# CHAPTER - 01 SOME BASIC CONCEPTS OF CHEMISTRY

#### **INTRODUCTION**

Chemistry deals with the composition, structure and properties of matter. These aspects can be best described and understood in terms of basic constituents of matter: atoms and molecules. That is why chemistry is called the science of atoms and molecules.

#### **IMPORTANCE OF CHEMISTRY**

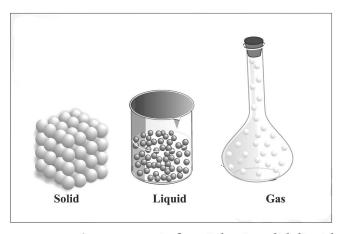
Chemists are interested in knowing how chemical transformations occur. Chemistry plays a central role in science and is often intertwined with other branches of science like physics, biology, geology etc. Chemistry also plays an important role in daily life. Many life saving drugs such as cisplatin and taxol, are effective in cancer therapy and AZT (Azidothymidine) used for helping AIDS victims, have been isolated from plant and animal sources or prepared by synthetic methods.

#### **NATURE OF MATTER**

Anything which has mass and occupies space is called **matter**. Everything around us, for example, book, pen, pencil, water, air, all living beings etc. are composed of matter.

#### **STATES OF MATTER**

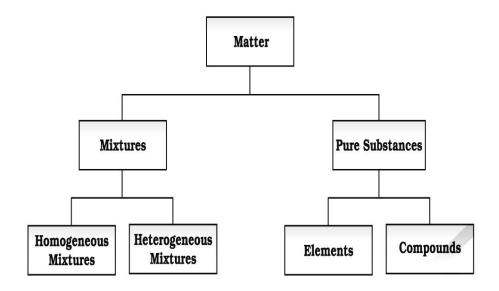
Matter can exist in three physical states viz. solid, liquid and gas. The constituent particles of matter in these three states can be represented as



Arrangement of particles in solid, liquid and gaseous state

#### **CLASSIFICATION OF MATTER**

At the macroscopic or bulk level, matter can be classified as mixtures or pure substances.



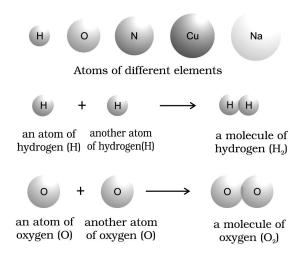
Classification of matter

In a homogeneous mixture, the components completely mix with each other and its composition is uniform throughout. Sugar solution, and air are thus, the examples of homogeneous mixtures. In contrast to this, in heterogeneous mixtures, the composition is not uniform throughout and sometimes the different components can be observed. For example, the mixtures of salt and sugar, grains and pulses along with some dirt (often stone) pieces, are heterogeneous mixtures.

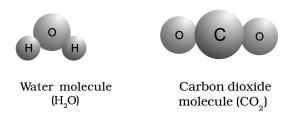
**Pure substances** have characteristics different from the mixtures. They have fixed composition, whereas mixtures may contain the components in any ratio and their composition is variable. Copper, silver, gold, water, glucose are some examples of pure substances. Glucose contains carbon, hydrogen and oxygen in a fixed ratio and thus, like all other pure substances has a fixed composition. Also, the constituents of pure substances cannot be separated by simple physical methods.

Pure substances can be further classified into **elements** and **compounds**. An **element** consists of only one type of particles. These particles may be **atoms** or **molecules**. Some elements such as sodium or copper, contain single atoms held together as their constituent particles whereas in some others, two or more atoms combine to give molecules of the element. Thus, hydrogen, nitrogen and oxygen gases consist of molecules in which two atoms combine to give their respective molecules.

When two or more atoms of different elements combine, the molecule of a compound is obtained. The examples of some compounds are water, ammonia, carbon dioxide, sugar etc.



A representation of atoms and molecules



A depiction of molecules of water and carbon dioxide

The atoms of different elements are present in a compound in a fixed and definite ratio and this ratio is characteristic of a particular compound. Also, the properties of a compound are different from those of its constituent elements. For example, hydrogen and oxygen are gases whereas the compound formed by their combination i.e., water is a liquid. It is interesting to note that hydrogen burns with a pop sound and oxygen is a supporter of combustion, but water is used as a fire extinguisher.

#### PROPERTIES OF MATTER AND THEIR MEASUREMENT

Every substance has unique or characteristic properties. These properties can be classified into two categories – physical properties and chemical properties.

