

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 : $1 \times 2 + 16 \times 1 = 18 \text{ amu} = 18 \text{ g/mol}$
- example: $NaCl$: $22.99 + 35.45 = 58.44 \text{ amu}$

$$\# \text{Molecular Weight} = \text{Formula Weight} = \text{Molar mass (g/mol)}$$

- example: calculate the formula weight for $Fe_2(SO_4)_3$
 $2 \times 55.8 + 3 \times 32.1 + 12 \times 16 = 399.9 \text{ amu}$

*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}
- Avogadro's NO. (N_A): The number of atoms in exactly 12g of C^{12}

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

*example: Na_2CO_3

$$1 \text{ mol } Na_2CO_3 = 6.022 \times 10^{23} \text{ unit of } Na_2CO_3$$

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

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

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

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

m.w $\text{Cl} = 35.45 \text{ amu}$

$$\text{mol} \times N_A = n$$

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

$$m = 0.166 \times 10^{-23} \times 35.45 = 5.90 \times 10^{-23} \text{ g}$$

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

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

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

$$\text{mw} = 1 \times 1 + 35.45 \times 1 = 36.45$$

* Mass Percentages from the Formula: $\Rightarrow 3.3$

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

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

$$* \text{ mol } \text{AB}_2 = \text{mol A} = 2 \text{ mol B} *$$

Questions:-

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

$$\text{m.w} = 2 \times 1.008 + 1 \times 32.07 + 4 \times 16 = 98.09 \text{ g/mol}$$

$$\% \text{H} = \frac{2 \times 1.008}{98.09} \times 100\% = 2.055\%$$

$$\% \text{O} = \frac{4 \times 16}{98.09} \times 100\% = 65.25\%$$

$$\% \text{S} = \frac{1 \times 32.07}{98.09} \times 100\% = 32.69\%$$

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

$$\text{Ag} = 107.9 \text{ g/mol} \quad \text{N} = 14 \text{ g/mol} \quad \text{O} = 16 \text{ g/mol}$$

$$\text{m.w} = 107.9 + 14 + 3 \times 16 = 169.9 \text{ g/mol}$$

$$\% \text{Ag} = \frac{107.9 \times 1}{169.9} \times 100\% = 63.5\%$$

$$\frac{63.5}{100} \times 3.4 \text{g} = \boxed{2.2 \text{g}}$$

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

$$\text{mass} = n \times \text{m.w}$$

$$= 12.4 \times 30.9 = 383.2 \text{g}$$

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

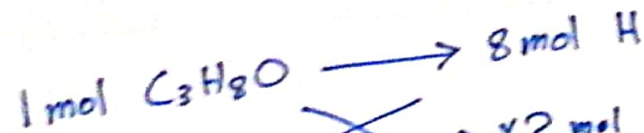
$$\text{NO. of atoms} = 2.1 \text{ mol} \times 6.022 \times 10^{23} \frac{\text{atom}}{\text{mol}} = 1.26 \times 10^{24} \text{ molecule}$$

Q5: How many H atoms are in 72.5g of $\text{C}_3\text{H}_8\text{O}$:

$$\text{C} = 12 \text{g/mol} \quad \text{H} = 1 \text{g/mol} \quad \text{O} = 16 \text{g/mol}$$

