nucleus on electrons.
      - In the example, the protons of the Cl atom exert a force of attraction on the electron of the H atom.

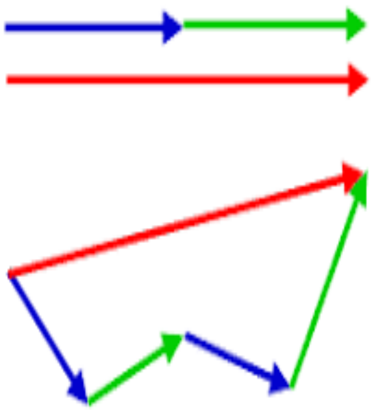


Dipole Moment has a Magnitude and a Direction

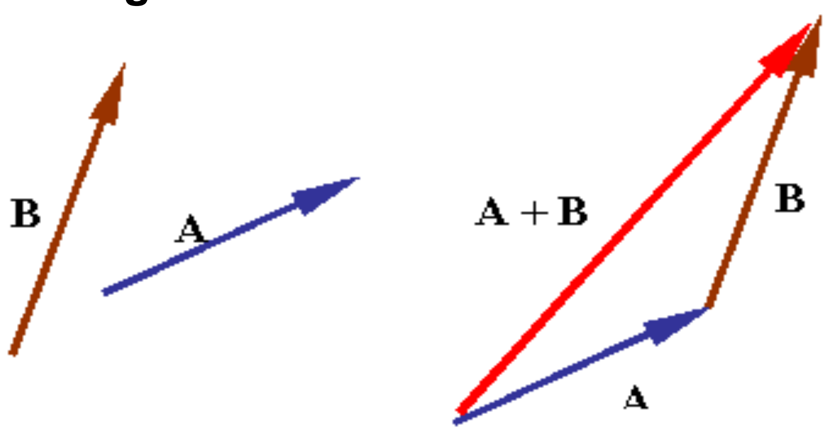
Dipole moments can be added



- Forces within a bond or within a molecule with many covalent bonds can be summed.
  - To add vectors, we chain the vectors by putting the tail of the next vector on the head of the previous vector
    - The resultant vector is then drawn from the tail of the first vector to the head of the last vector
      - This resultant vector is the <u>permanent dipole moment</u> in the bond or in the molecule.
        - When summing forces, they may cancel each other out, resulting in no <u>NET</u> (overall) force.
        - They may not cancel each other out resulting in a <u>NET</u> force with a certain Direction & Magnitude.
        - Ex: Below, adding vectors A and B results in the vector A+B



THE RED VECTORS ARE THE RESULT OF ADDING THE SMALLER COLORED ONES.



Polar vs Non-Polar Covalent Bonds

- **When forces in a covalent bond are added, they can either cancel each other out or result in a net bond dipole moment.**
  - **If the forces cancel each other out, the electrons being shared, are <u>shared equally</u>.**
    - **The bond is considered <u>non-polar</u>.**
    - **The vectors cancel each other out, leaving no overall dipole moment**
    - **<u>No dipole forms</u> (there are no equal and oppositely charged poles separated by a distance.**

Nonpolar covalent bond

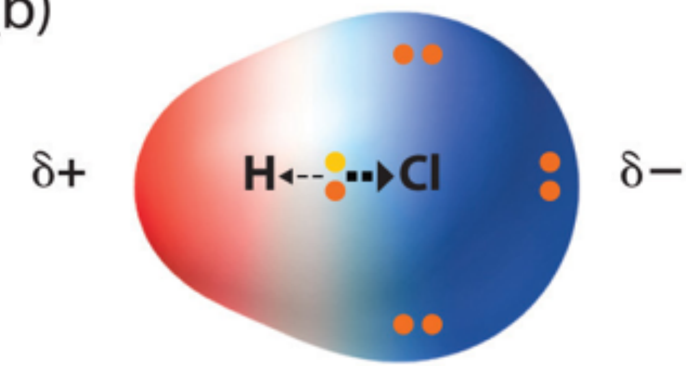
Bonding electrons shared equally between two atoms. No charges on atoms.

Polar vs Non-Polar Covalent Bonds

- When forces in a covalent bond are added, they can either cancel each other out or result in a net bond dipole moment.

- If the forces do not cancel each other out, the electrons being shared, are shared unequally.
    - The bond is considered polar.
    - The vectors do not cancel each other out, leaving an overall dipole moment
    - A dipole forms (there are no equal and oppositely charged poles separated by a distance.

(b)

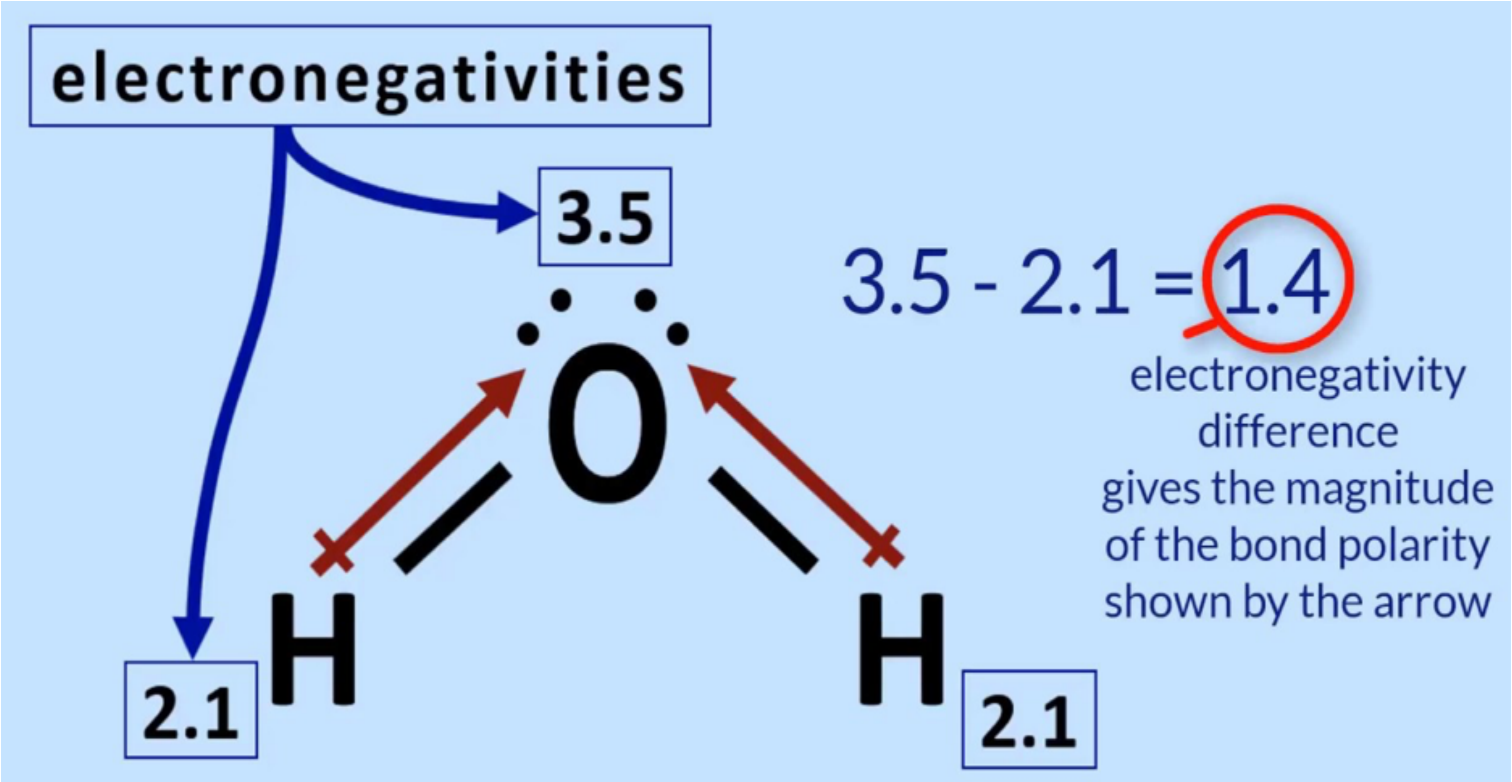


Polar covalent bond

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

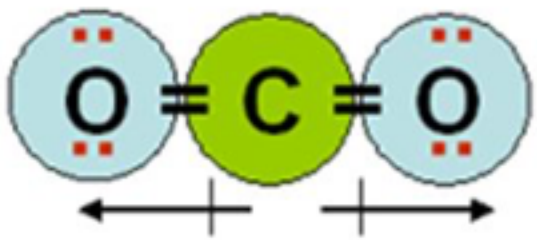
Polar vs Non-Polar Covalent Bonds

- **Whether a bond is non-polar or polar will depend on the <u>DIFFERENCE in Electronegativity</u> between the two atoms involved in the covalent bond.**



Molecules too can be nonpolar or polar not just individual covalent bonds!

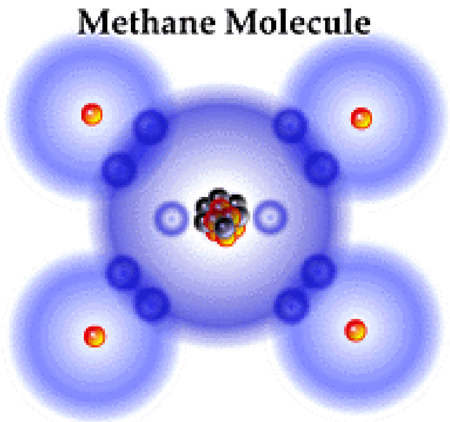
A molecule with **more than one polar bond** ***MIGHT NOT*** **have a permanent dipole moment** when the **charge separations are *symmetrically distributed*** so that the **resultant vector sums up to to *zero***.

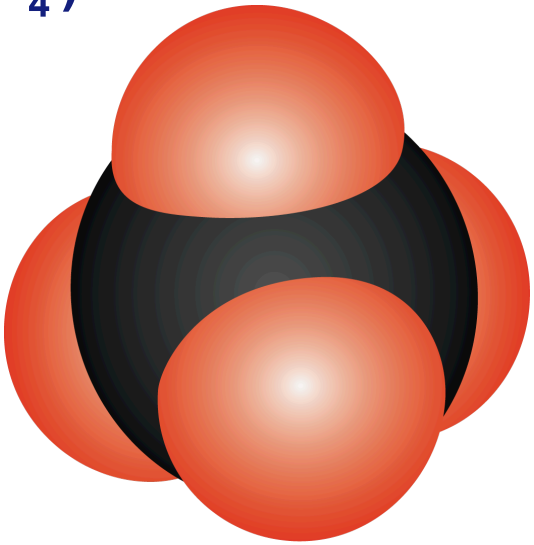


dipole moment = 0

Non-polar covalent bond & molecule

- Electrons in a covalent bond are **shared equally** by 2 atoms *- the atoms do not have an overall net charge*
  - *If all the covalent bonds in a molecule are non-polar, the molecule as a whole is **non-polar** (not a dipole)*
    - **Example:** Generic hydrocarbons = C_xH_x
      - Specific Example = methane (CH_4)

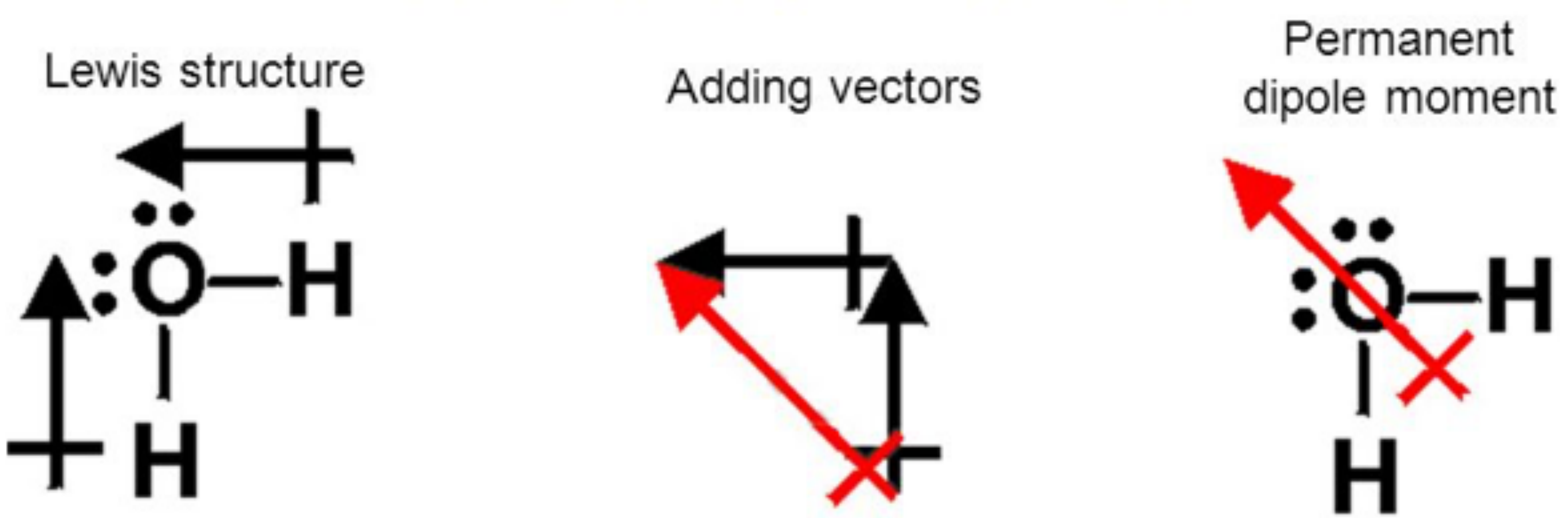




Balanced, stable, good building block, no permanent partial charges.

