Bonding, Lewis Structures____________ Z Ch 12.15, 13

"There are therefore Agents in Nature able to make the Particles of Bodies stick together by very strong Attractions. And it is the Business of Experimental Philosophy to find them out." **Isaac Newton, 1717**

"Two atoms may conform to the rule of eight, or the octet rule, not only by the transfer of electrons from one atom to another, but also by sharing one or more pairs of electrons. These electrons which are held in common by two atoms may be considered to belong to the outer shells of both atoms." **Gilbert Newton Lewis, 1916**

"We shall say that there is a chemical bond between two atoms or groups of atoms in case that the forces acting between them are such as to lead to the formation of an aggregate with sufficient stability to make it convenient for the chemist to consider it as an independent molecular species." **Linus Carl Pauling, 1939**

(Nobel Prize in Chemistry in 1954 "for his research into the nature of the chemical bond and its application to the elucidation of the structure of complex substances" and Nobel Peace Prize in 1962.)

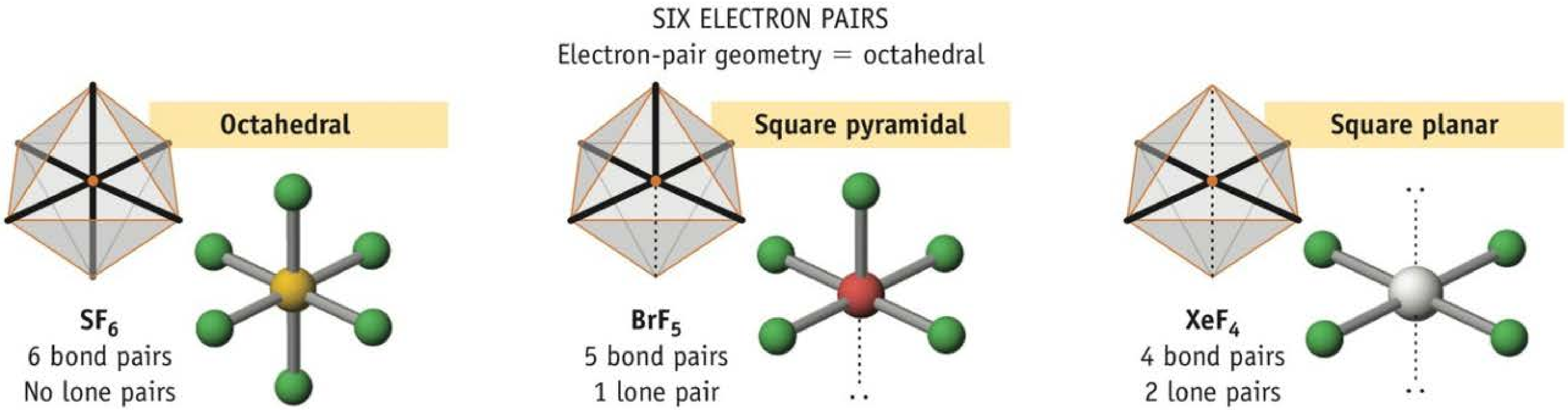
Quiz on Friday

Seven SIMPLE BONDING CONCEPTS

13.3 – Bond Polarity and Dipole Moments , 6) dipole moment
7) electronegativity and atomic size effects (EX 1 and 2)

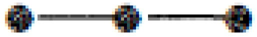
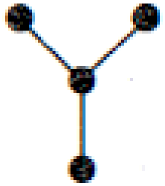
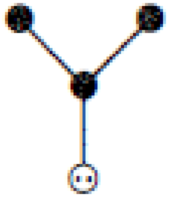
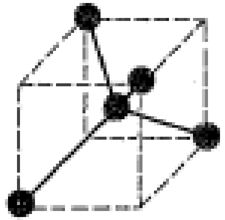
REVIEW FROM MONDAY

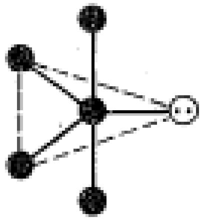
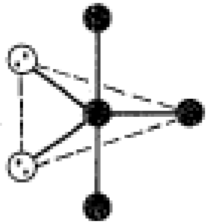
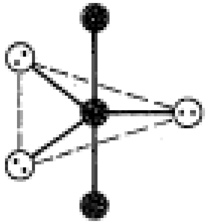
Electronic Geometry: Octahedral (SN=6)



REVIEW FROM MONDAY

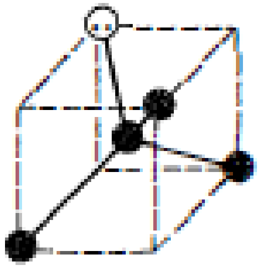
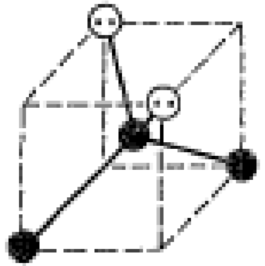
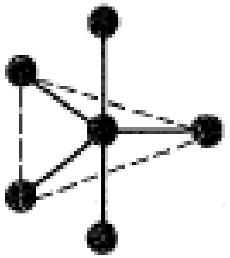
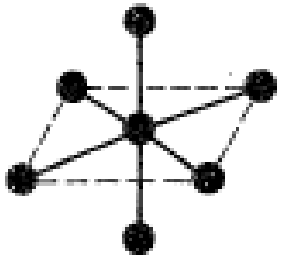
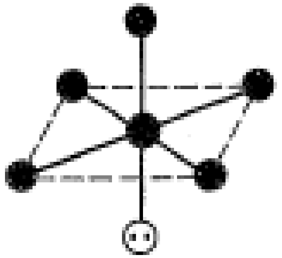
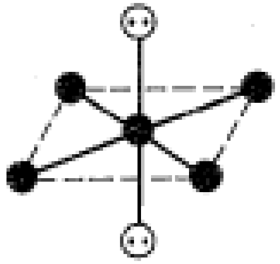
Lewis Structures and VSEPR

