1. Details of Module and its structure

Module Detail	
Subject Name	Chemistry
Course Name	Chemistry 01 (Class XI, Semester 01)
Module Name/Title	Some Basic Concepts of Chemistry: Part 4
Module Id	kech_10104
Pre-requisites	Laws of Chemical combination, Avagadro number, Atomic mass, Molecular mass
Objectives	After going through this module you will be able to: 1. Describe the terms – mole and molar mass. 2. Calculate the mass per cent of different elements constituting a compound. 3. Determine empirical formula and molecular formula for 4. A compound from the given experimental data. 5. Perform the stiochiometric calculations.
Keywords	Mole, Molar mass, Empirical formula, Molecular formula, Stiochiometry, Limiting Reagent, Mass%, Mole fraction, Molarity, Molality.

2. Development Team

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1. Mole Concept and Molar Masses

Atoms and molecules are extremely small in size. However, Avagadro's number, N_A (i.e. number of molecules present in one gram molecule of a substance) is 6.022×10^{23} which depicts that numbers in even a small amount of any substance is really very large. To handle such large numbers, a unit of similar magnitude is required. For example, generally we denote one dozen for 12 items, score for 20 items, gross for 144 items, one ton for 50 kilograms etc to count different substance. The idea of mole is used to count entities at the microscopic level (i.e. atoms/molecules/ particles, electrons, ions, etc). In SI system, mole (symbol, mol) was introduced as seventh base quantity for the amount of a substance. Hence, one mole of a substance is defined as, "the amount of a substance that contains as many particles or entities as there are atoms in exactly 12 g (or 0.012 kg) of the ^{12}C isotope".

It may be emphasised that the mole of a substance always contain the same number of entities irrespective of nature of substance. In order to determine this number precisely, the mass of a carbon– 12 atom was determined by a mass spectrometer and found to be equal to 1.992648 $\times 10^{-23}$ g. Knowing that one mole of carbon weighs 12g, the number of atoms in it is equal to:

$$\frac{12g/mol\ ^{12}C}{1.9924648\times10^{-23} g/^{12}C\ atom}$$

$= 6.0221367 \times 10^{23}$ atoms/mol

This number of entities in 1 mol is so important that it is given a separate name and symbol. It is known as '*Avogadro constant*', denoted by N_A in honour of Amedeo Avogadro. To really appreciate largeness of this number, let us write it with all the zeroes without using any powers of ten. 602213670000000000000000 Hence, so many units of either of the particles like atoms, molecules or any other particle constitute one mole of a particular substance. Therefore, we can say now that

1 mol of hydrogen atoms = 6.022×10^{23} atoms

1 mol of water molecules = 6.022×10^{23} water molecules

1 mol of sodium chloride = 6.022×10^{23} formula units of sodium chloride

In terms of mass, a mole is defined as *"the amount of the substance which has mass of equal to gram atomic mass for atomic substance and gram molecular mass for molecules"*. Having defined the mole, it is easier to know mass of one mole of the substance or the constituent units. *The mass of one mole of a substance in grams is called its molar mass*. The molar mass in grams is numerically equal to atomic/molecular/ formula mass in u.

For example, Molar mass of water = 18.02 g mol^{-1}

Molar mass of sodium chloride = 58.5 g mol^{-1}

Hence, from the above discussion it is found that a mole of a substance can be related to its mass or number of particles present in it or volume of a gas (Fig. 4.1 & 4.2).

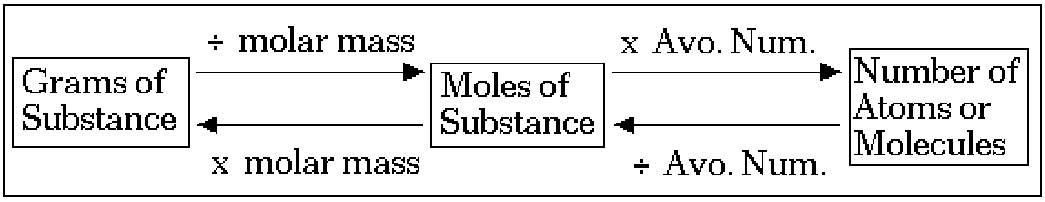

Fig. 4.1 Definition of a mole of a substance.

