Chapter 3: Calculations with Chemical Formulas and Equations

* 3.1: Molecular weight and Formula weight:-

- Molecular weight: sum of atomic weights of all atoms in a molecule (amu).
- Formula weight: sum of atomic weights of all atoms in a formula unit (amu).

→ example: H_2O : $1\times2 + 16\times1 = 18$ amu $= 18$ g/mol

→ example: NaCl : $22.99 + 35.45 = 58.44$ amu

Molecular Weight = Formula Weight = Molar mass (g/mol)

- example: calculate the formula weight for $Fe_2(SO_4)_3$

$$2\times55.8 + 3\times32.1 + 12\times16 = 399.9 \text{ amu}$$

*3.2: The Mole Concept:-

- Mole: quantity of given amount of a substance as the number of atoms in exactly 12 g of C^{12}
- Avogadros NO. (N_A): The number of atoms in exactly 12g of C^{12}

$$\boxed{1 \text{ mol} = N_A = 6.022 \times 10^{23} \text{ atoms, molecules,..}}$$

*example: $Na_{\underline{2}}CO_{\underline{3}}$

1mol Na_2CO_3 = 6.022×10^{23} unit of Na_2CO_3

$2 \times N_A = 1 \times N_A = 3 \times N_A$

- Molar Mass: mass of 1mole of substance, g/mol

$$\boxed{\text{mol} = \frac{\text{mass (g)}}{\text{molar mass (g/mol)}}}$$

Example: what is the mass in grams of a chlorine atom Cl?

m.w $Cl = 35.45$ amu

$$g\quad m = 0.166 \times 10^{-23} \times 35.45 = \boxed{5.90 \times 10^{-23}\, g}$$

$$mol \times N_A = n$$

$$mol = \frac{1 \text{ atom}}{6.022 \times 10^{23} \text{ atom/mol}} = 0.166 \times 10^{-23} \text{ mol } Cl$$

Example: what is the mass in grams of hydrogen chloride molecule, HCl?

$$\frac{1}{6022 \times 10^{23}} = 0.166 \times 10^{-23} \text{ mol}$$

$$m = 0.166 \times 10^{-23} \times 36.45 = \boxed{6.05 \times 10^{-23}\, g}$$

$$mw = 1 \times 1 + 35.45 \times 1 = 36.45$$

*Mass Percentages from the Formula: => 3.3

$$- \text{Mass } \%A = \frac{\text{Mass of A in the whole compound}}{\text{Mass of the whole compound}} \times 100\%$$

$$\boxed{\text{mass}\%A = \frac{\overset{mol}{n} \times \text{Molar Mass } A}{\text{Molar Mass compound}} \times 100\%}$$

$$* \text{ mol } AB_2 = \text{mol } A = 2 \text{ mol } B *$$

Questions:-

Q1: Calculate the Percent composition by mass of each of elements in (H_2SO_4): $H = 1.008\ g/mol$ $S = 32.07\ g/mol$ $O = 16\ g/mol$

$$m.w = 2\times1.008 + 1\times32.07 + 4\times16 = 98.09\ g/mol$$

$$\%H = \frac{2\times1.008}{98.09}\times100\% = 2.055\%$$

$$\%O = \frac{4\times16}{98.09}\times100\% = 65.25\%$$

$$\%S = \frac{1\times32.07}{98.09}\times100\% = 32.69\%$$

Q2: What is the mass of silver in 3.4g $AgNO_3$?

$Ag = 107.9\ g/mol$ $N = 14\ g/mol$ $O = 16\ g/mol$

$$m.w = 107.9 + 14 + 3\times16 = 169.9\ g/mol$$

$$\%Ag = \frac{107.9\times1}{169.9}\times100\% = 63.5\%$$

$$\frac{63.5}{100}\times3.4g = \boxed{2.2g}$$

Q3: Calculate th NO. of grams of Phosphorus (P) in 12.4 mole:

mass = n x m.w

$= 12.4 \times 30.9 = 383.2g$

Q4: How many molecules are there in 2.1 mol CO_2:

NO. of atoms $= 2.1 \text{ mol} \times 6.022 \times 10^{23} \frac{\text{atom}}{\text{mol}} = 1.26 \times 10^{24}$ ~~atom~~ molecule

Q5: How many H atoms are in 72.5g of C_3H_8O:

C = 12 g/mol   H = 1 g/mol   O = 16 g/mol

$m.w = 3 \times 12 + 8 \times 1 + 1 \times 16 = 60 \text{ g/mol}$

$mol = \frac{72.5}{60} = 1.21$

1 mol C_3H_8O ⟶ 8 mol H

1.21 mol // ⟶ X? mol H

$X = 8 \times 1.21 = 9.68 \text{ mol}$

$9.68 \text{ mol} \times \cancel{8}\, 6.022 \times 10^{23} \frac{\text{atom}}{\text{mol}} = \boxed{5.81 \times 10^{24} \text{ atom H}}$

* 3.4 : will be covered later

* 3.5 : Determining Formulas :

1] Molecular Formula : تعبير يظهر في عدد الذرات الحقيقي في المركب. ⇒ $C_6H_{12}O_6$ / H_2O

2] Empirical Formula : تعبير يبين أبسط صيغة لكتابة المركب. ⇒ CH_2O H_2O

	MF		EF
Example:	C_2H_2	→	CH
	$C_8H_{10}N_4O_2$	→	$C_4H_5N_2O$

⇒ determining <u>Empirical Formula</u> from the Percent :-

$\boxed{\text{mass Percent}} \rightarrow \boxed{\text{mol of each element}} \rightarrow \boxed{\text{mol ratio between elements}} \rightarrow \boxed{\text{Empirical Formula}} \rightarrow \boxed{\text{Molecular Formula}}$

IF we were asked about it

- Example: $C = 40.1\%$ $H = 6.6\%$ $O = 53.3\%$

assuming that there are 100 g of the compound:

	C	H	O
mass	40.1 g	6.6 g	53.3 g
mole	$\frac{3.34 \text{ mol}}{3.33}$	$\frac{6.6 \text{ mol}}{3.33}$	$\frac{3.33 \text{ mol}}{3.33}$
Ratio	1	2	1

⇒ devide all by the smallest value of moles.

Then the E.F is CH_2O

- Example: A sample of compound contain B and H, 6.444 g of B, 1.803 g of H, the M.W of compound (for M.F) is 30 g/mol, what is the M.F?

	B	H
mass	6.444 g	1.803 g
mole	$\frac{0.596 \text{ mol}}{0.596}$	$\frac{1.789 \text{ mol}}{0.596}$
ratio	1	3

E.F ⇒ BH_3

$$\boxed{L = \frac{M.W\ M.F}{M.W\ E.F}}$$

$$= \frac{30 \text{ g/mol}}{13.834 \text{ g/mol}} = 2.16 \approx 2$$

$$M.F = 2 \times (BH_3)$$
$$= B_2H_6$$

3.4: Elemental Analysis: Percentages of Carbon, Hydrogen, and Oxygen.

-Example: Acetic acid contains only C, H and O. A 4.24 mg sample of acetic acid is completely burned. It gives 6.21 mg of carbon dioxide and 2.54 mg of water. what is the mass Percentage of each element in acetic acid :-

H_2O 2.54 mg

CO_2 6.21 mg

$$CO_2 \Rightarrow \% C = \frac{1 \times 12}{44} * 100\% = 27.27\%$$

$$6.21 \text{ mg} \times 27.27\% = \boxed{1.69 \text{ mg}}$$

$$H_2O \Rightarrow \% H = \frac{2 \times 1.008}{18} * 100\% = 11.11\%$$

$$2.54 \text{ mg} \times 11.11\% = \boxed{0.28 \text{ mg}}$$

$$\text{mass of O} = 4.24 \text{ mg} - 0.28 \text{ mg} - 1.69 \text{ mg} = \boxed{2.27 \text{ mg}}$$

$$\% C \text{ in acetic acid} = \frac{1.69}{4.24} * 100\% = \boxed{39.85\%}$$

$$\% H \text{ " " "} = \frac{0.28}{4.24} \times 100\% = \boxed{6.6\%}$$

$$\% O \text{ " " "} = \frac{2.27}{4.24} \times 100\% = \boxed{53.53\%}$$

- **Example:** A sample of compound of Cl and O reacts with excess of H_2 to give 0.233g HCl and 0.403g H_2O. what is the E.F?