Molecules can also be nonpolar or polar not just individual covalent bonds!

The **permanent dipole moment** in water can be seen by adding together the **charge separation vectors of the two polar covalent O-H bonds.**

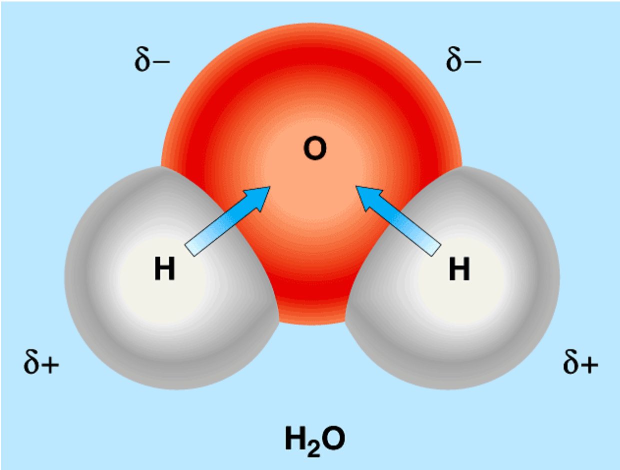


Polar covalent bonds & Molecules

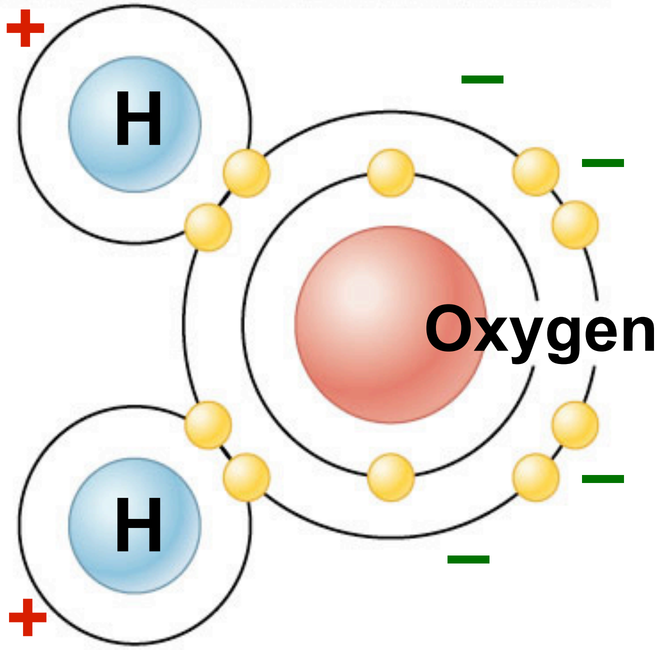
- Pair of electrons are **shared unequally** by 2 atoms

  Example: Water = H_2O

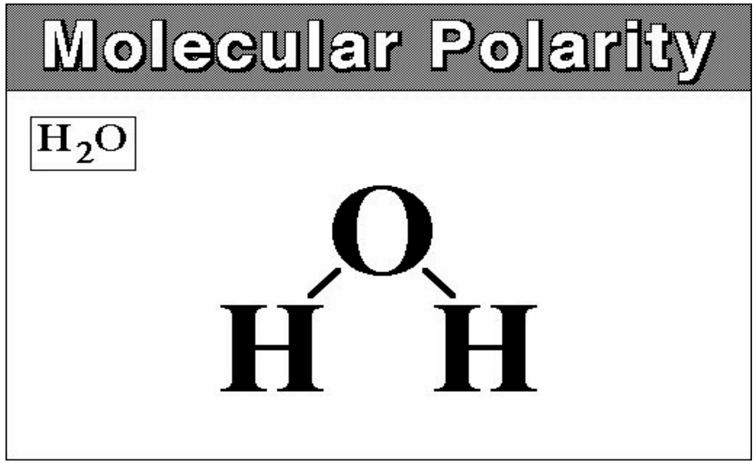
  - oxygen has stronger "attraction" for the electrons than hydrogen
  - oxygen has higher electronegativity



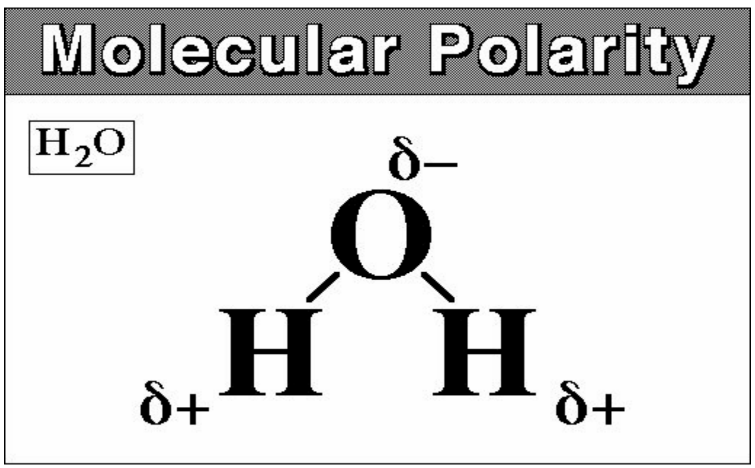
- Polar Molecules
  - Dipole moments (vectors existing in each polar bond) do not cancel each other out leaving a **net directional force acting on the electrons in the molecule** as a whole.
  - Water is a polar molecule
    - δ+ vs. δ– poles
    - leads to many interesting properties of water…



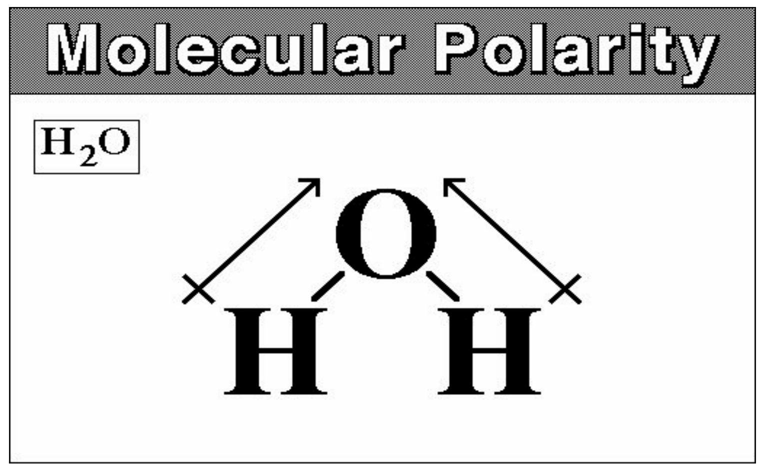
Why H2O is a POLAR MOLECULE with POLAR BONDS?



1. H2O's Structural Formula

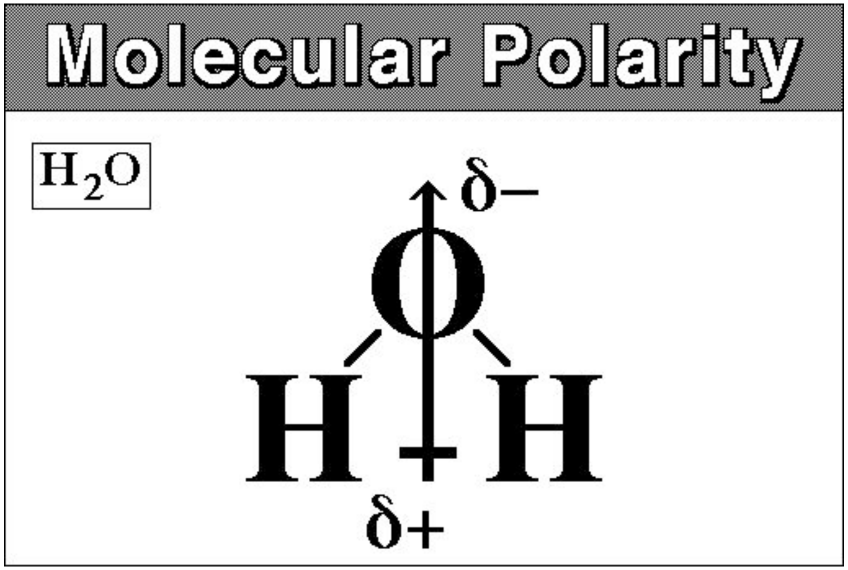


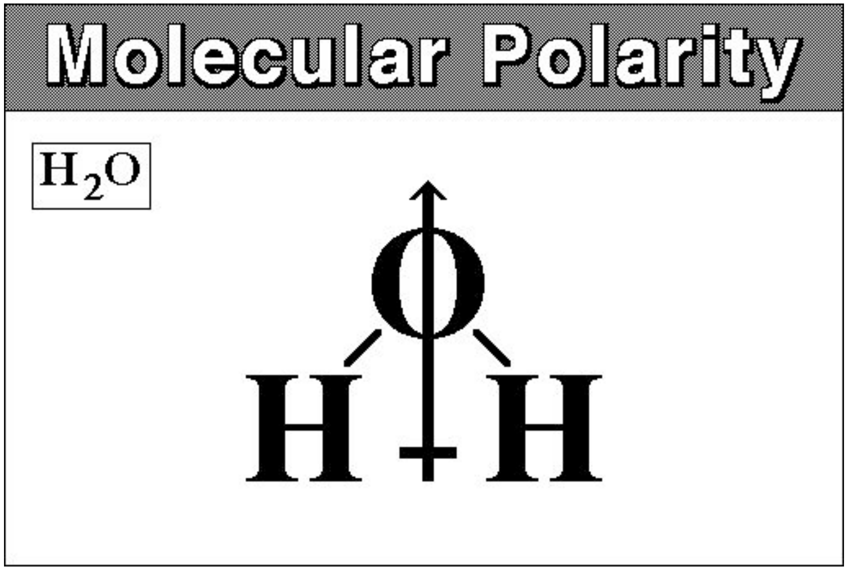
2. Atomic Partial Charges O has high EN & H has medium EN
(Determine if these are polar bonds)



3. Bond Dipole Moments
(They do not cancel each other out).

Why H_2O is a POLAR MOLECULE with POLAR BONDS?





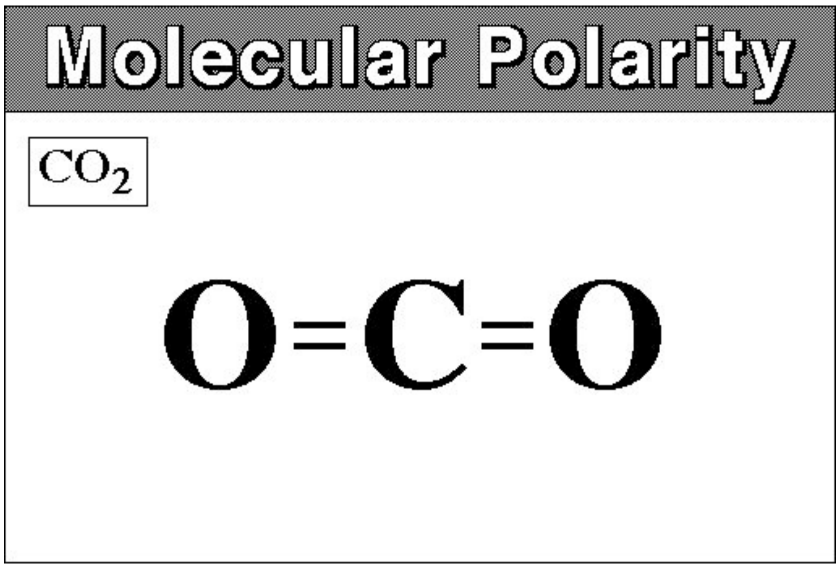
4. Molecular Partial Charges
(Adding the bond dipole Moments results in one molecular dipole moment. One end of the molecule more negative than the other)

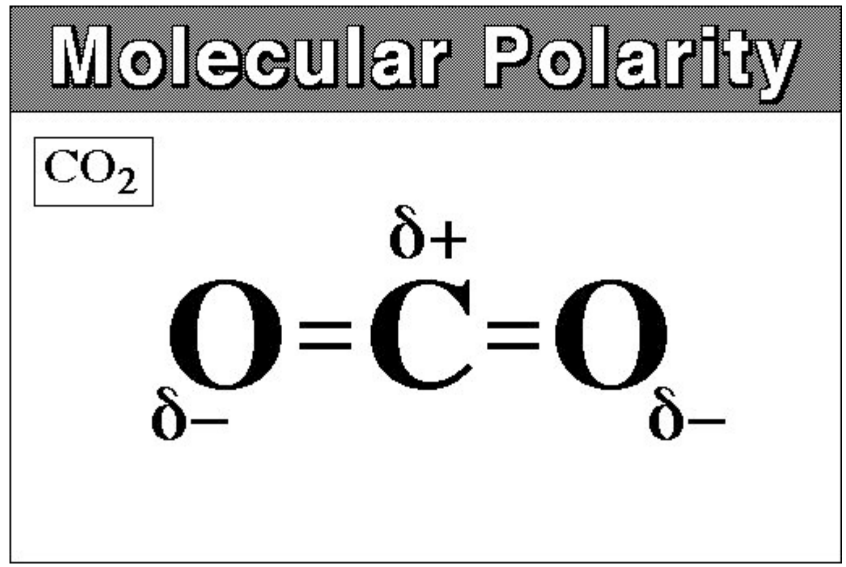
5. Molecular Dipole Moment
(Electron density is pulled to one end of the molecule, making one end slightly + and one end slightly -)

Warning:

A molecule is not automatically polar just because it has some polar bonds!