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

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



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

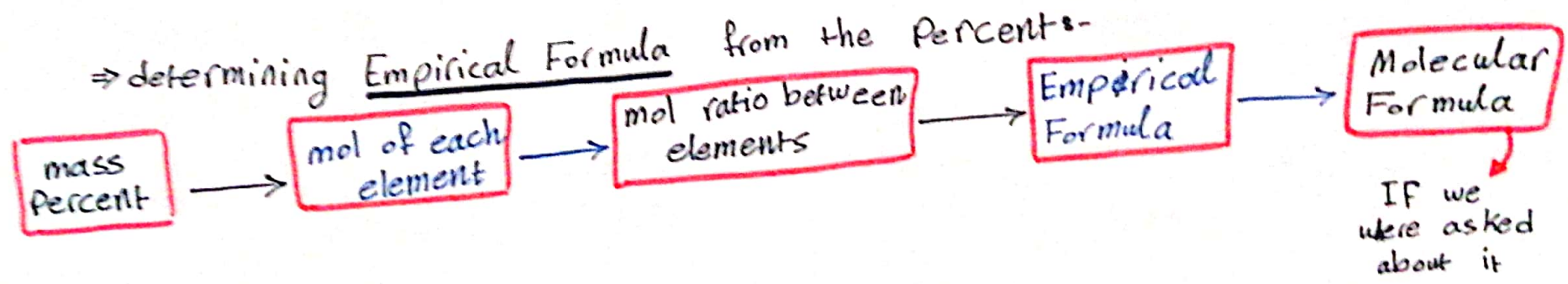
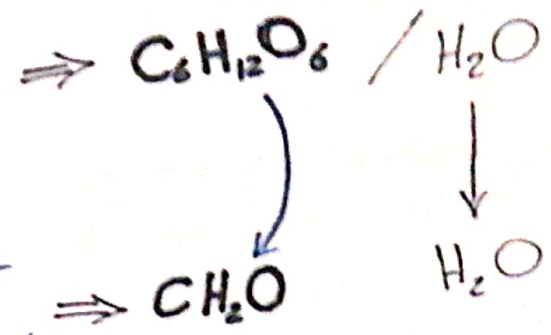
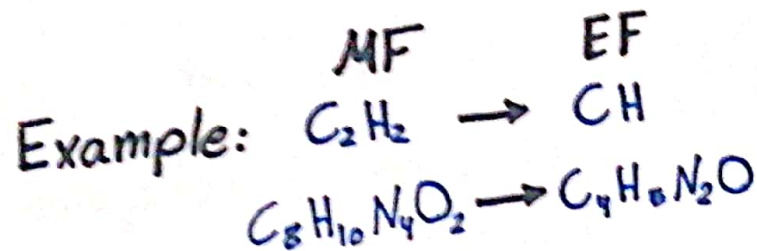
$$9.68 \text{ mol} \times 6.022 \times 10^{23} \frac{\text{atom}}{\text{mol}} = \boxed{5.81 \times 10^{24} \text{ atom H}}$$

* 3.4 : will be covered later

* 3.5 : Determining Formulas :

1] Molecular Formula : تعبير يظهر فيه عدد الذرات الحقيقي في المركب. $\Rightarrow C_6H_{12}O_6$

2] Empirical Formula : تعبير مبين أبسط صيغة لكتابة المركب. $\Rightarrow CH_2O$



- 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

⇒ divide all by the smallest value of moles.

Then the E.F is CH₂O

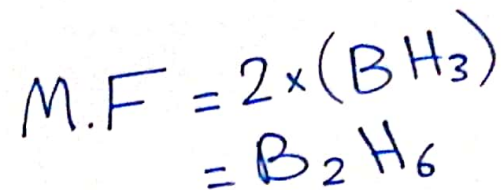
- Example: A sample of compound contain B and H, 6.444 g of B, 1.803 g of H, the M.W of compound (for M.F) is 30 g/mol, what is the M.F?

	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 ⇒ BH₃

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

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



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 :-

$$\text{CO}_2 \Rightarrow \% \text{C} = \frac{1 \times 12}{44} \times 100\% = 27.27\%$$

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

$$\text{H}_2\text{O} \Rightarrow \% \text{H} = \frac{2 \times 1.008}{18} \times 100\% = 11.11\%$$

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

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

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

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

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

H₂O 2.54 mg
CO₂ 6.21 mg

- 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?

