Periodic Properties of Atoms

Chapter 9

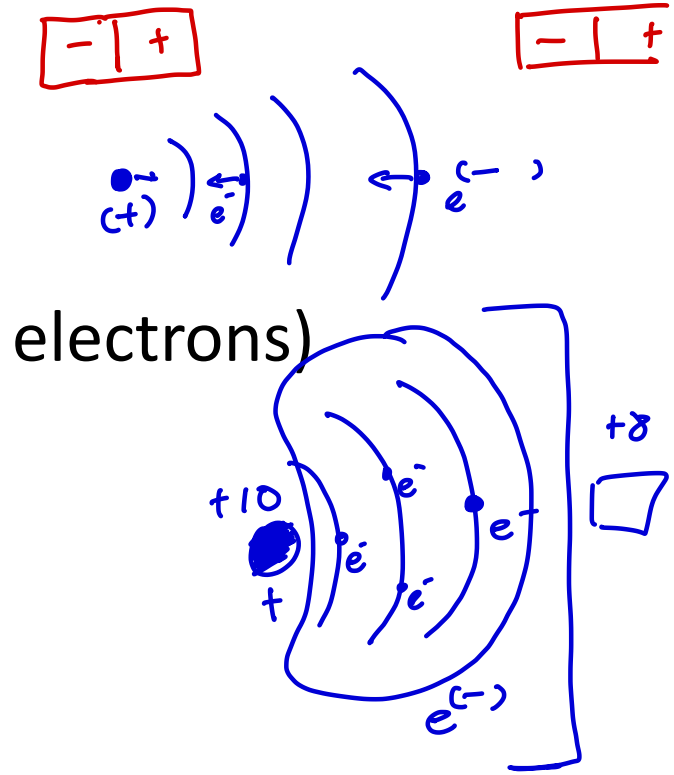
Effective Nuclear Charge (Z_{eff})

- Effective nuclear charge is the “positive charge” felt by valence electrons

$$Z_{eff} = Z - \sigma$$

Z is the actual nuclear charge

σ is the shielding constant (repulsive effect of other electrons)



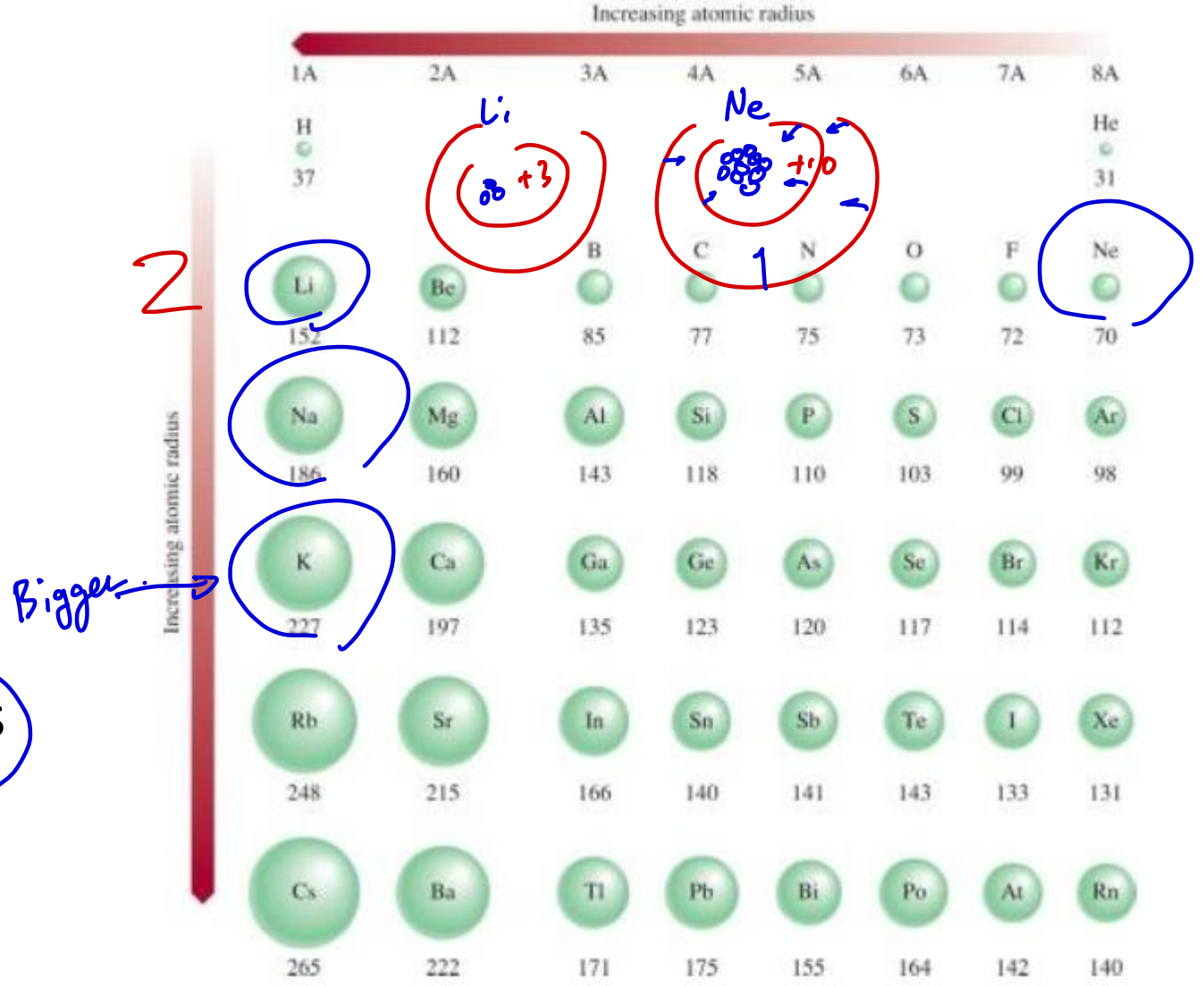
Atomic Radii

Horizonal Trend

- To the right → more P+ → electron cloud attracted to the center → smaller size

Vertical Trend

- Go down → more energy levels → bigger size



Ionic Size

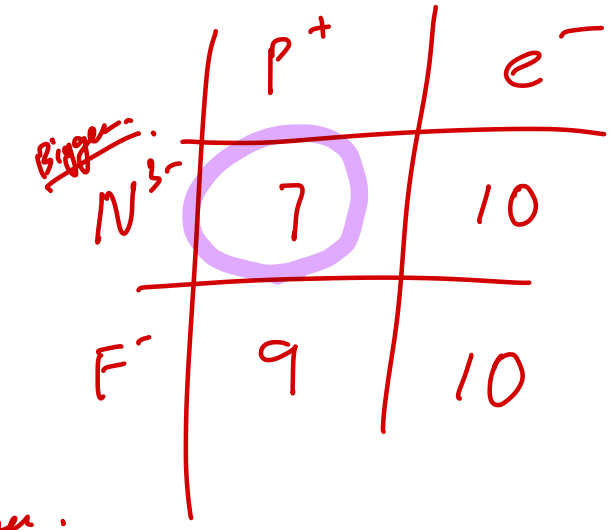
- Cation is always smaller than atom from which it formed.
- Anion is always larger than atom from which it is formed

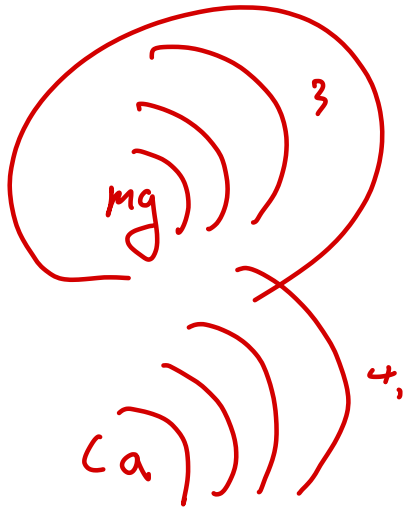
For each of the following pairs, indicate which one of the two species is larger

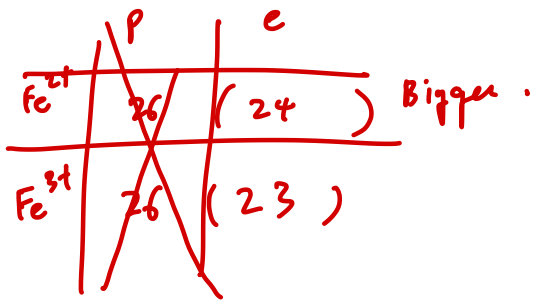
a) N^{3-} or F^-

b) Mg^{2+} or Ca^{2+}

c) Fe^{2+} or Fe^{3+}

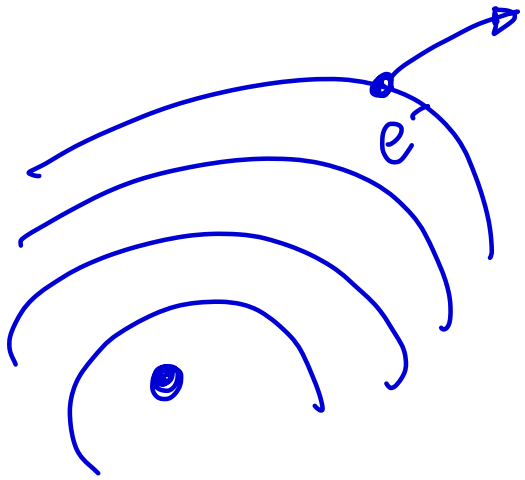






Ionization energy

- Maximum energy (KJ/mol) required to remove an electron from a gaseous atom in its ground state. + from the most outer energy level.
- You can remove one electron at a time
- Each succeeding ionization energy is larger than the preceding energy



$$Mg\,(g) \rightarrow Mg^{+}\,(g) + e^{-} \quad I_1 = 738\,kJ/mol$$

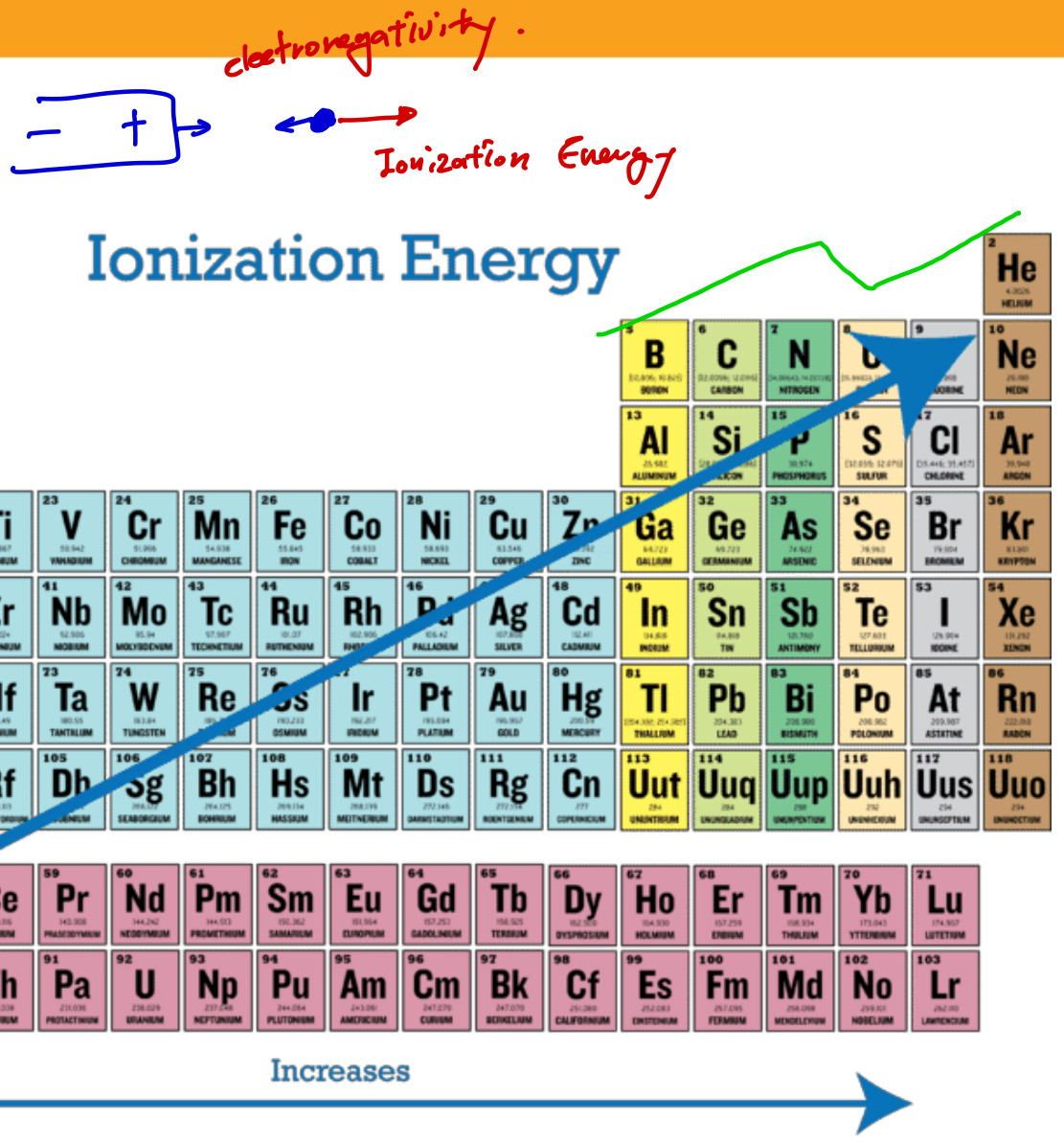
$$Mg^{+}\,(g) \rightarrow Mg^{2+}\,(g) + e^{-} \quad I_2 = 1451\,kJ/mol$$

Horizonal Trend

- To the right → more p+ → more attraction → need more energy to overcome the attraction when an e- is removed.

