Mathematical Tool in Chemistry

Measurable properties of gases

The characteristics of gases are described fully in terms of four parameters or measurable properties:

(i) The volume, V, of the gas.

(ii) Its pressure, P

(iii) Its temperature, T

(iv) The amount of the gas (i.e., mass or number of moles).

(1) Volume : (i) Since gases occupy the entire space available to them, the measurement of volume of a gas only requires a measurement of the container confining the gas.

(ii) Volume is expressed in litres (L), millilitres (mL) or cubic centimetres (cm^3), cubic metres (m^3) .

(iii) $1\ L = 1000\ mL$; $1\ mL = 10^{-3} L$; $1\ L = 1\ dm^3 = 10^{-3}\ m^3$

$1\ m^3 = 10^3\ dm^3 = 10^6 cm^3 = 10^6\ mL = 10^3\ L$

(2) Mass : (i) The mass of a gas can be determined by weighing the container in which the gas is enclosed and again weighing the container after removing the gas. The difference between the two weights gives the mass of the gas.

(ii) The mass of the gas is related to the number of moles of the gas i.e.

$$\text{moles of gas (n)} = \frac{\text{Mass in grams}}{\text{Molar mass}} = \frac{m}{M}$$

(3) Temperature : (i) Gases expand on increasing the temperature. If temperature is increased twice, the square of the velocity (v^2) also increases two times.

(ii) Temperature is measured in centigrade degree (ºC) or celsius degree with the help of thermometers. Temperature is also measured in Fahrenheit (ºF).

(iii) S.I. unit of temperature is kelvin (K) or absolute degree.

$$K = {}^{o}C + 273$$

(iv) Relation between ºF and ºC is $\frac{{}^{o}C}{5} = \frac{{}^{o}F - 32}{9}$

(4) Pressure : (i) Pressure of the gas is the force exerted by the gas per unit area of the walls of the container in all directions. Thus, Pressure (P) $= \frac{\text{Force(F)}}{\text{Area(A)}} = \frac{\text{Mass(m)} \times \text{Acceleration(a)}}{\text{Area(A)}}$

(ii) Pressure exerted by a gas is due to kinetic energy $(KE = \frac{1}{2}mv^2)$ of the molecules. Kinetic energy of the gas molecules increases, as the temperature is increased.

(iii) Pressure of a gas is measured by manometer or barometer.

(iv) Commonly two types of manometers are used :

(a) Open end manometer; (b) Closed end manometer

(v) The S.I. unit of pressure, the pascal (Pa), is defined as 1 newton per metre square. It is very small unit.

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

(vi) C.G.S. unit of pressure is dynes cm^{-2}.

(vii) M.K.S. unit of pressure is Newton m^{-2}. The unit Newton m^{-2} is sometimes called pascal (Pa).

(viii) Higher unit of pressure is bar, kPa or MPa.

$$1\ bar = 10^5 Pa = 10^5\ Nm^{-2} = 100KNm^{-2} = 100KPa$$

(ix) Several other units used for pressure are

Name	Symbol	Value
bar	bar	$1 bar = 10^5 Pa$
atmosphere	atm	$1 atm = 1.01325 \times 10^5 Pa$
Torr	Torr	$1 Torr = \frac{101325}{760} Pa = 133.322 Pa$
millimetre of mercury	mm Hg	$1 mm Hg = 133.322 Pa$

Prefixes used in the SI System

Multiple	Prefix	Symbol
10^{-24}	yocto	y
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	c
10^{-1}	deci	d
10	deca	D
10^{2}	hecto	h
10^{3}	kilo	k
10^{6}	mega	M
10^{9}	giga	G
10^{12}	tera	T
10^{15}	peta	P
10^{18}	exa	E
10^{21}	zeta	Z
10^{24}	yotta	Y

Equation of State :

Combining all the gas relations in a single expression which discribes relationship between pressure, volume and temperature, of a given mass of gas we get an expression known as equation of state.

$$\frac{PV}{T} = \text{constant (dependent on moles of the gas n).}$$

$$\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$$

Ideal gas Equation :

$$PV = nRT$$

This is the ideal gas equation as it is obeyed by the hypothetical gases called ideal gases under all conditions of temperature and pressure.