HCl 0.233g

H_2O 0.403g

in H_2O: $\%O = \frac{1 \times 16}{18} \times 100\% = 88.9\%$

mass (O) $= 88.9\% \times 0.403 = \boxed{0.358g}$

in HCl: $\%Cl = \frac{1 \times 35.45}{36.45} \times 100\% = 97.3\%$

mass (Cl) $= 97.3\% \times 0.233 = \boxed{0.227g}$

	Cl	O
mass	0.227	0.358
mole	$\frac{6.4 \times 10^{-3}}{6.4 \times 10^{-3}}$	$\frac{0.022}{6.4 \times 10^{-3}}$
ratio	[1	3.5] x2
	2	7

E.F $\Rightarrow \boxed{Cl_2O_7}$

- **Example:** A 0.67g sample of Cr is reacted with S. The resulting Chromium Sulfide has a mass of 1.2888g what is the E.F :

M.W Cr = 51.99 S = 32

mass of S
= 1.2888 - 0.67 = 0.62

	Cr	S
mass	0.67	0.62
mole	0.0129	0.0194
ratio	[1	1.5] x2
	2	3

E.F = Cr_2S_3

- **Example:** 0.6 g sample an unknown organic compound found to contain 0.24 g C, 0.04 g H, with the rest of O. If the M.W of the substance is 90 g/mol, what is the molecular formula:

mass of O = 0.6 − 0.24 − 0.04 = 0.28 g

	C	H	O
mass	0.24 g	0.04 g	0.28 g
mole	$\frac{0.02 \text{ mol}}{0.0175}$	$\frac{0.04 \text{ mol}}{0.0175}$	$\frac{0.0175 \text{ mol}}{\,}$ //
ratio	1.1	2.~~3~~	1

$E.F = CH_2O$

$\boxed{M.F = C_3H_6O_3}$

$L = \frac{90}{30} = 3$

* 3.6: Molar Interpretation of a chemical Equation:

- Stoichiometry: is the calculation of the quantities of reactants and products involved in a chemical reaction.

$$\underline{\underline{1}}\,N_2 + \underline{\underline{3}}\,H_2 \longrightarrow \underline{\underline{2}}\,NH_3$$

1 molecule N_2 + 3 molecules H_2 $\longrightarrow$ 2 molecules NH_3 molecular interpretation

1 mol N_2 + 3 mol H_2 $\longrightarrow$ 2 mol NH_3 molar interpretation

$$\underset{N_2}{1 \times 28.0\,g} + \underset{H_2}{3 \times 2.02\,g} \longrightarrow \underset{NH_3}{2 \times 17.0\,g}$$ mass interpretation

* 3.7: Amount of substances in a chemical Reaction:

$$\text{Mass of A} \xrightarrow[\text{mass A}]{\div\text{molar}} \text{mol A} \xrightarrow[\text{ratio}]{\text{stoichiometric}} \text{mol B} \xrightarrow[\text{B}]{\times\text{ molar mass}} \text{mass of B}$$

$$2A + 3B \longrightarrow A_2B_3$$

Example: How many grams of Iron can be produced from 1g Fe_2O_3:

$$\underset{1.00g}{Fe_2O_3} + 3CO \longrightarrow \underset{g=??}{2Fe} + 3CO_2$$

$$g\ Fe_2O_3 \longrightarrow \text{mol } Fe_2O_3 \longrightarrow \text{mol Fe} \longrightarrow g\ Fe$$

$$\frac{1.00g\,Fe_2O_3}{160\ \cancel{g}/mol} = 6.25 \times 10^{-3}\ \cancel{mol} \times \frac{2mol\ Fe}{\cancel{1mol}\ Fe_2O_3} = 0.0125\ \cancel{mol}\ Fe \times 55.8\frac{g}{\cancel{mol}} = 0.6975g$$

Example: How many grams of HCl react with 5.00g of manganese dioxide, according to this equation:

$$4\,HCl + MnO_2 \longrightarrow 2H_2O + MnCl_2 + Cl_2$$

g = ??   5.00g

$$\frac{5.00\text{g } MnO_2}{86.9\text{ g/mol}} \times \frac{4\text{ mol HCl}}{1\text{ mol } MnO_2} \times 36.45\text{ g/mol} = \boxed{8.40\text{ g HCl}}$$

* In every chemical reaction mass and atoms are conserved.

* 3.8: Limiting Reactant; Theoritical and Percentage Yields.

- limiting reactant: reactant that is entirely consumed when reaction goes to completion.

$$\Rightarrow \; 2H_2 + O_2 \longrightarrow 2H_2O$$

0.5 mol   0.5 mol

$H_2 \longrightarrow 0.5\text{ mol } H_2 \times \dfrac{2\text{ mol } H_2O}{2\text{ mol } H_2} = 0.5\text{ mol } H_2O$

→ Then H_2 is the limiting reactant, and O_2 is excess.

