ABD ELHAFIDH UNIVERSITY CENTER
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PROCESS ENGINEERING

MINERAL CHEMISTRY

Chapter I: Review of Some Important Definitions

I .1.The mole:

During the application of chemistry, chemists have to calculate the number of atoms, ions, or molecules, referred to as chemical units, at the microscopic level, present in the used samples at the macroscopic level. For example, when we want to buy sugar, we need to take a package of one kilogram or more; it's impossible to buy it per piece or unit. Using the same logic (due to the small size and weight of atoms, molecules, or particles), we determine the quantity of atoms, molecules, or particles through a package or bundle.

Figure 1: Sugar

Example: the number of iron atoms in a sample with a mass of 3.5 g is 3.8 x 10^{-22} atoms. These large numbers led chemists to invent a new unit to facilitate calculations, which is the mole. The mole is defined as the number of entities (atoms, molecules, or particles) in one package, and it is represented by the symbol 'n'. The unit for the mole is mol. The Avogadro's number ($\mathcal{N}_{\mathcal{A}}$), which is the number of atoms in 12 grams of carbon-12, is equal to 6.02 x 10^{-23} units. Therefore, **the amount of substance** in a chemical sample is the number of moles present in that sample

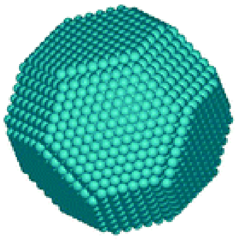

Figure 2: Atomes

$$\boldsymbol{n} = \frac{\boldsymbol{N}}{\mathcal{N}_A}\begin{cases} n: the\ amount\ of\ substance \\ N: number\ of\ unites \\ N_A: Avogadro\ number\ 6{,}02214.10^{23} \end{cases}$$

I.2.MOLAR MASS :

In chemistry, we often need to determine the amount of substance in samples, but we can't measure it directly. Instead, we calculate it starting from mass (which can be easily obtained using a balance). The molar mass is the quantity that relates mass to the amount of substance, symbolized by $\mathcal{M}$, and its unit is grams per mole (g/mol).

$$\boldsymbol{m} = \boldsymbol{N} \times \boldsymbol{m}_{unit}$$

$$m = n \times\ N_A\ \times m_{unit}$$

$$m = n \times \mathcal{M}$$

$$\mathcal{M} = \frac{m}{n}$$

I.1 .2. ATOMIC MASS

The molar mass of an element is the mass of one mole of atoms of that element, taking into account the masses of its isotopes and their relative abundance in nature, as found in a sample. Molar mass is specific to each element and can be found in the periodic table. It is expressed in grams per mole (g/mol).

For example, if we want to calculate the molar mass of carbon (C), we consider the presence of different isotopes of carbon (such as C-12, C-13, and C-14) and calculate the average atomic mass based on their natural abundance. The molar mass of carbon is approximately 12.01 g/mol.

These values are crucial because they help convert quantities measured in mass to quantities measured in moles and vice versa. This is useful in chemistry for various calculations and determining the amounts needed for chemical reactions.