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 = $\boxed{0.227g}$

HCl 0.233g
H₂O 0.403g

	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	$\left[\frac{1}{2} \right]$	$\left[\frac{3.5}{7} \right] \times 2$



- 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.:

$$\text{M.W Cr} = 51.99$$

$$\text{S} = 32$$

$$\begin{aligned} &\text{mass of S} \\ &= 1.2888 - 0.67 = 0.62 \end{aligned}$$

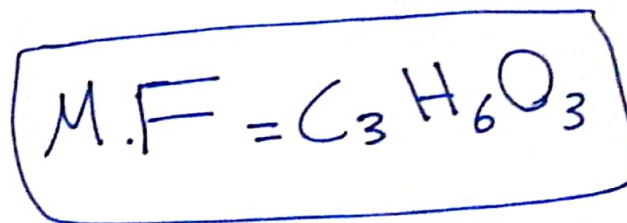
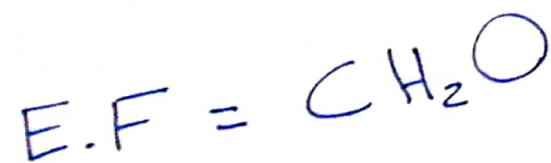
	Cr	S
mass	0.67	0.62
mole	0.0129	0.0194
ratio	[1	1.5] x 2
	2	3



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

$$\text{mass of O} = 0.6 - 0.24 - 0.04 = 0.28\text{g}$$

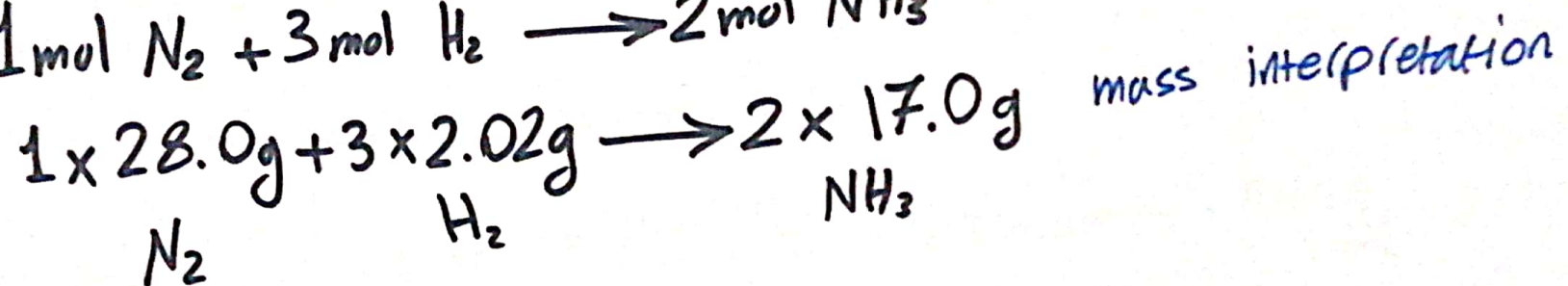
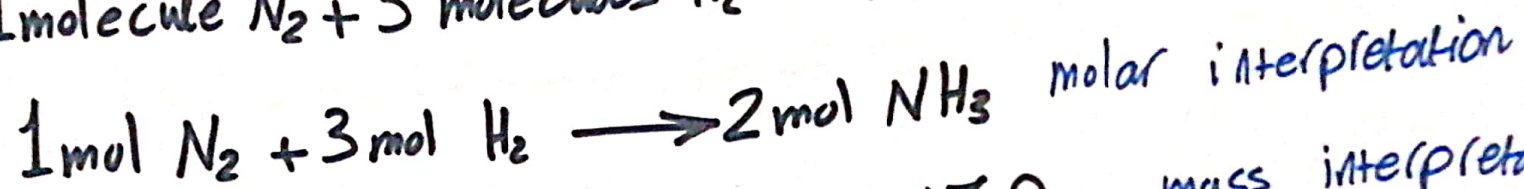
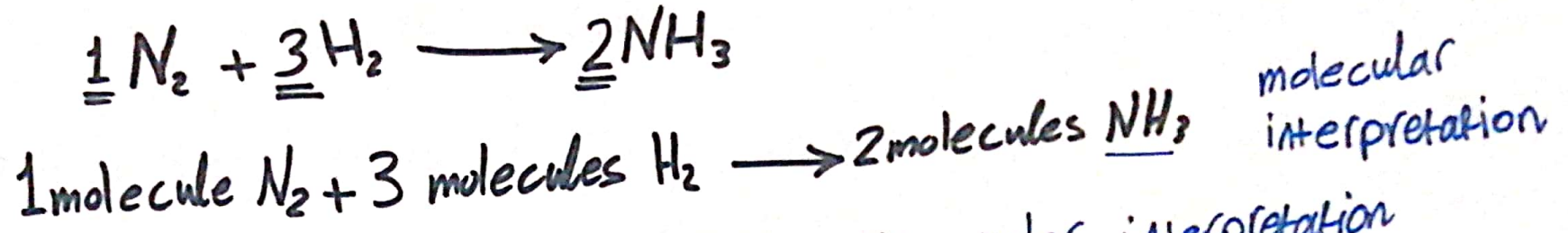
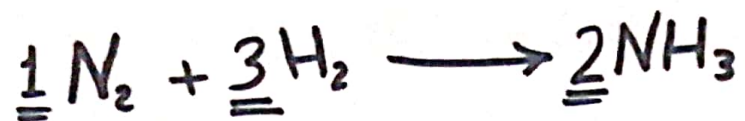
	C	H	O
mass	0.24g	0.04g	0.28g
mole	$\frac{0.02\text{ mol}}{0.0175}$	$\frac{0.04\text{ mol}}{0.0175}$	$\frac{0.0175\text{ mol}}{1}$
ratio	1.1	2.33	1