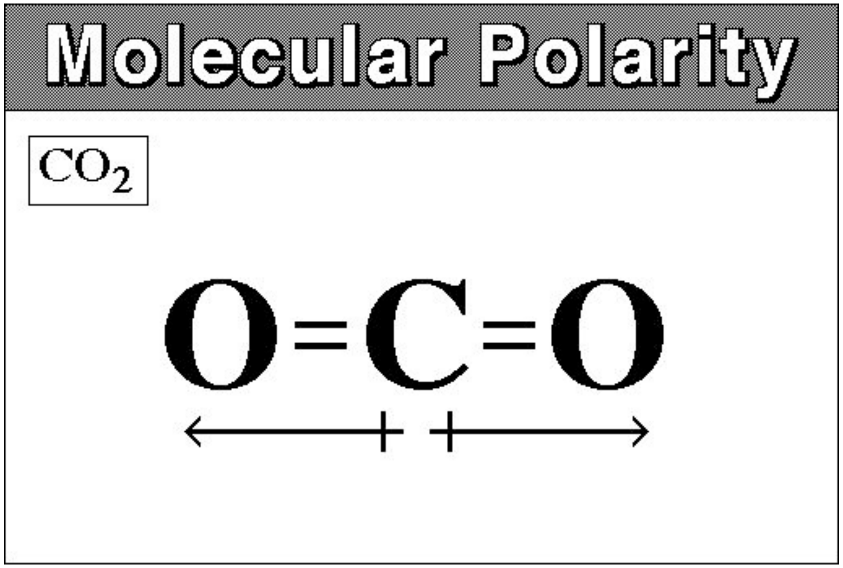
CO_2 is NON-POLAR MOLECULE with POLAR BONDS

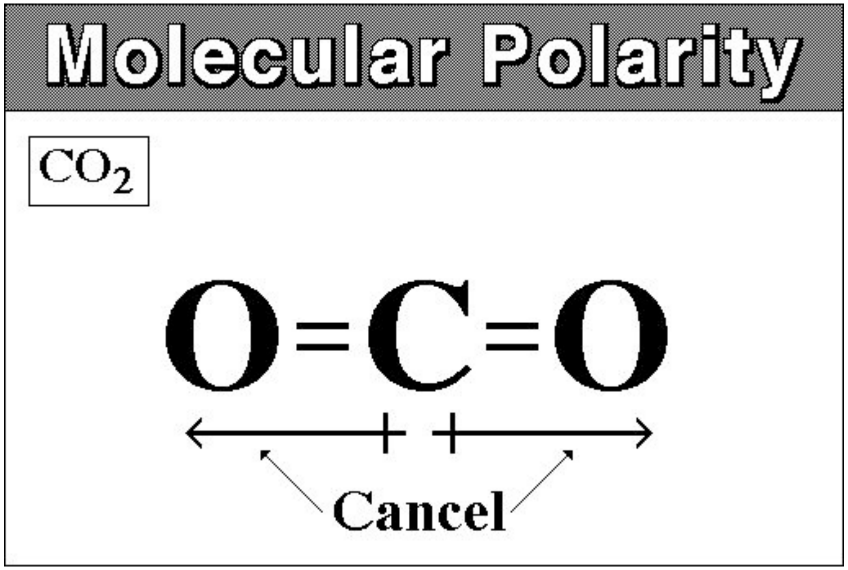




1. **CO2's Structural Formula**
2. **Partial Charges. O has high EN & C has medium EN**

CO_2 is NON-POLAR MOLECULE with POLAR BONDS





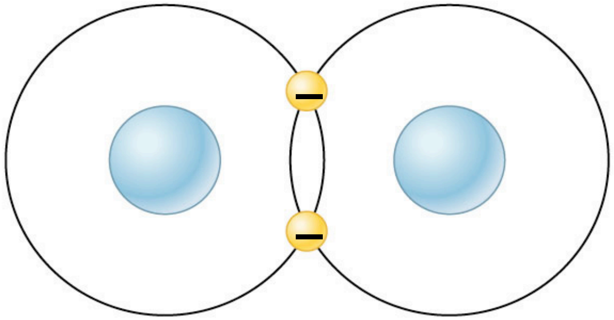
3. **Bond Dipole Moments**
(The two C-O bonds are determined to be polar based on ΔEN)

4. **Bond Dipole Moments cancel out leaving NO Molecular Dipole Moment**
(Ends of CO2 both have same partial charge, negative, so it's NONPOLAR)

Biological Bonds

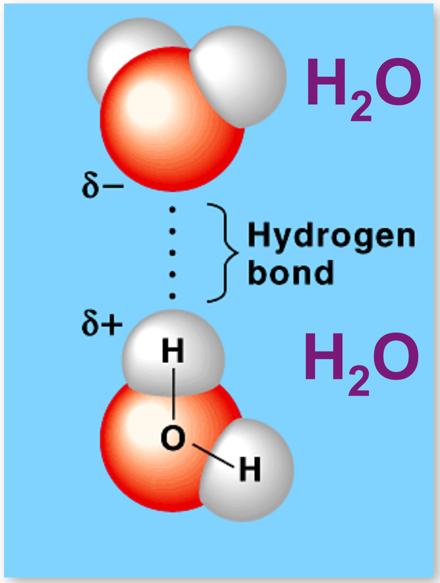
- Strong bonds
  - Covalent bonds
  - Ionic bond
- Weak bonds are equally important!
  - Van der Waals Forces
    - Van der Waals forces are caused by **attraction between DIPOLES** (*i.e.* molecules with positive and negative 'ends' either permanent or induced).
    - There are three sorts (although A-level chemistry and biology texts often erroneously equate Van Der Waals forces with London Dispersion Forces only).
  - Hydrogen bonds are one example of Van der Waals Forces
    - **Attraction between a δ⁺ H (covalently bonded to N, O, F) and a δ⁻ atom on another molecule)**

Covalent bond



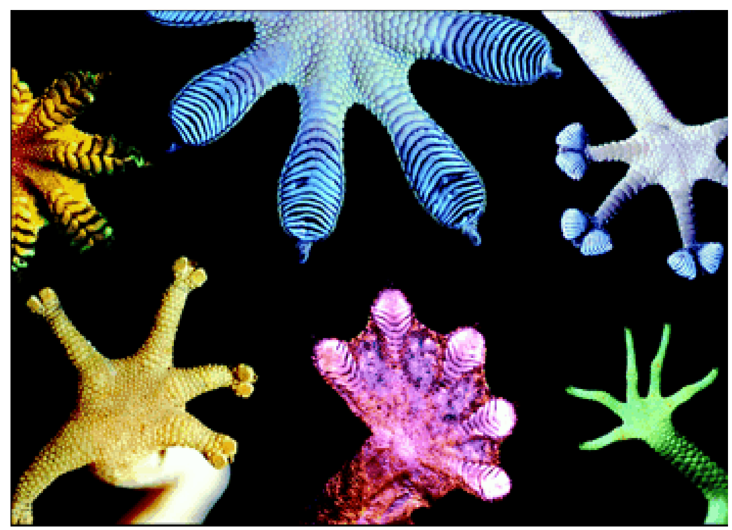
H_2 (hydrogen gas)

Hydrogen bond



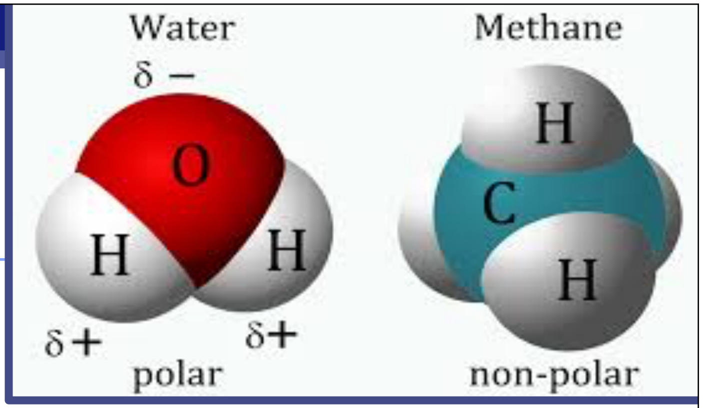
Van Der Waals Forces

- Electrons are not constantly symmetrically distributed even in nonpolar molecules.
  - At times, they accumulate in one area or another even if only temporarily.
- So there are ever-changing regions of + and - charges that can cause neighboring molecules to weakly stick to each other at times.

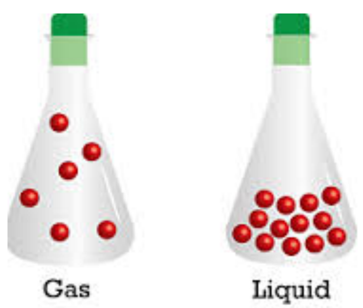


- **Types of Van Der Waals Forces:**
  1. Temporary Dipole - Induced Dipole Forces
     - A.K.A. London Dispersion Forces
  2. Dipole - Induced Dipole Forces
  3. Dipole - Dipole Forces
     - Including Hydrogen Bonding

Recall that Nonpolar molecules are not permanent dipoles



- **Polar molecules have an imbalanced electron density distribution and thus charge distribution** *- there are regions that are on average more permanently positively & negatively charged.*
- **Non-polar molecules have a more symmetrical electron density distribution.**
  - **They will be neutral and exhibit no net dipole moment.**
    - **Because nonpolar molecules lack any regions that display a more permanent net charge, non-polar molecules are not attracted easily to one another.**
      - **Besides being made up of covalent bonds (strong intramolecular attractions), they do not exhibit many intermolecular attractions.**
        - **Because there is always some thermal energy in a substance causing atoms to vibrate or molecules to collide randomly, nonpolar substances tend to form liquids and then gases at lower temperatures than polar substances - there aren't any permanent charges that cause these nonpolar molecules to attract one another more regularly and hold them more closely together for longer in the presence of increasing kinetic energy as happens with polar substances.**

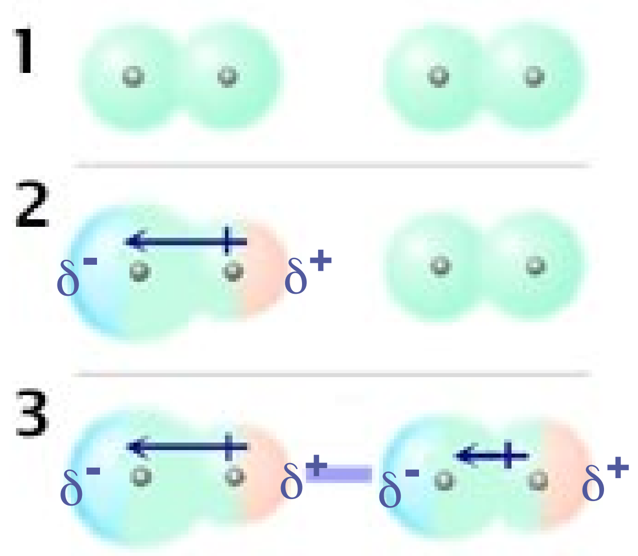


1. HOW LONDON DISPERSION FORCES FORM

These are attractions between ALL molecules (including NONPOLAR molecules).

Dispersion forces or London Dispersion forces are a result of electrostatic attraction between temporary & induced dipoles caused by the temporary variations in electron density around atoms and molecules.

1. **The electron cloud and *average* e^- distribution of two non-polar molecules has a certain symmetry or 'evenness'.**
2. **However at any *instant* the electrons in an atom or molecule may be at one end, producing a temporary dipole moment.**
3. **This temporary dipole moment can induce a dipole moment in nearby molecules causing them to be attracted to the first molecule.**



LONDON DISPERSION FORCES

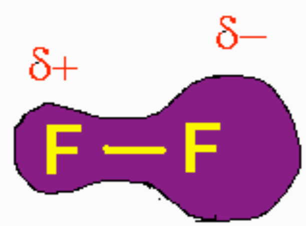
EXAMPLE: Consider the non-polar molecule F_2.

Here, electrons are shared equally but are constantly in motion.

At times, the bonding electrons end up around one nuclei and not the other.

Thus one end of the molecule becomes partially negatively charged, while the other becomes partially positively charged, forming a TEMPORARY DIPOLE.

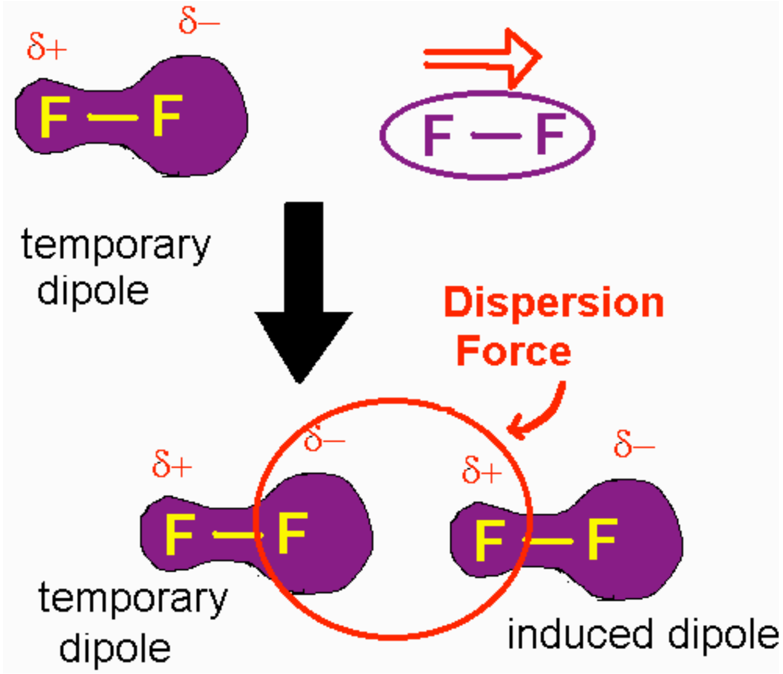
* on average, the electrons are shared equally between the two nuclei

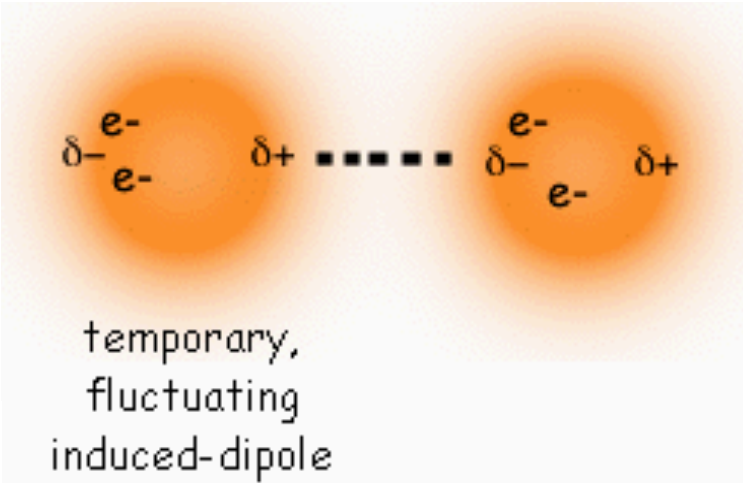


*occasionally, the shared electrons "spend more time" around one nucleus, making it partially negatively charge

LONDON DISPERSION FORCES

These temporary dipoles can attract or repel the electron clouds of nearby non-polar molecules, shifting the electron distribution in the neighboring molecule and producing a momentary induced dipole.