SN	Number of lone pairs	Molecular shape	Example
2	0	 linear	BeH_2, CO_2
3	0	 trigonal planar	SO_3, BF_3
3	1	 angular	SO_2, O_3
4	0	 tetrahedral	CH_4, CF_4, SO_4^{2-}

SN	Number of lone pairs	Molecular shape	Example
5	1	 sawhorse seesaw	SF_4
5	2	 T-shaped	ClF_3
5	3	 linear	XeF_2, I_3^-, IF_2^-

REVIEW FROM MONDAY

Lewis Structures and VSEPR (Beyond Octets)

4	1	 trigonal pyramidal	NH_3, PF_3, $AsCl_3$
4	2	 angular	H_2O, H_2S, SF_2
5	0	 trigonal bipyramidal	PF_5, PCl_5, AsF_5
6	0	 octahedral	SF_6, PF_6^-, SiF_6^{2-}
6	1	 square pyramidal	IF_5, BrF_5
6	2	 square planar	XeF_4, IF_4^-

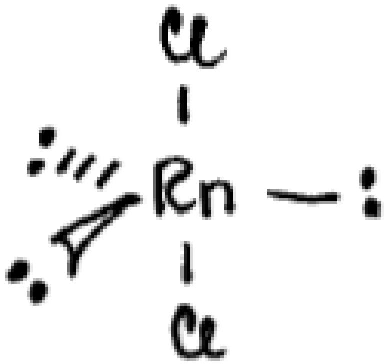
5) VSE (Valence Shell Expansion)

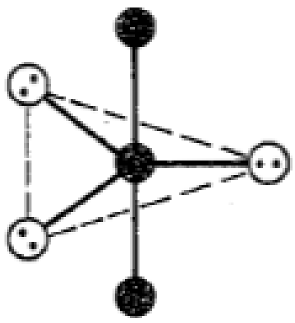
$RnCl_2$

VAL = 8 + 2(7) = 22
STAB = 3(8) = 24
BOND = 24 – 22 = 2/2 = 1 BP
LONE = 22 – 2 = 20/2 = 10 LP
2 Rn – Cl bonds => VSE =>
2 BP, 9 LP (6 on Cl)

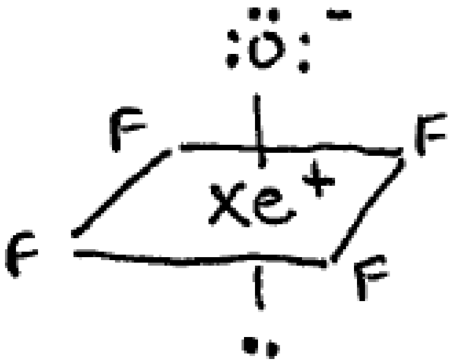
$XeOF_4$

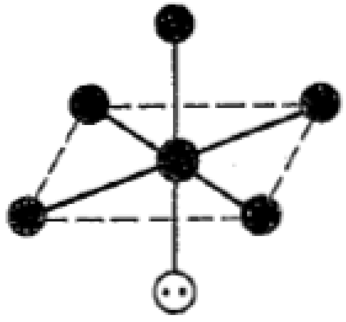
VAL = 8 + 6 + 4(7) = 42
STAB = 6(8) = 48
BOND = 48 – 42 = 6/2 = 3 BP
LONE = 42 – 6 = 36/2 = 18 LP
need 5 bonds => 5 BP => 2 VSE expansions
5 BP, 16 LP (15 on O,F)





linear





square pyramidal

Seven SIMPLE BONDING CONCEPTS

1) Lewis structures
2) Resonance
3) Formal charge
4) Valence Shell Electron Pair Repulsion (VSEPR) Theory
5) Valence shell expansion (VSE)
6) Bond and molecular polarity
7) Effect of electronegativity and atomic size on bond angles

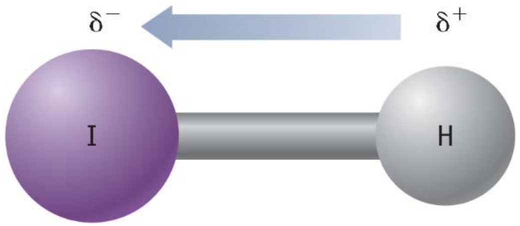
Molecular Polarity

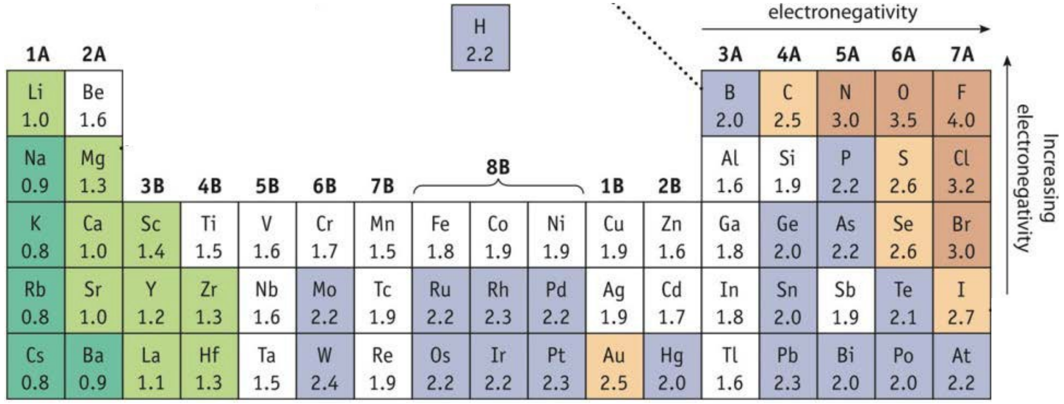
For a molecule to be polar it must

1. have a polar bond (bond between atoms of different electronegativities)
2. bond polarities must add to give a net polarity (dipole) for the molecule
3. a dipole moment is a vector