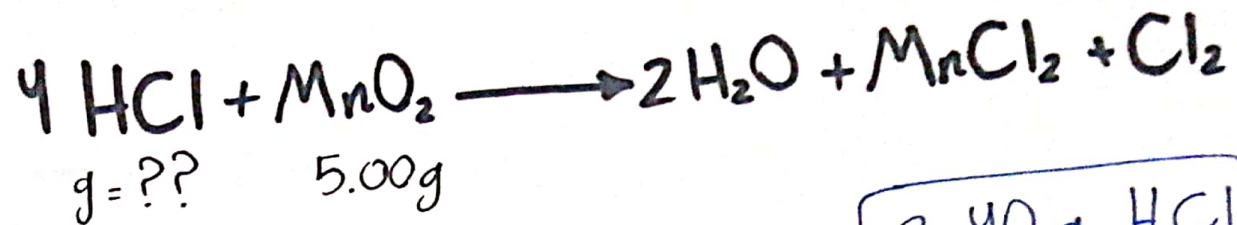
$$L = \frac{90}{30} = 3$$

* 3.6: Molar Interpretation of a chemical Equation:

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



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

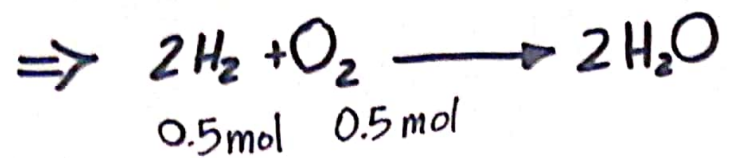


$$\frac{5.00\text{g MnO}_2}{86.9\text{g/mol}} \times \frac{4\text{ mol HCl}}{1\text{ mol MnO}_2} \times 36.45\text{ g/mol} = \boxed{8.40\text{ g HCl}}$$

* In every chemical reaction mass and atoms are conserved.

* 3.8: Limiting Reactant; Theoretical and Percentage Yields.