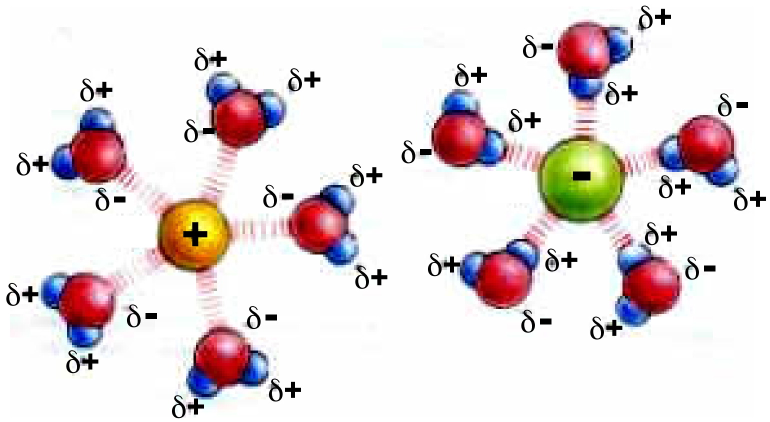


These dipoles may exist for only a fraction of a second but a force of attraction between them also exist for that fraction of time.

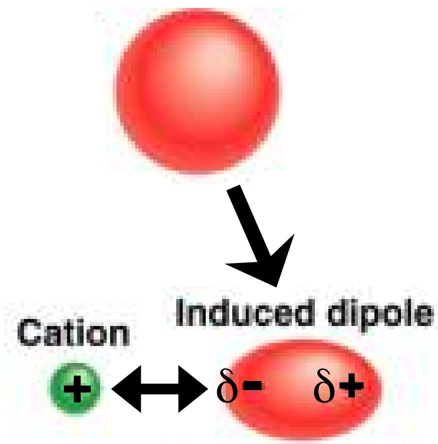
A quick review of the effects of Ions

Before discussing Permanent Dipole-Induced Dipole forces, let's review two other inter-molecular forces involving ions:

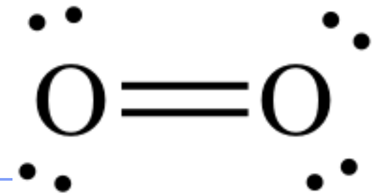
- **Ion - Dipole Forces:**
  - When an ion nears a polar molecule, oppositely charged partial charges in the molecule are attracted to the ion.



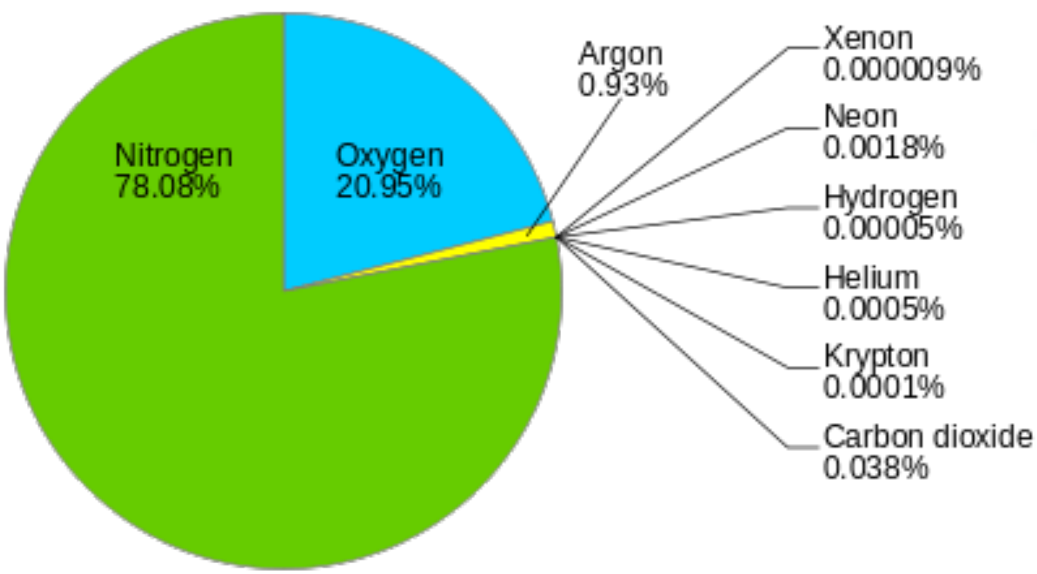
- **Ion-Induced Dipole Force:**
  - Weak attraction results when an ION INDUCES A TEMPORARY DIPOLE IN NONPOLAR MOLECULES by disturbing the arrangement of electrons in the nonpolar species.

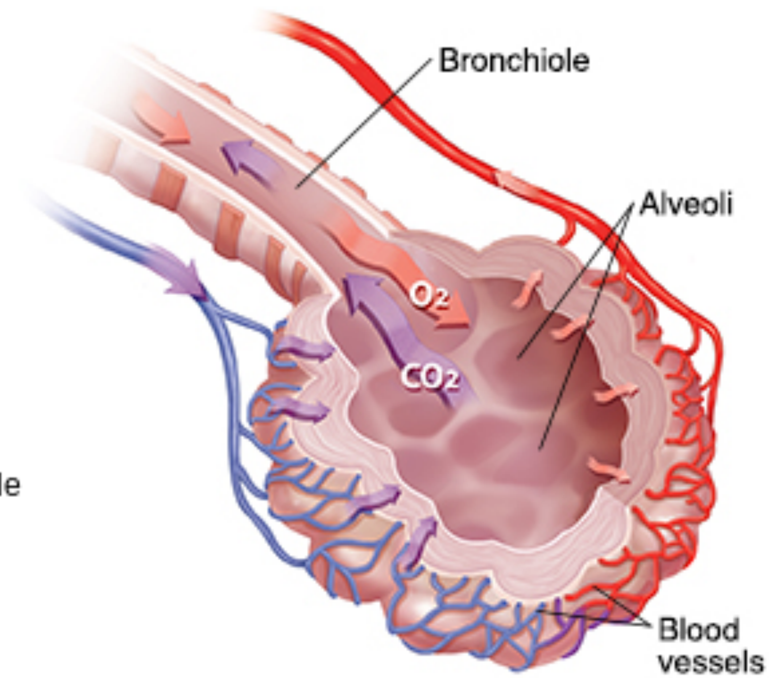


Ion - Induced Dipole Forces

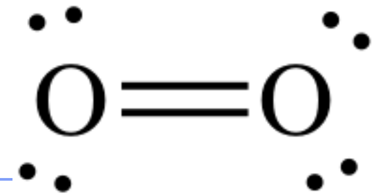


- How do humans carry oxygen to the cells of the body?
  - Oxygen ($O2$) is a non-polar molecule
    - It has no permanent dipole moment given that both O atoms are equally electronegative.
  - Air is filled with 21% $O2$ gas.
    - We inhale air bringing the air into our lung cavity in order to bring $O2$ gas close to blood vessels that surround our lung tissue

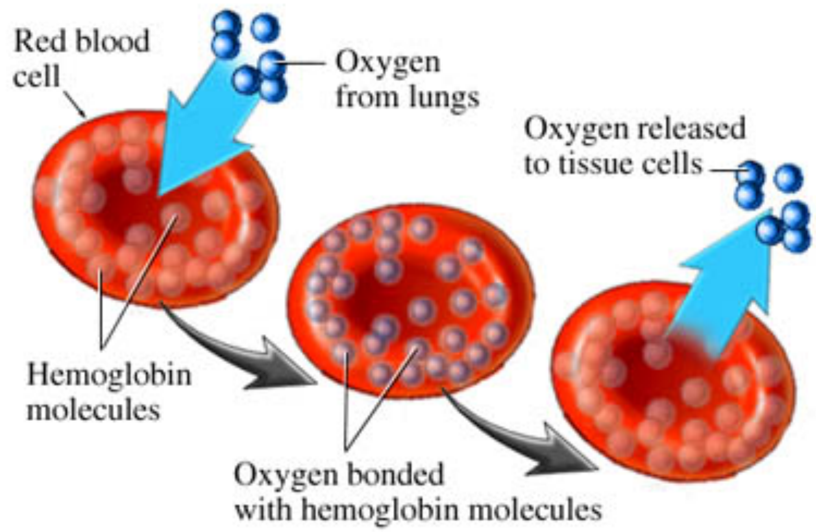




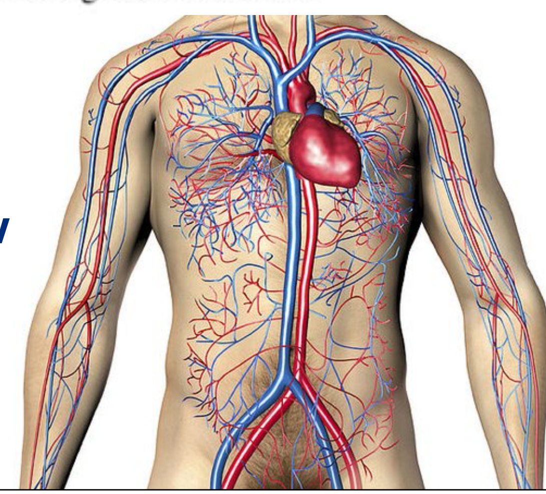
Ion - Induced Dipole Forces



- It's the job of red blood cells to carry oxygen to all cells
  - Red blood cells are filled with a transport protein known as hemoglobin

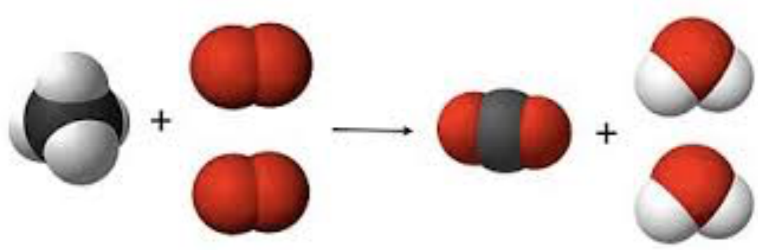


    - When you inhale air high in oxygen content, oxygen molecules diffuse through the lung into the surrounding blood vessels, diffusing into red blood cells where they attach to hemoglobin proteins.
    - As the heart pumps blood through the body, red blood cells carry oxygen throughout the body
    - The oxygen molecules will detach from hemoglobin when they reaches body cells low in oxygen, the oxygen gas diffusing out of the red blood cell, out of the blood vessel, and into the body cells.