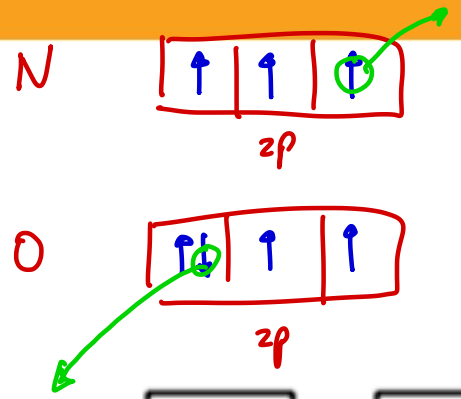
Vertical Trend

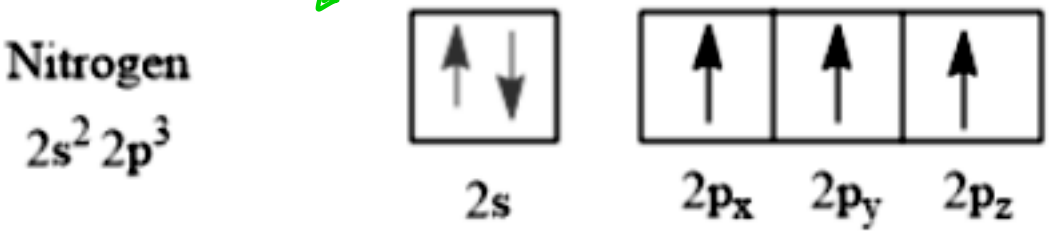
- Go down → More layers of electron → the valence electron is further away from the center (less attraction) AND there are more electrons in between the nucleus and the valence electron (less attraction) → need less energy to overcome the attraction when an e- is removed.

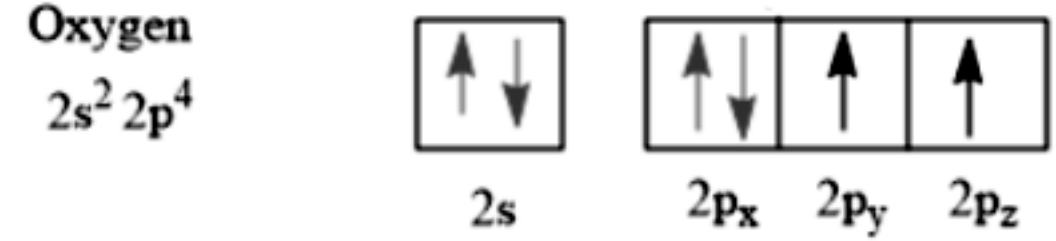


Exception in Ionization Energy Trend

P orbital is stable when it is half-filled or fully filled. P orbital in Nitrogen is already at the stable state. So removing an electron from there is difficult (takes more energy). However, P orbital in Oxygen has one extra from the stable state. So removing an electron actually helps it to go back to the stable state. So it is easier (takes less energy)







Electron Affinity (EA)

- Electron affinity is the amount of energy released when an electron is added to a neutral atom or molecule in the gaseous state to form a negative ion

Ex)

$F_{(g)} + e^- \rightarrow F^-(g)$ $\Delta H = -328$ kJ/mol (negative sign = release)

Amount of energy released is 328 kJ/mol when the electron is gained. Meaning, that much energy is needed to detach the electron from F.

Large EA means the negative ion is very stable.

Electron affinity

- amount of energy that is released when an electron attaches to the atom

Electronegativity

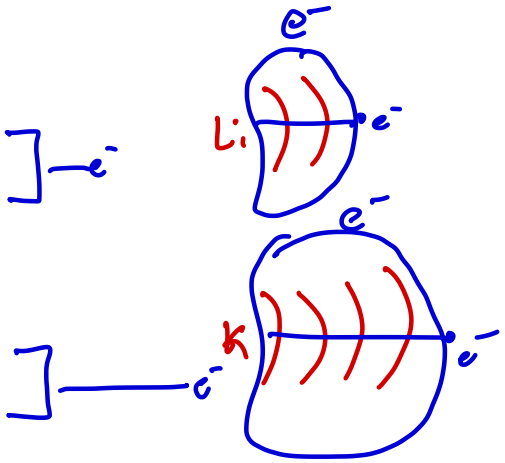
- quantification of a molecules ability to attract an electron and form a covalent bond.
- Cannot be measured scientific means. It depends on the molecule that it is bonded to.

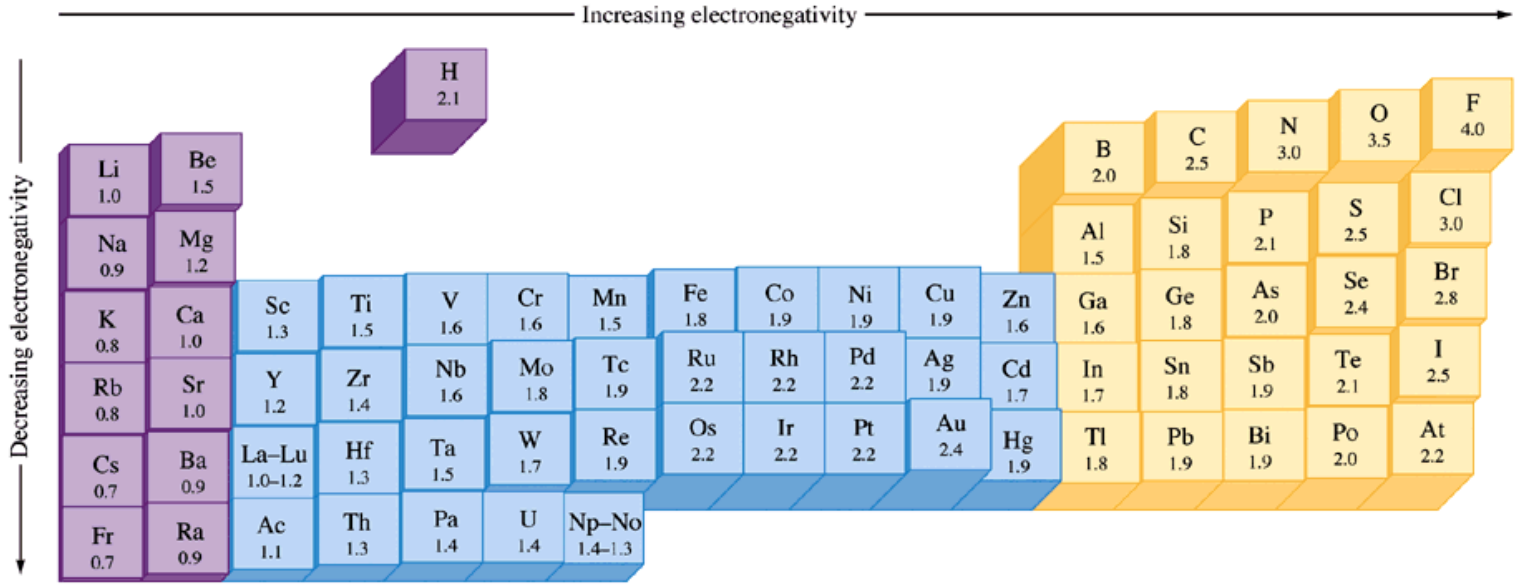
Horizonal Trend

- To the right → more p+ → more attraction

Vertical Trend

- Go down → More layers of electron → the valence electron is further away from the center (less attraction) AND there are more electrons in between the nucleus and the valence electron (less attraction)





CHAPTER 10

Chemical Bonding

Types of Bonds

international.

Intermolecular forces are attractive forces between molecules

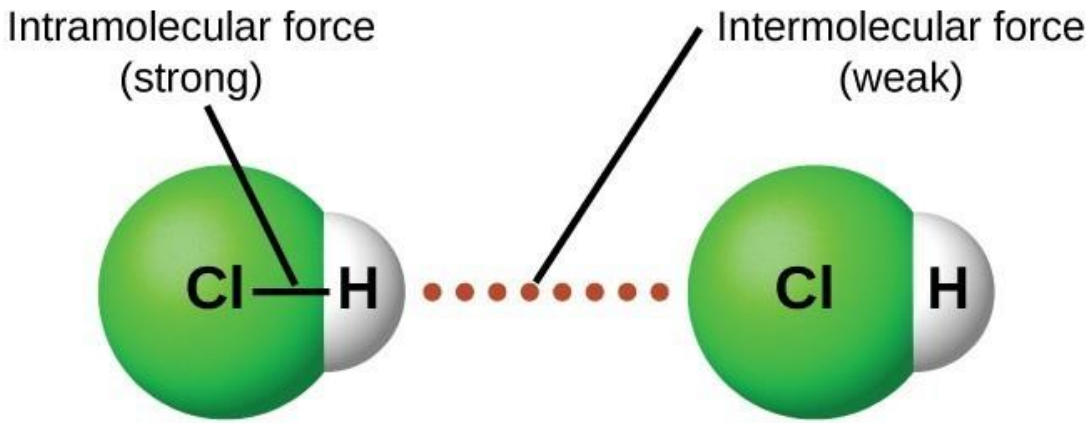
Intramolecular forces hold atoms together in a molecule

Intermolecular vs Intramolecular

41 kJ to vaporize 1 mole of water (inter)

930 kJ to break all O-H bonds in 1 mole of water (intra)

Generally, intermolecular forces are much weaker than intramolecular forces



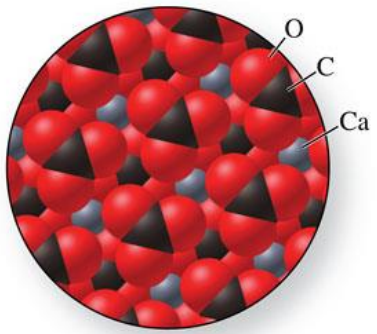
Types of bonds

Chemical bond

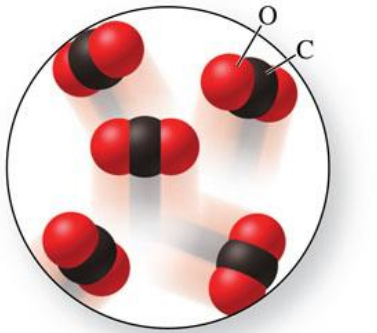
- A force that holds atoms together in a molecule or compound

Two types of chemical bonds

- Ionic Bonds
- Covalent Bonds



A $CaCO_3$



B CO_2

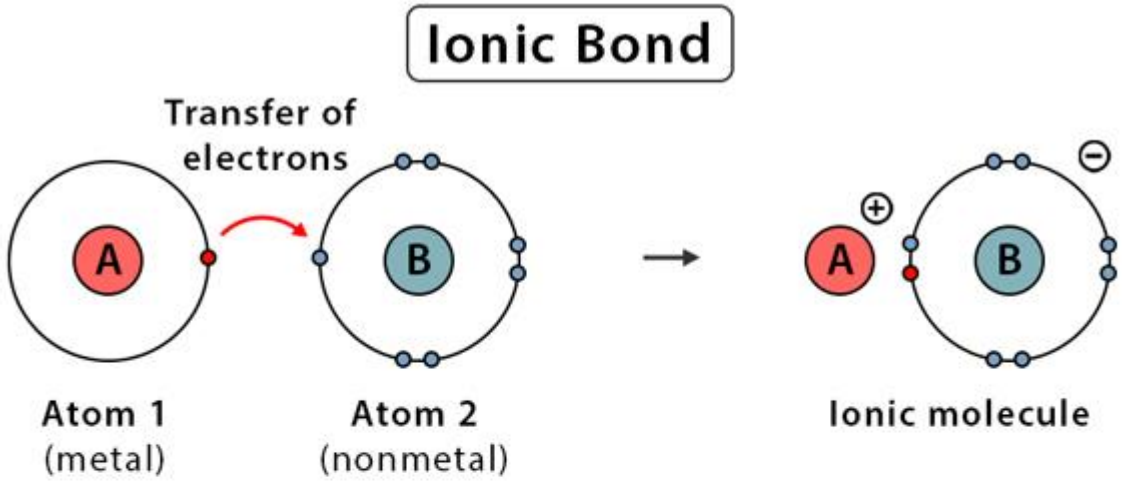
TABLE 8.2 | General Properties of Ionic and Covalent Substances