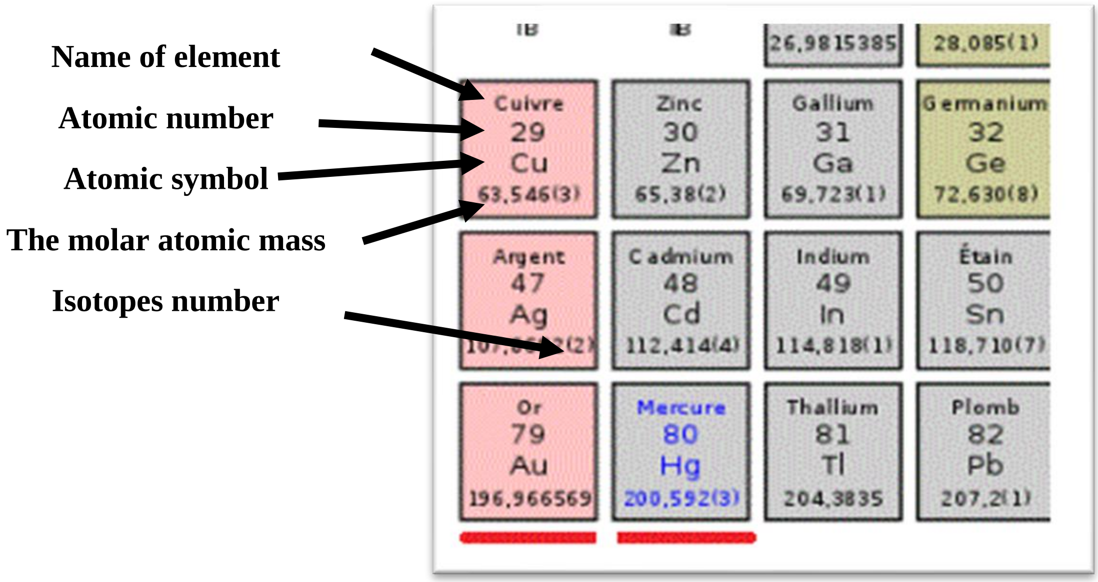

Figure 3: Part of periodic table

Example: Chlorine exists in nature in the form of two isotopes, -^{35}Cl ($\mathcal{M}$=35, 75,77%) و^{37} Cl ($\mathcal{M}$=35 ; 24, 23%)

$$\mathcal{M} = 35 \times 0{,}7577 + 37 \times 0{,}2423 = 35{,}453\, g/mol$$

I .2.2. MOLAR MOLECULAR MASS:

The molecular molar mass represents the mass of one mole of molecules. It is equal to the sum of the atomic molar masses of the elements that constitute the molecule

Exemple:

$\mathcal{M}(H_2O) = 2 \times \quad (\mathrm{H}) + \quad (\mathrm{O}) = 2 \times 1 + 16 = 18\mathrm{g/mol}$

Activity:

The weight of the water in a cup of water is 150 g. Calculate the quantity of substance as well as the number of water molecules.

$$\boldsymbol{n = \frac{m}{\mathcal{M}} = \frac{150}{18} = 8,3 mol}$$

$$\boldsymbol{N = n \times \mathcal{N}A = 8,3 \times 6,023.10^{23} = 5.10^{24} molucules}$$

I.5. MOLAR VOLUME OF GASES:

At a specific temperature and pressure, the molar volume of a gas is not dependent on its nature but is related to the quantity of substance (n). This is known as Avogadro's Law. The molar volume is denoted as V_m and is expressed in liters per mole (L/mol)

- For a temperature of 20°C and at atmospheric pressure (1 atm or 1013 hPa), the molar volume for gases, denoted as V_m, is 24 L/mol (standard conditions for temperature and pressure).
- For a temperature of 0°C and at atmospheric pressure (1 atm), the molar volume for gases is V_m = 22.4 L/mol (normal conditions regarding pressure and temperature).
- As the pressure increases or the temperature decreases, the molar volume decreases, following the principles of the ideal gas law. (PV=nRT)

$$\boldsymbol{V_m = \frac{V}{n}}$$

Activity:

1. Calculate the Molar Mass of Methane (CH_4).
2. Calculate the Volume Occupied by 13.4 moles of Methane at 0°C and 1013 hPa
3. Calculate the Corresponding Mass.

$$\boldsymbol{\mathcal{M} = \quad \mathcal{M}_C + 4\,\mathcal{M} \quad H = \ 12 + (4 \times 1) = 16 g/mol}$$

$$V = V_m \times n = 22,4 \times 13,4 = 300,16L$$

$$m = n \times \mathcal{M} = 13,4 \times 16 = 214,4g$$

I.3. The fraction or percentage.:

The fraction or percentage is a value used in chemistry or metallurgy to express the composition of a compound or alloy.