Ion - Induced Dipole Forces

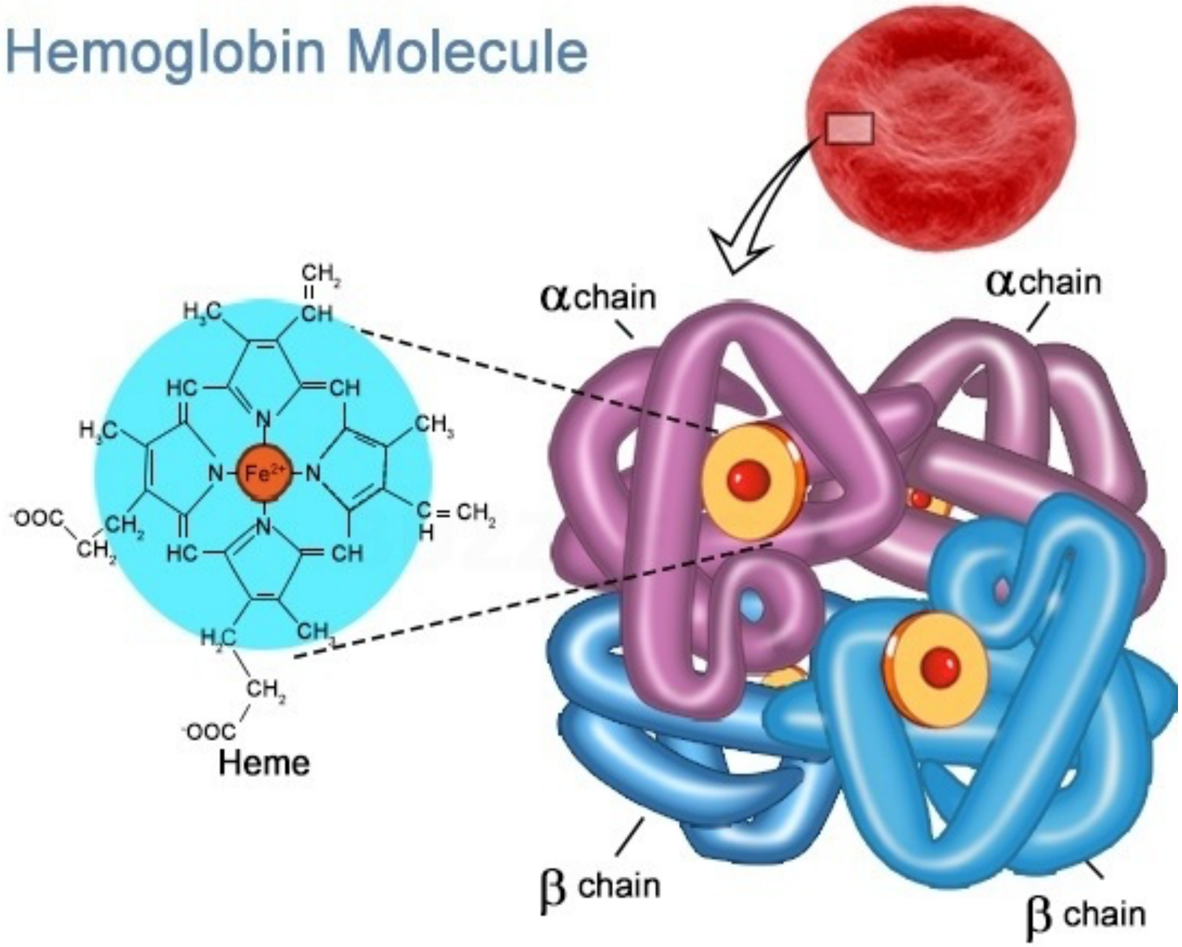
- To be efficient, oxygen must quickly bind to hemoglobin in the lung and yet also easily detach from hemoglobin when the red blood cell reaches tissues, ideally without requiring a lot of effort or energy.
  - Recall: Chemical reactions involve breaking strong intramolecular forces (ionic & covalent bonds) in order to rearrange atoms of reactants into new products.
    - Breaking covalent and ionic bonds between atoms isn't easy - it takes an input of energy or the use of additional substances, called catalysts.
      - If oxygen bound to hemoglobin through covalent or strong ionic bonds, it would be hard to release the oxygen when red blood cells reach body tissues.
        - Oxygen thus bonds through a weaker intermolecular force: an Ion - Induced Dipole Force



$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$

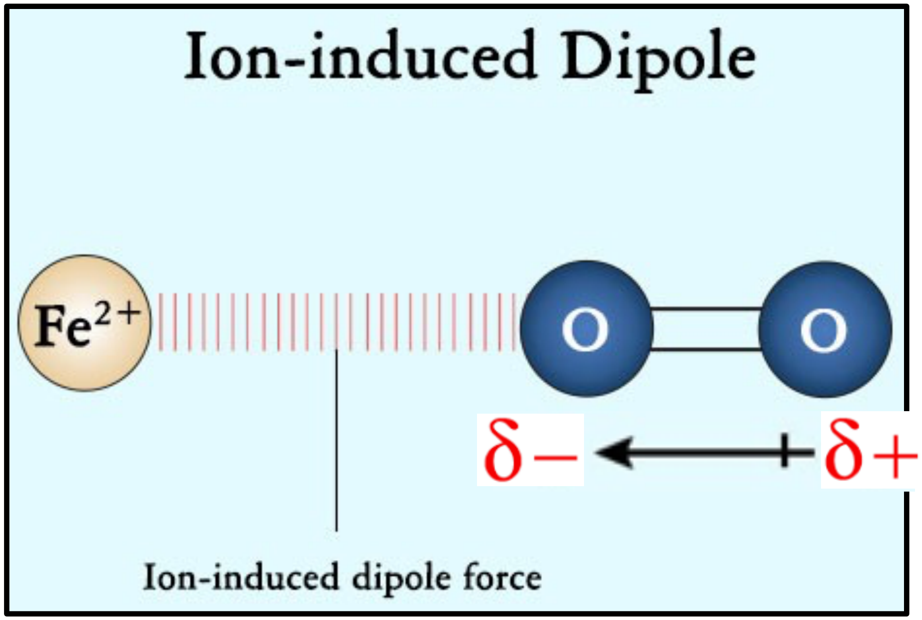
Ion - Induced Dipole Forces

- Hemoglobin is a protein made up of four large molecules or subunits, two alpha chains and two beta chains.
  - At the center of each of the 4 subunits or chains, you will find an Iron Cation



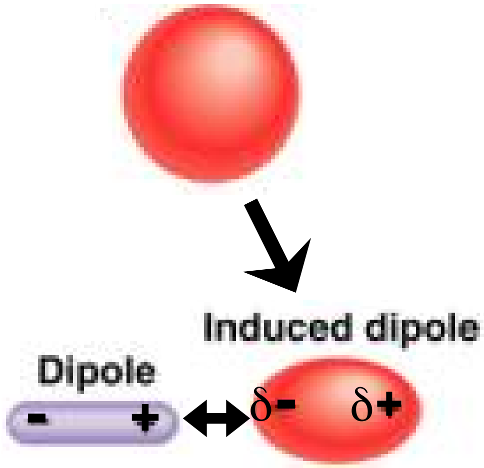
Ion - Induced Dipole Forces

- When O_2 molecules diffuse into the red blood cells and pass near the 4 Fe2+ ions on each hemoglobin transport protein, the strong positive charge of the Fe2+ cation, causes an induced dipole to form in the O_2 molecule.
  - The O_2 molecule now experiences a weak intermolecular force of attraction between it and the Fe2+ ion.
    - The resulting ion-induced dipole force holds O_2 onto the hemoglobin.
  - Since this force of attraction is much weaker than any strong covalent/ionic bond, O2 can easily detach from hemoglobin in order to diffuse into body cells low in oxygen.



2. Permanent Dipole - Induced Dipole Forces

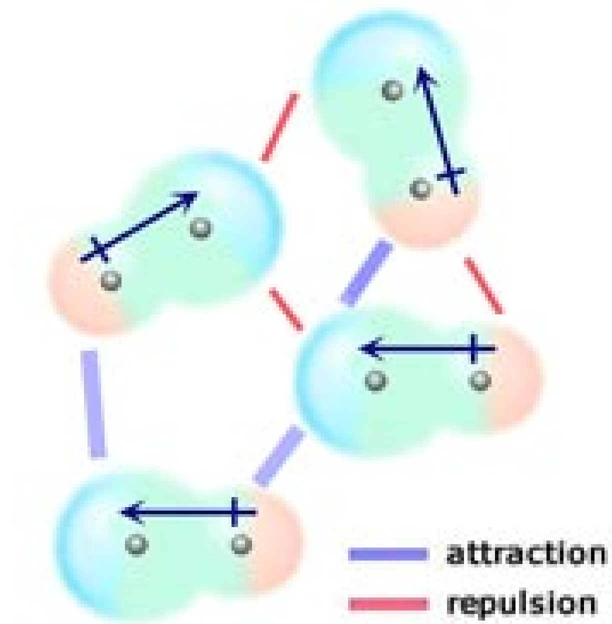
- **Dipole - Induced Dipole Forces:**
  - A polar molecule (a molecule with a *permanent dipole*) produces an electric field which can distort the electron cloud of a nearby non-polar molecule, inducing a dipole.

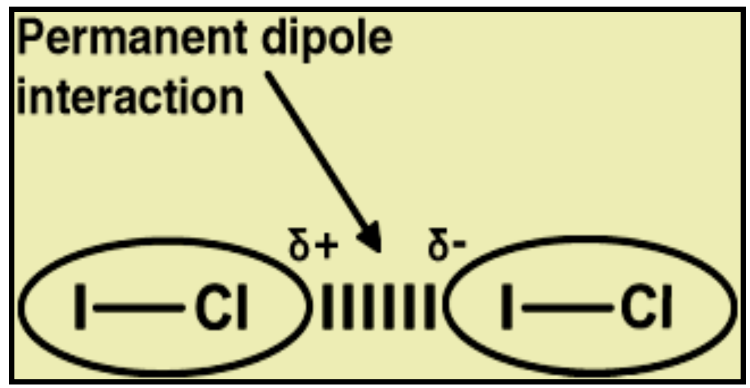


  - This will cause the an attraction between the molecules. This type of force is responsible for the solubility of oxygen (a non-polar molecule) in water (polar).
  - When the induced dipole moves away, it looses its temporary polarity going back to a non-polar molecule till it passes by another polar molecule and the process starts over again.

3. Permanent Dipole-Dipole Forces

If two neutral POLAR molecules, each having a permanent dipole moment, come together such that their oppositely charged ends align, they will be attracted to each other.

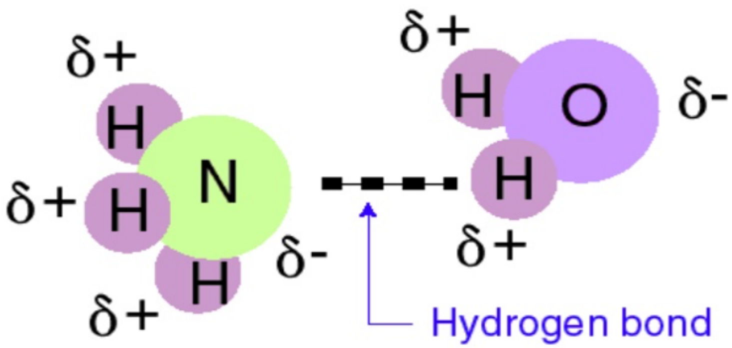


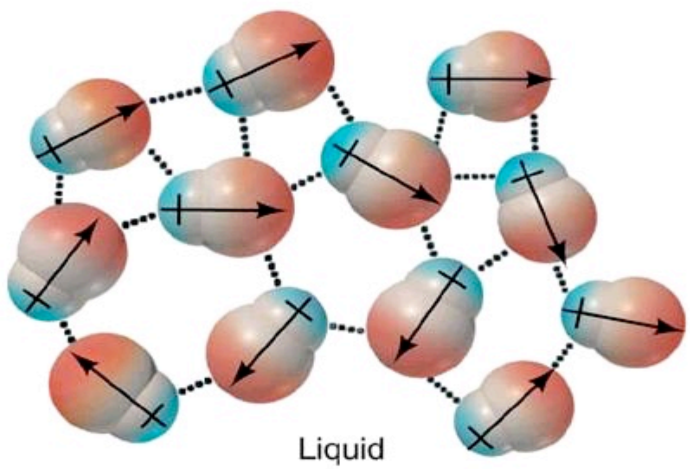


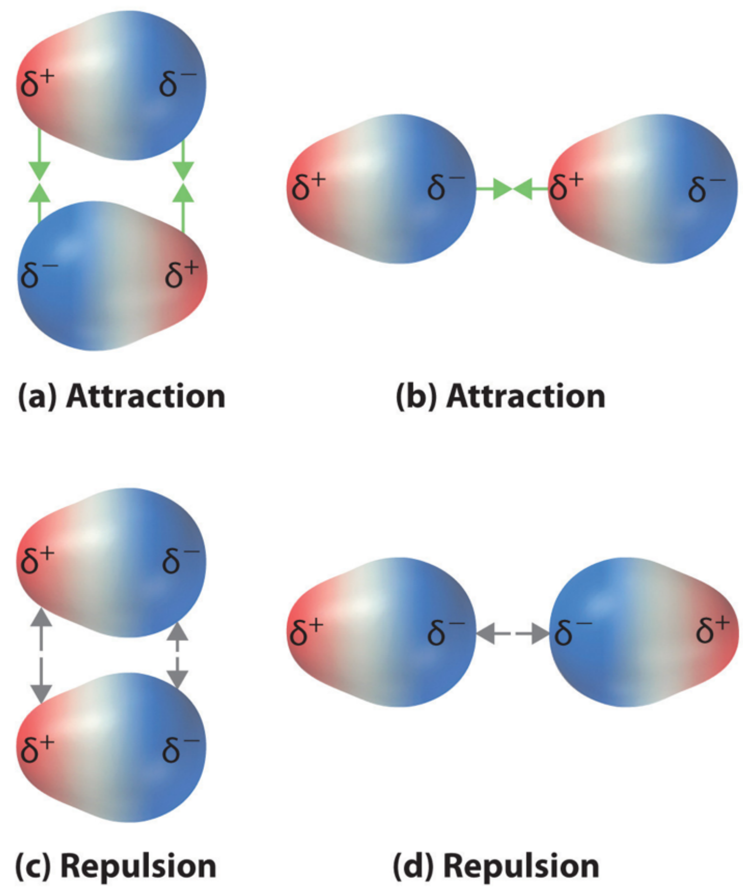
A special type of dipole-dipole interaction is *hydrogen bonding.*

Permanent Dipole-Dipole Forces

Polar molecules arrange themselves (rotate) in ways that <u>maximize the attractions</u> between opposite charges and <u>minimize the repulsions</u> between like charges.