However there is no gas that is perfectly ideal. But the gases may show nearly ideal behaviour under the conditions of low pressure and high temperature and are called real gases.

$$\frac{PV}{nT} = \text{constant} \qquad \text{[universal constant]}$$

$$= R \qquad \text{(ideal gas constant or universal gas constant)}$$

Experimentally

$$\boxed{\begin{aligned} R &= 8.314 \text{ J/Kmole} \approx 25/3 \\ &= 1.987 \text{ cal/mole} \approx 2 \\ &= 0.08 \text{ Latm/mole} \approx 1/12 \end{aligned}}$$

Density and molar Mass of a Gaseous Substance :

Ideal gas equation is $PV = nRT$ ....(i)

On rearranging the above equation, we get

$$\frac{n}{V} = \frac{P}{RT} \quad \text{....(ii)}$$

Putting the value of 'n' from equation (iii) in equation (ii), we get

$$\frac{m}{MV} = \frac{P}{RT} \quad \text{....(iv)}$$

Replacing $\frac{m}{V}$ in eq. (iv) with d (density)

$$\frac{d}{M} = \frac{P}{RT}$$

Rarranging the above equation, we get $M = \frac{dRT}{P}$

Energy, Wavelength Calculation

Energy of one photon is given by

$E_0 = h\nu$ (ν- Frequency of light)

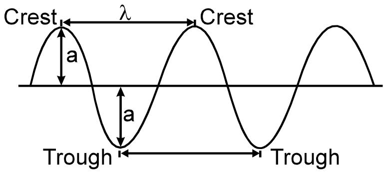
$h = 6.625 \times 10^{-34}$ J-Sec (h - Planck const.)

$E_0 = \frac{hc}{\lambda}$ (c - speed of light)

(λ - wavelength)

Order of magnitude of $E_o = \frac{10^{-34} \times 10^{8}}{10^{-10}} = 10^{-16}$ J

- **Wavelength** of a wave is defined as the distance between any two consecutive crests or troughs. It is represented by λ (lambda) and is expressed in Å or m or cm or nm (nanometer) or pm (picometer).
  $1 \text{ Å} = 10^{-8} \text{ cm} = 10^{-10} \text{ m}$
  $1 \text{ nm} = 10^{-9} \text{ m}$, $1 \text{ pm} = 10^{-12} \text{ m}$



- **Wave number** is defined as the number of waves present in 1 cm length. Evidently, it will be equal to the reciprocal of the wavelength. It is represented by $\bar{\nu}$ (read as nu bar).

$$\bar{\nu} = \frac{1}{\lambda}$$

If λ is expressed in cm, $\bar{\nu}$ will have the units cm^{-1}.

pH scale :

- Acidic strength means the tendency of an acid to give H_3O^+ or H^+ ions in water.
  So greater the tendency to give H^+ , more will be the acidic strength of the substance.
- Basic strength means the tendency of a base to give OH^- ions in water.
  So greater the tendency to give OH^- ions, more will be basic strength of the substance.

- The concentration of H^+ ions is written in a simplified form introduced by Sorenson known as pH scale.
  pH is defined as negative logarithm of activity of H^+ ions.
  $\therefore$ $pH = -\log a_{H^+}$ (where a_{H^+} is the activity of H^+ ions)
- Activity of H^+ ions is the concentration of free H^+ ions or H_3O^+ ions in a Solution.
- For dilute Solutions $[H^+] \le 1M$ concentration can be taken as activity of H^+ ions while for higher concentrations the activity would be much less than the concentration itself, so it is calculated experimentally.
- The pH scale was marked from 0 to 14 with central point at 7 at 25°C taking water as solvent.
- If the temperature is changed, the pH range of the scale will also change. For ***Example***

0 – 14	at 25°C	Neutral point, pH = 7
0 –13	at 80°C ($K_w = 10^{-13}$)	Neutral point, pH = 6.5

- pH can also be negative or > 14

Concentration terms :

The following concentration terms are used to expressed the concentration of a solution. These are

- Molarity (M)
- Molality (m)
- Mole fraction (x)
- % calculation
- ppm

- Remember that all of these concentration terms are related to one another. By knowing one concentration term you can also find the other concentration terms. Let us discuss all of them one by one.

Molarity (M) :

The number of moles of a solute dissolved in 1 L (1000 ml) of the solution is known as the molarity of the solution.

$$\text{i.e., Molarity of solution} = \frac{\text{number of moles of solute}}{\text{volume of solution in litre}}$$

Let a solution is prepared by dissolving w g of solute of mol.wt. M in V ml water.

$$\therefore \quad \text{Number of moles of solute dissolved} = \frac{w}{M}$$

$$\therefore \quad \text{V ml water have } \frac{w}{M} \text{ mole of solute}$$

$$\therefore \quad \text{1000 ml water have } \frac{w \times 1000}{M \times V_{ml}} \qquad \therefore \quad \text{Molarity (M)} = \frac{w \times 1000}{(\text{Mol. wt of solute}) \times V_{ml}}$$

Some other relations may also useful.

$$\text{Number of millimoles} = \frac{\text{mass of solute}}{(\text{Mol. wt. of solute})} \times 1000 = (\text{Molarity of solution} \times V_{ml})$$

- Molarity of solution may also given as :

$$\frac{\text{Number of millimole of solute}}{\text{Total volume of solution in ml}}$$