Physical properties are those properties which can be measured or observed without changing the identity or the composition of the substance. Some examples of physical properties are colour, odour, melting point, boiling point, density etc. The measurement or observation of chemical properties require a chemical change to occur. The examples of chemical properties are characteristic reactions of different substances; these include acidity or basicity, combustibility etc.

#### **Measurement of properties**

Any quantitative observation or measurement is represented by a number followed by units in which it is measured. For example length of a room can be represented as 6 m; here 6 is the number and m denotes metre – the unit in which the length is measured.

Two different systems of measurement, i.e. the English System and the Metric System were being used in different parts of the world. The metric system which originated in France in late eighteenth century, was more convenient as it was based on the decimal system. The need of a common standard system was being felt by the scientific community. Such a system was established in 1960 known as SI system.

#### The International system of units (SI)

The International System of Units (in French Le Systeme International d'Unités – abbreviated as SI) was established by the 11th General Conference on Weights and Measures (CGPM from Conference Generale des Poidset Measures). The CGPM is an inter governmental treaty organization created by a diplomatic treaty known as Metre Convention which was signed in Paris in 1875.

Base Physical Quantities and their Units

Base Physical Quantity	Symbol for Quantity	Name of SI Unit	Symbol for SI Unit
Length	l	metre	m
Mass	m	kilogram	kg
Time	t	second	s
Electric current	I	ampere	A
Thermodynamic temperature	T	kelvin	K
Amount of substance	n	mole	mol
Luminous intensity	$I_{_{\mathcal{O}}}$	candela	cd

Each modern industrialized country including India has a National Metrology Institute (NMI) which maintains standards of measurements. This responsibility has been given to the National Physical Laboratory (NPL), New Delhi.

Prefixes used in the SI System

Multiple	Prefix	Symbol
10-24	yocto	у
10-21	zepto	z
$10^{-18}$	atto	a
$10^{-15}$	femto	f
$10^{-12}$	pico	p
10-9	nano	n
10-6	micro	μ
10-3	milli	m
$10^{-2}$	centi	$\mathbf{c}$
10-1	deci	d
10	deca	da
$10^{2}$	hecto	h
$10^{3}$	kilo	k
$10^{6}$	mega	M
$10^{9}$	giga	G
$10^{12}$	tera	T
1015	peta	P
$10^{18}$	exa	E
$10^{21}$	zeta	Z
$10^{24}$	yotta	Y

#### Some Important physical properties

#### 1) Mass and weight

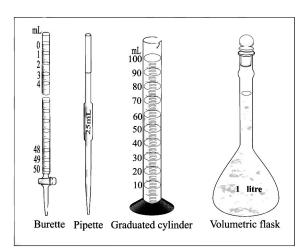
Mass of a substance is the amount of matter present in it while weight is the force exerted by gravity on an object. The mass of a substance is constant whereas its weight may vary from one place to another due to change in gravity.

The mass of a substance can be determined very accurately in the laboratory by using an analytical balance.

The SI unit of mass is kilogram. However, its fraction gram (1 kg = 1000 g), is used in laboratories due to the smaller amounts of chemicals used in chemical reactions.

#### 2) Volume

Volume has the units of (lengths)<sup>3</sup>. So in SI system, volume has units of m<sup>3</sup>. But again, in chemistry laboratories, smaller volumes are used. Hence, volume is often denoted in cm<sup>3</sup> or dm<sup>3</sup> units.



Some volume measuring devices

$$1L = 10^{-3} \,\mathrm{m}^3 = 10^3 \,\mathrm{(cm^3 \ cc \ mL)} = 1 \,\mathrm{dm^3}$$

#### 3) Density

Density of a substance is its amount of mass per unit volume. So SI units of density can be obtained as follows:

SI unit of density = 
$$\frac{\text{SI unit of mass}}{\text{SI unit of volume}} = \frac{\text{kg}}{\text{m}^3} \text{ or kg m}^{-3}$$

This unit is quite large and a chemist often expresses density in g cm<sup>-3</sup>, where mass is expressed in gram and volume is expressed in cm<sup>3</sup>.

#### 4) Temperature

There are three common scale to measure temperature - °C (degree celsius). °F (degree fahrenheit) and K(kelvin). Here, K is the SI unit.

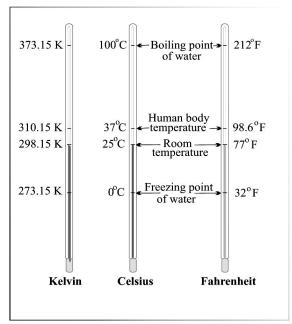
Generally, the thermometer with celsius scale are calibrated from 0° to 100° where these two temperatures are the freezing point and the boiling point of water respectively. The fahrenheit scale is represented between 32° to 212°.

