MATHEMATICAL CONVERSIONS 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*	$1bar = 10^5\,Pa$
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.

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

= R (ideal gas constant or universal gas constant)

Experimentally

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

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)

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

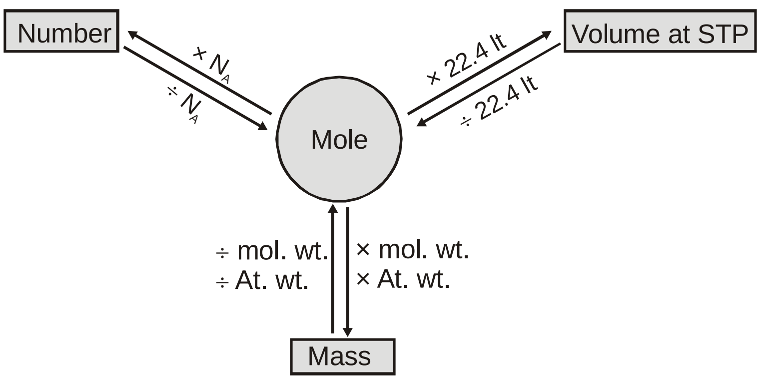
Rarranging the above equation, we get $M = \frac{dRT}{P}$

Mole Calculation

A mole is the amount of a substance that contains as many entities (atoms, molecules or other particles) as there are atoms in exactly 0.012 kg (or 12 g) of the carbon-12 isotope.

From mass spectrometer we found that there are 6.023×10^{23} atoms present in 12 g of C-12 isotope.

The number of entities in 1 mol is so important that it is given a separate name and symbol known as Avogadro constant denoted by N_A.



- **Note : In modern practice gram-atom and gram-molecule are termed as mole.**

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)

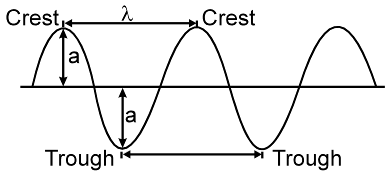
(λ - wavelength)

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 Å = 10^{-8} cm = 10^{-10} m

  1 nm = 10^{-9} m, 1 pm = 10^{-12} 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 $[H^+] \leq 1M$ 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

Now **$pH = -\log[H^+] = 7$** and **$pOH = -\log[OH^-] = 7$** for water at 25° (experimental)

$$\left.\begin{array}{ll} pH = 7 = pOH & \Rightarrow \text{neutral} \\ pH < 7 \text{ or } pOH > 7 & \Rightarrow \text{acidic} \\ pH > 7 \text{ or } pOH < 7 & \Rightarrow \text{Basic} \end{array}\right\} \text{at } 25°C$$

Oxidation Number

Oxidation Number

- It is an imaginary or apparent charge developed over atom of an element when it goes from its elemental free state to combined state in molecules.

- It is calculated on basis of an arbitrary set of rules.

- It is a relative charge in a particular bonded state.

- In order to keep track of electron-shifts in chemical reactions involving formation of compounds, a more practical method of using oxidation number has been developed.

- In this method, it is always assumed that there is a complete transfer of electron from a less electronegative atom to a more electronegative atom.

Rules governing oxidation number

The following rules are helpful in calculating oxidation number of the elements in their different compounds. It is to be remembered that the basis of these rule is the electronegativity of the element .

- **Fluorine atom :**

  Fluorine is most electronegative atom (known). It always has oxidation number equal to –1 in all its compounds

- **Oxygen atom :**

  In general and as well as in its oxides , oxygen atom has oxidation number equal to –2.

In case of (i) peroxide (e.g. H_2O_2 , Na_2O_2) is –1,

(ii) super oxide (e.g. KO_2) is –1/2

(iii) ozonide (e.g. KO_3) is –1/3

(iv) in OF_2 is + 2 & in O_2F_2 is +1

- **Hydrogen atom :**

  In general, H atom has oxidation number equal to +1. But in metallic hydrides (e.g. NaH, KH), it is –1.

- **Halogen atom :**

  In general, all halogen atoms (Cl, Br , I) have oxidation number equal to –1. But if halogen atom is attached with a more electronegative atom than halogen atom, then it will show positive oxidation numbers.

  e.g. $K\overset{+5}{Cl}O_3$, $\overset{+5}{HI}O_3$, $H\overset{+7}{Cl}O_4$, $K\overset{+5}{Br}O_3$

- **Metals :**

  (a) Alkali metal (Li , Na, K, Rb, ...) always have oxidation number +1

  (b) Alkaline earth metal (Be , Mg , Ca ....) always have oxidation number +2.

  (c) Aluminium always has +3 oxidation number

Note : Metal may have negative or zero oxidation number

- Oxidation number of an element in free state or in allotropic forms is always zero

  e.g. $\overset{0}{O_2}$, $\overset{0}{S_8}$, $\overset{0}{P_4}$,$\overset{0}{O_3}$

- Sum of the oxidation numbers of atoms of all elements in a molecule is zero.