- Molarity is a unit that depends upon temperature. It varies inversely with temperature .
  Mathematically : Molarity decreases as temperature increases.

$$\text{Molarity} \propto \frac{1}{\text{temperature}} \propto \frac{1}{\text{volume}}$$

- If a particular solution having volume V_1 and molarity = M_1 is diluted upto volume V_2 mL than
  $M_1V_1 = M_2V_2$
  M_2 : Resultant molarity

- If a solution having volume V_1 and molarity M_1 is mixed with another solution of same solute having
  volume V_2 mL & molarity M_2
  then $M_1V_1 + M_2V_2 = M_R (V_1 + V_2)$
  M_R = Resultant molarity = $\frac{M_1V_1 + M_2V_2}{V_1 + V_2}$

Solved Examples

Example-1 149 g of potassium chloride (KCl) is dissolved in 10 Lt of an aqueous solution. Determine the molarity of the solution (K = 39, Cl = 35.5)

Solution Molecular mass of KCl = 39 + 35.5 = 74.5 g

$\therefore$ Moles of KCl = $\frac{149 \text{ gm}}{74.5 \text{ gm}} = 2$

$\therefore$ Molarity of the solution = $\frac{2}{10} = 0.2$ M

Molality (m) :

The number of moles of solute dissolved in1000 g (1 kg) of a solvent is known as the molality of the solution.

i.e., molality = $\frac{\text{number of moles of solute}}{\text{mass of solvent in gram}} \times 1000$

Let Y g of a solute is dissolved in X g of a solvent. The molecular mass of the solute is M_0. Then Y/M_0 mole of the solute are dissolved in X g of the solvent. Hence

Molality = $\frac{Y}{M_0 \times X} \times 1000$

- ***Molality is independent of temperature changes.***

Solved Examples

Example-2 225 g of an aqueous solution contains 5 g of urea. What is the concentration of the solution in terms of molality. (Mol. wt. of urea = 60)

Solution Mass of urea = 5 g

Molecular mass of urea = 60

Number of moles of urea = $\frac{5}{60} = 0.083$

Mass of solvent = (255 – 5) = 250 g

$\therefore$ Molality of the solution = $\frac{\text{Number of moles of solute}}{\text{Mass of solvent in gram}} \times 1000 = \frac{0.083}{250} \times 1000 = 0.332.$

Mole fraction (x) :

The ratio of number of moles of the solute or solvent present in the solution and the total number of moles present in the solution is known as the mole fraction of substances concerned.

Let number of moles of solute in solution = n

Number of moles of solvent in solution = N

$\therefore$ Mole fraction of solute $(x_1) = \dfrac{n}{n+N}$

$\therefore$ Mole fraction of solvent $(x_2) = \dfrac{N}{n+N}$

also $x_1 + x_2 = 1$

- Mole fraction is a pure number. It will remain independent of temperature changes.

% calculation :

The concentration of a solution may also expressed in terms of percentage in the following way.

- **% weight by weight (w/w) :** It is given as mass of solute present in per 100 g of solution.

i.e. $\% \text{ w/w} = \dfrac{\text{mass of solute in gm}}{\text{mass of solution in gm}} \times 100$

- **% weight by volume (w/v) : It is given as mass of solute present in per 100 ml of Solution.**

i.e., $\% \text{ w/v} = \dfrac{\text{mass of solute in gm}}{\text{volume of solution in ml}} \times 100$

- **% volume by volume (v/v) : It is given as volume of solute present in per 100 ml Solution.**

i.e., $\% \text{ v/v} = \dfrac{\text{volume of solute in ml}}{\text{volume of solution in ml}} \times 100$

Solved Examples

Example-3 0.5 g of a substance is dissolved in 25 g of a solvent. Calculate the percentage amount of the substance in the solution.

Solution Mass of substance = 0.5 g

Mass of solvent = 25 g

$\therefore$ percentage of the substance (w/w) = × 100 = 1.96

Example-4 20 cm^3 of an alcohol is dissolved in80 cm^3 of water. Calculate the percentage of alcohol in solution.

Solution Volume of alcohol = 20 cm^3

Volume of water = 80 cm^3

$\therefore$ Percentage of alcohol = × 100 = 20.

Parts Per Million (ppm)

When the solute is present in very less amount, then this concentration term is used. It is defined as the number of parts of the solute present in every 1 million parts of the solution. ppm can both be in terms of mass or in terms of moles. If nothing has been specified, we take ppm to be in terms of mass. Hence, a 100 ppm solution means that 100 g of solute is present in every 1000000 g of solution.

$$\text{ppm}_A = \frac{\text{mass of A}}{\text{Total mass}} \times 10^6 = \text{mass fraction} \times 10^6$$