(Source: http://www.chemteam.info/Mole/Avogadro-Number-CalcsII-1.GIF)

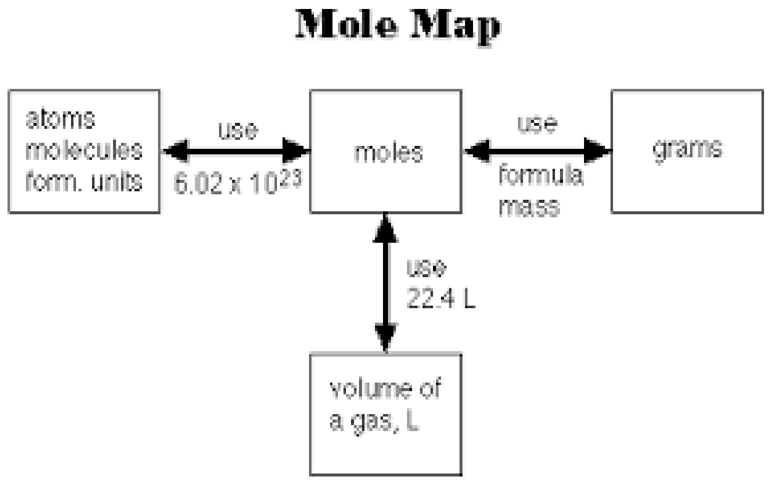

Fig. 4.2 Relationship of mole of a substance with number of particles present in it, mass of the substance and volume of a gas

(Source: http://3.bp.blogspot.com/_9fh8OjpL7M4/TPiawRO23UI/AAAAAAAAACA/cI9YCsmPgpU/s1600/molemap.gif)

2. Percentage Composition

Until now, we were dealing with the number of entities present in a given sample. But many a time, the information regarding the percentage of a particular element present in a compound is required. For example, if an unknown or new compound given, the first question that would ask is: what is its formula or what are its constituents and in what ratio are they present in the given compound? Even for known compounds also, such information verifies whether the given sample contains the same percentage of elements as is present in a pure sample. Hence, in this way purity of a substance can be checked by analysing this data.

Example: Water (H_2O) molecule. Since water contains hydrogen and oxygen, the percentage composition of both these elements can be calculated as follows:

$$\text{Mass \% of an element} = \frac{\textit{mass of that element in the compound}}{\textit{molar mass of the compound}} \times 100$$

Since, molar mass of water = 18.02 g

$$\text{Mass \% of hydrogen} = \frac{2 \times 1.008}{18.02} \times 100 = 11.18\%$$

$$\text{Mass \% of oxygen} = \frac{16.00}{18.02} \times 100 = 88.79\%$$

Example: What is the percentage of carbon, hydrogen and oxygen in ethanol?

Molecular formula of ethanol is: C_2H_5OH,

Molar mass of ethanol = (2×12.01 + 6×1.008 + 16.00) g = 46.068 g

$$\text{Mass per cent of carbon} = \frac{2 \times 12.01}{46.068} \times 100 = 52.14\%$$

$$\text{Mass per cent of hydrogen} = \frac{6 \times 1.008}{46.068} \times 100 = 13.13\%$$

$$\text{Mass per cent of oxygen} = \frac{1 \times 16.00}{46.068} \times 100 = 34.73\%$$

Empirical Formula for Molecular Formula: The percent composition data also depicts the formulas for the substance. An *empirical formula* of a compound is the chemical formula which represents the simplest whole number ratio of various atoms present in a compound. If the mass per cent of various elements present in a compound is known, its empirical formula can be determined. On the other hand, the *molecular formula* of a compound represents the exact number of different types of atoms present in a molecule of a compound. Molecular formula can further be obtained if the molar mass is known. Some of the examples to illustrate the difference between empirical and molecular formula is listed below:

Compound	Empirical Formula	Molecular Formula
Benzene	CH	C_6H_6
Hydrogen peroxide	HO	H_2O_2
Glucose	CH_2O	$C_6H_{12}O_6$

Following example will illustrate the calculations involving the determination of empirical and molecular formula of a compound.

Example: A compound contains 4.07 % hydrogen, 24.27 % carbon and 71.65 % chlorine. Its molar mass is 98.96 g. What are its empirical and molecular formulas?

Step 1. Conversion of mass per cent to grams: Since we are having mass per cent, it is convenient to use 100 g of the compound as the starting material. Thus, in the 100 g sample of the above compound, 4.07g hydrogen is present, 24.27g carbon is present and 71.65 g chlorine is present.

Step 2. Convert into number moles of each element: Divide the masses obtained above by respective atomic masses of various elements.

Moles of hydrogen = $\frac{4.07\,g}{1.008\,g}$ = 4.04

Moles of carbon = $\frac{24.27\,g}{12.01\,g}$ = 2.021

Moles of chlorine = $\frac{71.65\,g}{35.453\,g}$ = 2.021

Step 3. Divide the mole value obtained above by the smallest number: Since 2.021 is smallest value, division by it gives a ratio of 2:1:1 for H:C:Cl. In case the ratios are not whole numbers, then they may be converted into whole number by multiplying by the suitable coefficient.