The temperatures on two scales are related to each other by the following relationship:

$${}^{0}F = \frac{9}{5} ({}^{0}C) + 32$$

The kelvin scale is related to celsius scale as follows:

$$K = {}^{\circ}C + 273.15$$



Thermometers using different temperature scales

It is interesting to note that temperature below 0 °C (i.e. negative values) are possible in Celsius scale but in Kelvin scale, negative temperature is not possible.

#### 5) Pressure (p)

$$p = \frac{\text{force}}{\text{area}}$$

SI unit =  $kg m^{-1}s^{-2} = Nm^{-2} = Pa$ 

1 atm = 1.013 bar = 760 mmHg (torr) = 101325 Pa ( $\approx 10^5$  Pa Nm<sup>-2</sup> or kg m<sup>-1</sup>s<sup>-2</sup>)

Atmospheric pressure can be measured by barometer ( $p = h\rho g$ )

Gas pressure can be measured by manometer (open end as well as closed end)

#### **UNCERTAINTY IN MEASUREMENT**

#### **Scientific Notation**

scientific notation for such numbers, i.e., exponential notation in which any number can be represented in the form  $N \times 10^n$  where n is an exponent having positive or negative values and N is a number (called digit term) which varies between 1.000... and 9.999....

eg: Avogadro number is 6.022 × 10<sup>23</sup>

#### **Multiplication and Division**

These two operations follow the same rules which are there for exponential numbers, i.e.

$$(5.6 \times 10^{5}) \times (6.9 \times 10^{8}) = (5.6 \times 6.9) (10^{5+8})$$

$$= (5.6 \times 6.9) \times 10^{13}$$

$$= 38.64 \times 10^{13}$$

$$= 3.864 \times 10^{14}$$

$$(9.8 \times 10^{-2}) \times (2.5 \times 10^{-6}) = (9.8 \times 2.5) (10^{-2+(-6)})$$

$$= (9.8 \times 2.5) (10^{-2-6})$$

$$= 24.50 \times 10^{-8} = 2.450 \times 10^{-7}$$

$$\frac{2.7 \times 10^{-3}}{5.5 \times 10^{4}} = (2.7 \div 5.5) (10^{-3-4}) = 0.4909 \times 10^{-7} = 4.909 \times 10^{-8}$$

#### Addition and subtraction

For these two operations, first the numbers are written in such a way that they have same exponent. After that, the coefficient are added or subtracted as the case may be.

Thus, for adding  $6.65 \times 10^4$  and  $8.95 \times 10^3$ .

 $6.65 \times 10^4 + 0.895 \times 10^4$  exponent is made same for both the numbers.

Then, these numbers can be added as follows

$$(6.65 + 0.895) \times 10^4 = 7.545 \times 10^4$$

Similarly, the subtraction of two numbers can be done as shown below:

$$2.5 \times 10^{-2} - 4.8 \times 10^{-3}$$
  
=  $(2.5 \times 10^{-2}) - (0.48 \times 10^{-2})$   
=  $(2.5 - 0.48) \times 10^{-2} = 2.02 \times 10^{-2}$ 

#### **Significant Figures**

#### **Precision & Accuracy**

**Precision** refers to the closeness of various measurements for the same quantity. However, **accuracy** is the agreement of a particular value to the true value of the result. For example, if the true value for a result is 2.00 g and a student 'A' takes two measurements and reports the results as 1.95 g and 1.93 g. These values are precise as they are close to each other but are not accurate. Another student repeats the experiment and obtains 1.94 g and 2.05 g as the results for two measurements. These observations are neither precise nor accurate. When a third student repeats these measurements and reports 2.01g and 1.99g as the result. These values are both precise and accurate.

Data to Illustrate Precision and Accuracy

Measurements/g			
	1	2	Average (g)
Student A	1.95	1.93	1.940
Student B	1.94	2.05	1.995
Student C	2.01	1.99	2.000

#### Significant figures

The uncertainty in the experimental or the calculated values is indicated by mentioning the number of significant figures. Significant figures are meaningful digits which are known with certainty. The uncertainty is indicated by writing the certain digits and the last uncertain digit. Thus, if we write a result as 11.2 mL, we say the 11 is certain and 2 is uncertain and the uncertainty would be +1 in the last digit. Unless otherwise stated, an uncertainty of +1 in the last digit is always understood.

There are certain rules for determining the number of significant figures.