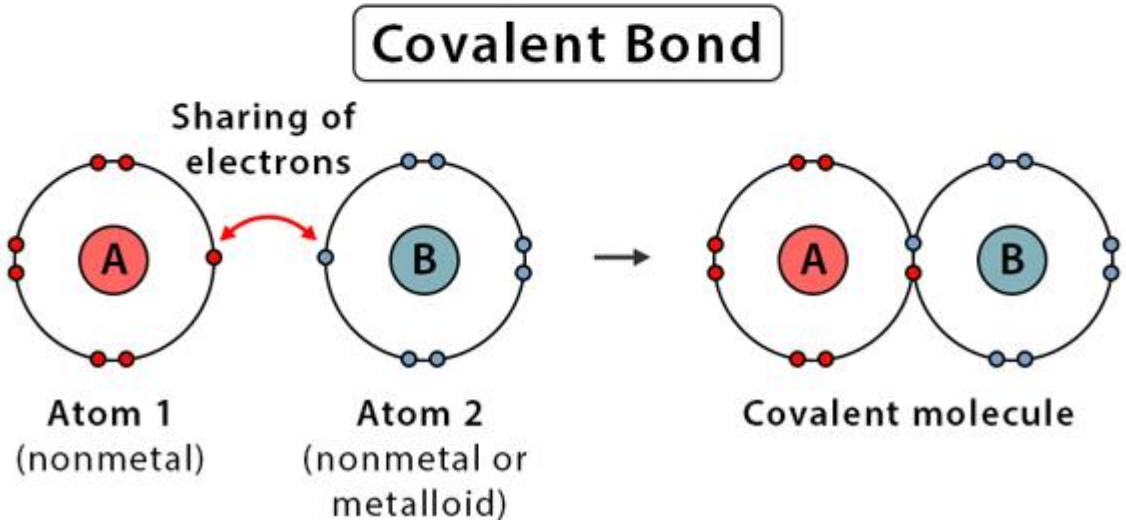
Ionic	Covalent
Crystalline solids	Gases, liquids, or solids
Hard and brittle solids	Brittle and weak solids, or soft and waxy solids
Very high melting point	Low melting point
Very high boiling point	Low boiling point
Good electrical conductor when molten or in solution	Poor conductor of electricity and heat
Often soluble in water but not in carbon tetrachloride	Often soluble in carbon tetrachloride but not in water

Ionic and Covalent

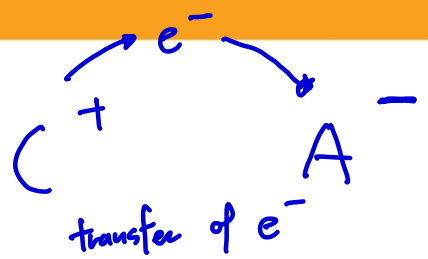
- In ionic compounds, ions are held together by electrostatic forces – forces between oppositely charged ions.

- In molecular compounds, atoms are held together by covalent bonds in which electrons are shared.

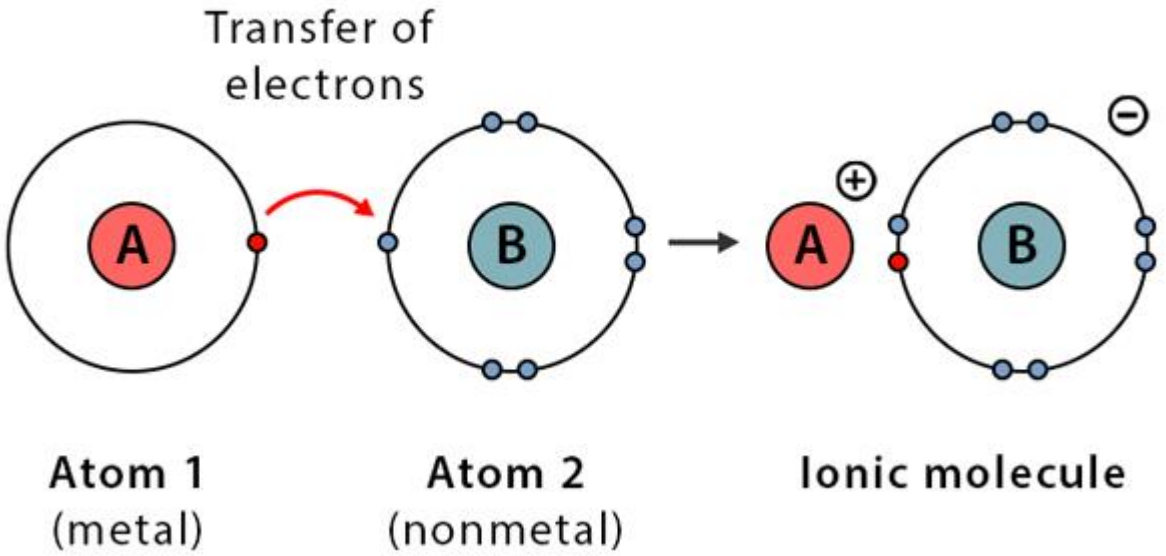




Ionic Bonds



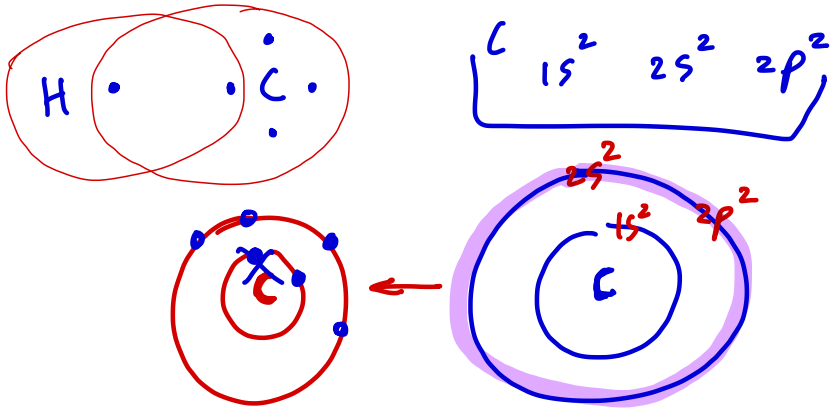
- A bond created by electrostatic attraction between oppositely charged ions
- Occurs between a metal and a nonmetal
- Electrons transferred between the cation (positively charged ion) and the anion (negatively charged ion)
- Extremely strong bonds

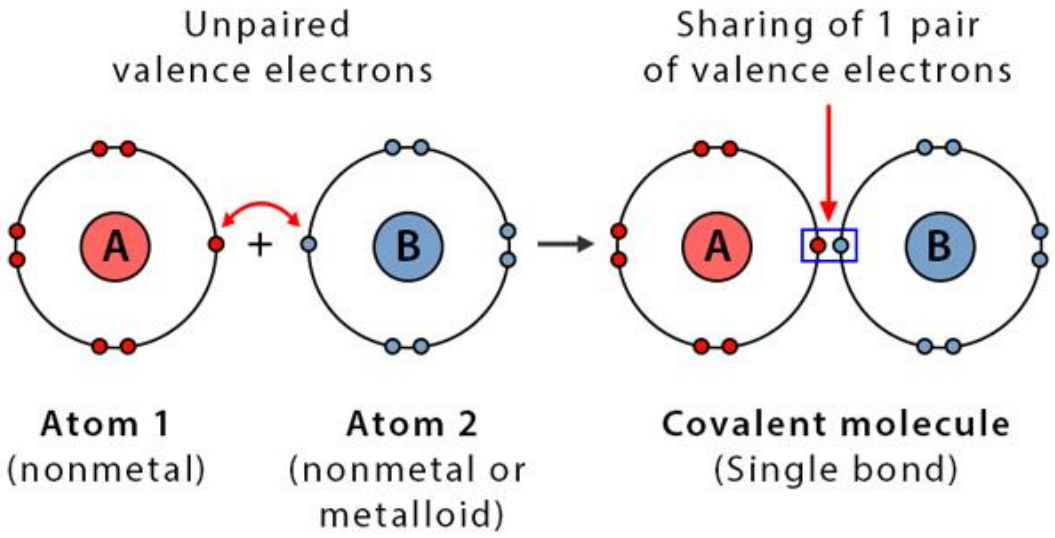


- Metals lose electrons, forming a positive charge, to become cations.
- Nonmetals gain electrons, forming a negative charge, to become anions.
- Formation of ions and ionic bonds relates to an element's electron configuration.
- Many main-group elements either lose or gain electrons to become isoelectronic with a noble gas (i.e. have the same electron configuration). As ions, they are known as the common ions.

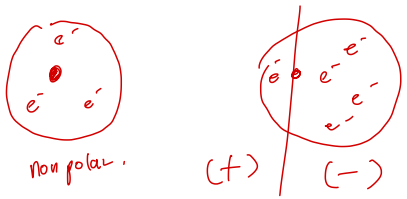
Covalent Bonds

- A bond created by the sharing of electrons between atoms
- Occurs between two nonmetals
- Electrons typically shared in pairs
- Weaker bonds than ionic bonds

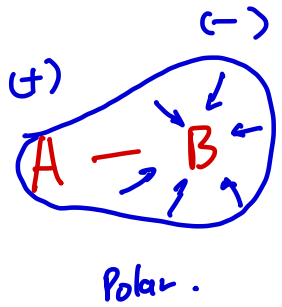


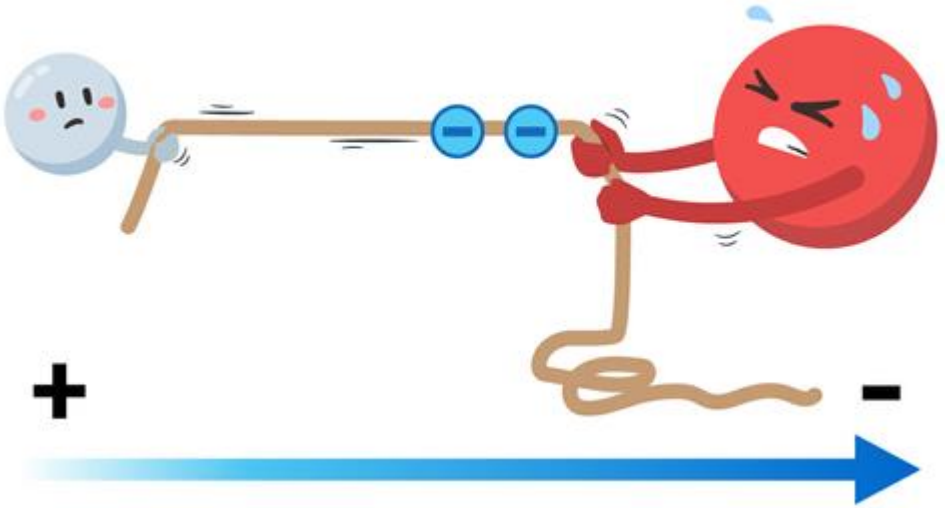


Polarity



The degree of transfer of electrons in a covalently bonded molecule composed of different element's atoms.