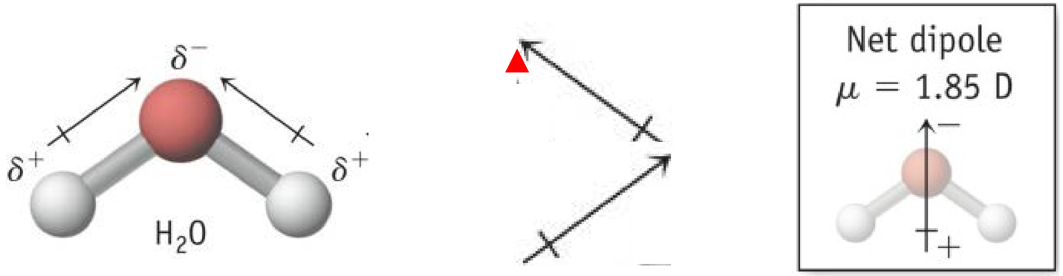
$$\mu = \Sigma\, Q_i \boldsymbol{r}_i$$

Consider HI: I is more electronegative than H so the dipole points from H (δ+) to I (δ-)



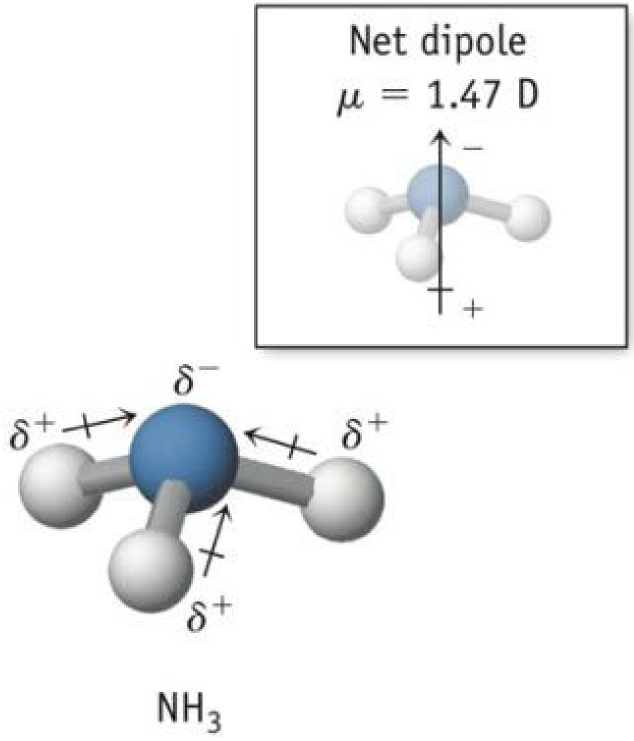


In water each O – H bond is polar with the dipole pointing from H (δ+) to O (δ-). Then the two bond dipoles need to be vectorially added to give the net dipole for the molecule

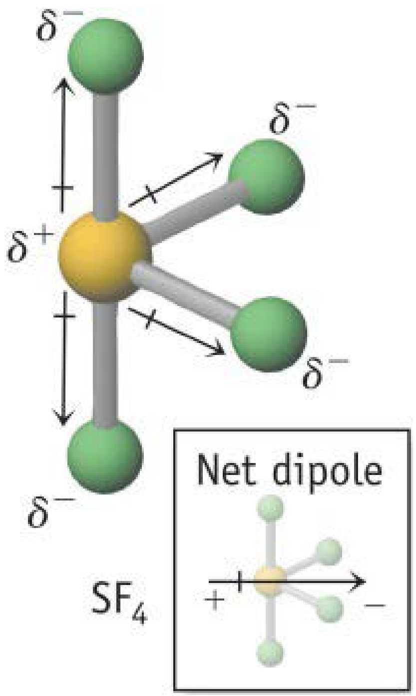


Molecular Polarity

ammonia, NH_3



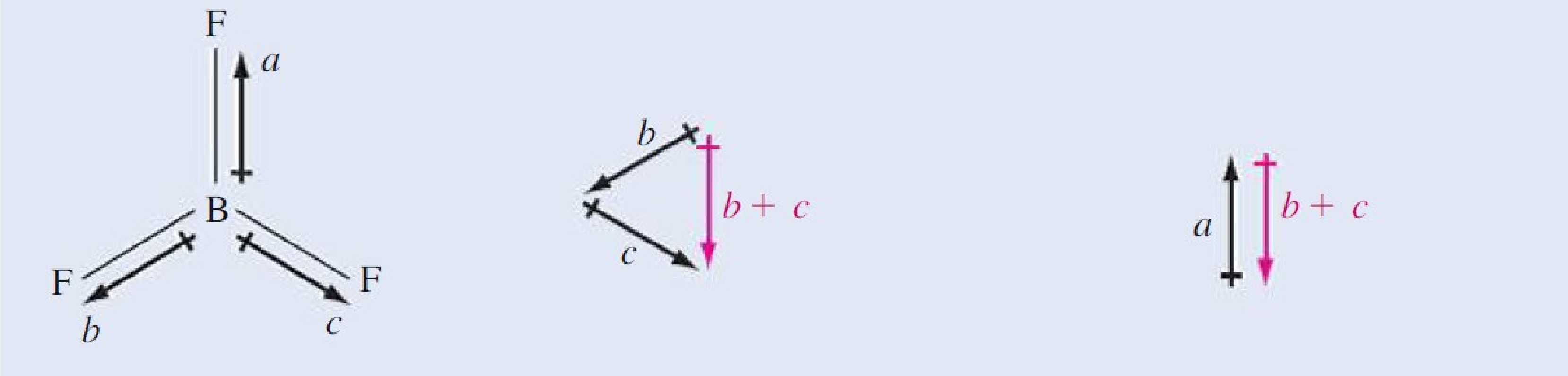
sulfur tetrafluoride, SF_4



Molecule with Polar Bonds May Not be Polar

The addition of bond dipoles can be extended to more than two. Consider BF_3

1. draw the Lewis structure
2. determine the electronic geometry and then the molecular geometry (determines bond dipoles)
3. sketch the structure (three dimensional if needed
4. vectorially add the bond dipoles