- Sum of the oxidation numbers of atoms of all elements in an ion is equal to the charge on the ion.

- If the group number of an element in modern periodic table is ***n,*** then its oxidation number may vary from

  (n – 10) to ***(n – 18)*** (but it is mainly applicable for p-block elements)

  e.g. N- atom belongs to 15th group in the periodic table, therefore as per rule, its oxidation number may vary from

  –3 to +5 ($\overset{-3}{N}H_3$,$\overset{+2}{N}O$, $\overset{+3}{N_2}O_3$, $\overset{+4}{N}O_2$, $\overset{+5}{N_2}O_5$)

- The maximum possible oxidation number of any element in a compound is never more than the number of electrons in valence shell.(but it is mainly applicable for p-block elements)

Oxidising and reducing agent

- **Oxidising agent or Oxidant :**

  Oxidising agents are those compounds which can oxidise others and reduce itself during the chemical reaction. Those reagents in which for an element, oxidation number decreases or which undergoes gain of electrons in a redox reaction are termed as oxidants.

  e.g. $KMnO_4$, $K_2Cr_2O_7$, HNO_3, conc.H_2SO_4 etc are powerful oxidising agents .

- **Reducing agent or Reductant :**

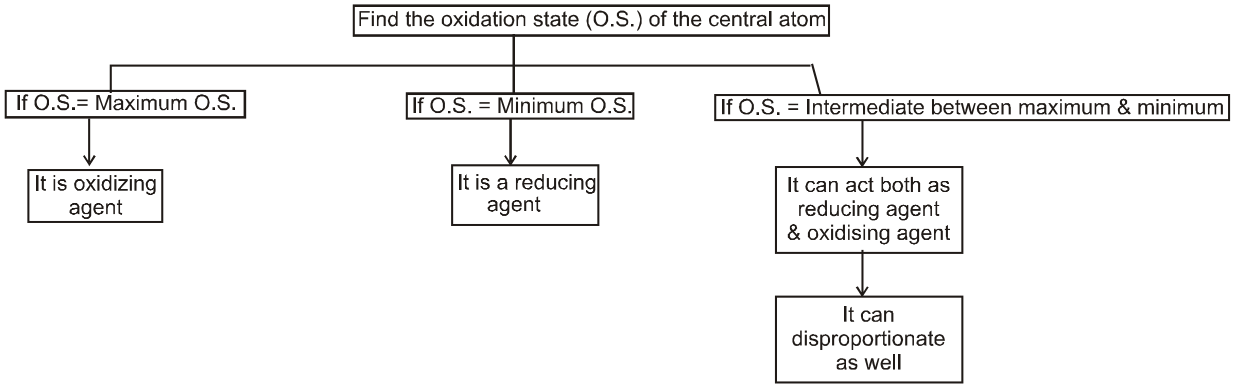
  Reducing agents are those compounds which can reduce other and oxidise itself during the chemical reaction. Those reagents in which for an element, oxidation number increases or which undergoes loss of electrons in a redox reaction are termed as reductants.

  e.g. KI , $Na_2S_2O_3$ etc are the powerful reducing agents.

  Note : ***There are some compounds also which can work both as oxidising agent and reducing agent***

  e.g. H_2O_2, NO_2^-

HOW TO IDENTIFY WHETHER A PARTICULAR SUBSTANCE IS AN OXIDISING OR A REDUCING AGENT



Redox reaction

A reaction in which oxidation and reduction simultaneously take place is called a redox reaction

In all redox reactions, the total increase in oxidation number must be equal to the total decrease in oxidation number.

e.g. $10\overset{+2}{Fe}SO_4 + 2K\overset{+5}{Mn}O_4 + 8H_2SO_4 \longrightarrow 5\overset{+3}{Fe_2}(SO_4)_3 + 2\overset{+2}{Mn}SO_4 + K_2SO_4 + 8H_2O$

Disproportionation Reaction :

A redox reaction in which same element present in a particular compound in a definite oxidation state is oxidized as well as reduced simultaneously is a disproportionation reaction.

Disproportionation reactions are a special type of redox reactions. One of the reactants in a disproportionation reaction always contains **an element that can exist in at least three oxidation states**. The element in the form of reacting substance is in the intermediate oxidation state and both higher and lower oxidation states of that element are formed in the reaction. For example :

$$2H_2\overset{-1}{O_2}\ (aq) \longrightarrow 2H_2\overset{-2}{O}\ (\ell) + \overset{0}{O_2}\ (g)$$

$$\overset{0}{S_8}\ (s) + 12OH^-(aq) \longrightarrow 4\overset{-2}{S}{}^{2-}\ (aq) + 2\overset{+2}{S_2}O_3^{2-}\ (aq) + 6H_2O\ (\ell)$$

$$\overset{0}{Cl_2}\ (g) + 2OH^-(aq) \longrightarrow \overset{+1}{Cl}O^-(aq) + \overset{-1}{Cl}{}^-(aq) + H_2O\ (\ell)$$