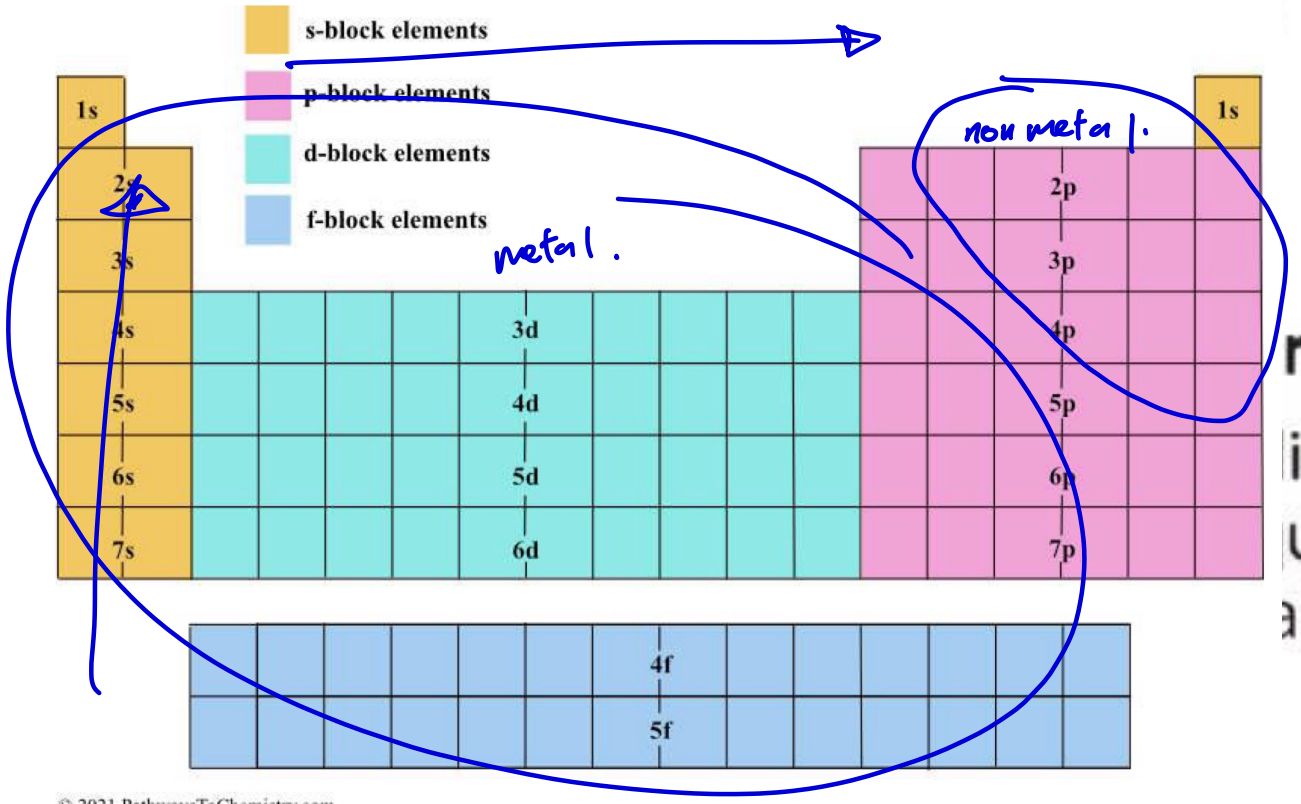
Polar vs. Nonpolar

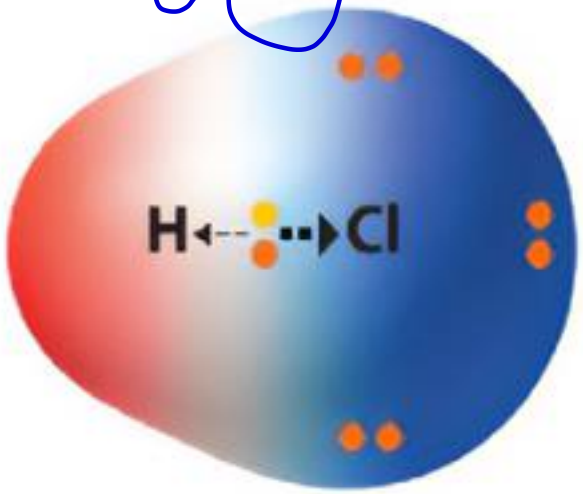
Polar covalent

- Unequal sharing (or a partial transfer) of electrons
- Occurs when different elements are covalently bonded to one another
  - Why different elements?
    - Because different elements have different electronegativities
- Typically shorter bonds
- Stronger bonds due to their increased ionic character

Nonpolar covalent

- Equal sharing (no transfer) of electrons
- Occurs only when all of the atoms in a molecule belong to the same element
- Typically longer bonds
- Weaker bonds

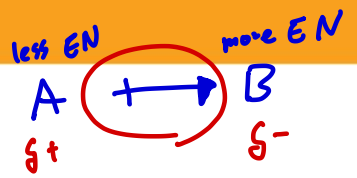




r covalent bond

ing electrons shared
ually between two atoms.
al charges on atoms.

Dipole Moment

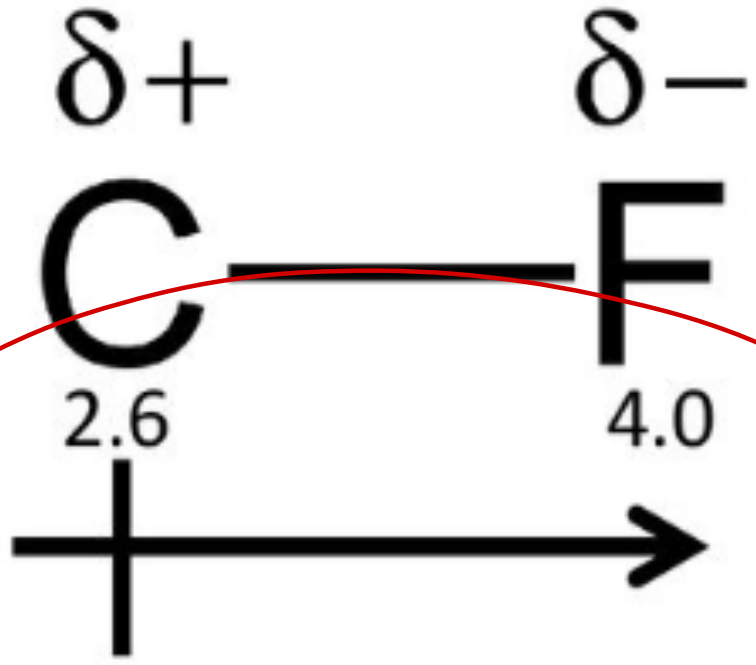


δ (delta) means "partial"

δ+ "partially positive"

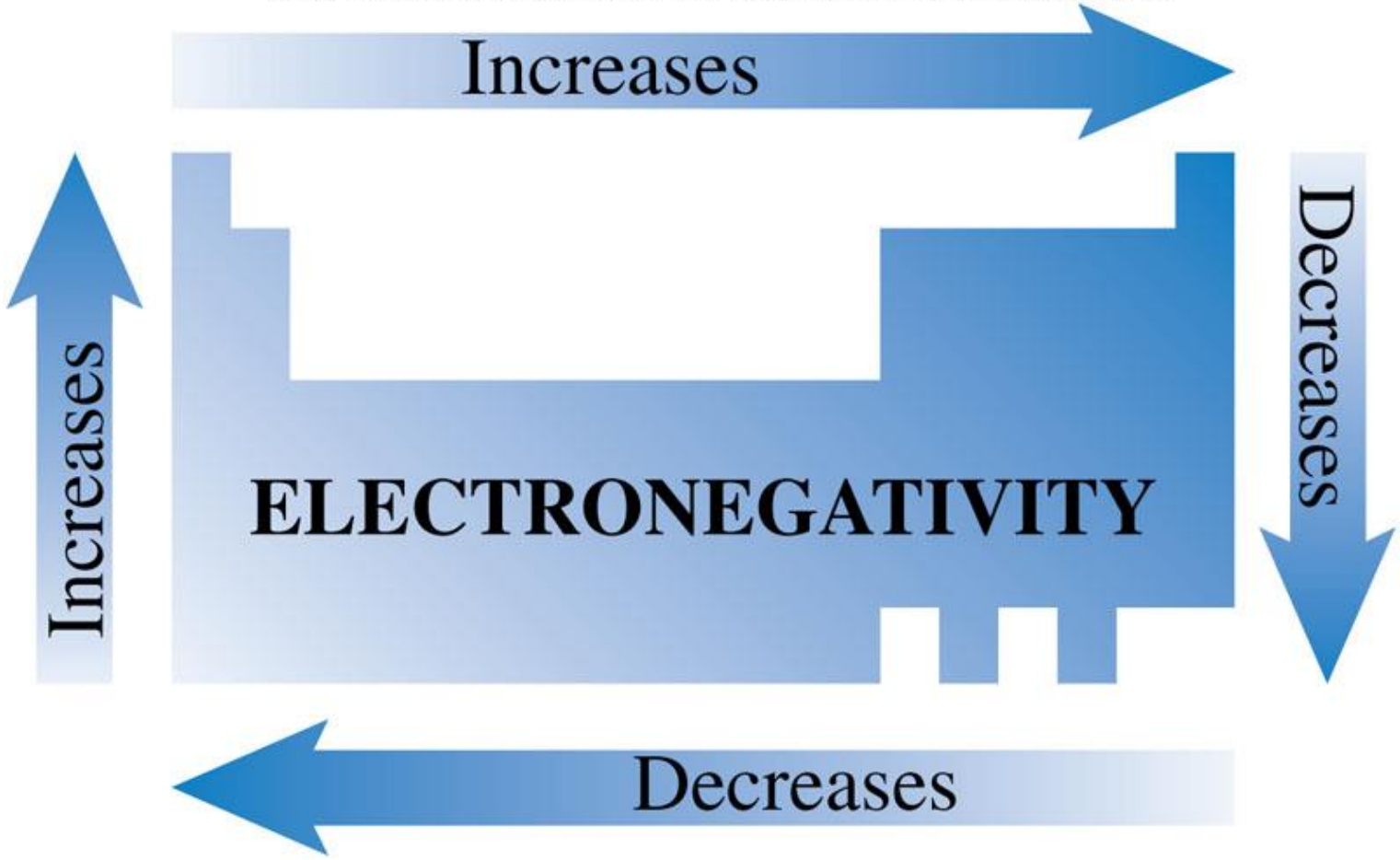
δ- "partially negative"

- Arrow points toward negative side (more electronegative)
- Cross is at the positive side



$4.0 - 2.6 = 1.4$

Electronegativity Trends



Which of the following molecules have polar bonds? If a bond is polar, which atom has a partial negative charge?

1. SO_2 $S \rightarrow O$
2. N_2 $N - N$
3. H_2S
4. CCl_4

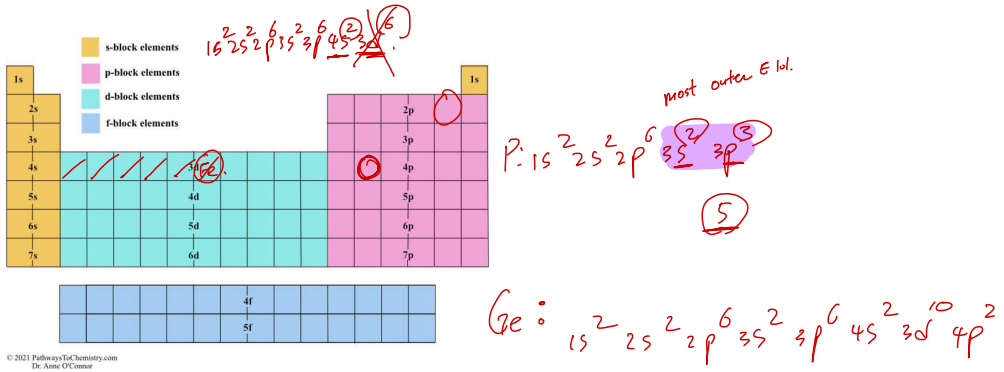
Lewis Dot Structure

Valence electrons

Most outer shell E lvl.

- Valence electrons are the most outer shell electrons of an atom. The valence electrons are the electrons that participate in chemical bonding.
- Valence electron of a transition metal is 2. why?

Group	e^- configuration	# of valence e^-
1A	ns^1	1
2A	ns^2	2
3A	ns^2np^1	3
4A	ns^2np^2	4
5A	ns^2np^3	5
6A	ns^2np^4	6
7A	ns^2np^5	7

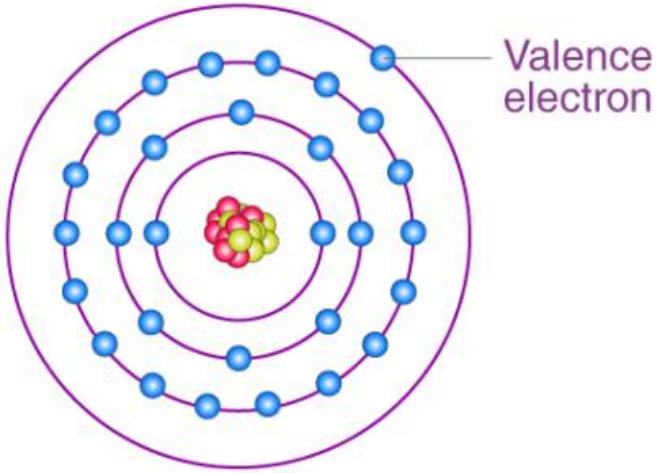


$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10}$

most outer E lvl.