Step 4. Write empirical formula by mentioning the numbers after writing the symbols of respective elements: CH_2Cl is, thus, the empirical formula of the above compound.

Step 5. Writing molecular formula: (a) Determine empirical formula mass Add the atomic masses of various atoms present in the empirical formula

For CH_2Cl, empirical formula mass is 12.01 + 2 × 1.008 + 35.453 = 49.48 g

(b) Divide Molar mass by empirical formula mass

$$\frac{Molar\,mass}{Empirical\,mass} = \frac{98.96\,g}{49.48\,g} = 2 = n$$

(c) Multiply empirical formula by n obtained above to get the molecular formula

Empirical formula = CH_2Cl, n = 2. Hence, molecular formula is $C_2H_4Cl_2$.

3. Stoichiometry and Stoichiometric Calculations

The word ‘stoichiometry’ is derived from two Greek words - stoicheion (meaning element) and metron (meaning measure). Stoichiometry, thus, deals with the calculation of masses (sometimes volumes also) of the reactants and the products involved in a chemical reaction. Before understanding how to calculate the amounts of reactants required or the products produced in a chemical reaction, let us study what information is available from the balanced chemical equation for a given reaction.

Let us consider the combustion of methane. A balanced equation for this reaction is:

CH_4 (g) + $2O_2$ (g) → CO_2 (g) + 2 H_2O (g)

Here, methane and dioxygen are called reactants and carbon dioxide and water are called products. Note that all the reactants and the products are gases in the above reaction and this has been indicated by letter (g) in the brackets next to its formula. Similarly, in the case of solids and liquids, (s) and (l) are written respectively.

The coefficients 2 for O_2 and H_2O are called stoichiometric coefficients. Similarly the coefficient for CH_4 and CO_2 is one in each case. They represent the number of molecules (and moles as well) taking part in the reaction or formed in the reaction.

Thus, according to the above chemical reaction.

1. One mole of CH_4(g) reacts with two moles of O_2(g) to give one mole of CO_2(g) and two moles of H_2O(g)

2. One molecule of CH_4(g) reacts with 2 molecules of O_2(g) to give one molecule of CO_2(g) and 2 molecules of H_2O(g)

3. 22.7 L of CH_4(g) reacts with 45.4 L of O_2(g) to give 22.7 L of CO_2(g) and 45.4 L of H_2O(g)

4. 16g of CH_4(g) reacts with 2×32g of O_2(g) to give 44 g of CO_2(g) and 2×18 g of H_2O (g).

From these relationships, the given data can be interconverted as follows :

mass ⇌ moles ⇌ no. of molecules and $\frac{Mass}{Volume} = Density$

Example: Calculate the amount of water (g) produced by the combustion of 16 g of methane.

The balanced equation for combustion of methane is:

$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(g)$

(i) 16 g of CH_4 corresponds to one mole.

(ii) From the above equation, 1 mol of CH_4 (g) gives 2 mol of H_2O (g).

2 mol of water (H_2O) = 2 × (2+16) = 2 × 18 = 36 g

1 mol H_2O = 18 g H_2O ⇒ $\frac{18\, g\, H_2O}{1\, mol\, H_2O} = 1$

Hence, 2 mol H_2O × $\frac{18\, g\, H_2O}{1\, mol\, H_2O}$ = 2 × 18 g H_2O = 36 g H_2O

Example: How many moles of methane are required to produce 22 g CO_2 (g) after combustion?

According to the chemical equation, CH_4 (g) + $2O_2$ (g) → CO_2 (g) + 2 H_2O (g)

44 g CO_2 (g) is obtained from 16 g CH_4 (g) [because 1 mol CO_2(g) is obtained from 1 mol of CH_4 (g)]

mole of CO_2 (g) = 22 g CO_2 (g) × $\frac{1\, mol\, CO_2(g)}{44\, g\, CO_2(g)}$ = 0.5 mol CO_2 (g)

Hence, 0.5 mol CO_2 (g) would be obtained from 0.5 mol CH_4 (g) or 0.5 mol of CH_4 (g) would be required to produce 22 g CO_2 (g).