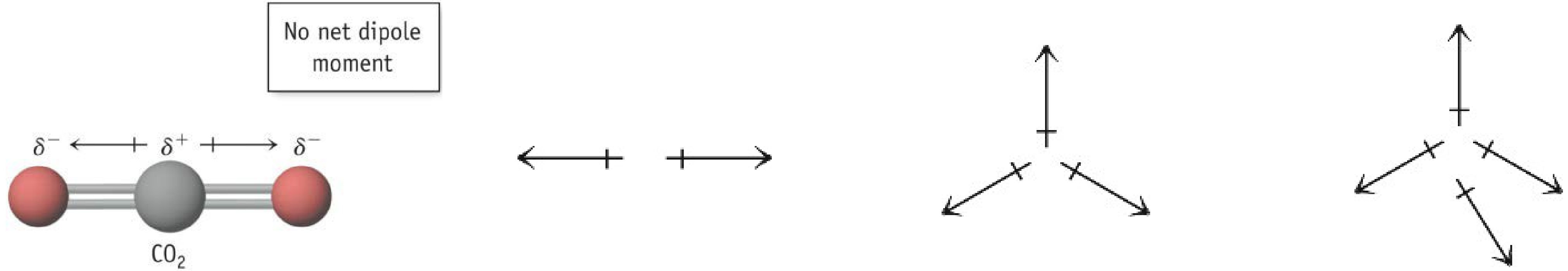


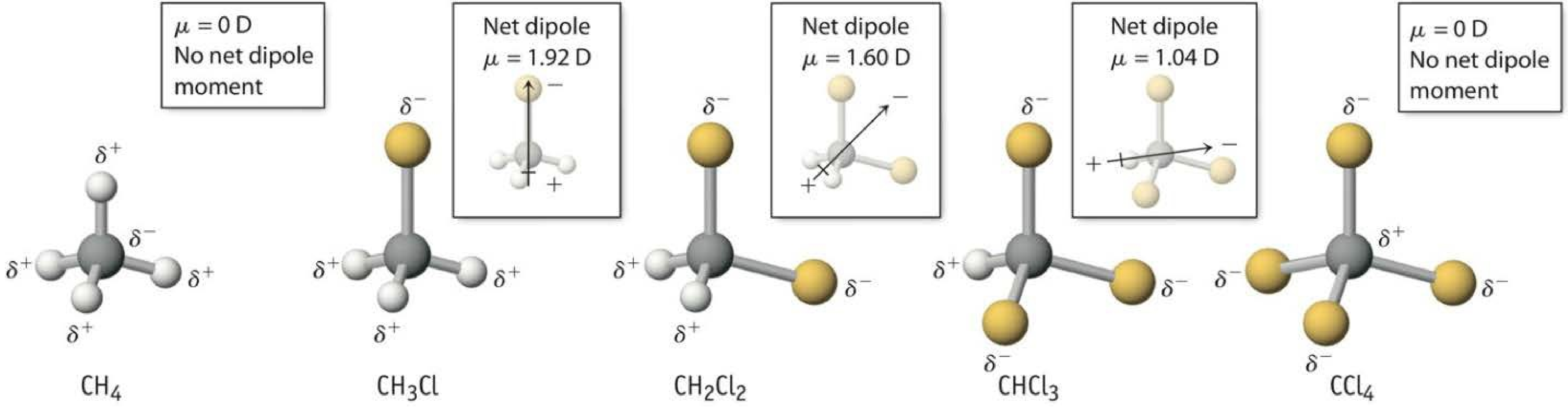
The bond dipoles are labeled *a*, *b*, and *c*.

Add *b* and *c* “head-to-tail” to form the vector sum *b* + *c*.

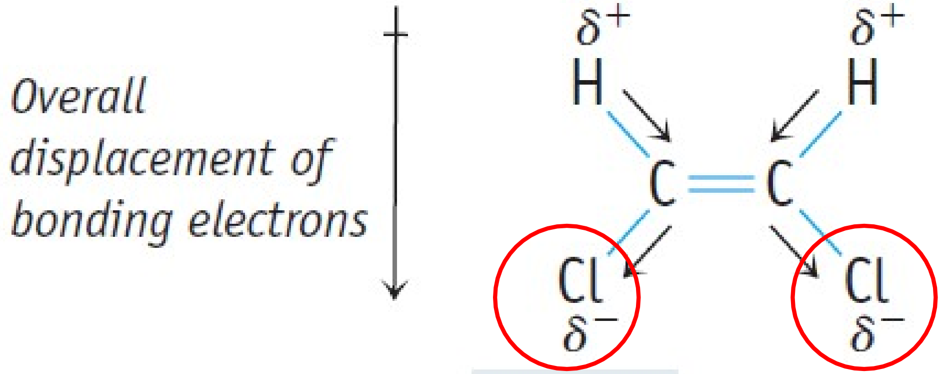
The vector sum of *a* and *b* + *c* is a vector of zero length (no dipole).