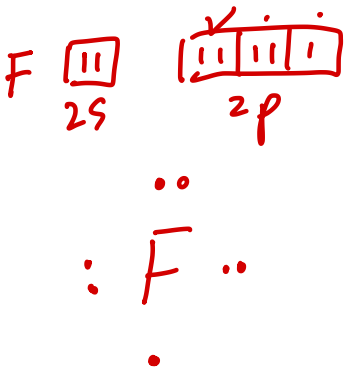
P: $1s^2 2s^2 2p^6 3s^2 3p^3$

Ge: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^2$



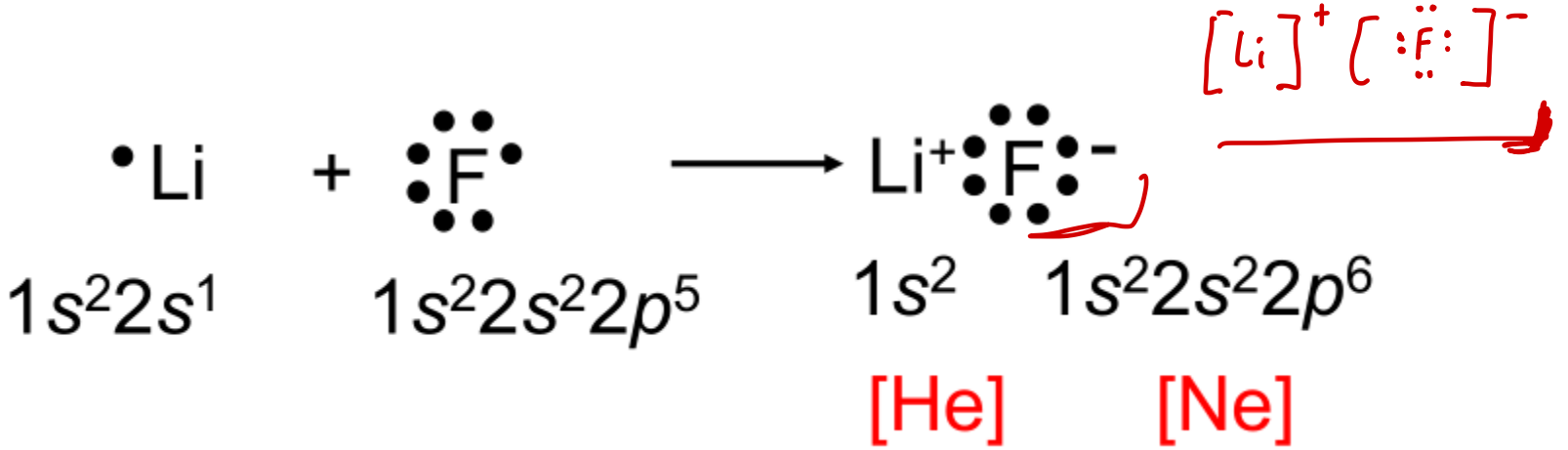
Lewis Periodic Table Showing Outer Shell (Valence) Electrons

1	2	3	4	5	6	7	8
H•							•He•
Li•	•Be•	•B•	•C•	•N•	•O•	:F•	:Ne:
Na•	•Mg•	•Al•	•Si•	•P•	•S•	:Cl•	:Ar:
K•	•Ca•	•Ga•	•Ge•	•As•	•Se•	:Br•	:Kr:
Rb•	•Sr•	•In•	•Sn•	•Sb•	•Te•	:I•	:Xe:
Cs•	•Ba•						

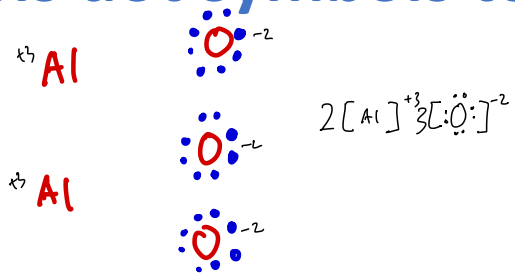


The Ionic Bond

- Ionic Bond: the electrostatic force that holds ions together in an ionic compound. (formed by a metal and a non-metal)

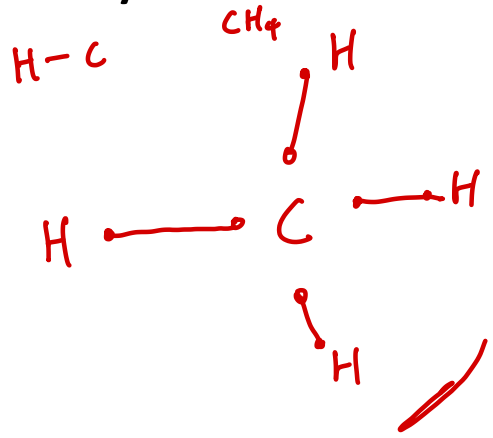


Use Lewis dot symbols to show the formation of aluminum oxide (Al_2O_3)

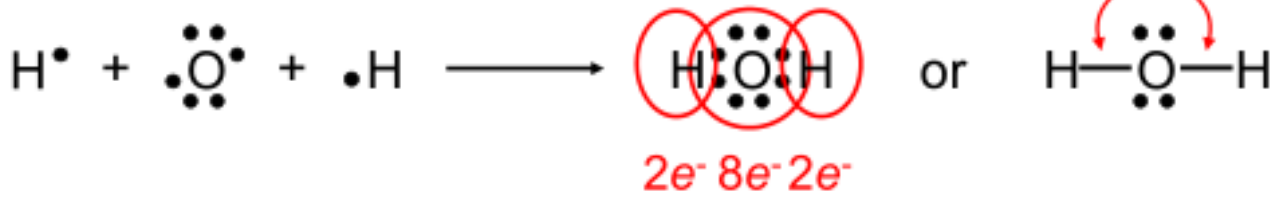


Covalent Bond

- A Covalent bond is a chemical bond in which two or more electrons are shared by two atoms.

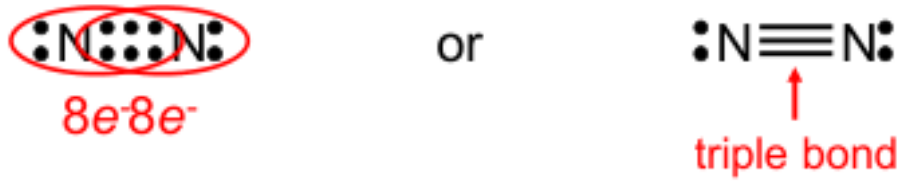


Lewis structure of water



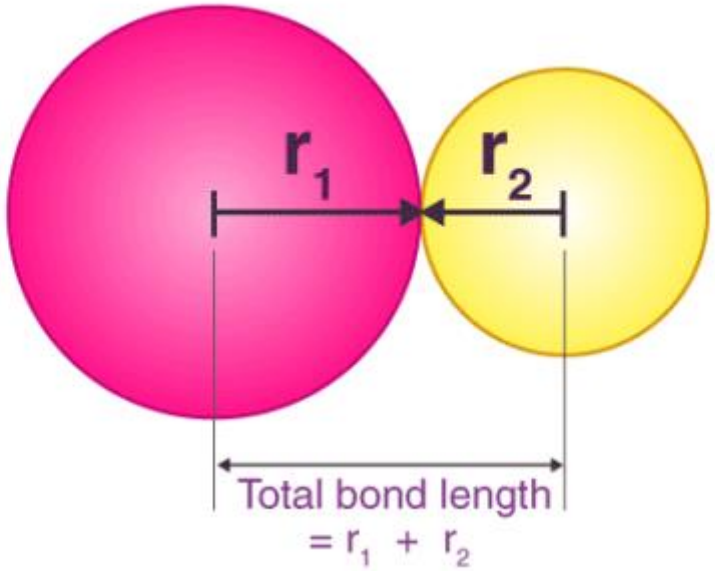
Double bond – two atoms share two pairs of electrons

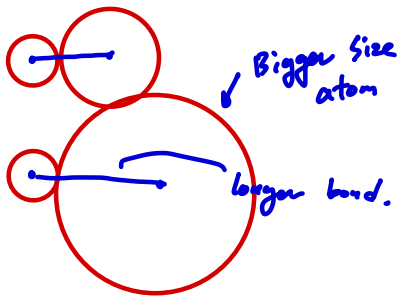
Triple bond – two atoms share three pairs of electrons



Lengths of Covalent Bonds

- Bond length depends on the size of the elements
- Bond length gets shorter with more bonds
  - Triple bond < Double < Single
- Shorter the length, stronger it gets





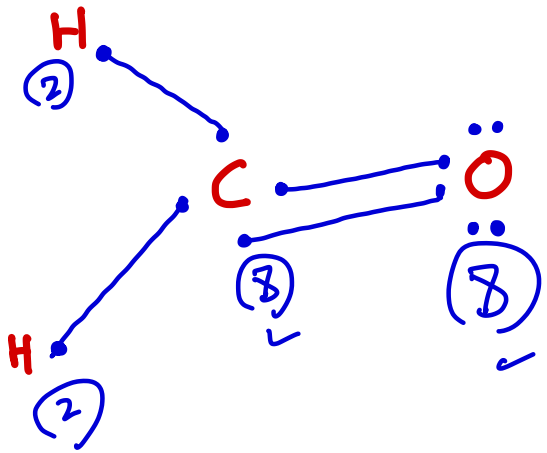
Average Bond Lengths of Some Common Single, Double, and Triple Bonds

Bond Type	Bond Length (pm)
C—H	107
C—O	143
C=O	121
C—C	154
C=C	133
C≡C	120
C—N	143
C=N	138
C≡N	116
N—O	136
N=O	122
O—H	96

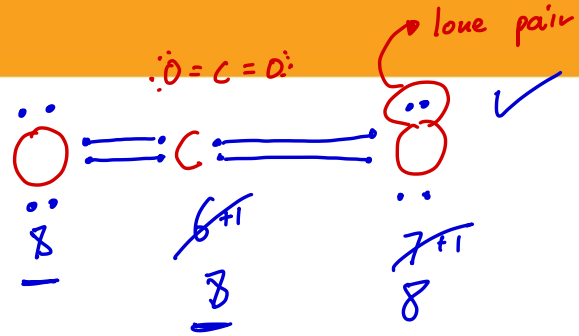
Steps for Writing Lewis Structures

1. Write an atomic skeleton.
2. Place all the valence electrons
3. Connect two electrons to make a single bond
4. Check by the octet rule—if it doesn't satisfy it, try double bond or transfer e-
   - Octet Rule – having 8 electrons per element