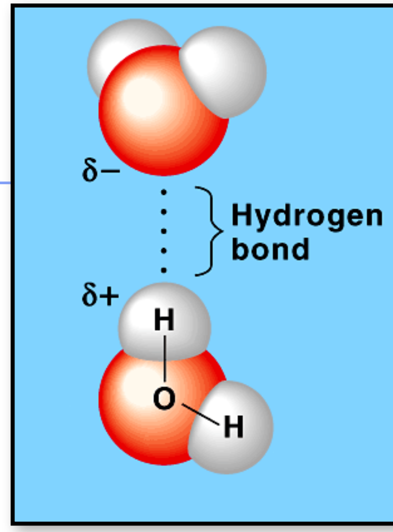


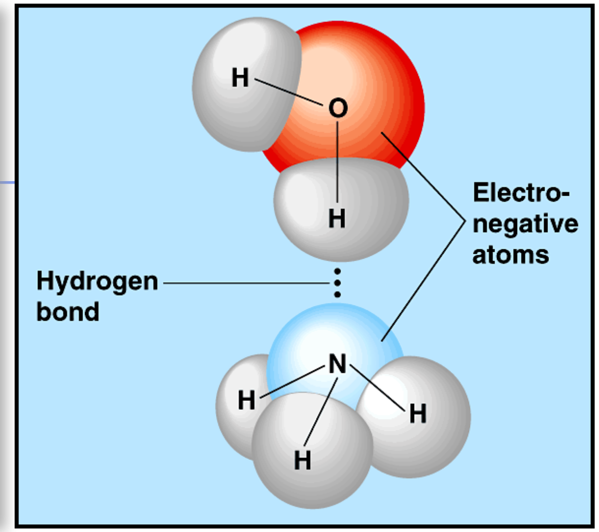




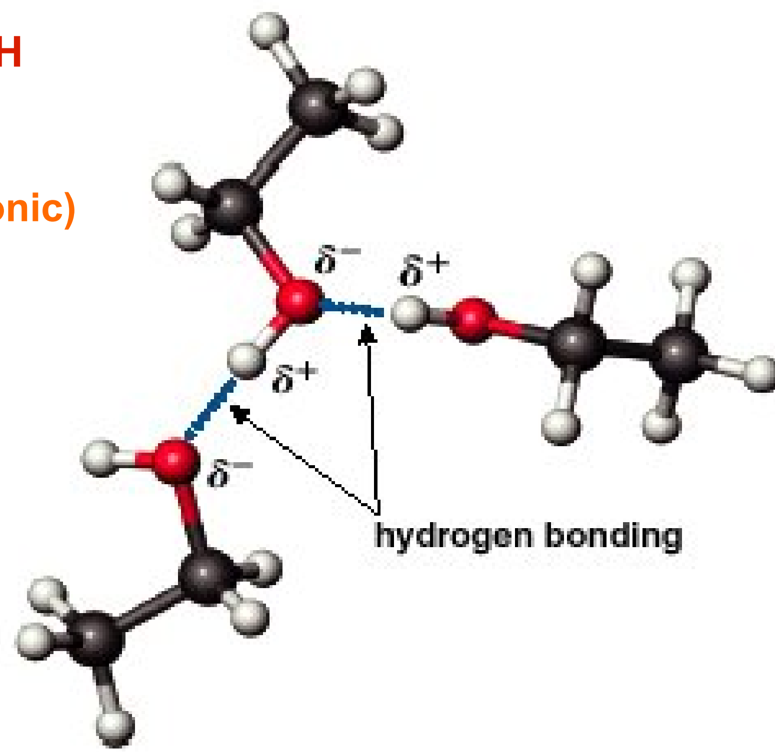
Hydrogen bonding -

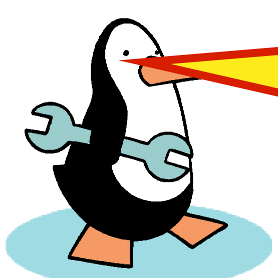
A special case of dipole-dipole interaction





- Polar water results in intermolecular attractions
  - Attraction between a partially positive H in one H_2O molecule to a partially negative O in another H_2O
  - Can also occur wherever an -OH or -NH group exists in a larger molecule
- <u>Weak bond</u> (10x weaker than covalent or ionic)
- Bonds can be broken but there is <u>strength in numbers</u>



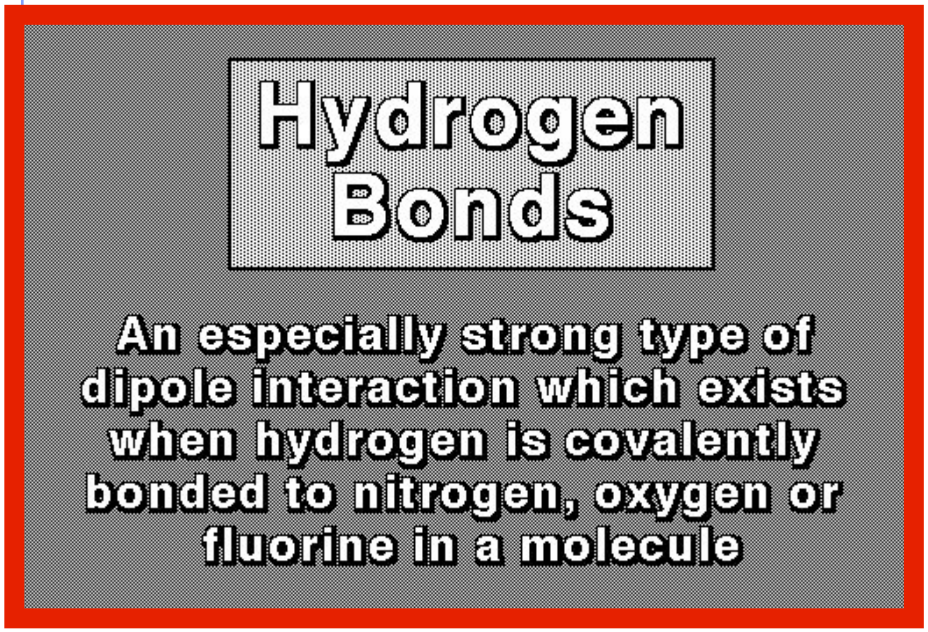


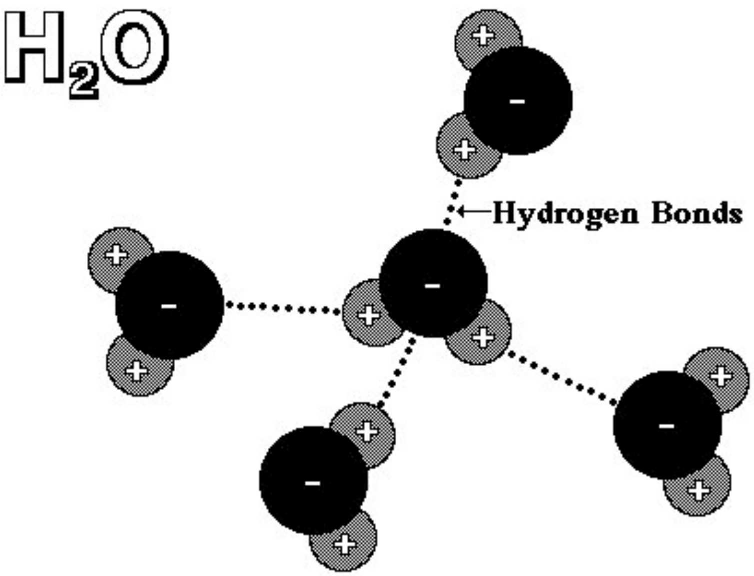
Water's polarity is responsible for <u>Hydrophobic & Hydrophilic Interactions</u> as we will learn

H–

HYDROGEN BONDING

Hydrogen Bonding = A special type of dipole force (permanent dipole – permanent dipole interaction)





HYDROGEN BONDING

Hydrogen Bonds are about **15 to 100 times weaker than covalent bonds** BUT they are the **strongest type of dipole interaction (van der Waals force)** – about **10x** stronger than normal dipole forces (the attraction seen between polar molecules) for **two reasons:**

Hydrogen Bonds	Hydrogen Bonds
Nitrogen, oxygen and fluorine are all very electronegative, so a covalent bond between any of them and hydrogen tends to be very polarized	Also, hydrogen, nitrogen, oxygen and fluorine are small atoms, so the negative end of one dipole can approach very close to the positive end of another dipole, and vice versa

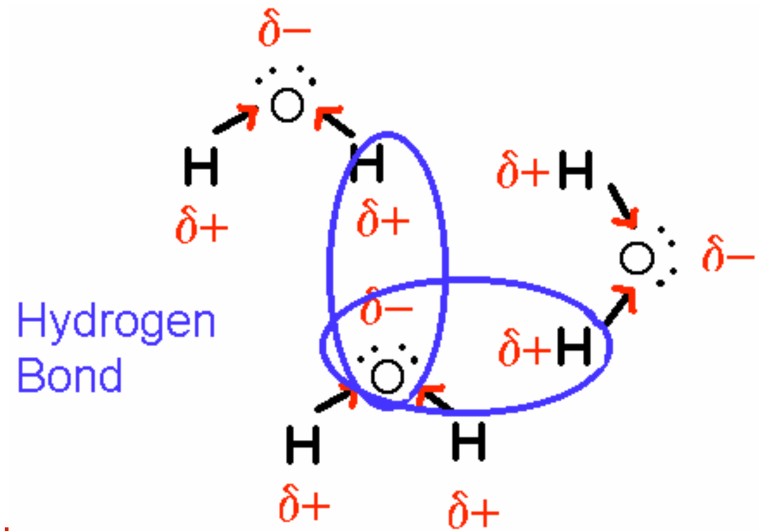
HYDROGEN BONDING

Why do Hydrogen Bonds Form?

Because of the GREAT electronegativity of O, N, and F, the electrons shared between each atom and H are more strongly attracted to the O, N, or F atom.

The shared electrons "spend more time" around the O, N, or F compared to the H, forming a VERY polar bond.

The O, N, and F atoms become partially negatively charged, more so that in just any other polar molecule, but still they do not gain a full negative charge (the shared electrons do spend some "time" around the H nucleus).

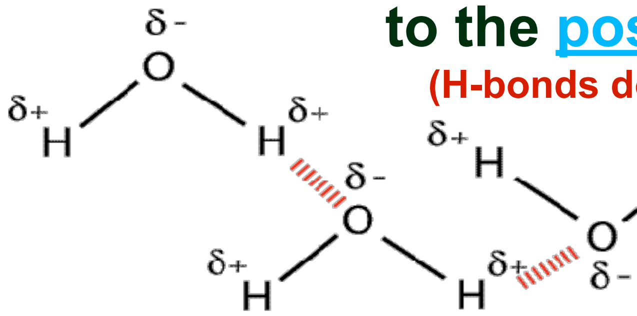


Between molecules, now the δ^- end on the O, N, or F is attracted to the δ^+ end on the H.

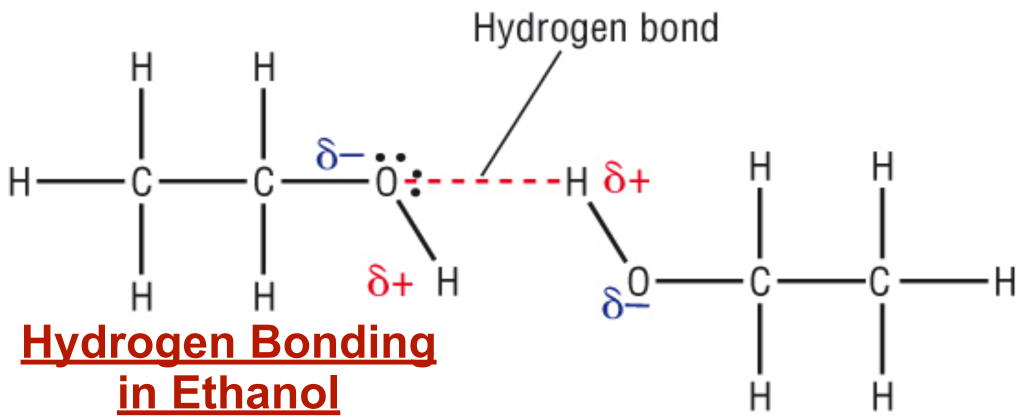
HYDROGEN BONDING

A hydrogen bond is formed when the negative end of one molecule becomes oriented to and semi-attracted to the positive end of another molecule.

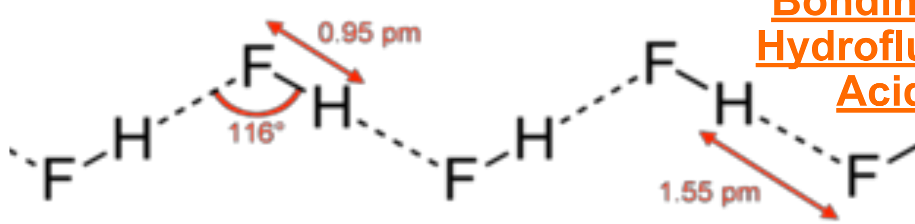
(H-bonds do not just form between water molecules!)