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



$$\text{H}_2 \longrightarrow 0.5 \text{ mol H}_2 \times \frac{2 \text{ mol H}_2\text{O}}{2 \text{ mol H}_2} = 0.5 \text{ mol H}_2\text{O}$$

\Rightarrow Then H_2 is the limiting reactant, and O_2 is excess.

$$\text{O}_2 \longrightarrow 0.5 \text{ mol O}_2 \times \frac{2 \text{ mol H}_2\text{O}}{1 \text{ mol O}_2} = 1.0 \text{ mol H}_2\text{O}$$

Example: Zinc metal reacts with hydrochloric acid by the following reaction:
 $\text{Zn} + 2\text{HCl} \longrightarrow \text{ZnCl}_2 + \text{H}_2$ if 0.30 mol Zn is added to Hydrochloric acid containing 0.52 mol HCl, How many moles of H_2 are Produced?

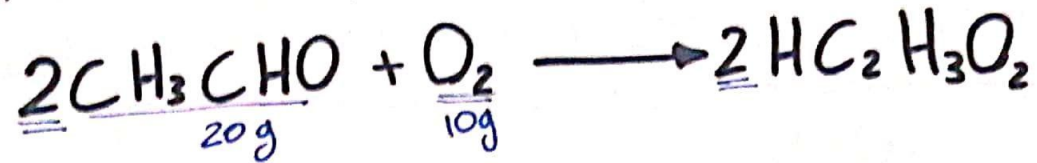
$$0.30 \text{ mol Zn} \times \frac{1 \text{ mol H}_2}{1 \text{ mol Zn}} = 0.30 \text{ mol H}_2$$

$$0.52 \text{ mol HCl} \times \frac{1 \text{ mol H}_2}{2 \text{ mol HCl}} = 0.26 \text{ mol H}_2 \checkmark$$

HCl is a limiting reactant

$$\boxed{0.26 \text{ mol H}_2}$$

Example: In laboratory 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?



(a) $\frac{20\text{g CH}_3\text{CHO}}{44\text{ g/mol}} \times \frac{2\text{ mol HC}_2\text{H}_3\text{O}_2}{2\text{ mol CH}_3\text{CHO}} = \underline{\underline{0.454\text{ mol HC}_2\text{H}_3\text{O}_2}}$ ✓

CH_3CHO is limiting reactant.

$\frac{10\text{g O}_2}{32\text{ g/mol}} \times \frac{2\text{ mol HC}_2\text{H}_3\text{O}_2}{1\text{ mol O}_2} = 0.625\text{ mol HC}_2\text{H}_3\text{O}_2$

mass of ~~CH_3CHO~~ $\text{HC}_2\text{H}_3\text{O}_2 = 0.454 \times 60 = \boxed{27.24\text{g}}$

(b) $0.454\text{ mol} \times \frac{1\text{ mol O}_2}{2\text{ mol HC}_2\text{H}_3\text{O}_2} = \underline{\underline{0.227\text{ mol O}_2}}$

mass $\text{O}_2 = 0.227 \times 32 = 7.264\text{g}$

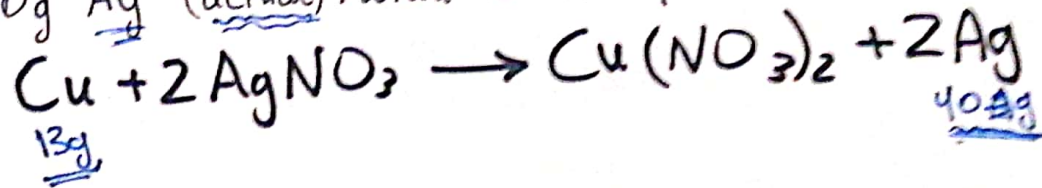
excess = $10.0\text{g} - 7.264\text{g} = \boxed{2.736\text{g}}$

* 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.

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

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



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

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

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



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

$$\frac{1.54 \times 10^3 \text{ g}}{181.8 \text{ g/mol}} \times \frac{2 \text{ mol V}}{1 \text{ mol V}_2\text{O}_5} = \underline{\underline{16.9}}$$

V_2O_5 limiting reactant

$$\text{mass V} = 16.9 \times 50.9 = \underline{\underline{860.2 \text{ g}}}$$

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

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