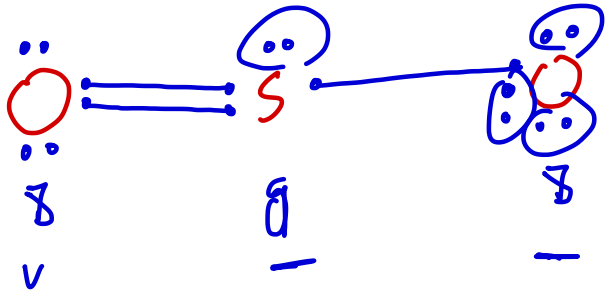
H_2CO

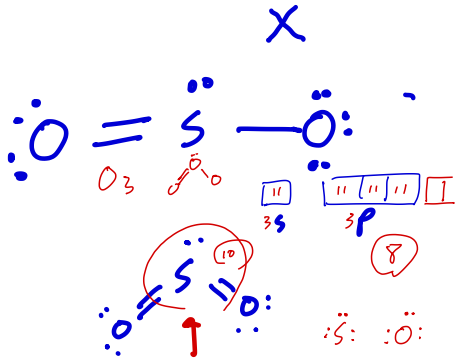


CO_2

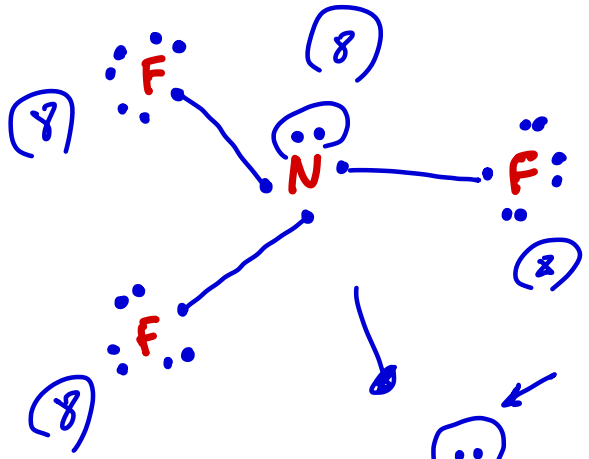


SO_2

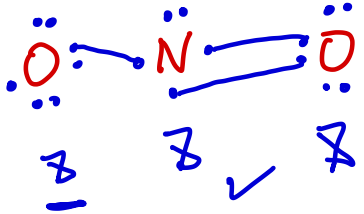




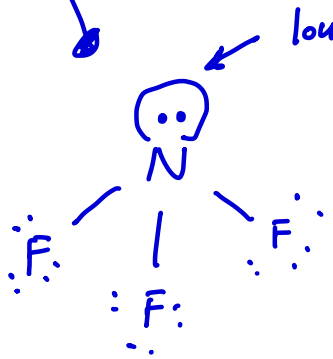
NF_3



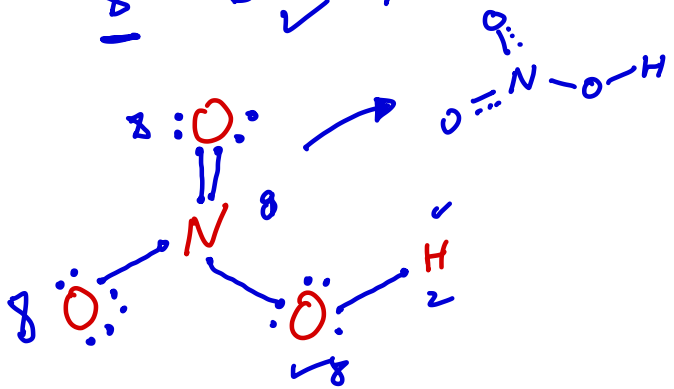
NO_2^-



H_2O

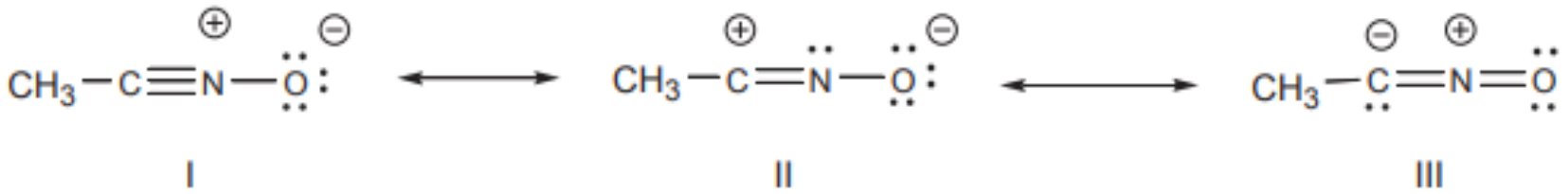


HNO_3



Resonance

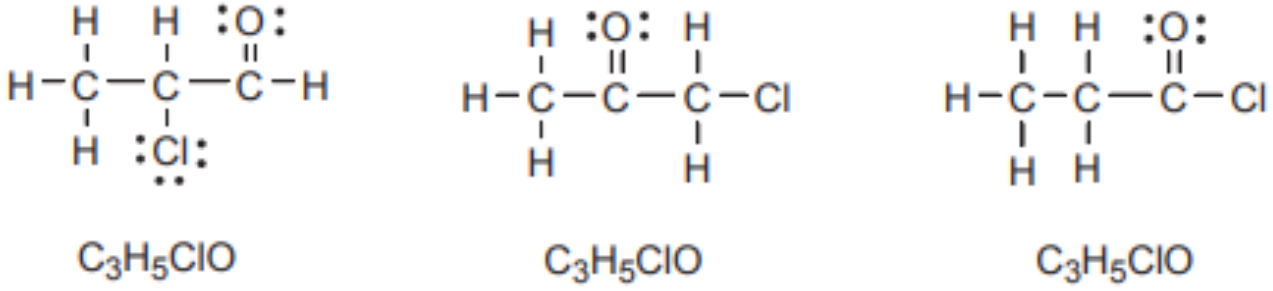
- Same formula, different e- location



I II III

Isomers

- Same formula, different atom location



C_3H_5ClO C_3H_5ClO C_3H_5ClO

Which of the following has resonance? For those that do, how many resonance structures do they have?

NO_3^-

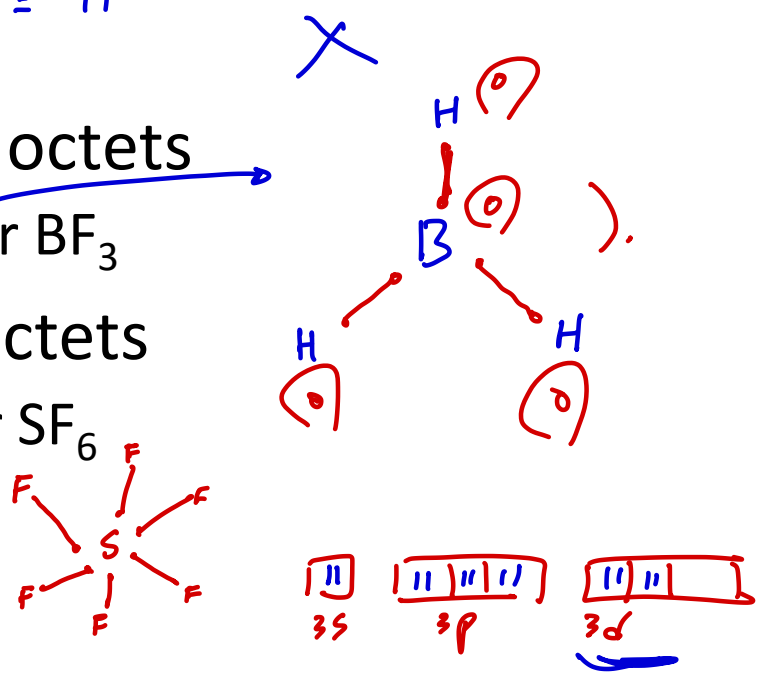
CH_4

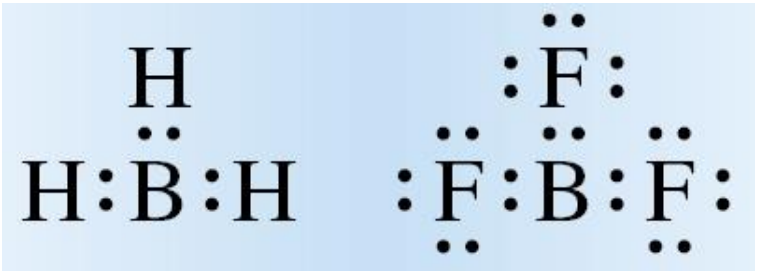
H_2CO

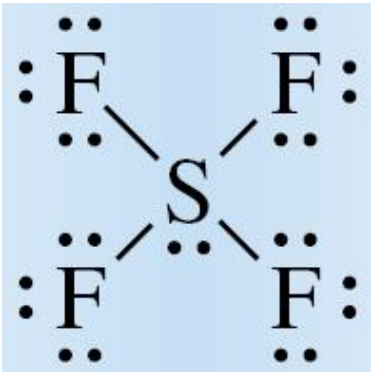
HNO_3

Exceptions to the Octet Rule

- Molecules with an odd number of electrons
  - e.g. NO
- Incomplete octets
  - e.g. BH_3 or BF_3
- Expanded octets
  - e.g. SF_4 or SF_6

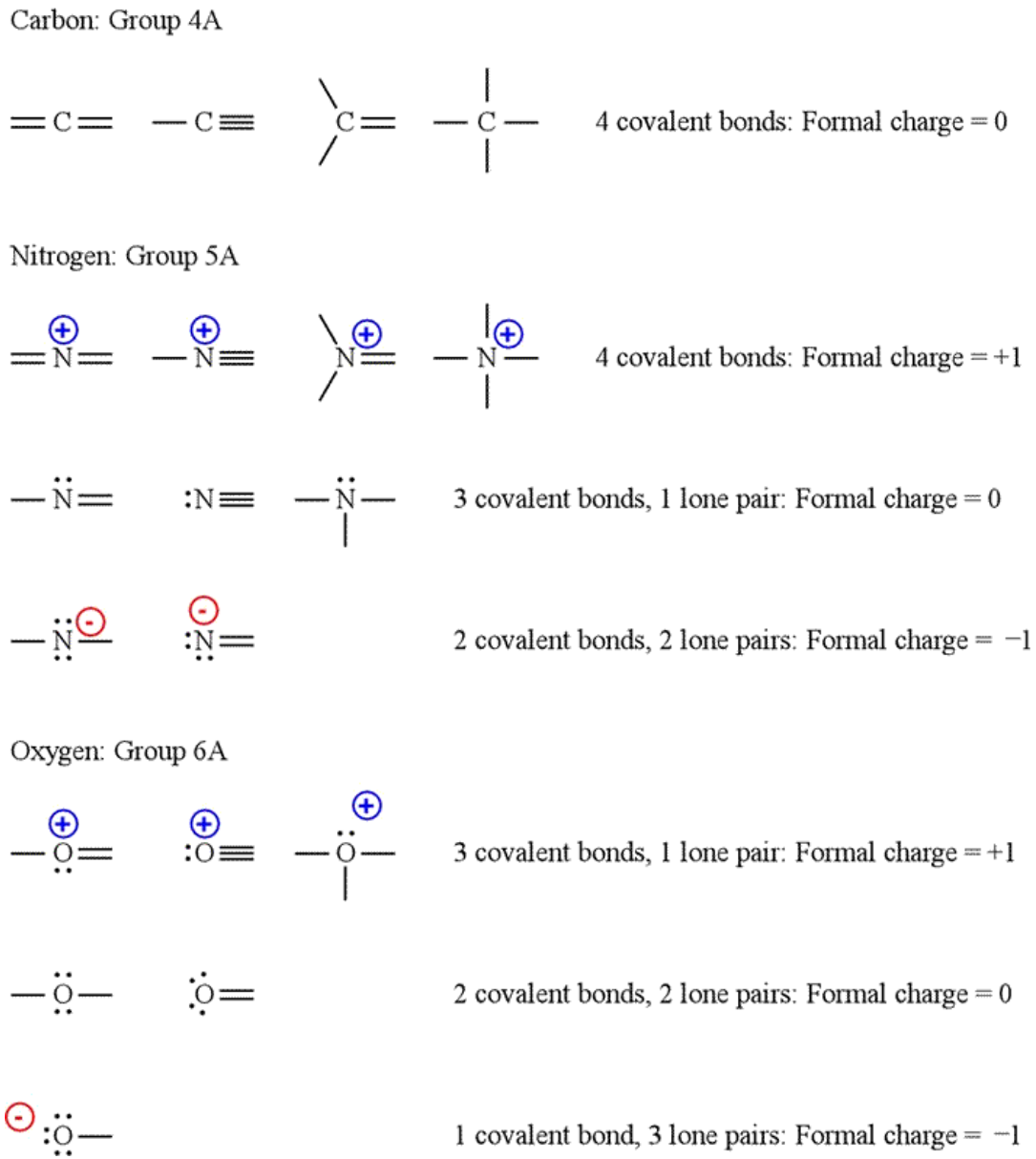






Formal Charge

- Formal charge = number of valence electrons - (number of lone-pair electrons + 1/2 number of bonding electrons)
  - "lone pair electrons" are also known as "nonbonding pairs" or "unshared pairs".
- The sum of formal charges of the Lewis structure of a molecule or ion must be equal to the net charge on the molecule or ion.



