Quantitative analysis of organic compound (from last class)

Determining the empirical experimental formula:

- Definition: empirical formula is ratio of atoms to each other in a molecular formula
- Three steps to calculate the empirical formula:
  i) divide each percentage (%) by the atomic weight of element → crude ratio
  ii) divide all crude ratio by the smallest crude ratio → refined ratio
  iii) Multiply the refined ratio by an integer value to get integral ratio

% Composition	Crude ratio	Refined ratio	Integral ratio
65.1 % C	65.1 / 12.0 = 5.42	5.42 / 1.63 = 3.34	3.34 x 3 = 10
8.83 % H	8.83 / 1.01 = 8.76	8.76 / 1.63 = 5.39	5.39 x 3 = 16
26.1 % O	26.1 / 16.0 = 1.63	1.63 / 1.63 = 1.00	1.00 x 3 = 3

From the integral ratio, the empirical formula is $C_{10}H_{16}O_3$. Using this formula an empirical weight can be calculated.

C $10 \times 12 = 120$ g/mol
H $16 \times 1 = 16$ g/mol
O $3 \times 16 = 48$ g/mol

$C_{10}H_{16}O_3$ = 184 g/mol

Note: suppose the molecular weight is given as 368 g/mol, then the molecular formula is obtained by multiplying the integral ratios by a factor of 2 and it would be $C_{20}H_{32}O_6$.

Gas Law: (different kinds of units for pressure and volume can be used provided the value of the gas constant is adjusted to those units)

PV = nRT P=Pressure in mmHg
V=Volume in L
n=moles
T=temperature in °K; °K and °C are same size but 0 °K = minus 273 °C

R is a constant $\frac{0.082\ L \cdot atm.}{Mol\ .\ °K}$

Sample Question- What volume will 3 mL of N_2 gas occupy at standard pressure and temperature (STP) ?

Standard Pressure is 1 atmosphere or 760 mm Hg; Standard temperature is 273 °K

$\frac{P_1V_1}{P_2V_2} = \frac{nRT_1}{nRT_2}$ divide equations to give $\frac{P_1V_1}{P_2V_2} = \frac{T_1}{T_2}$

$P_1 = 760$ mmHg $T_1 = 273$ °K

$P_2 = 750$ mmHg $T_2 = 298$ °K $V_2 = 3$ mL

Solve for V_1

$$V_1 = \frac{T_1P_2V_2}{T_2P_1} = \frac{(273\ °K)(750\ mmHg)(3\ mL)}{(298\ °K)(760\ mmHg)}$$

= 2.71 mL is the answer

Question: How many moles of N_2 is 2.71 mL at STP and what is its mass ?

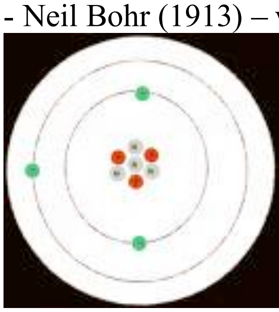
NOTE: 1 mole of an ideal gas occupies 22.4 L at STP.

$$2.71 \times 10^{-3}\ L \times \frac{1\ mole}{22.4\ L} = 1.21 \times 10^{-4}\ \text{moles of } N_2$$

1.21×10^{-4} mol × 28 g/mol = 3.4 mg of N_2

Atomic theory:

- Neil Bohr (1913) – won his Nobel prize for his atomic theory – NOT fully correct



- the neutrons and protons occupy a dense central region called the nucleus
- the electrons orbit the nucleus much like planets orbiting the Sun

- de Broglie (1924) – his 12 page PhD thesis won him the Nobel prize
  - he proposed that ordinary "particles" such as electrons and protons could behave as both particles and waves (wave-particle duality)

- the orbitals of an atom are described by wave functions (mathematical equations) – they have no direct physical meaning but when squared, provide electron density
- ψ = orbital

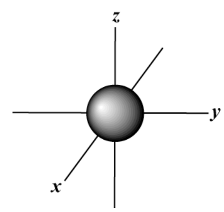
- (orbital)^2 = electron density distribution

Note. Often the electron density distribution is called an "orbital" by chemists

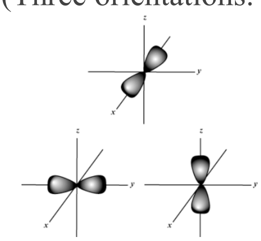
For hydrogen (H) atom: >95% of electron density is found within 1Å = 10^{-8} cm

Orbitals:

1. S-orbital - spherical shaped (electron density)



2. p-orbital - dumbbell-shaped (Three orientations: placed on the x, y and z-axis)



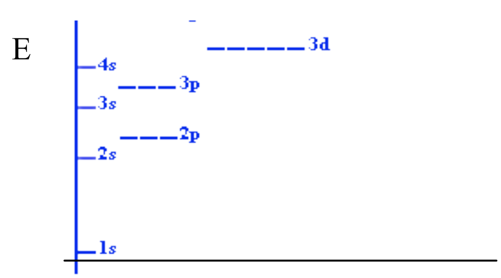
Basic principles:

- like charges repel each other
- unlike charges attract each other
- atoms want to be in inert gas electron configuration (isoelectronic with inert gas)

Atoms	Protons (+)	Neutrons	1s electrons	2s electrons	2p electrons
H	1	0	1		
He	2	2	2		
Li	3	3	2	1	