3.1. Limiting Reagent: Number of times, the reactions are carried out when the reactants are not present in the amounts as required by a balanced chemical reaction. In such situations, one reactant is in excess over the other. The reactant which is present in the lesser amount gets consumed after sometime and after that no further reaction takes place whatever be the amount of the other reactant present. Hence, the reactant which gets consumed, limits the amount of product formed and is, therefore, called the limiting reagent. Therefore, the limiting reactant or reagent is defined as *"the reactant which reacts completely in the reaction"*. In performing stoichiometric calculations, the concept of limiting reagent should taken into care.

Example: 50.0 kg of N_2 (g) and 10.0 kg of H_2 (g) are mixed to produce NH_3 (g). Calculate the NH_3 (g) formed. Identify the limiting reagent in the production of NH3 in this situation.

A balanced equation for the above reaction is written as follows:

Calculation of moles: $N_2 (g) + 3H_2 (g) \rightleftharpoons 2NH_3 (g)$

$$\text{moles of } N_2 = 50.0 \text{ kg } N_2 \times \frac{1000\, g\, N_2}{1\, kg\, N_2} \times \frac{1\, mol\, N_2}{28.0\, g\, N_2} = 17.86\times10^2 \text{ mol}$$

$$\text{moles of } H_2 = 10.00 \text{ kg } H_2\times \frac{1000\, g\, H_2}{1\, kg\, H_2} \times \frac{1\, mol\, H_2}{2.016\, g\, H_2} = 4.96\times10^3 \text{ mol}$$

According to the above equation, 1 mol N_2 (g) requires 3 mol H_2 (g), for the reaction. Hence, for 17.86×10^2 mol of N_2, the moles of H_2 (g) required would be

$$17.86\times10^2 \text{ mol } N_2 \times \frac{3\, mol\, H_2(g)}{1\, mol\, N_2(g)} = 5.36\times10^3 \text{ mol } H_2$$

But we have only 4.96×10^3 mol H_2. Hence, dihydrogen is the limiting reagent in this case. So NH_3(g) would be formed only from that amount of available dihydrogen i.e., 4.96×10^3 mol.

Since 3 mol H_2(g) gives 2 mol NH_3(g)

$$4.96\times10^3 \text{ mol } H_2 \text{ (g)} \times \frac{2\, mol\, NH_3(g)}{3\, mol\, H_2(g)} = 3.30\times10^3 \text{ mol } NH_3 \text{ (g)}$$

3.30×10^3 mol NH_3 (g) is obtained.

If they are to be converted to grams, it is done as follows:

1 mol NH_3 (g) = 17.0 g NH_3 (g)

$$3.30\times10^3 \text{ mol } NH_3\text{(g)} \times \frac{17.0\, g\, NH_3(g)}{1\, mol\, NH_3(g)} = 3.30\times10^3\times17 \text{ g } NH_3\text{(g)}$$

$$= 56.1\times10^3 \text{ g } NH_3 = 56.1 \text{ kg } NH_3$$

3.2. Reactions in Solutions: A majority of reactions in the laboratories are carried out in solutions. Therefore, it is important to understand as how much amount of substance is present in the solution. The concentration of a solution or the amount of substance present in its given volume can be expressed in any of the following ways.

1. Mass per cent or weight per cent (w/w %)
2. Mole fraction
3. Molarity
4. Molality

Let us now study each one of them in detail.

3.2.1. Mass per cent or Weight percent (w/w %): Mass percent of a solute in a solution is the mass of the solute in grams present in 100 g of the solution. It is obtained by using the following relation:

$$\text{Mass percent} = \frac{Mass\ of\ the\ solute}{Mass\ of\ solution} \times 100$$

Example: A solution is prepared by adding 2 g of a substance A to 18 g of water. Calculate the mass per cent of the solute.

$$\text{Mass per cent of A} = \frac{Mass\ of\ A}{Mass\ of\ solution} \times 100$$

$$= \frac{2g}{2\,g\,of\ A + 18\,of\ water} \times 100 = (2/20) \times 100$$

= 10 %

3.2.2. Mole Fraction (x): Mole fraction is the ratio of number of moles of a particular component to the total number of moles of the solution. If a substance 'A' dissolves in substance 'B' and their number of moles are n_A and n_B respectively; then the mole fractions of A and B are given as

Mole fraction of A (x_A),

$$= \frac{Number\ of\ moles\ of\ A}{Number\ of\ moles\ of solution} = \frac{n_A}{n_A + n_B}$$

and, Mole fraction of B (x_B),

$$= \frac{Number\ of\ moles\ of\ B}{Number\ of\ moles\ of solution} = \frac{n_B}{n_A + n_B}$$

3.2.3. Molarity (M): It is the commonly used unit to express the concentration of the solution. Molarity of a solution is defined as the number of moles of the solute dissolved in one litre of the solution. Molarity of the solution is denoted by M. Thus,

$$\text{Molarity (M)} = \frac{Moles\ of solute}{Volume\ of\ solution\ (in\ litres)}$$

$$= \frac{n_A \times 1000}{V\ (ml)} = \frac{w_A \times 1000}{M \times V\ (ml)}$$

where, w_A represent the mass of solute A in grams and M is its molecular mass.