Using Formal Charge

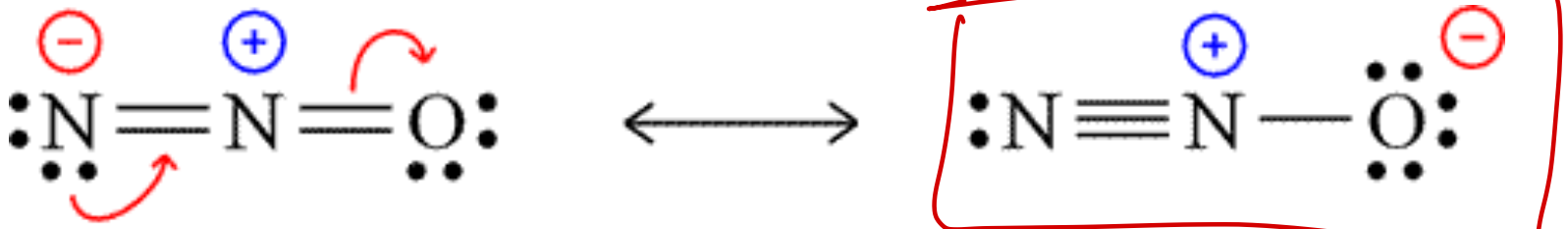
- Having zero formal charge means it has the right amount of electrons for that element.
  - Negative formal charge = excess electrons
  - Positive formal charge = missing electrons
- In case of non-zero formal charge
  - More electronegative elements = negative formal charge
  - Less electronegative elements = positive formal charge

FC : # Ve⁻ (unlone e⁻) − (lone pair e⁻ (dots) + ½ bonding e⁻ (lines))

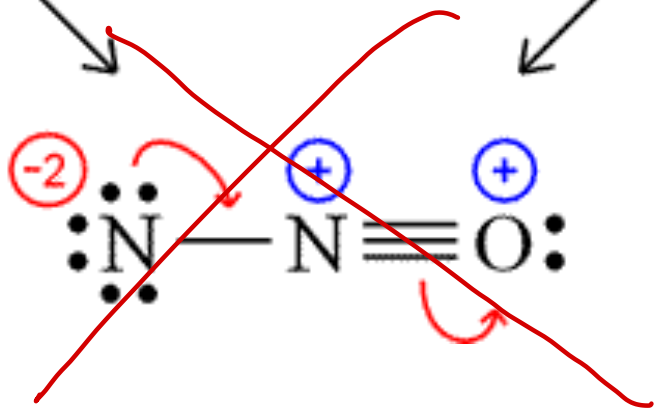
= 5 − (4 + ½ 4)

5 − 6 = −1

5 − (4 + 2)



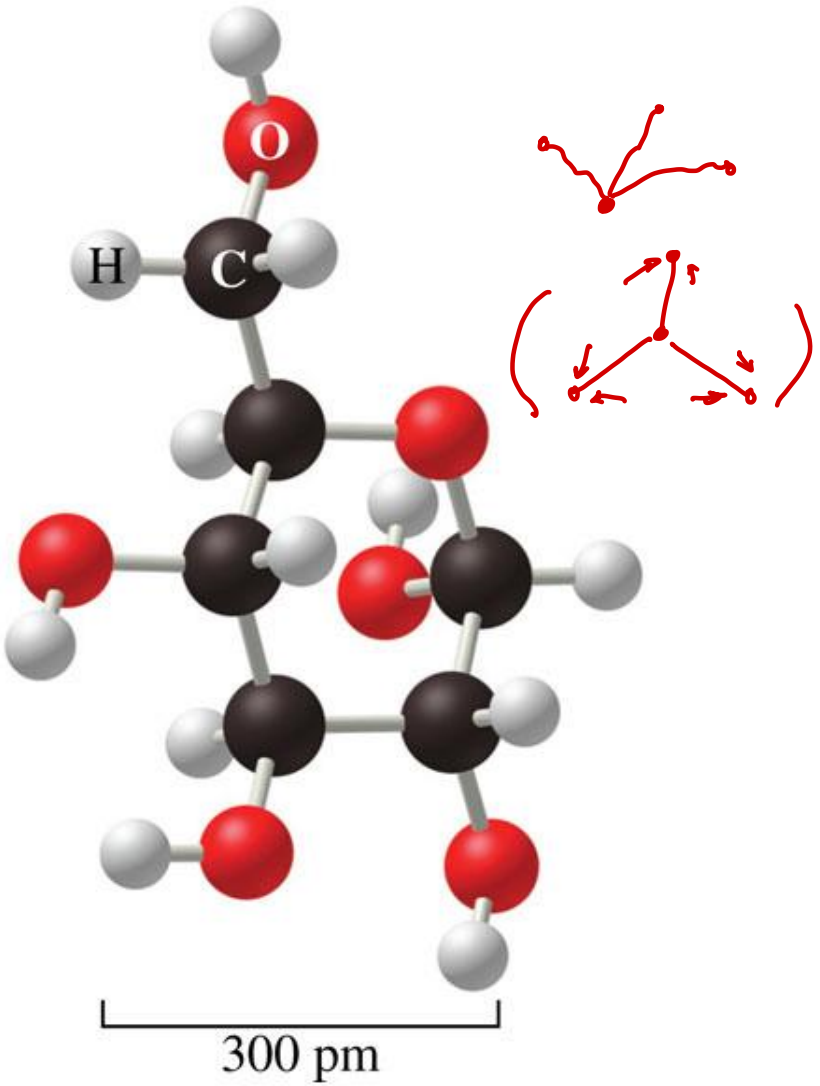
N	less EN	(+)
O	more EN	(−)

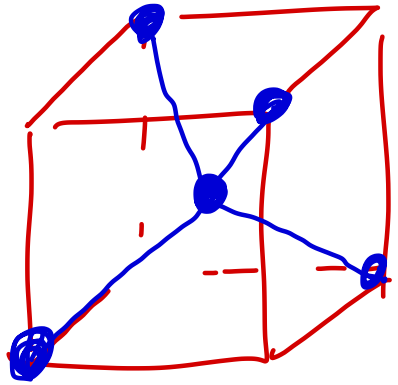


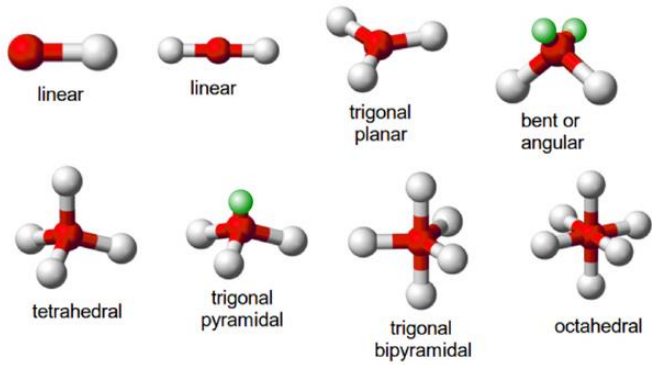
Shapes of Molecules

Predicting Shapes of Molecules

- A simple model used with Lewis structures allows us to predict shapes of molecules.
- **Valence-Shell Electron-Pair Repulsion Theory (VSEPR theory)** is based on the fact that negative charges repel one another.
  - Valence electron pairs (bonding or nonbonding) repel one another and take up positions that maximize their distance and angles between them.

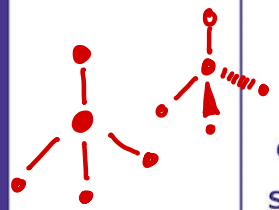






Number of Electron Dense Areas	Electron-Pair Geometry	Molecular Geometry				
		No Lone Pairs	1 lone Pair	2 lone Pairs	3 lone Pairs	4 lone Pairs
2	Linear	Linear				
3	Trigonal planar	Trigonal planar	Bent			
4	Tetrahedral	Tetrahedral	Trigonal pyramidal	Bent		
5	Trigonal bipyramidal	Trigonal bipyramidal	Sawhorse	T-shaped	Linear	
6	Octahedral	Octahedral	Square pyramidal	Square planar	T-shaped	Linear

CN	Number of Lone Electron Pairs							
	0	e.g.	1	e.g.	2	e.g.	3	e.g.
2	 linear	CO_2						
3	 trigonal planar	BCl_3 SO_3	  angled	SO_2 NO_2^- O_3	  linear	O_2		
4	 tetrahedral	CH_4 SO_4^{2-}	  trigonal pyramidal	NH_3	  angled	H_2O	  linear	HCl
5	 trigonal bipyramidal	PCl_5	  bisphenoidal (seesaw)	SF_4	  T-shaped	ClF_3	  linear	I_3^-
6	 octahedral	SF_6	  square pyramidal	ClF_5	  square planar	ICl_4^-		

CN	Number of Lone Electron Pairs							
	0	e.g.	1	e.g.	2	e.g.	3	e.g.
2	 linear	CO_2						
3	 trigonal planar	BCl_3 SO_3	 angled Bent	SO_2 NO_2^- O_3	linear	O_2		
4	 tetrahedral	CH_4 SO_4^{2-}	 trigonal pyramidal	NH_3	angled	H_2O	linear	HCl
5	trigonal bipyramidal	PCl_5	bisphenoidal (seesaw)	SF_4	T-shaped	ClF_3	linear	I_3^-
6	octahedral	SF_6	square pyramidal	ClF_5	square planar	ICl_4^-		

Practice

PF_5	CS_2	BrO_3^-
NH_4^+	SCl_4	BrF_5
BF_3	SCl_6	PH_3
NF_3	SO_4^{2-}	CO_3^{2-}
$SiCl_4$	ClO_3^-	CH_2O
NO_3^-	O_3	CCl_4
AlH_3	SO_2	SO_3
CO	$CHCl_3$	BrF_3
H_2S	I_3^-	H_3O^+

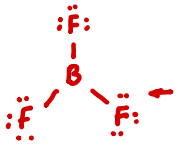
PF_5

40 electrons
tbp
tbp

NH_4^+

8 electrons
Td
Td

BF_3



24 electrons
trigonal planar
trigonal planar

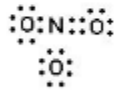
NF_3

26 electrons
Td
trigonal pyr.

$SiCl_4$

32 electrons
Td
Td

NO_3^-



24 electrons
trigonal planar
trigonal planar

AlH_3

6 electrons
trigonal planar
trigonal planar

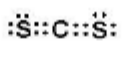
CO

10 electrons
linear
linear

H_2S

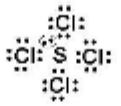
8 electrons
Td
bent

CS_2



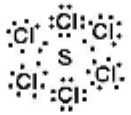
16 electrons
linear
linear

SCl_4



34 electrons
tbp
see-saw

SCl_6



48 electrons
Oh
Oh

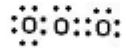
SO_4^{2-}

32 electrons
Td
Td

ClO_3^-

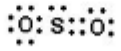
26 electrons
Td
trigonal pyr.

O_3



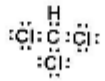
18 electrons
trigonal planar
bent

SO_2



18 electrons
trigonal planar
bent

$CHCl_3$



26 electrons
Td
Td

I_3^-

22 electrons
tbp
linear

BrO_3^-

26 electrons
Td
trigonal pyr.

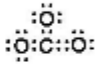
BrF_5

42 electrons
Oh
square pyr.

PH_3

8 electrons
Td
trigonal pyr.

CO_3^{2-}

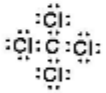


24 electrons
trigonal planar
trigonal planar

CH_2O

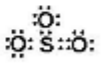
12 electrons
trigonal planar
trigonal planar

CCl_4



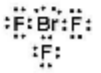
32 electrons
Td
Td

SO_3



24 electrons
trigonal planar
trigonal planar

BrF_3



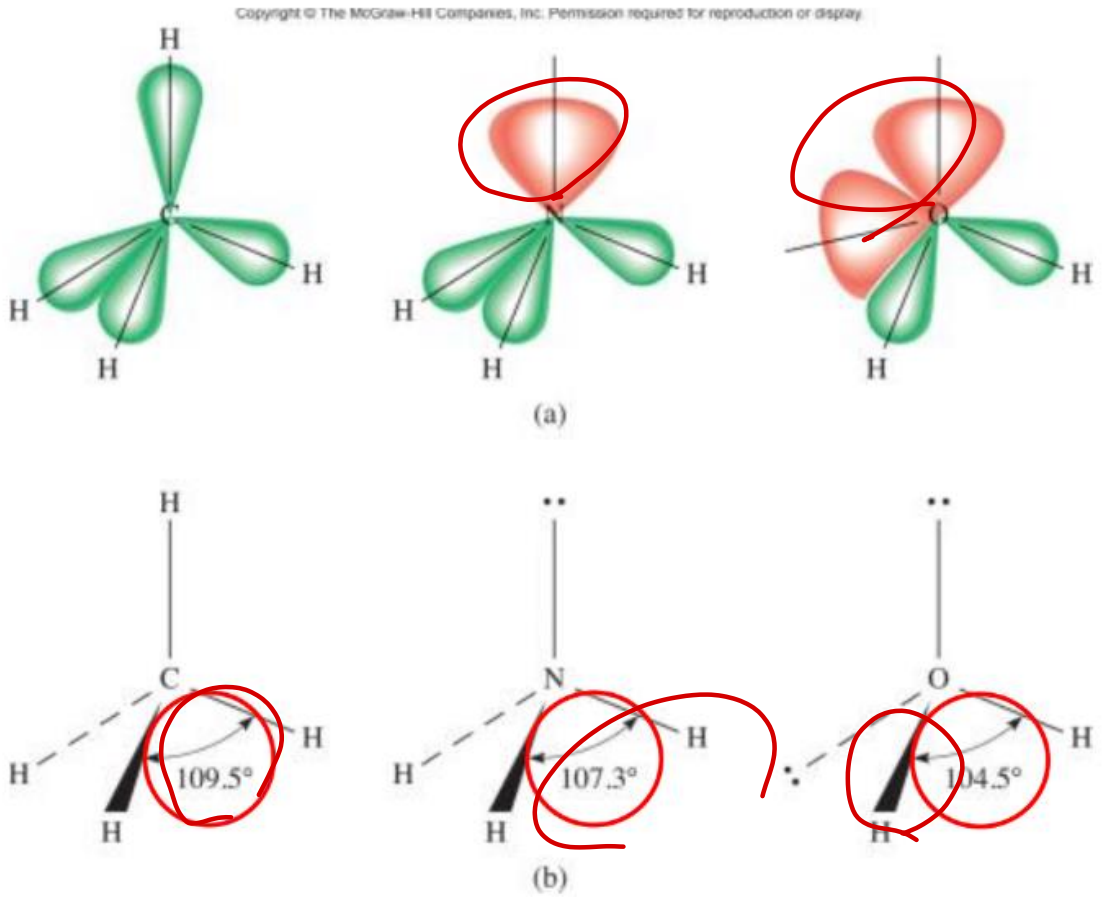
28 electrons
tbp
T-shaped

H_3O^+

8 electrons
Td
trigonal pyr.