Molecule with Polar Bonds May Not be Polar

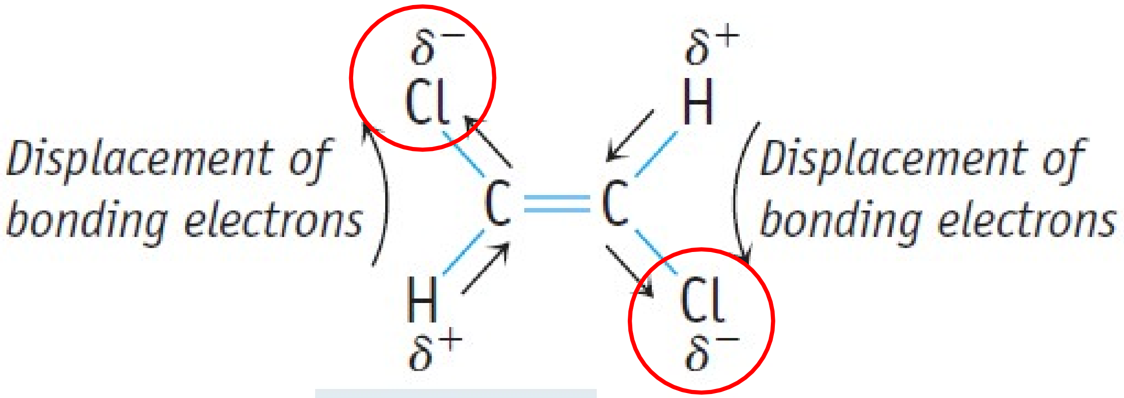




Molecular Polarity for Organic Molecules



A, polar, displacement of bonding electrons to one side of the molecule



B, not polar, no net displacement of bonding electrons to one side of the molecule

Electronegativity and Atomic Size Effects

In a bond between elements of differing electronegativity, the **more electronegative element pulls the bonding pair electrons more strongly to itself**. If a central atom is surrounded by atoms of large electronegativity, the bonding electrons are drawn away from the central atom, reducing the repulsive effect of these electrons and leading to smaller bond angles. On the other hand, if the central atom has a large electronegativity, bonding electrons are pulled toward it, increasing electronic repulsions and a larger bond angle results.

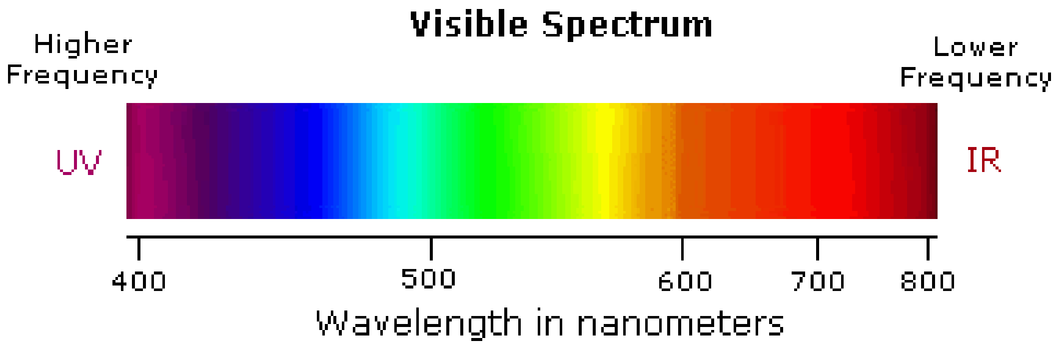
In comparing a bond containing a larger atom to one containing a smaller atom, the **bond with the larger atom naturally has its bonding pair of electrons further removed** from it just due to its size. So a molecule with a large central atom would tend to have smaller bond angles than a smaller central atom.

Electronegativity and Atomic Size Effects

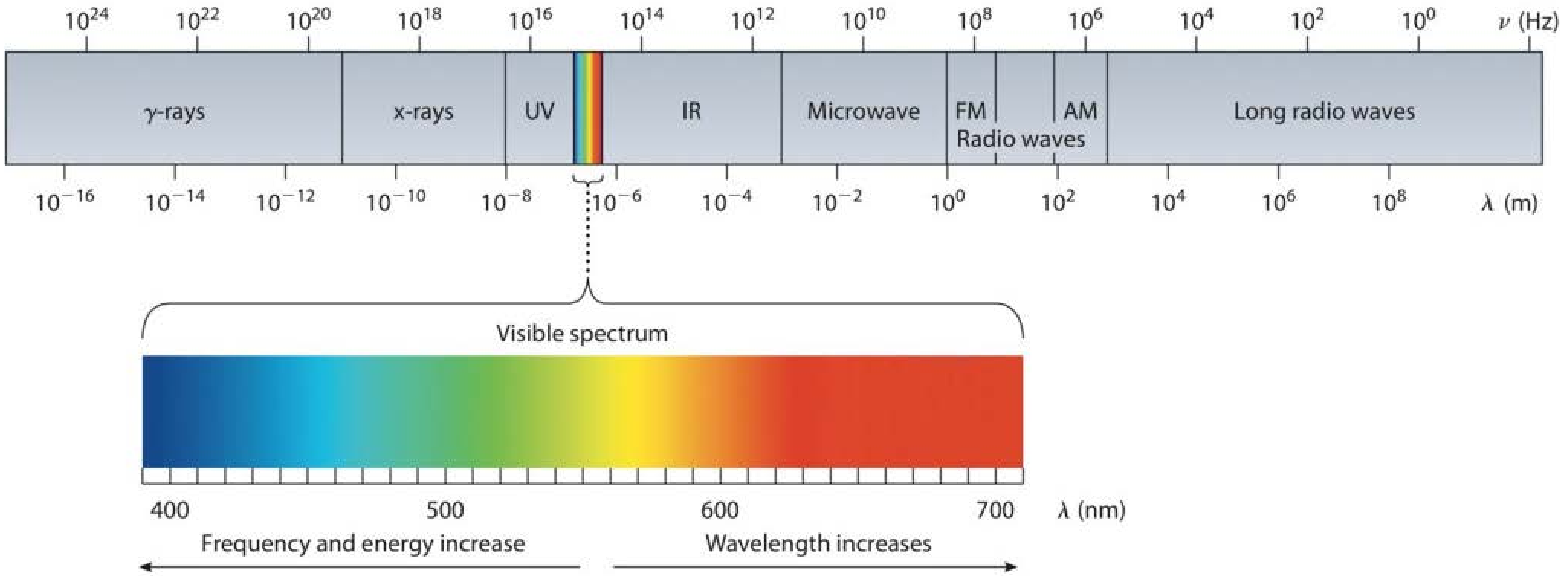
EX 1. Determine the stronger acid in the following pairs and explain why.