The concentration of a solution can be determined using other solution of known concentration. For example, we have 1 M solution of a substance, say NaOH and we want to prepare a 0.2 M solution from it. 1 M NaOH means 1 mol of NaOH present in 1 litre of the solution. For 0.2 M solution we require 0.2 moles of NaOH in 1 litre solution.

Hence, we have to take 0.2 moles of NaOH and make the solution to 1 litre. Now how much volume of concentrated (1M) NaOH solution be taken which contains 0.2 moles of NaOH can be calculated as follows: If 1 mol is present in 1 L or 1000 mL then 0.2 mol is present in

(1000 mL/1 mol) × 0.2 mol = 200 mL

Thus, 200 mL of 1M NaOH are taken and enough water is added to dilute it to make it 1 litre.

Indeed for such calculations, a general formula can be used which is given as:

$M_1 \times V_1 = M_2 \times V_2$

where, M and V are molarity and volume respectively.

In the above mentioned example, M_1 is equal to 0.2; V_1 = 1000 mL and, M_2 = 1.0; V_2 is to be calculated. Substituting the values in the formula:

$0.2 \text{ M} \times 1000 \text{ mL} = 1.0 \text{ M} \times V_2$

$V_2 = 200 \text{ mL}$

Note that the number of moles of solute (NaOH) was 0.2 in 200 mL and it has remained the same, i.e., 0.2 even after dilution (in 1000 mL) as we have changed just the amount of solvent (i.e. water) and have not done anything with respect to NaOH. But keep in mind the concentration.

Example: Calculate the molarity of NaOH in the solution prepared by dissolving its 4 g in enough water to form 250 mL of the solution.

Since, molarity (M) = (No. of moles of solute)/(Volume of solution in litres)

$$= \frac{Mass\ of\ NaOH}{Molar\ mass\ of\ NaOH \times Volume\ of\ solution}$$

$$= \frac{4\,g}{40\frac{g}{mol} \times 0.250\,l} = \text{ 0.4 mol/l or M}$$

Note that molarity of a solution depends upon temperature because volume of a solution is temperature dependent.

3.2.4. Molality (m): Molality of a solution is defined as the number of moles of solute dissolved in one kilo-gram of solvent. It is denoted by m and expressed as:

Molality (m) = (No. of moles of solute)/(Mass of solvent in kg)

$$= \frac{n_A \times 1000}{w_B(g)} = \frac{w_A \times 1000}{M \times w_B(g)}$$

where, w_A represent the mass of solute A in grams, M is its molecular mass and w_B is the mass of the solvent in gram. Molality is temperature independent quantity.

Example: The density of 3 M solution of NaCl is 1.25 g mL^{-1}. Calculate molality of the solution.

M = 3 mol L^{-1}

Mass of NaCl in 1 L solution = 3 × 58.5 = 175.5 g

Mass of 1L solution = 1000 × 1.25 = 1250 g (since density = 1.25 g mL^{-1})

Mass of water in solution = 1250 –175.5 = 1074.5 g

Molality = (No. of moles of solute)/(Mass of solvent in kg)

= (3 mol)/(1.0745 kg)

= 2.79 m

Often in a chemistry lab, a solution of a desired concentration is prepared by diluting a solution of known higher concentration. The solution of higher concentration is also known as stock solution. Note that molality of a solution does not change with temperature since mass remains unaffected with temperature.

4. Summary

In this module, we studied about the concept of mole of a substance and association with different stoichiometric and concentration calculations. The numbers of atoms, molecules or any other particles present in a given system are expressed in the terms of Avogadro constant (6.022×10^{23}). This is known as 1 mol of the respective particles or entities. Chemical reactions represent the chemical changes undergone by different elements and compounds. A balanced chemical equation provides a lot of information. The coefficients indicate the molar ratios and the respective number of particles taking part in a particular reaction. The quantitative study of the reactants required or the products formed is called stoichiometry. Using stoichiometric calculations, the amount of one or more reactant(s) required to produce a particular amount of product can be determined and vice-versa. The amount of substance present in a given volume of a solution is expressed in number of ways, e.g., mass per cent, mole fraction, molarity and molality.