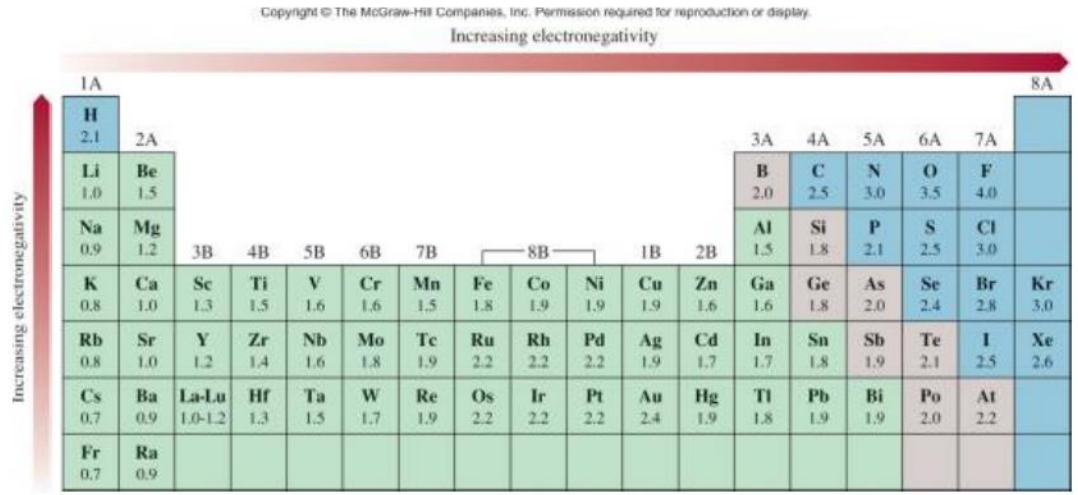
Change in Bond Angle

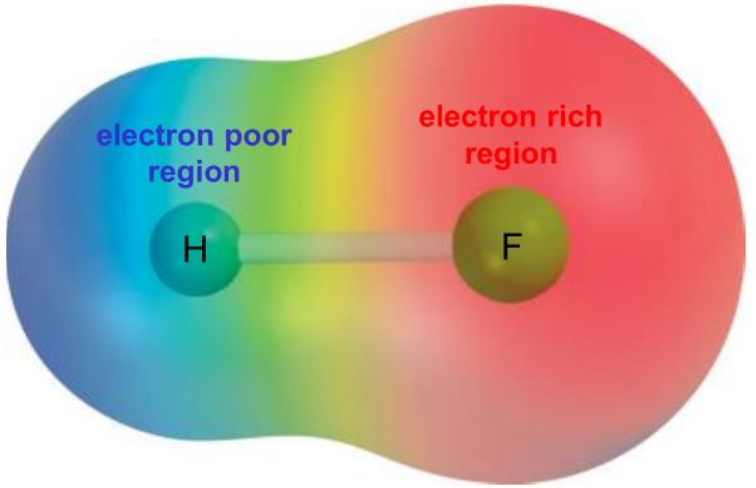
- Lone pairs pushes the other elements
- A shoelementsrter bond pushes the other elements
- Larger elements pushes the smaller elements



Electronegativity in Molecular Bonding

- Polar covalent bond, or polar bond is a covalent bond with greater electron density around one of the two atoms. This occurs due to uneven electronegativity.



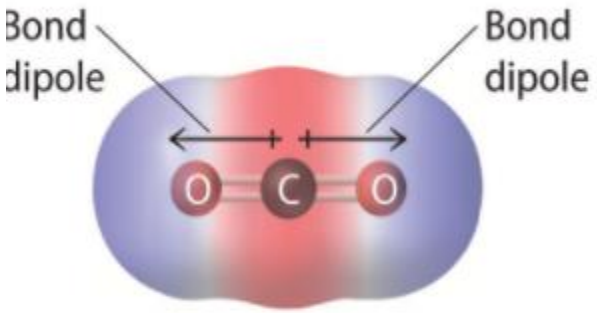


- If one element has much stronger electronegativity, it will just take away the electron from the other element (transfer of e-)
- When they have similar electronegativity, they will share that electron.

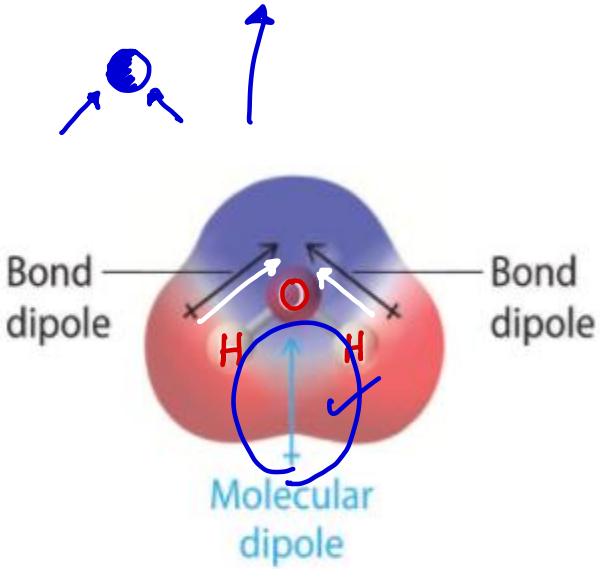
Difference	Bond Type
0	Covalent
≥ 2	Ionic
0 < and <2	Polar Covalent

Net Dipole

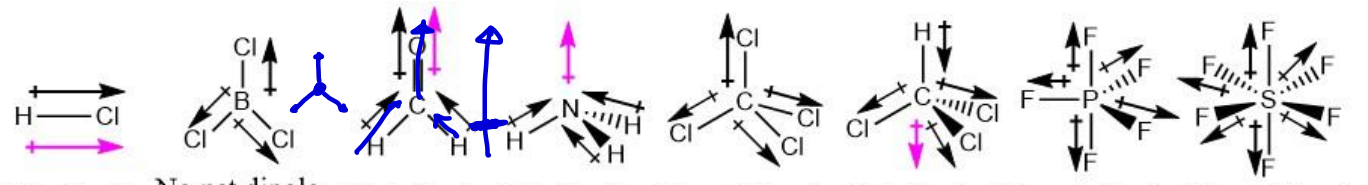
- Sum of dipole moments of the molecule = net dipole
- A molecule can have a polar bond, but it may not possess a dipole moment if it is in a symmetrical geometry

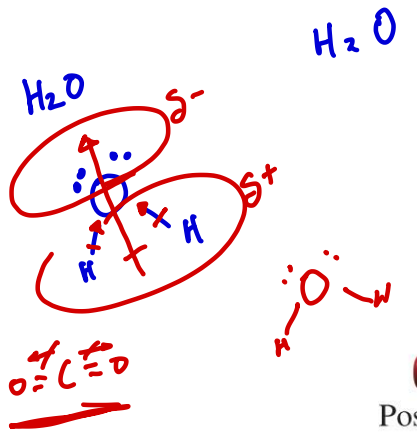


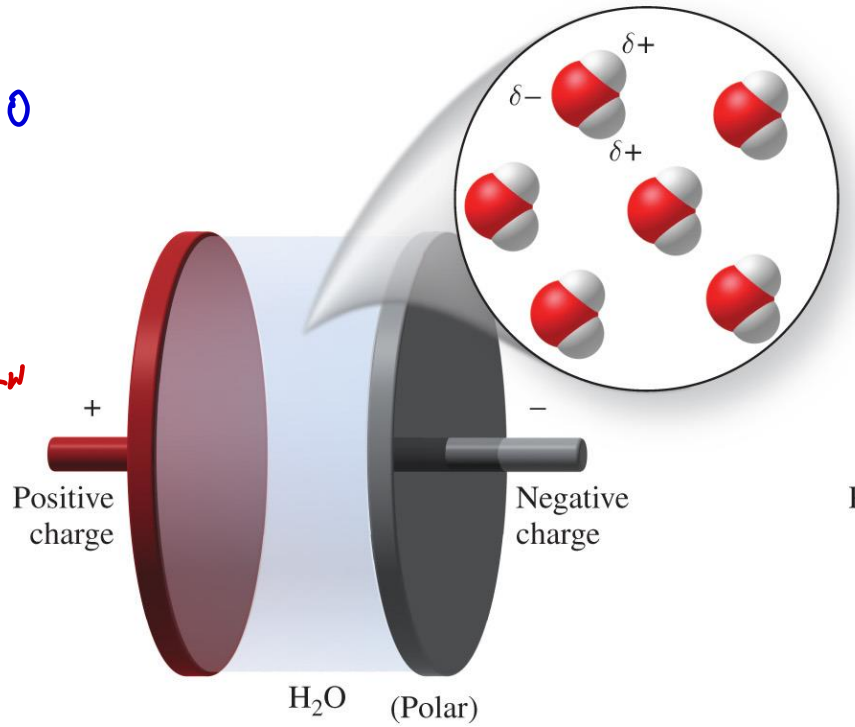
(a) No net dipole moment

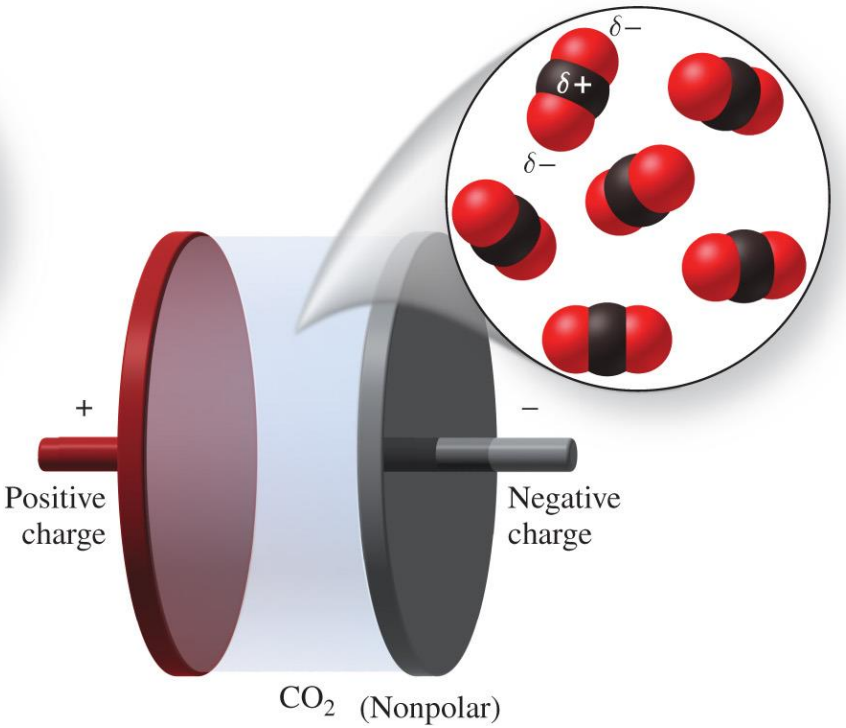


(b) Net dipole moment









- NH_3
- BH_3
- CS_2
- H_2S
- CH_2Cl_2