- (1) All non-zero digits are significant. For example in 285 cm, there are three significant figures and in 0.25 mL, there are two significant figures.
- (2) Zeros preceding to first non-zero digit are not significant. Such zero indicates the position of decimal point. Thus, 0.03 has one significant figure and 0.0052 has two significant figures.
- (3) Zeros between two non-zero digits are significant. Thus, 2.005 has four significant figures.
- (4) Zeros at the end or right of a number are significant provided they are on the right side of the decimal point. For example, 0.200 g has three significant figures.

But, if otherwise, the terminal zeros are not significant if there is no decimal point. For example, 100 has only one significant figure, but 100. has three significant figures and 100.0 has four significant figures. Such numbers are better represented in scientific notation. We can express the number 100 as  $1\times10^2$  for one significant figure,  $1.0\times10^2$  for two significant figures and  $1.00\times10^2$  for three significant figures.

(5) Counting numbers of objects, for example, 2 balls or 20 eggs, have infinite significant figures as these are exact numbers and can be represented by writing infinite number of zeros after placing a decimal i.e.,

2 = 2.000000 or 20 = 20.000000

In numbers written in scientific notation, all digits are significant e.g.,  $4.01 \times 10^2$  has three significant figures, and  $8.256 \times 10^{-3}$  has four significant figures.

#### Addition and substraction of significant figures

The result cannot have more digits to the right of the decimal point than either of the original numbers.

12.11

18.0

1.012

31.122

Here, 18.0 has only one digit after the decimal point and the result should be reported only up to one digit after the decimal point which is 31.1

#### Multiplication and division of significant figures

In these operations, the result must be reported with no more significant figures as are there in the measurement with the few significant figures.

 $2.5 \times 1.25 = 3.125$ 

Since 2.5 has two significant figures, the result should not have more than two significant figures, thus, it is 3.1.

#### Rounding off the numbers

- 1. If the rightmost digit to be removed is more than 5, the preceding number is increased by one. for example, 1.386 If we have to remove 6, we have to round it to 1.39
- 2. If the rightmost digit to be removed is less than 5, the preceding number is not changed. For example, 4.334 if 4 is to be removed, then the result is rounded upto 4.33.
- 3. If the rightmost digit to be removed is 5, then the preceding number is not changed if it is an even number but it is increased by one if it is an odd number. For example, if 6.35 is to be rounded by removing 5, we have to increase 3 to 4 giving 6.4 as the result. However, if 6.25 is to be rounded off it is rounded off to 6.2.

#### **Dimensional Analysis**

Often while calculating, there is a need to convert units from one system to other. The method used to accomplish this is called factor label method or unit factor method or dimensional analysis.

#### LAWS OF CHEMICAL COMBINATIONS

The combination of elements to form compounds is governed by the following five basic laws.

#### 1) Laws of conservation of mass

It states that matter can neither be created nor destroyed.

This law was put forth by Antoine Lavoisier. He performed careful experimental studies for combustion reactions for reaching to the above conclusion.

#### 2) Law of Definite Proportions

This law was given by, a French chemist, Joseph Proust. He stated that a given compound always contains exactly the same proportion of elements by weight.

Proust worked with two samples of cupric carbonate — one of which was of natural origin and the other was synthetic one. He found that the composition of elements present in it was same for both the samples

	% of copper	% of oxygen	% of carbon
Natural Sample	51.35	9.74	38.91
Synthetic Sample	51.35	9.74	38.91

It is sometimes also referred to as Law of definite composition.

#### 3) Law of multiple proportions

This law was proposed by Dalton in 1803. According to this law, if two elements can combine to form more than one compound, the masses of one element that combine with a fixed mass of the other element, are in the ratio of small whole numbers.

For example, hydrogen combines with oxygen to form two compounds, namely, water and hydrogen peroxide.

 $\begin{array}{ccc} \text{Hydrogen} + \text{Oxygen} \rightarrow \text{Water} \\ & 2g & 16g & 18g \\ \text{Hydrogen} + \text{Oxygen} \rightarrow \text{Hydrogen Peroxide} \\ & 2g & 32g & 34g \end{array}$ 

Here, the masses of oxygen (i.e. 16 g and 32 g) which combine with a fixed mass of hydrogen (2g) bear a simple ratio, i.e. 16 : 32 or 1 : 2.

# 4) Gay Lussac's Law of Gaseous Volumes

This law was given by Gay Lussac. He observed that when gases combine or are produced in a chemical reaction they do so in a simple ratio by volume provided all gases are at same temperature and pressure.

Thus, 100 mL of hydrogen combine with 50 mL of oxygen to give 100 mL of water vapour.