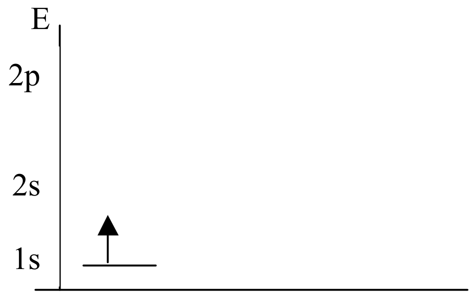
Abbreviation of electron - e^-

Energy (E) level diagram for an atom:

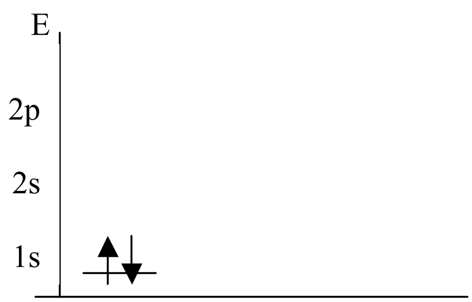


Rules for filling electron – AUFBAU rule (Build up Principle):

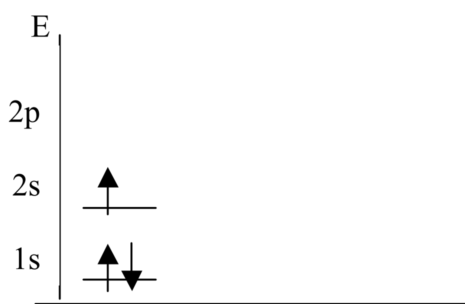
- add electron to lowest energy orbital available
- maximum two electron per orbital (each having opposite spin quantum number)
- Pauli Exclusion principle
- fill 1 electron into each orbital of same energy (degenerate orbital), then add second electron - Hund rule



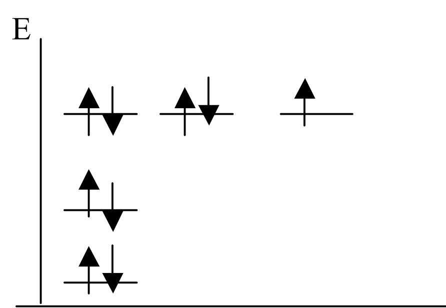
Helium (He)



Lithium (Li)



Fluorine (F)



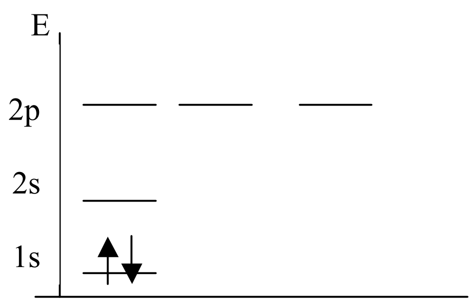
- all elements want inert gas configuration (e.g. Ne) and from above diagrams both Li and F are unhappy with unfilled orbitals (not in inert gas configuration)

Bonding - Ionic

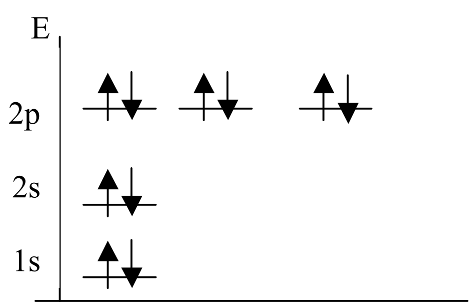
- isoelectronic = same electron configuration
- Li could lose 1e$^-$ from 2s orbital to be isoelectronic to He (as Li$^+$) and F could gain 1e$^-$ to be isoelectronic to Ne (as F$^-$)

$$Li^o \quad + \quad F^o \rightarrow Li^+ \quad + \quad F^-$$

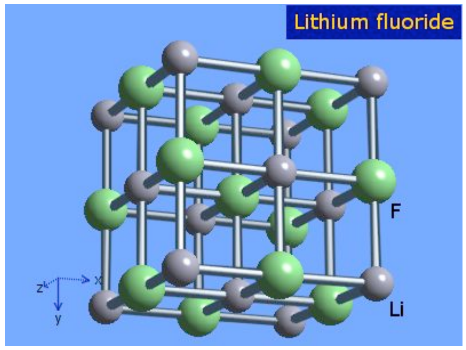
Li$^+$ (cation)



F$^-$ (anion)



- in space these ions would be attracted to each other
- in solution they might be separated due to solvation (e.g. water would surround)
- in solid, they would form a crystalline solid structure

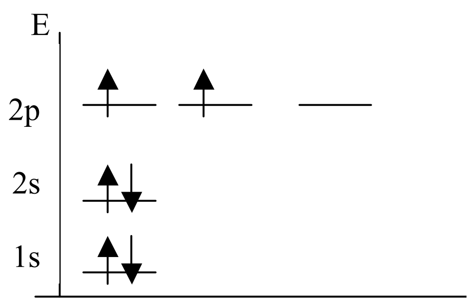


Bonding – Covalent and hybridisation

Electronic configuration of carbon (C):

- atomic number = 6
- atomic weight = 12 (also has 6 neutrons)
- other isotopes of carbon
    - ^{13}C ($6p^+$, 7n) is a stable isotope, 1.1 % natural abundance
    - ^{14}C ($6p^+$, 8n) is radioactive, $t_{1/2}$ = 5700 yrs, ^{14}C dating of organic material

Carbon (C)



- need to gain or lose $4e^-$ to get inert gas configuration – but this gives unfavourable charge buildup:

- C^{4+} isoelectronic with He

- C^{4-} isoelectronic with Ne

- so, carbon makes 4 bonds to share $4e^-$ (covalent bonding)