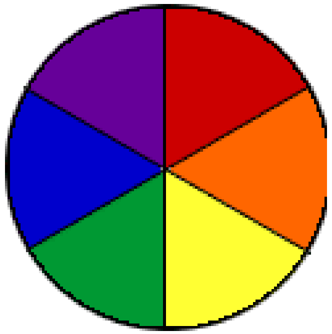
a) H_3PO_3 or H_3PO_4	more lone O atoms
b) CH_4 or NH_3	N more electronegative
c) $H_2AsO_4^-$ or $HAsO_4^{2-}$	easier to remove H^+ from singly charged anion
d) HIO or HClO	Cl more electronegative
e) H_2Se or H_2Te	Te larger

Absorption and Emission of Ultraviolet and Visible Radiation

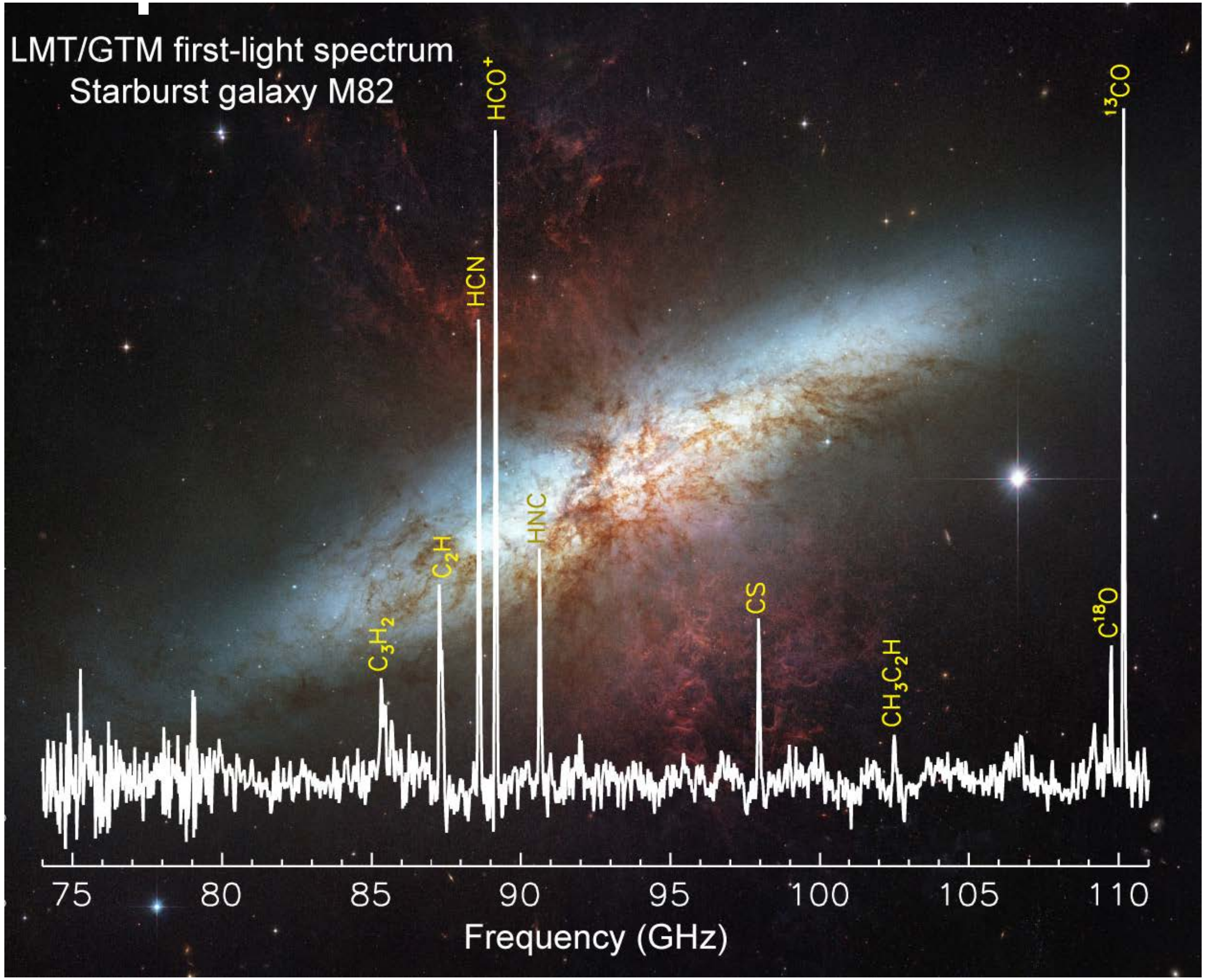


- Violet: 400 - 420 nm
- Indigo: 420 - 440 nm
- Blue: 440 - 490 nm
- Green: 490 - 570 nm
- Yellow: 570 - 585 nm
- Orange: 585 - 620 nm
- Red: 620 - 780 nm