Hydrogen + Oxygen  $\rightarrow$  Water 100 mL 50 mL 100 mL

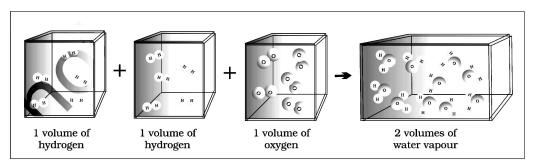
Thus, the volumes of hydrogen and oxygen which combine together (i.e. 100 mL and 50 mL) bear a simple ratio of 2:1.

Gay-Lussac's discovery of integer ratio in volume relationship is actually the law of definite proportions by volume. The Gay-Lussac's law was explained properly by the work of Avogadro

#### 5) Avogadro Law

Avogadro proposed that equal volumes of gases at the same temperature and pressure should contain equal number of molecules. Avogadro made a distinction between atoms and molecules.

Each box contains equal number of molecules. In fact, Avogadro could explain the above result by considering the molecules to be polyatomic. If hydrogen and oxygen were considered as diatomic as recognised now, then the above results are easily understandable.



Two volumes of hydrogen react with One volume of oxygen to give Two volumes of water vapour

Also volume directly proportional to number of molecules keeping T and P are constants.

#### **DALTON'S ATOMIC THEORY**

In 1808, Dalton published 'A New System of Chemical Philosophy' in which he proposed the following:

- 1. Matter consists of indivisible atoms.
- 2. All the atoms of a given element have identical properties including identical mass. Atoms of different elements differ in mass.
- 3. Compounds are formed when atoms of different elements combine in a fixed ratio.
- 4. Chemical reactions involve reorganisation of atoms. These are neither created nor destroyed in a chemical reaction.

Dalton's theory could explain the laws of chemical combination.

#### ATOMIC AND MOLECULAR MASSES

#### **Atomic mass**

The atomic mass or the mass of an atom is actually very-very small because atoms are extremely small. Today, we have sophisticated techniques e.g., mass spectrometry for determining the atomic masses fairly accurately. But, in the nineteenth century, scientists could determine mass of one atom relative to another by experimental means, as has been mentioned earlier. Hydrogen, being lightest atom was arbitrarily assigned a mass of 1 (without any units) and other elements were assigned masses relative to it. However, the present system of atomic masses is based on carbon - 12 as the standard and has been agreed upon in 1961. Here, Carbon - 12 is one of the isotopes of carbon and can be represented as 12C. In this system, 12C is assigned a mass of exactly 12 atomic mass unit (amu) and masses of all other atoms are given relative to this standard. One atomic mass unit is defined as a mass exactly equal to onetwelfth the mass of one carbon - 12 atom.

And 1 amu =  $1.66056 \times 10^{-24}$  g

Mass of an atom of hydrogen = 1.6736 × 10<sup>-24</sup> g

Thus, in terms of amu, the mass of hydrogen atom =  $\frac{1.6736 \times 10^{-24} \text{g}}{1.66056 \times 10^{-24} \text{g}} = 1.0078 \text{ amu} = 1.0080 \text{ amu}$ 

Today, 'amu' has been replaced by 'u' which is known as unified mass.

#### Relative atomic mass (RAM)

RAM = 
$$\frac{\text{mass of an atom of element}(w_1)}{\text{mass of an atom of}^{12}C} \times 12$$

#### Gram atomic mass (GAM or 1 g atom)

It is mass of one mole of atoms

eg: atomic mass of C is 12 u

GAM of C is 12 g

#### **Average Atomic Mass**

Many naturally occurring elements exist as more than one isotope. When we take into account the existence of these isotopes and their relative abundance (per cent occurrence), the average atomic mass of that element can be computed. For example, carbon has the following three isotopes with relative abundances and masses as shown against each of them.

Isotope	Relative Abundance (%)	Atomic Mass (amu)
12C	98.892	12
13C	1.108	13.00335
14C	$2 \times 10^{-10}$	14.00317

From the above data, the average atomic mass of carbon will come out to be :

$$(0.98892)(12 \text{ u}) + (0.01108)(13.00335 \text{ u}) + (2 \times 10^{-12})(14.00317 \text{ u}) = 12.011 \text{ u}$$

Similarly, average atomic masses for other elements can be calculated. In the periodic table of elements, the atomic masses mentioned for different elements actually represented their average atomic masses.

#### New scale versus conventional scale

On changing scale, relative atomic mass changes but actual mass never changes

#### Molecular mass

Molecular mass is the sum of atomic masses of the elements present in a molecule. It is obtained by multiplying the atomic mass of each element by the number of its atoms and adding them together.