1. **The molar fraction x:**

$$x_i = \frac{n_i}{n_t} \text{ (the molar percentage (or molar ration) } x_i(\%) = \frac{n_i}{n_t} \times 100)$$

2. **The mass fraction P:**

$$P_i = \frac{m_i}{m_t} \text{(mass percentage (or mass ratio)} P_i\% = \frac{m_i}{m_t} \times 100)$$

3. **Volume fraction φ :**

$$\varphi_i = \frac{V_i}{V_t} \text{(Volume ration } \varphi_i\% = \frac{V_i}{V_t} \times 100)$$

Activity:

The solution of clogged pipes contains 10% by mass of sodium hydroxide (NaOH) solution. Calculate the mass present in 1 liter of sodium hydroxide solution with a mass of 1220 g.

$$P_i\% = \frac{m_i}{m_t} \times 100 \Rightarrow m_i = \frac{P_i \times m_t}{100} = \frac{10 \times 1220}{100} = 122\text{g}$$

4. **The relation between the molar fraction and the mass fraction:**

$$x_i = \frac{n_i}{\sum_i n_i} = \frac{m_i / \mathcal{M}i}{\sum_i m_i / \mathcal{M}i} = \frac{P_i m_t / \mathcal{M}i}{\sum_i P_i m_i / \mathcal{M}i}$$

$$x_i = \frac{P_i / \mathcal{M}i}{\sum_i P_i / \mathcal{M}i}$$

I .4.the density and specific gravity:

I .1.4.density:

Density or Volumetric mass, or mass-to-volume ratio, is the proportion of the mass (m) of a given sample to its volume (V). It represents the mass per unit volume occupied by the substance (at specific temperature and pressure).

$$\rho = \frac{m}{V}\ (kg/m^3, Kg/L, ou\ g/cm^3 ...)$$

I.4.2. specific gravity:

A. Density of solid and liquid materials with respect to water:

It is determined by comparing a certain mass of the substance with the mass of the same volume of water.

$$d = \frac{m_{sample}}{m_{water}} = \frac{\rho_{sample} \times V}{\rho_{water} \times V} = \frac{\rho_{sample}}{\rho_{water}} (no\ unit)$$

$$\rho_{water} = 1kg/L$$

B. Density of gases with respect to air:

Air and gases are taken under the same conditions of temperature and pressure.

$$d = \frac{\rho_{gaz}}{\rho_{air}}\ (\rho_{air} = 1,293g/L)$$

In normal conditions (T= 0°C et P=101325 Pa)

$$\rho_{air} = \frac{m_{air}}{V_{air}} = \frac{m_{air}/n}{V_{air}/n} = \frac{\mathcal{M}_{air}}{V_m}$$

$$\mathcal{M}_{air} = \rho_{air} \times V_m = 1,293 \times 22,4 = 29g/mol$$

$$\mathcal{M}_{air} = 29g/mol$$

$$d = \frac{\rho_{gas}}{\rho_{air}} = \frac{m_{gas}/V}{m_{air}/V} = \frac{m_{gas}}{m_{air}} = \frac{m_{gas}/n}{m_{air}/n}$$

$$d = \frac{\mathcal{M}_{gas}}{\mathcal{M}_{air}} = \frac{\mathcal{M}_{gas}}{29}$$

activity:

calculate the volumetric mass of the given substances:

1. Kerosene (Liquid Fuel) with a specific gravity of 0.78.
2. Concrete with a specific gravity of 2.5
3. Carbon Dioxide with a density of 1.53 at 0 degrees Celsius

1. $d = \frac{\rho_{substance}}{\rho_{water}} \Rightarrow \rho_{kerosene} = d \times \rho_{water} = 0,78 \times 1 = 0,78Kg/L$
2. $\rho_{concrete} = d \times \rho_{water} = 2,5 \times 1 = 2,5Kg/L$
3. $\rho_{CO_2} = d \times \rho_{air} = \frac{\mathcal{M}_{CO2}}{29} \times \rho_{air} = \frac{(12+2.16)}{29} \times 1,293 = 1,962g/L$

I .5.THE MATERIAL BALANCE:

The material balance is a concept in chemistry and chemical engineering that involves accounting for the mass of substances during a chemical reaction or a process. It is based on the principle of conservation of mass, which states that mass is neither created nor destroyed in a chemical reaction; it is merely rearranged.