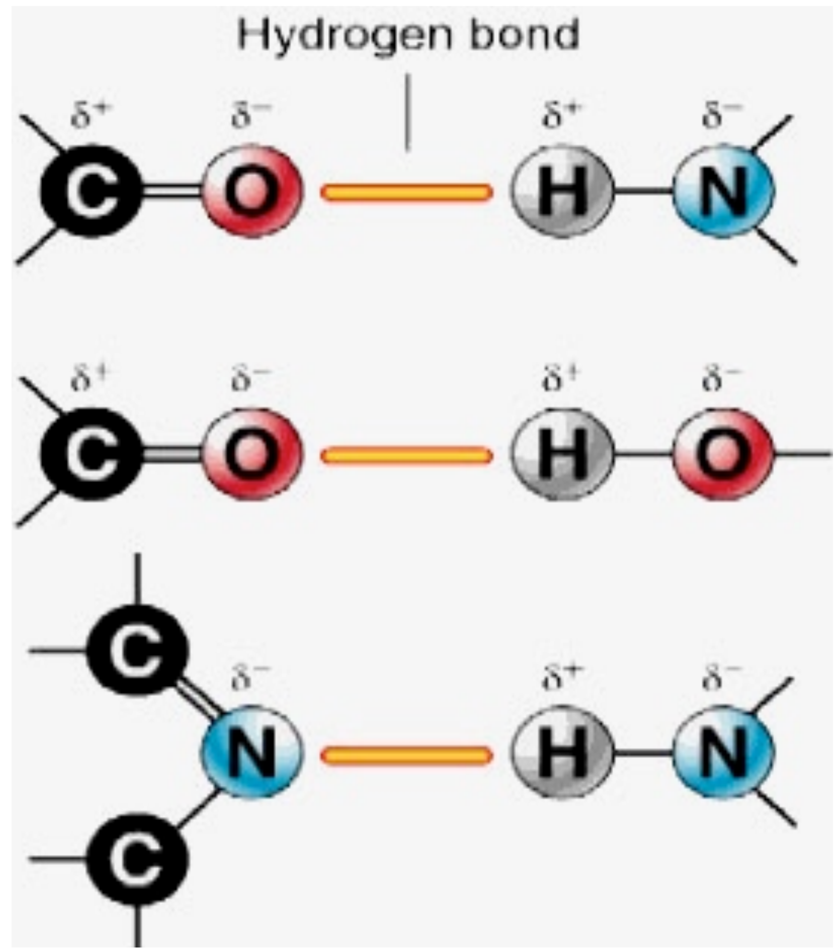
Hydrogen Bonding in Water

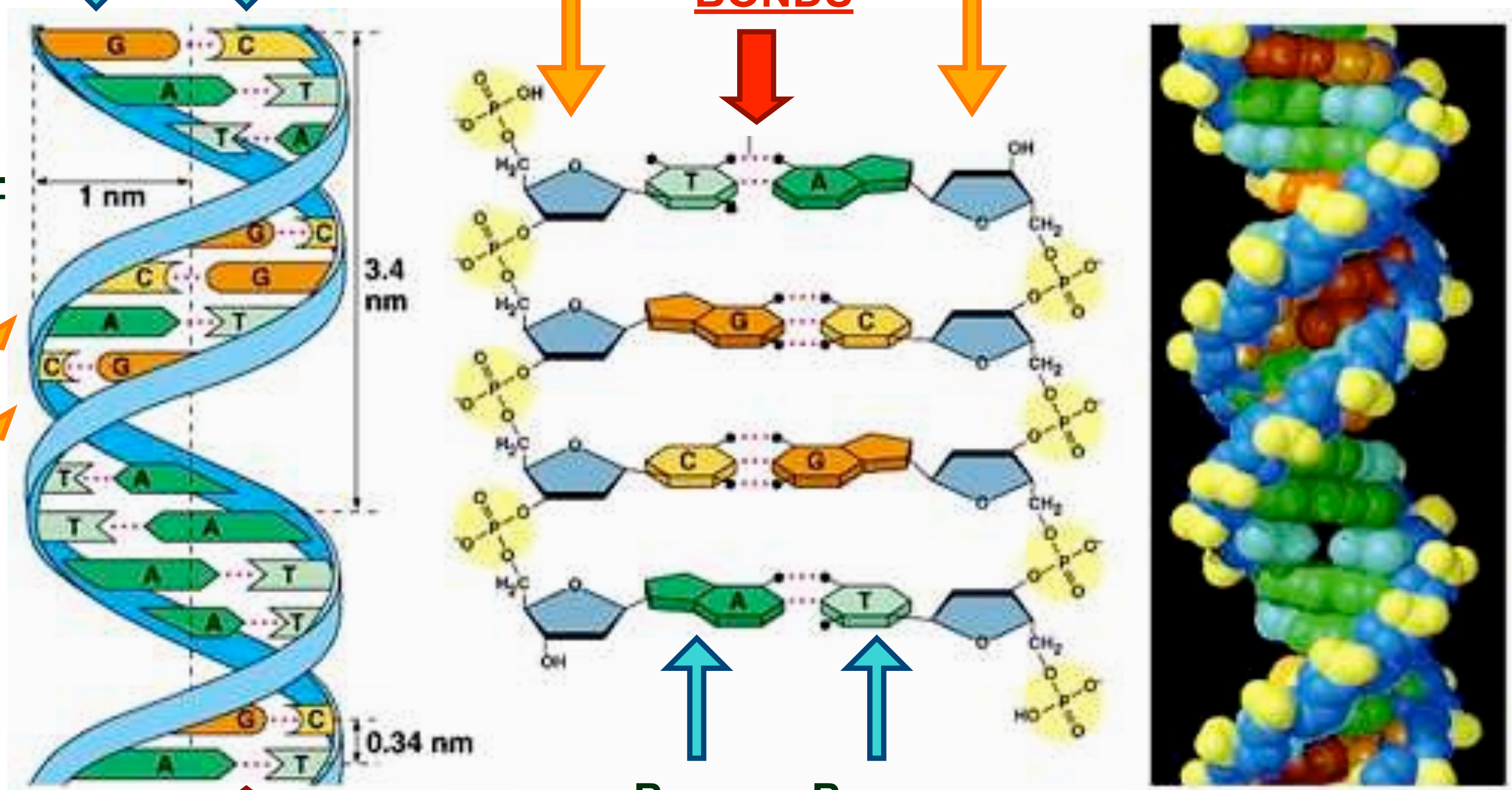


Hydrogen Bonding in Ethanol



Hydrogen Bonding in Hydrofluoric Acid

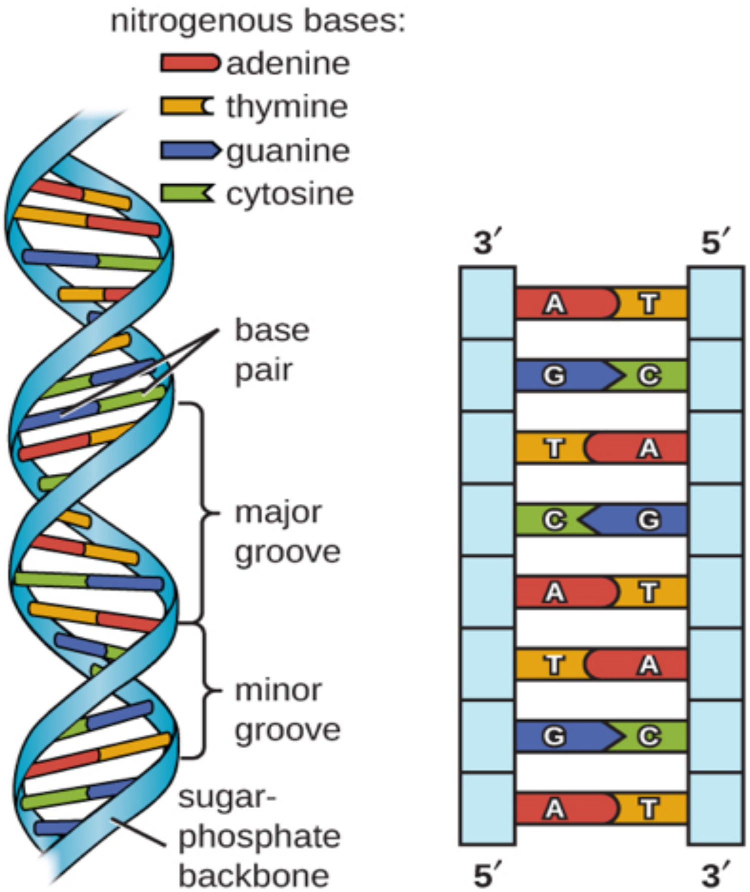


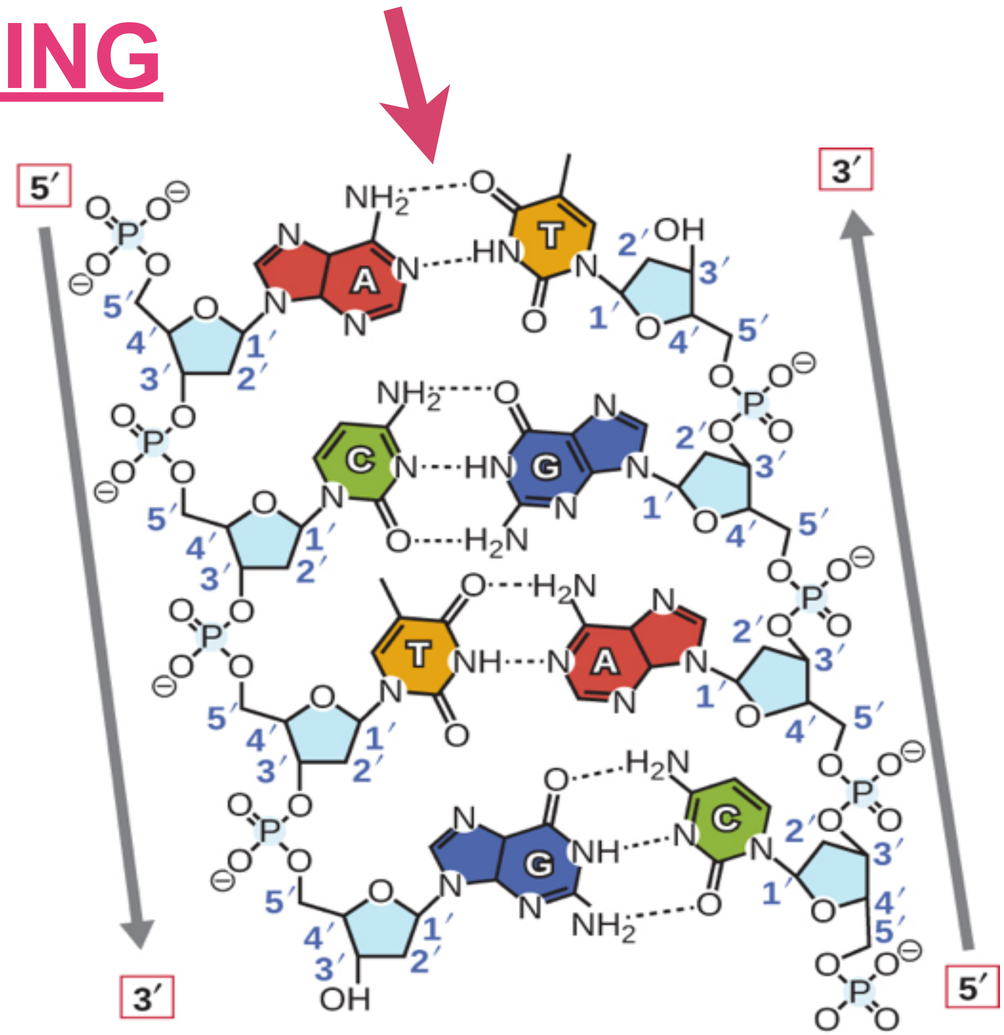


These 2 DNA strands are held together by HYDROGEN BONDS between nearby atoms in DNA molecules.

A

HYDROGEN BONDING



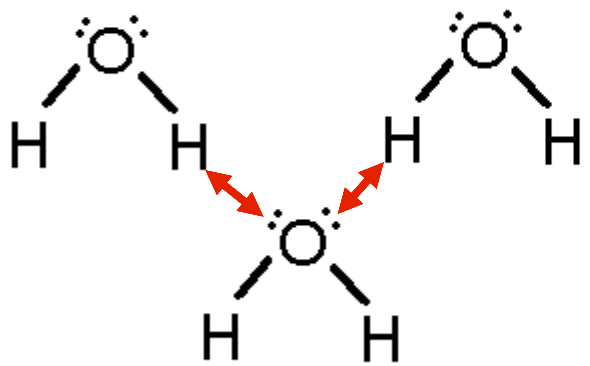


Hydrogen bonds are the strongest of the intermolecular forces but weak when compared to a fully ionic (full + and - charge) attraction or compared to a covalent bond. Even so, given great numbers, Hydrgen Bonds can be quite strong and provide a significant level of stabilization to large molecules such as proteins and nucleic acids (DNA or RNA).

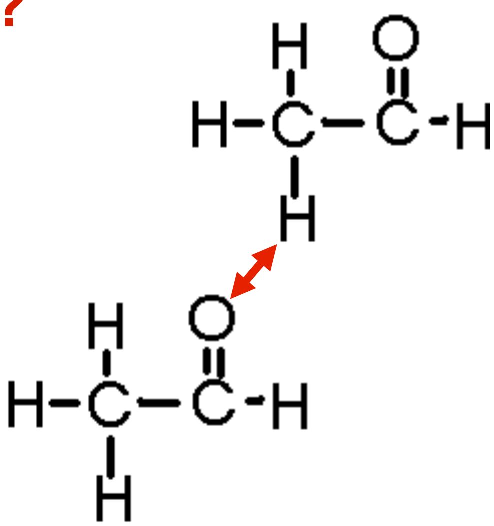
HYDROGEN BONDING OR NO HYDROGEN BONDING?

In order for hydrogen bonds to form between molecules, hydrogen MUST be bonded to nitrogen, oxygen or fluorine in the SAME molecule. ***The hydrogen bonds though occur BETWEEN molecules!!!***

Look at the following groups of molecules: Which would qualify as having hydrogen bonds?