Molecular mass of methane,

$$(CH_4) = (12.011 \text{ u}) + 4 (1.008 \text{ u})$$

= 16.043 u

# Gram molecular mass (GMM or 1 g molecule)

It is mass of one mole of molecules

eg: molecular mass of CO2 is 44 u

GMM of CO<sub>2</sub> is 44 g

#### **Formula Mass**

Some substances such as sodium chloride do not contain discrete molecules as their constituent units. In such compounds, positive (sodium) and negative (chloride) entities are arranged in a three-dimensional structure.

The formula such as NaCl is used to calculate the formula mass instead of molecular mass as in the solid state sodium chloride does not exist as a single entity.

Thus, formula mass of sodium chloride = atomic mass of sodium + atomic mass of chlorine

$$= 23.0 u + 35.5 u = 58.5 u$$

GFM of NaC
$$l = 58.5 g$$

# Structure for NaCl

#### **MOLE CONCEPT AND MOLAR MASSES**

One mole is 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. The mass of a carbon–12 atom was determined by a mass spectrometer and found to be equal to 1.992648 ×  $10^{-23}$  g. Knowing that one mole of carbon weighs 12 g, the number of atoms in it is equal to :

$$\frac{12 \text{ g/mol}^{12}\text{C}}{1.992648 \times 10^{-23} \text{ g/}^{12}\text{C atom}} = 6.0221367 \times 10^{23} \text{ atoms/mol}$$

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.

We can, therefore, say that 1 mol of hydrogen atoms = 6.022×10<sup>23</sup> atoms

1 mol of water molecules = 6.022×10<sup>23</sup> water molecules

1 mol of sodium chloride =  $6.022 \times 10^{23}$  formula units of sodium chloride

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.

Molar mass of water = 18.02 g mol<sup>-1</sup>

Molar mass of sodium chloride = 58.5 g mol-1

#### **STP and SATP**

#### **STP (Standard temperature and pressure)**

 $T = 0^{\circ} C = 273 K$ 

p = 1bar

If p is 1 atm the condition is NTP (normal temperature and pressure)

#### SATP (Standard ambient temperature and pressure)

$$T = 25^{\circ} C = 298 K$$

p = 1bar

#### **Molar volume**

Volume occupied by 1 mole of any gas at standard conditions of T and P is called molar volume.

Molar volume at STP = 22.7 L

Molar volume at NTP = 22.4 L

Irrespective of the pressure we can take molar volume as 22.4 L for doing calculations.

#### Vapour density of a gas (VD)

$$VD = \frac{Density of gas}{Density of standard gas} = \frac{D_{gas}}{D_{H}}$$

# Relation between molecular mass and VD of gas

$$VD = \frac{\text{molecular mass of a gas}}{2}$$

If the standard gas is methane (CH<sub>4</sub>)

Then, 
$$VD = \frac{\text{molecular mass of a gas}}{16}$$

# Molar mass of mixture of gases (M<sub>mix</sub>)

$$M_{\text{mix}} = \frac{n_1 M_1 + n_2 M_2}{n_1 + n_2}$$

# **Summary of mole concept**

44 g 
$$CO_2$$
 = 1 mol of  $CO_2$  = 6.022 × 10<sup>23</sup> molecules of  $CO_2$   
= 1 × 6.022 × 10<sup>23</sup> C atoms  
= 2 × 6.022 × 10<sup>23</sup> O atoms  
= 3 × 6.022 × 10<sup>23</sup> atoms  
= 22 × 6.022 × 10<sup>23</sup> electrons = 22.4 L at STP (only for gases)

#### Number of moles (n)

$$n = \frac{given \ mass(w)}{molar \ mass(M)}$$

$$n = \frac{given \ volume \ at \ STP(V)}{molar \ Volume \ at \ STP(V_m)}$$

$$n = \frac{given \text{ number of molecules at } STP(N)}{avogadros \text{ number}(N_A)}$$

#### PERCENTAGE COMPOSITION

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

eg: Molar mass of water = 18.02 g

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

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

# **Empirical formula for molecular formula**

An empirical formula represents the simplest whole number ratio of various atoms present in a compound whereas the molecular formula shows the exact number of different types of atoms present in a molecule of a compound.

#### Relation between empirical formula and molecular formula

Molecular formula =  $(empirical formula)_n$  where  $n = \frac{molecular mass}{empirical mass}$ 

#### 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.

#### **Balancing a chemical equation**

According to the law of conservation of mass, a balanced chemical equation has the same number of atoms of each element on both sides of the equation. Many chemical equations can be balanced by trial and error.

Let us take combustion of propane, C<sub>3</sub>H<sub>8</sub>. This equation can be balanced in steps.