In practical terms, a material balance involves tracking the quantities of reactants and products involved in a chemical process. This is often done through chemical equations, where the coefficients represent the stoichiometry of the reaction. The goal is to ensure that the total mass of the reactants equals the total mass of the products.

Material balances are essential in various fields, including chemical engineering, environmental science, and analytical chemistry. They help in designing and optimizing chemical processes, understanding reaction kinetics, and assessing the efficiency of a given reaction or system.

$$aA + bB \leftrightarrow cC + dD$$

$$\frac{|\Delta \boldsymbol{n_A}|}{\boldsymbol{a}} = \frac{|\Delta \boldsymbol{n_B}|}{\boldsymbol{b}} = \frac{\Delta \boldsymbol{n_C}}{\boldsymbol{c}} = \frac{\Delta \boldsymbol{n_D}}{\boldsymbol{d}}$$

Therefore, the change in each quantity of substance for the reactants can be expressed in terms of a quantity called the reaction progress, represented by $\boldsymbol{x}$, and expressed in moles (mol), as follows:$n_i = n_{i0} \pm v_i x \ (v; stoichiometry\ coefficient\ )$

In order to perform the molar balance, it is necessary to create a table (progress table) containing the progress of the consumed reactant quantities and the quantities of the products formed during three states.

Chemical equation	$\boldsymbol{aA}$ +	$\boldsymbol{bB}$ ↔	$\boldsymbol{cC}$	$\boldsymbol{dD}$
t=0	n_{A0}	n_{B0}	0	0
t	n_{A0}-ax	n_{B0}-bx	Cx	dx
Tmax	n_{A0}-ax_{max}	n_{B0}-bx_{max}	cx_{max}	dx_{max}

We say that the transformation is:

- ***Complete*** when at least one of the reactants (limiting reactant) disappears entirely; the other reactants may still be present in the final state (excess reactant).

- ***Maximal***: When the final progress is less than the maximum progress, the transformation is classified as ***incomplete***.
- ***Under stoichiometric conditions***: When all reactants disappear completely.
- Most chemical reactions are not complete, and this is referred to as a state of equilibrium, characterized by the equilibrium constant.
- $K = \frac{[A]^a[B]^b}{[C]^c[D]^d}\begin{cases} if\ K < 10^{-4}\ weak\ reaction \\ if\ 10^{-4} < K < 10^4\ reaction\ in\ equilibrium\ state \\ if\ K > 10^4, complete\ reaction \end{cases}$

I.5.1. THE RATIO PROGRESS

The final progress rate, denoted by τ, is equal to the ratio of the final progress to the maximum progress:

$$\boldsymbol{\tau} = \frac{x_{final}}{x_{maximal}}\begin{cases} \boldsymbol{non\ complet\ reaction, O}\ \leq \tau < 1 \\ \boldsymbol{complet\ reaction, \tau = 1} \end{cases}$$

The ratio progress is:

$$\boldsymbol{\tau}\% = \frac{x_{final}}{x_{max}} \times \mathbf{100}\begin{cases} \boldsymbol{non\ complete\ reaction, O}\ \leq \tau\% < 100 \\ \boldsymbol{complete\ reaction, \tau = 100} \end{cases}$$

❖ In case of complete reaction:

$$x_{max} = \frac{n_{limiting\ reactant}}{\boldsymbol{coefficient\ of\ limitant\ reactant}} = x_{final}$$

❖ **In case of non-complete reaction**

Experimental parameters, such as pH, concentration, absorption, determine the final progress empirically

I.5.2. CONVERSION RATE:

The conversion rate of reactant A is equal to the ratio of the number of moles of A reacted during the chemical reaction to the initial number of moles of A (A_0) present. Therefore, we can write

$$\boldsymbol{X_A} = \frac{\boldsymbol{n_{i,0} - n_i}}{\boldsymbol{n_{i,0}}}$$

The conversion percentage:

$$\boldsymbol{X_A}\% = \frac{\boldsymbol{n_{i,0} - n_i}}{\boldsymbol{n_{i,0}}} \times \mathbf{100}$$