$O_2 \longrightarrow 0.5\text{ mol } O_2 \times \dfrac{2\text{ mol } H_2O}{1\text{ mol } O_2} = 1.0\text{ mol } H_2O$

Example: Zinc metal reacts with hydrochloric acid by the following reaction:

$Zn + 2HCl \longrightarrow ZnCl_2 + H_2$ if **0.30** mol **Zn** is added to Hydrochloric acid containing **0.52** mol **HCl**, How many moles of H_2 are Produced?

$\boxed{0.26\text{ mol } H_2}$

$0.30\,\cancel{\text{mol Zn}} \times \dfrac{1\text{ mol } H_2}{\cancel{1\text{ mol Zn}}} = 0.30\text{ mol } H_2$

$0.52\,\cancel{\text{mol HCl}} \times \dfrac{1\text{ mol } H_2}{2\,\cancel{\text{mol HCl}}} = 0.26\text{ mol } H_2$ ✓

HCl is a limiting reactant

Example: In alaboratory test of this reaction 20.0g CH_3CHO and 10.0g O_2 were put into reaction vessel, a. How many grams of acetic acid can be produced by this reaction? b. How many grams of excess reactant remain after the reaction is complete?

$$\underset{20g}{2CH_3CHO} + \underset{10g}{O_2} \longrightarrow 2HC_2H_3O_2$$

(a)

$\frac{20g\ CH_3CHO}{44\ g/mol} \times \frac{2mol\ HC_2H_3O_2}{2mol\ CH_3CHO} = 0.454\ mol\ HC_2H_3O_2$ ✓

CH_3CHO is limiting reactant.

$\frac{10g\ O_2}{32\ g/mol} \times \frac{2\ mol\ HC_2H_3O_2}{1\ mol\ O_2} = 0.625\ mol\ HC_2H_3O_2$

mass of ~~CH_3CHO~~ $HC_2H_3O_2$ $= 0.454 \times 60 = \boxed{27.24g}$

(b) $0.454\ mol \times \frac{1mol\ O_2}{2mol\ HC_2H_3O_2} = 0.227\ mol\ O_2$

mass $O_2 = 0.227 \times 32 = 7.264g$

excess $= 10.0g - 7.264g = \boxed{2.736g}$

* Percentage Yield:-

- Theoretical yield: amount of product can be obtained by a reaction from given amount of reactant.

- Actual yield: amount of product obtained experimentally.

$$\boxed{\text{Percentage Yield} = \frac{\text{Actual Yield}}{\text{Theoretical Yield}} \times 100\%}$$

Example: In a particular reaction between copper metal and silver nitrate 13g Cu produced 40g Ag (actual). what is the percent Yield of silver in this reaction?

$$\underset{13g}{Cu} + 2AgNO_3 \longrightarrow Cu(NO_3)_2 + \underset{40g}{2Ag}$$

$$\frac{13\ \cancel{g}\ Cu}{63.5\ \cancel{g/mol}} \times \frac{2\ \cancel{mol\ Ag}}{1\ \cancel{mol\ Cu}} \times \frac{107.9\ g/\cancel{mol}\ Ag}{\cancel{mol}} = \boxed{44.1g\ Ag}$$

$$\text{Percentage Yield} = \frac{40}{44.1} \times 100\% = \boxed{90.7\ \%}$$

Example: Industrially vanadium metal (V) can be obtained by reacting

$$5Ca + V_2O_5 \longrightarrow 5CaO + 2V$$

In one process 1.54×10^{3} g of V_2O_5 react with 1.96×10^{3} g of Ca, Calculate Percent yield if 803 g of V are obtained?

$$\frac{1.54 \times 10^3 \text{ g}}{181.8\ \cancel{50.9}\text{ g/mol}} \times \frac{2 \text{ mol V}}{1 \text{ mol } V_2O_5} = \cancel{60.5} \ 16.9$$

V_2O_5 limiting reactant

mass V = 16.9 × 50.9 = 860.2 g

$$\frac{1.96 \times 10^3 \text{ g}}{40 \text{ g/mol}} \times \frac{2 \text{ mol V}}{5 \text{ mol Ca}} = 19.6$$

$$\text{Percentage Yield} = \frac{803}{860.2} \times 100\% = \boxed{93.3\%}$$