#### Step 1

Write down the correct formulas of reactants and products. Here propane and oxygen are reactants, and carbon dioxide and water are products.

$$C_3H_8(g) + O_2(g) \rightarrow CO_2(g) + H_2O(\ell)$$
 unbalanced equation

#### Step 2

Balance the number of C atoms: Since 3 carbon atoms are in the reactant, therefore, three  $CO_2$  molecules are required on the right side.

$$C_3H_8(g) + O_2(g) \rightarrow 3CO_2(g) + H_2O(\ell)$$

#### Step 3

Balance the number of H atoms: on the left there are 8 hydrogen atoms in the reactants however, each molecule of water has two hydrogen atoms, so four molecules of water will be required for eight hydrogen atoms on the right side.

$$C_3H_8(g) + O_2(g) \rightarrow 3CO_2(g) + 4H_2O(\ell)$$

#### Step 4

Balance the number of O atoms : There are ten oxygen atoms on the right side ( $3 \times 2 = 6$  in  $CO_2$  and  $4 \times 1 = 4$  in water). Therefore, five  $O_2$  molecules are needed to supply the required ten oxygen atoms.

$$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(\ell)$$

#### Step 5

Verify that the number of atoms of each element is balanced in the final equation. The equation shows three carbon atoms, eight hydrogen atoms, and ten oxygen atoms on each side.

#### **Limiting Reagent**

The reactant which gets consumed, limits the amount of product formed and is, therefore, called the **limiting reagent**.

The other reagent, a part of which remains unreacted is known as excess reagent

# **Equivalent mass**

Equivalent mass of an element is the mass of the element which combine with or displaces 1.008 parts by mass of hydrogen or 8 parts by mass of oxygen or 35.5 parts of chlorine by mass.

a) Equivalent mass of an element

$$E_{element} = \frac{Atomic\ mass}{Valency}$$

b) Equivalent mass of an acid,

$$\mathsf{E}_{\mathsf{acid}} = \frac{\mathsf{molecular\ mass}}{\mathsf{basicity}}$$

Basicity is the number of replaceable H<sup>+</sup> ion from one molecule of acid

Eg: Basicity of HCI = 1

Basicity of  $H_2SO_4 = 2$ 

c) Equivalent mass of a base;

$$E_{base} = \frac{Molecular \, mass}{Acidity}$$

Acidity is the number of replaceable OH- ions from one molecule of the base.

Eg: Acidity of NaOH = 1

Acidity of Ca(OH)<sub>2</sub> = 2

d) Equivalent mass of a salt;

$$E_{salt} = \frac{formula\ mass}{total + ve\ charge\ on\ cation}$$

e) Equivalent mass of an ion;

$$E_{ion} = \frac{formula\ mass}{charge}$$

f) Equivalent mass of an oxidising or reducing agent

$$E_{_{O.A/R.A}} = \frac{Molecular\,mass}{Number\,\,of\,\,electron\,\,transferred\,\,per\,\,mole}$$

Generally,

Equivalent mass = 
$$\frac{\text{Molecular mass}}{\text{n-factor}}$$

Here n-factor = valency, basicity, acidity, total +ve charge, number of electrons transferred per mole

#### **Reactions in solutions**

- Solutions are homogeneous mixture of two or more than two components
- ♦ The component present usually in largest quantity and doesnot undergo a phase change is called solvent which is denoted as 1, while the component present in small amount and undergo a phase change is called solute, which is denoted as 2.
- Binary solution solutions consists of two components only one solute and one solvent
- ♦ Physical state of solution = physical state of solvent

#### **Expressing concentration of solutions (Concentration Terms)**

Concentration of a solution means the amount of solute in solution. The major concentration techniques are

#### 1) Mass percentage (w/w)

$$\frac{W}{W} = \frac{\text{Mass of one component}}{\text{Total mass of solution}} \times 100$$

10 % (w/w) aqueous solution of glucose means 10 g glucose dissolved in 90 g water results in 100 g of glucose solution

The unit is commonly used in industrial chemical application.

eg: Commercial bleaching solution contains 3.62 % (w/w) aqueous solution of sodium hypochlorite.

#### 2) Volume percentage (v/v)

$$\frac{V}{V} = \frac{\text{Volume of one component}}{\text{total volume of solution}}$$

10 % (v/v) aqueous solution of ethanol means 10 mL of ethanol dissolved in water such that the total volume of the solution is 100 mL.