I.5.3. REACTION YIELD

The chemical reaction yield is the ratio of the actual amount of the obtained product to the maximum amount of that product if all reactants were converted to products.

$$\boldsymbol{R}\,\% = \frac{\boldsymbol{Actual\ quantity\ of\ the\ product}}{\boldsymbol{Maximum\ quantity}} \times \mathbf{100}$$

Activity:

What is the material balance for the following reaction, as well as the percentage of progress, conversion, and yield?

$$2Ag^{+}_{(aq)} + Cu_{(s)} \rightarrow Cu^{2+}_{(aq)} + 2Ag_{(s)} \begin{cases} n_{0,Ag} = 10^{-3}mol \\ n_{0,Cu} = 4.10^{-3}mol \end{cases}$$

The obtained mass of silver is equal to 0.067 g

reaction	$2Ag^{+}_{(aq)}$	$+ Cu_{(s)}$	$\rightarrow Cu^{2+}_{(aq)}$	$+ 2Ag_{(s)}$
t_0	10^{-3}	$4.\ 10^{-3}$	0	0
t	10^{-3}-2x	$4.\ 10^{-3}$-x	x	2x
t max	10^{-3}-$2x_{max}$	$4.\ 10^{-3}$-x_{max}	x_{max}	$2x_{max}$

$$\boldsymbol{n_{Ag}} = \frac{\boldsymbol{m}}{\boldsymbol{M}} = \frac{\mathbf{0,067}}{\mathbf{107,87}} = \mathbf{6,21}.\,10^{-4}\text{mol} = 2x_{\text{final}}$$

$$\boldsymbol{x_{final}} = \frac{\mathbf{6,21}.\,10^{-4}}{\mathbf{2}} = \mathbf{3,11}.\,10^{-4}\text{mol}$$

For t_{final}:

$$[\boldsymbol{Ag}^{+}] = 10^{-3} - 6{,}21.\,10^{-4} = 3{,}79.\,10^{-4}\text{mol}$$

$$n_{Cu} = 4..\,10^{-3} - 3{,}11.\,10^{-4} = 3{,}689\ 10^{-3}\text{mol}$$

$$[Cu^{+2}] = 3{,}11.\,10^{-4}\text{mol}$$

Progress ratio

First, we have to find the limiting reactant:

1. Ag+:$10^{-3} - 2x_{\text{max},1} = 0$ =>, $x_{max,1} = \frac{10^{-3}}{2} = 5.\,10^{-4}$mol

2. Cu:$4.10^{-3} - \mathrm{x}_{\mathrm{max},2} = 0 => x_{max,2} = 4.10^{-3}$ mol

the limiting reactant is Ag+<= $x_{max,1} < x_{max,2}$

$$\boldsymbol{\tau} = \frac{\boldsymbol{x_{final}}}{\boldsymbol{x_{max}}} \times \mathbf{100} = \frac{\mathbf{3,11..}10^{-4}}{\mathbf{5.}10^{-4}} \times \mathbf{100} = \mathbf{62,1}\%$$

The conversion ratio

1. **silver**

$$\boldsymbol{X_{Ag+}}\% = \frac{\boldsymbol{n_{i,0}} - \boldsymbol{n_i}}{\boldsymbol{n_{i,0}}} \times \mathbf{100} = \frac{\mathbf{10^{-3}} - \mathbf{3,79.}10^{-4}}{\mathbf{10^{-3}}} \times \mathbf{100} = \mathbf{62,1}\%$$

2. **cupper**

$$\boldsymbol{X_{Cu}}\% = \frac{\boldsymbol{n_{i,0}} - \boldsymbol{n_i}}{\boldsymbol{n_{i,0}}} \times \mathbf{100} = \frac{\mathbf{4.10^{-3}} - 3{,}689\ 10^{-3}}{\mathbf{4.10^{-3}}} \times \mathbf{100} = \mathbf{7,77}\%$$

3. **the reaction yield**

$$\boldsymbol{R}\ \% = \frac{\mathbf{6,21.}10^{-4}}{\mathbf{10^{-3}}} = \mathbf{62,1}\%$$