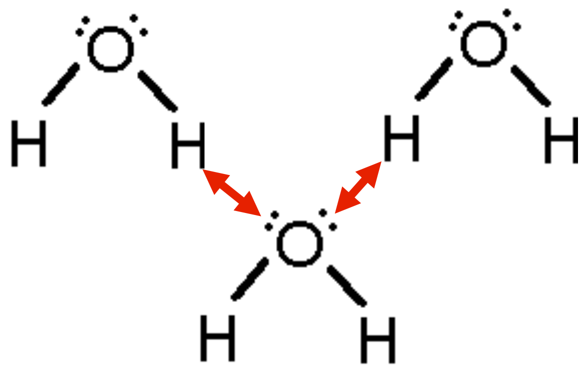


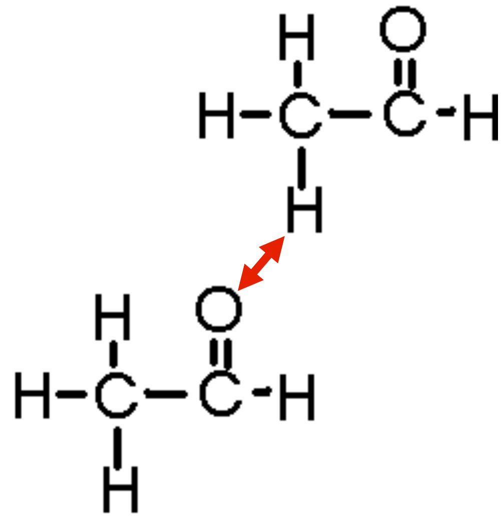
water



acetaldehyde

HYDROGEN BONDING OR NO HYDROGEN BONDING?

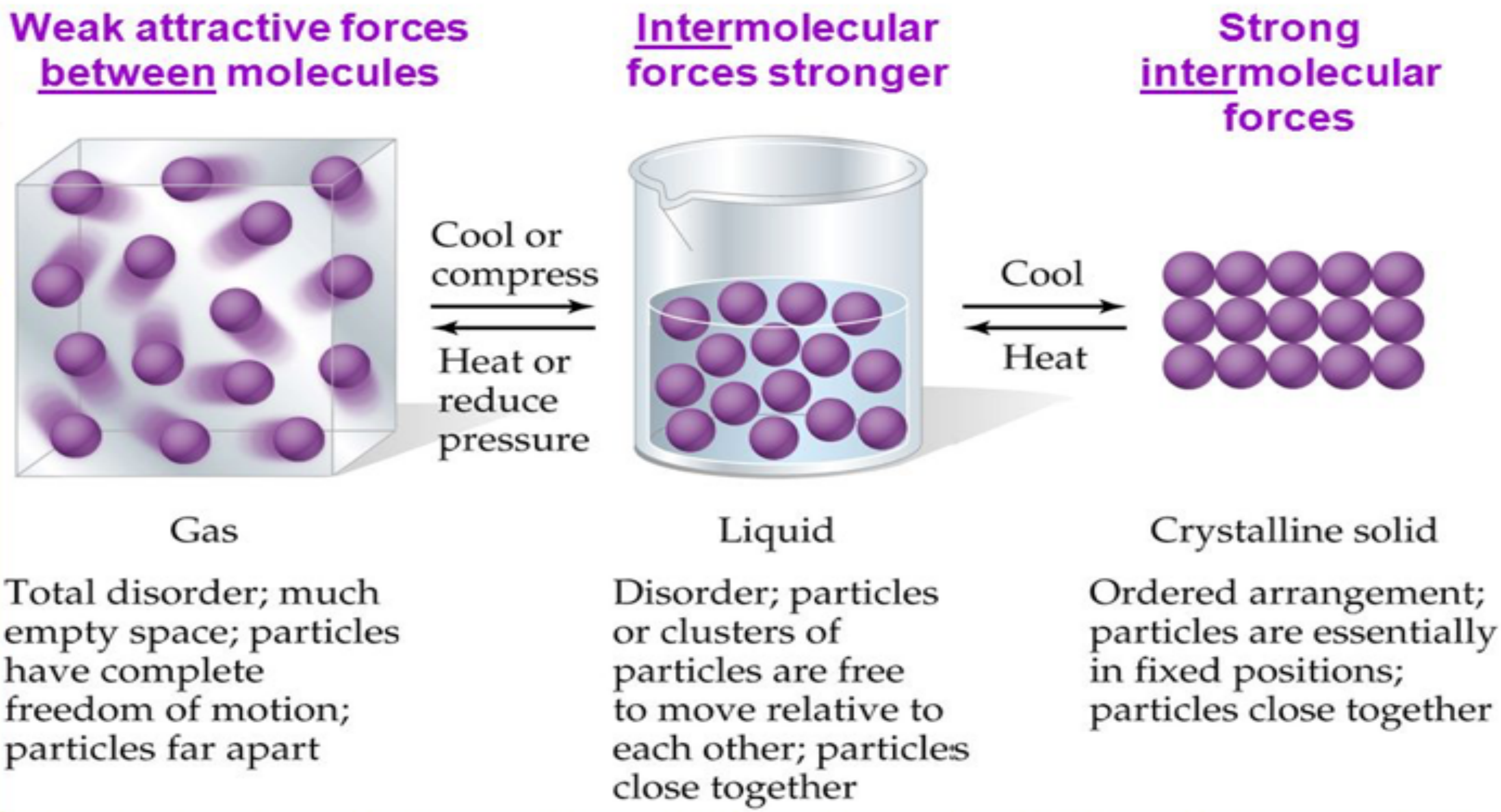




In water, H is bonded directly to O. **Thus, water would qualify as having hydrogen bonds between different water molecules in a sample.**

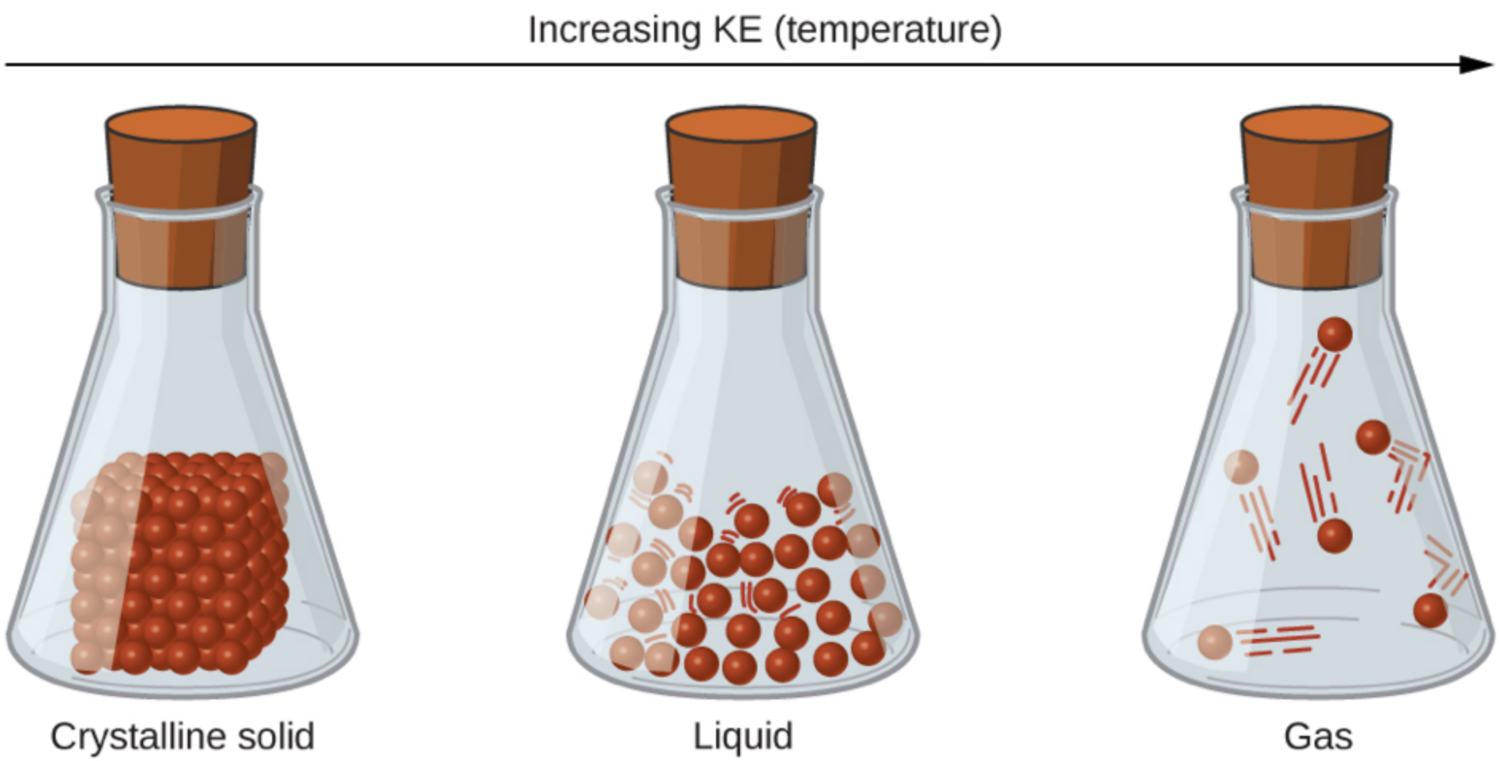
Even though acetaldehyde contains both H and O, the bond shown is NOT a hydrogen bond, as the H atom in the above molecule is not directly bonded to the O atom, leaving the H in the top acetaldehyde molecule neutral. This H then is will not attract the partially negatively charged O atom in the lower acetaldehyde molecule!

While the existence of any temporary or permanent intermolecular forces cause molecules or ions to attract one another, kinetic energy in the system causes particles to vibrate, collide, and want to disperse in space.

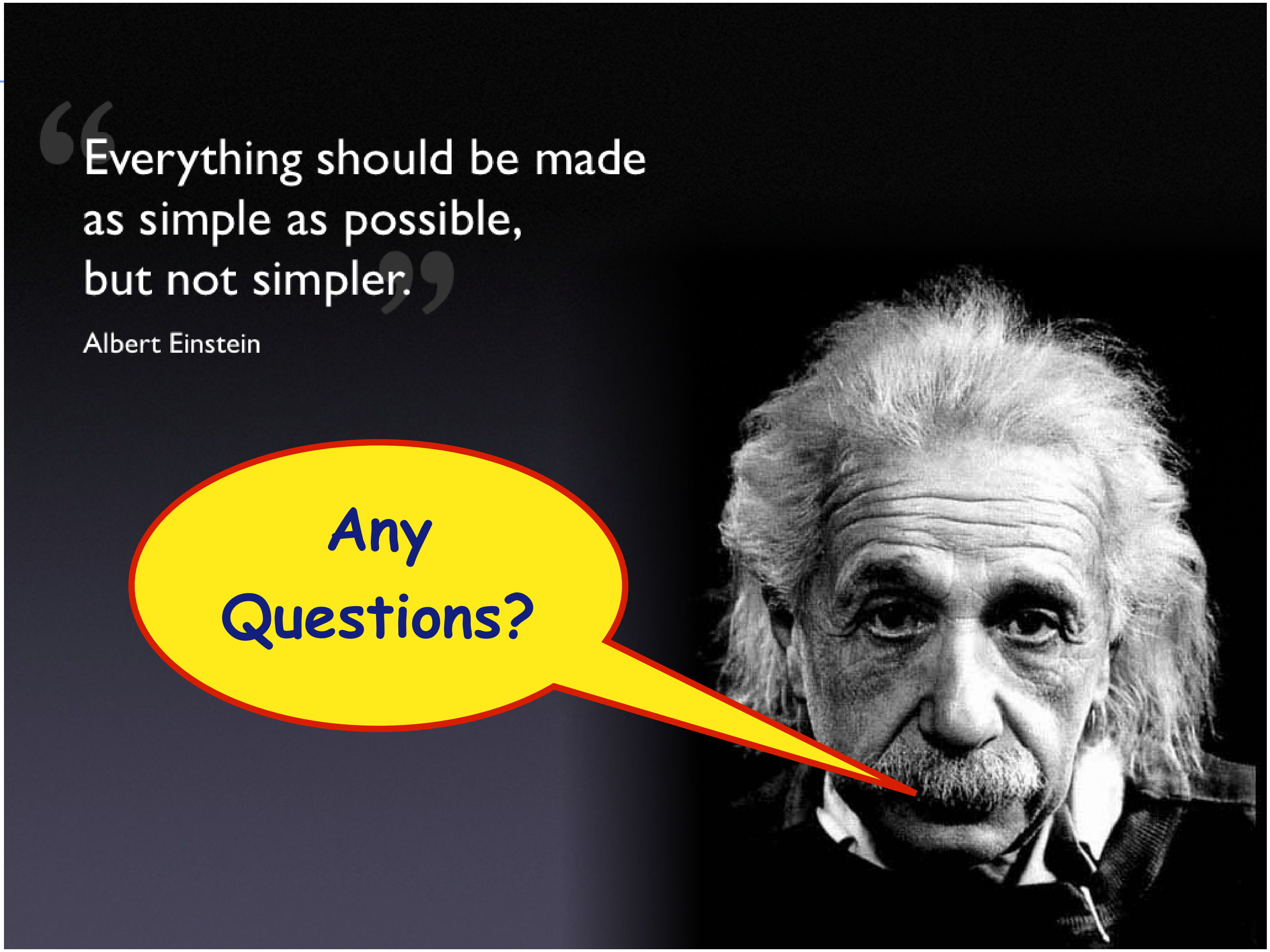


The state of a substance depends largely on the balance between the kinetic energies of the particles and the interparticle energies of attraction.

The State of Matter depends on the amount of KE and the strengths of the IMFs present.



Substances that exhibit weaker or occasional, temporary intermolecular forces, change from solid to liquid to gas with the addition of less kinetic energy (at lower temperatures) compared to substances that exhibit stronger or more permanent intermolecular forces as more kinetic energy is needed for the latter to be able to overcome their intermolecular forces of attraction in order to be able to slide past one another in liquid or move far away from one another in gas.


"Everything should be made
as simple as possible,
but not simpler."
Albert Einstein
Any
Questions?