This unit is also used in chemical induction

eg : A 35 % (v/v) solution of ethylene glycol (anti freeze) is used in cars for cooling the engine which lowers the freezing point of water to 255.4 K (-17.6 $^{\circ}$  C)

#### 3) Mass by volume percentage (w/v)

$$\frac{W}{V} = \frac{Mass of solute}{Volume of solution in mL} \times 100$$

5% (w/v) aqueous solution of NaCl means 5 g NaCl dissolved in enough water so that the final volume of the solution is 100 mL

This unit is used in medicine and pharmacy.

# 4) Parts per million (ppm)

This unit is commonly used when the solute is present in trace quantities

$$ppm = \frac{Number of parts of the component}{Total number of parts of all components of solution} \times 10^{6}$$

The term 'part' may be mass or volume.

In terms of mass

$$ppm = \frac{mass of one component}{total mass of solution} \times 10^{2} \times 10^{4} = mass \% \times 10^{4}$$

ie, ppm = mass 
$$\% \times 10^4$$

volume % × 10<sup>4</sup>

$$1ppm = 1mg L^{-1} = 1\mu g mL^{-1}$$

# 5) Strength (S)

$$S = \frac{Mass of solute(g)}{Volume of solution(L)} gL^{-1}$$

5 g L-1 aqueous solution of NaCl means 5 g NaCl is present in 1 L solution

# 6) Mole fraction $(\chi)$

$$\chi = \frac{Number\ of\ moles\ of\ the\ component}{Total\ number\ of\ moles\ of\ all\ the\ components}$$

For a binary solution

$$\chi_1 = \frac{n_1}{n_1 + n_2}$$
 and  $\chi_2 = \frac{n_2}{n_1 + n_2}$ 

OR 
$$\chi_1 = \frac{w_1}{w_1} \frac{M_1}{M_1 + w_2}$$
 and  $\chi_2 = \frac{w_2}{w_1} \frac{M_2}{M_1 + w_2} \frac{M_2}{M_2}$ 

Also 
$$\chi_1 + \chi_2 = 1$$

Generally, in a given solution sum of all the mole fraction is unity ie,

$$\chi_1 + \chi_2 + \dots + \chi_i = 1$$

#### 7) Molality (m)

$$m = \frac{\text{Number of moles of solute}}{\text{Mass of solvent in kg}} = \frac{n_2}{w_1} = \frac{w_2}{M_2 \cdot w_1}$$

If w₁ is in g,

$$m = \frac{w_2.1000}{M_2.w_1} \text{mol kg}^{-1}(m)$$

x molal (x m) aqueous solution of NaOH means x mol. NaOH dissolved in 1 kg water

#### 8) Molarity (M)

$$M = \frac{Number of moles of solute}{Volume of solution in L} = \frac{n_2}{v} = \frac{w_2}{M_2 v}$$

If v is in mL,

$$M = \frac{w_2.1000}{M_2.V} mol L^{-1}(M)$$

x molar (x M) aqueous solution of NaOH means x mol NaOH present in 1 L solution

# 9) Normality (N)

$$N = \frac{Number of gram equivalent of solute}{Volume of solution in L} = \frac{n_{g,eq}}{v} = \frac{w_2}{E_2 \cdot v}$$

 $E_2$  = Equivalent mass of solute

If v is in mL

$$N = \frac{w_2.1000}{E_2.V} eqL^{-1}(N)$$

x normal (x N) aqueous solution of H<sub>2</sub>SO<sub>4</sub> means x gram equivalents of H<sub>2</sub>SO<sub>4</sub> present in 1 L solution

#### <u>NOTE</u>

Seminormal = 
$$\frac{N}{2}$$

Decinormal = 
$$\frac{N}{10}$$
 etc

#### 1) Relation between m and M

$$M = \frac{1000M}{1000d - MM_{_2}}$$
 , Where  $\mathrm{M_{_2}}$  is molar mass of solute

# 2) Relation between N and M

$$N = n$$
-factor  $\times M$ 

$$n_{a-eq} = (n - factor) n moles$$



Acidity of base

Basicity of acid

Number of electrons transferred per mole etc

#### 3) Molarity equation

a) Dilution formula

$$M_1V_1 = M_2V_2$$

# b) Reaction formula

$$\frac{M_1 V_1}{n_1} = \frac{M_2 V_2}{n_2}$$

Here  $\rm n_{\scriptscriptstyle 1}$  and  $\rm n_{\scriptscriptstyle 2}$  are the stoichiometric coefficients of reactants or products

# 4) Normality equation

For both dilution and reaction, normality equation is

$$N_1V_1 = N_2V_2$$

e, 1 equivalent of reactant A requires 1 equivalent of reactant B

OR

1 equivalent of reactant A produces 1 equivalent of product B