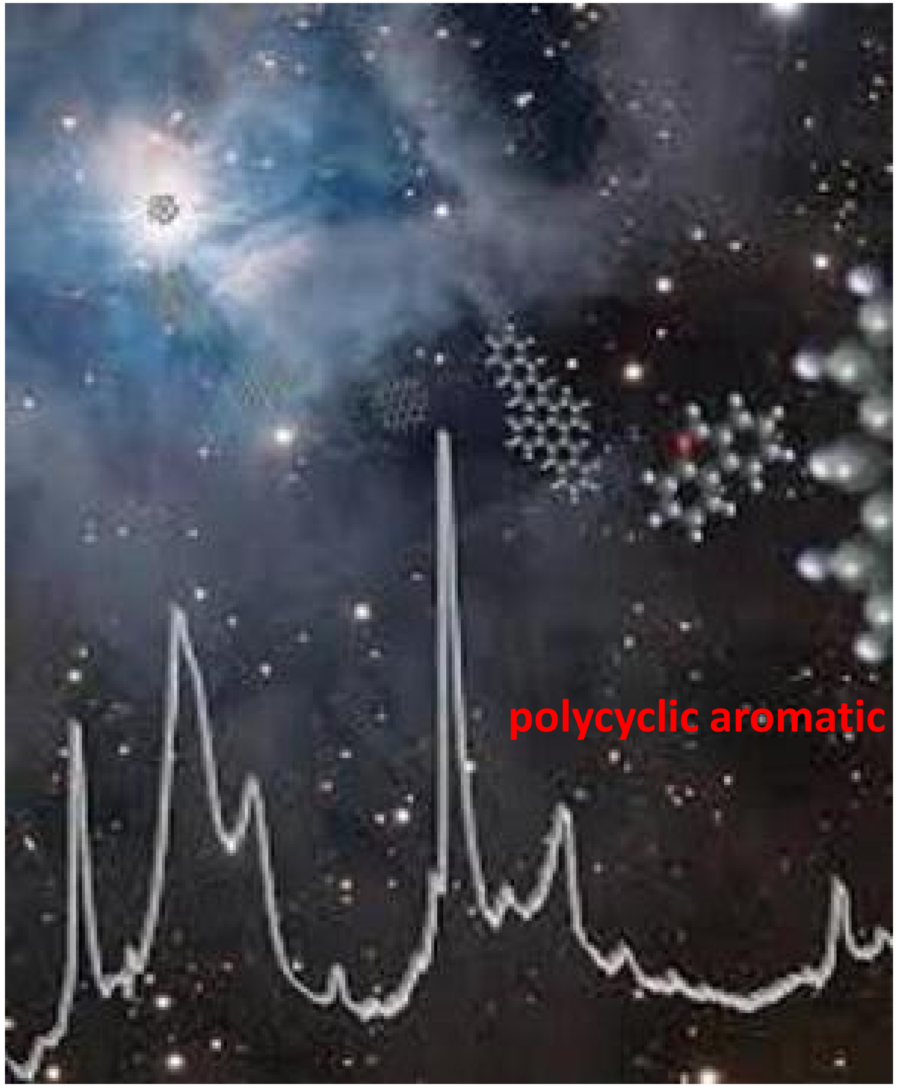




color wheel



LMT/GTM first-light spectrum
Starburst galaxy M82
HCO^+
^{13}CO
HCN
HNC
C_2H
C_3H_2
CS
CH_3C_2H
$C^{18}O$
75
80
85
90
95
100
105
110
Frequency (GHz)

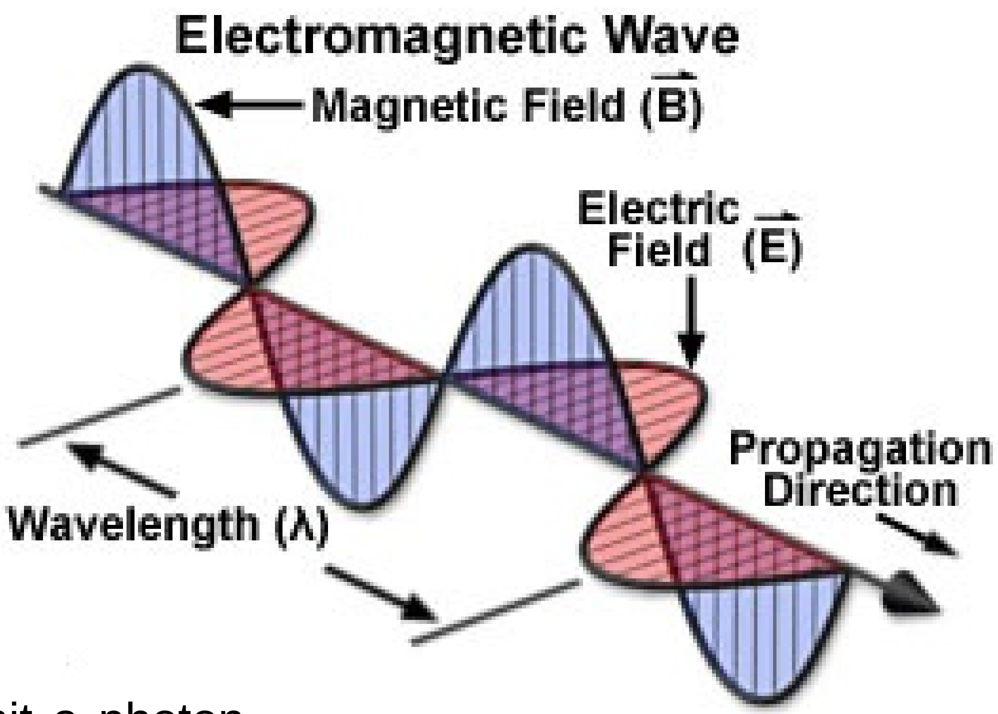


Infrared Emission from Iris Nebula

UV/VIS Emission from Cat’s Eye Nebula

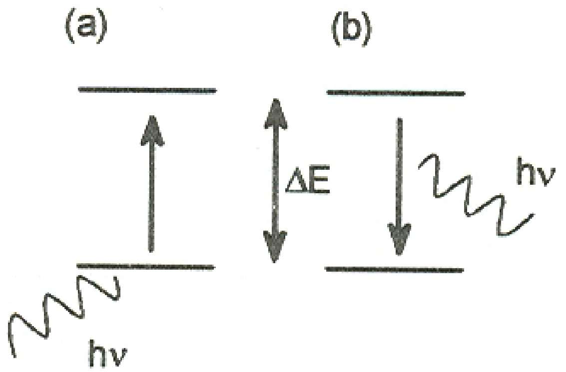
(Hubble Space Telescope) red (H), blue (O), green (singly ionized N atoms)

Basic Theory

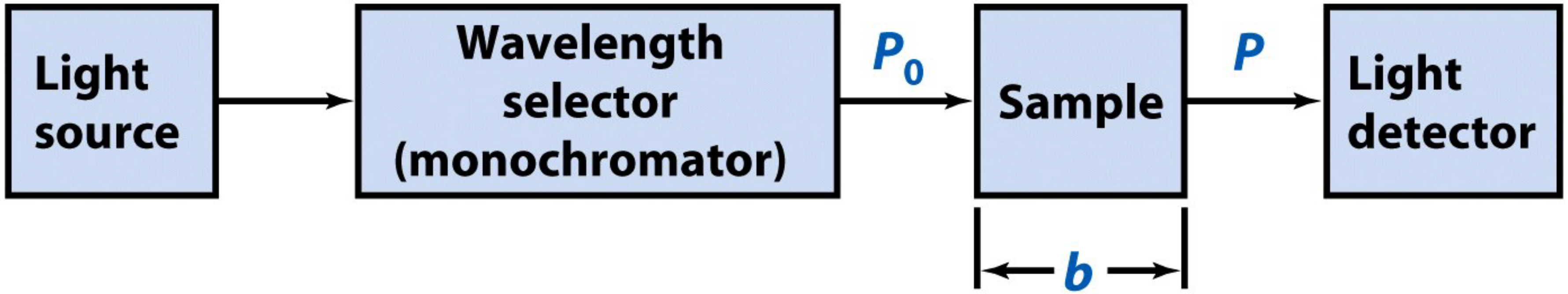


To a) absorb or b) emit a photon of electromagnetic radiation the sample must exhibit periodic motion whose frequency matches that of the absorbed radiation.

$$\Delta E_{sample} = E_{photon} = h\nu = hc/\lambda$$



Basic Experiment (black box lab exp)



$$T = \frac{P}{P_0}$$

transmittance

$$A = \log\left(\frac{P_0}{P}\right) = -\log T$$

absorbance

$$A = \varepsilon bc$$

Beer's Law

1A (1)	2A (2)	3B (3)	4B (4)	5B (5)	6B (6)	7B (7)	(8)	8B (9)	(10)	1B (11)	2B (12)	3A (13)	4A (14)	5A (15)	6A (16)	7A (17)	8A (18)
1 **H** 1.008																	2 **He** 4.0026
3 **Li** 6.94	4 **Be** 9.0122											5 **B** 10.81	6 **C** 12.011	7 **N** 14.007	8 **O** 15.999	9 **F** 18.998	10 **Ne** 20.180
11 **Na** 22.990	12 **Mg** 24.305											13 **Al** 26.982	14 **Si** 28.085	15 **P** 30.974	16 **S** 32.06	17 **Cl** 35.45	18 **Ar** 39.95
19 **K** 39.098	20 **Ca** 40.08	21 **Sc** 44.956	22 **Ti** 47.867	23 **V** 50.942	24 **Cr** 51.996	25 **Mn** 54.938	26 **Fe** 55.85	27 **Co** 58.933	28 **Ni** 58.693	29 **Cu** 63.55	30 **Zn** 65.4	31 **Ga** 69.723	32 **Ge** 72.63	33 **As** 74.922	34 **Se** 78.97	35 **Br** 79.904	36 **Kr** 83.80
37 **Rb** 85.468	38 **Sr** 87.62	39 **Y** 88.906	40 **Zr** 91.22	41 **Nb** 92.906	42 **Mo** 95.95	43 **Tc** (97/8)	44 **Ru** 101.1	45 **Rh** 102.91	46 **Pd** 106.42	47 **Ag** 107.87	48 **Cd** 112.41	49 **In** 114.82	50 **Sn** 118.71	51 **Sb** 121.76	52 **Te** 127.6	53 **I** 126.90	54 **Xe** 131.29
55 **Cs** 132.91	56 **Ba** 137.33	57 **La** 138.91	72 **Hf** 178.5	73 **Ta** 180.95	74 **W** 183.84	75 **Re** 186.21	76 **Os** 190.2	77 **Ir** 192.22	78 **Pt** 195.08	79 **Au** 196.97	80 **Hg** 200.59	81 **Tl** 204.38	82 **Pb** 207.2	83 **Bi** 208.98	84 **Po** (209)	85 **At** (210)	86 **Rn** (222)
87 **Fr** (223)	88 **Ra** (226)	89 **Ac** (227)	104 **Rf** (267)	105 **Db** (268)	106 **Sg** (269)	107 **Bh** (271)	108 **Hs** (277)	109 **Mt** (276/7)	110 **Ds** (281)	111 **Rg** (282)	112 **Cn** (285)	113 **Nh** (286)	114 **Fl** (289)	115 **Mc** (290)	116 **Lv** (293)	117 **Ts** (294)	118 **Og** (294)

Lanthanides	58 **Ce** 140.12	59 **Pr** 140.91	60 **Nd** 144.24	61 **Pm** (145)	62 **Sm** 150.4	63 **Eu** 151.96	64 **Gd** 157.3	65 **Tb** 158.93	66 **Dy** 162.50	67 **Ho** 164.93	68 **Er** 167.26	69 **Tm** 168.93	70 **Yb** 173.05	71 **Lu** 174.97
Actinides	90 **Th** 232.04	91 **Pa** 231.04	92 **U** 238.03	93 **Np** (237)	94 **Pu** (244)	95 **Am** (243)	96 **Cm** (247)	97 **Bk** (247)	98 **Cf** (251)	99 **Es** (252)	100 **Fm** (257)	101 **Md** (258)	102 **No** (259)	103 **Lr** (262)