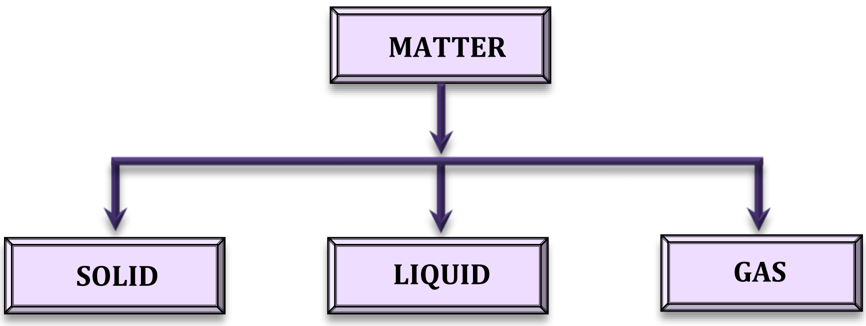
01 Some Basic Concepts of Chemistry

All of the objects around you - this book, your pen or pencil, and the things of nature such as rocks, water and plant and animal substances - constitute the matter of the universe. Each of the particular kinds of matter, such as a certain kind of paper or plastic or metal, is referred to as a material. We can define chemistry as the science of the composition and structure of materials and of the changes that material undergoes.
Because chemistry deals with all materials, it is a subject of enormous breadth. It would be difficult to exaggerate the influence of the chemistry on modern science and technology. In the section that follows, we will take a brief glimpse at basic concepts of chemistry.

Classification of Matter:

Matter: Matter is anything that has mass and occupies space.
Two ways of classifying matter.
I. Physical classification
II. Chemical classification

I. Physical classification:



(i)	Particles are very closely packed in ordered manner.	Particles are less closely packed.	Particles are farthest apart
(ii)	No freedom of movement of particles	Particles can move around to some extent	Movement of particles is very easy and fast
(iii)	Definite shape and volume	Definite volume, indefinite shape	indefinite shape and volume
(iv)	Exists at low T and high P	Exists at intermediate P & T	Exists at high T and low P

Note: For same substance:
- Solid and Liquid co-exist at ***MELTING POINT***.
- Liquid and gas co-exist at ***BOILING POINT***.
- Solid and gas co-exist at ***SUBLIMATION POINT***.
- Solid, liquid and gas co-exist at ***TRIPLE POINT***.

II. Chemical classification:

MATTER

- **Pure substances**
  - Have fixed composition
  - Cannot be separated by physical methods
  - **Elements**
    - Made of only one type of atoms

    Ex. : S_8, P_4, O_3
    $C_{(diamond)}$
    $C_{(graphite)}$
    Hg(l), I_2(s)
    Br_2(l)
  - **Compounds**
    - Made of two or more types of atoms/ions
    - **Ionic**

      Ex. : NaCl(s)
    - **Covalent**

      Ex. : CH_4(g)
- **Mixtures**
  - Variable composition
  - Can be separated by physical methods to pure substances
  - **Homogeneous (solutions)**
    - Have uniform composition and density through out

    Ex. : Mixture of gases
    or NaCl + H_2O
    or Glucose + H_2O
    or Alloys
  - **Heterogeneous**
    - Are not uniform in composition and/or density

    Ex. : Graphite+Diamond
    or Fe + FeO
    or Sand + H_2O

Note : PHASE : It is the state of matter uniform in density and composition.

- Homogeneous mixtures have single phase while heterogeneous mixtures are multi-phase.

  Ex : NaCl + H_2O mixture has one phase

  Ex : Graphite + Diamond mixture has 2 phases.

Illustration 1:

Match the column :

Column-I		Column-II	
(A)	Element	(P)	Can't be decomposed into simpler substances by physical decomposition
(B)	Compound	(Q)	Can be decomposed into simpler substances by chemical methods.
(C)	Mixture	(R)	Can't be decomposed into simpler substances by chemical methods
(D)	H_2O	(S)	Uniform composition
(E)	Fe(s) + S(s) in powdered form	(T)	Consists of one type of atoms
(F)	Sea water	(U)	Consists of 2 or more type of atoms.

Solution:

(A) → (R) & (T), (P), (S)
(B) → (Q) & (U), (S), (P)
(C) → (U), (Q)
(D) → (Q) & (U), (S), (P)
(E) → (U), (Q)
(F) → (U), (Q)

Note :

(i) Mixtures can be separated by both physical and chemical methods.
(ii) Compounds can only be broken by chemical methods.

Illustration 2:

$2HgO \xrightarrow{\Delta} 2Hg + O_2 \uparrow$

How many phases do you observe in the above given reaction at room temperature ?

Solution:

(3)

$HgO \longrightarrow$ solid, $Hg \longrightarrow$ liquid, $O_2 \longrightarrow$ gas

Properties of Matter and their Measurement:

Chemists broadly classified properties into two kinds, namely physical properties and chemical properties in order to characterize a particular sample of matter. physical properties are those properties which can be measured or observed without changing the identity or the composition of the substance.

Chemical properties are those which can be measured only by a chemical reaction. these cannot be determined just by viewing or touching the substance. chemical properties shows the kind of reaction in which a substance can take part e.g ., acidity or basicity, combustibility, reactivity etc.

There are many properties of matter which are capable of being measured or quantitative in nature e.g., length, area, volume etc. such quantities are measured with some fixed standard. for example, if we want to know the length of a piece of paper, we shall lay the piece of paper parallel to a centimeter scale and will count the number of marking on the scale. suppose the number of marking is 15.2, this means that the piece of paper is 15.2 times longer than one unit of measurement but it is senseless to say the paper is 15.2, until we add centimeter, a unit of length to 15.2 i.e., 15.2 cm. this presentation is appropriate and called **physical quantity**. therefore, a measured physical quantity is expressed in two parts, a **numerical coefficient** and a **unit**. either of them are meaningless without each other.

A unit is the standard of reference chosen to measure or express any physical quantity.

The International System of Units (S.I.):

SI system is a modification of metric system and has seven base units pertaining to the seven fundamental scientific quantities.

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	l_v	Candela	cd

Some specific properties of substances:

Deliquescence :

The property of certain compounds of taking up the moisture present in atmosphere and becoming wet when exposed, is known as deliquescence. These compounds are known as deliquescent. Sodium hydroxide, potassium hydroxide, anhydrous calcium chloride, anhydrous magnesium chloride, anhydrous ferric chloride, etc., are the examples of deliquescent compounds.

Hygroscopicity :

Certain compounds combine with the moisture of atmosphere and are converted into hydroxides or hydrates. Such substances are called hygroscopic. Anhydrous copper sulphate, quick lime (CaO), anhydrous sodium carbonate, etc., are of hygroscopic nature.

Efflorescence :

The property of some crystalline substances of losing their water of crystallisation on exposure and becoming powdery on the surface is called efflorescence and such salts are known as efflorescent. The examples are : Ferrous sulphate ($FeSO_4.7H_2O$), sodium carbonate ($Na_2CO_3.10H_2O$), sodium sulphate ($Na_2SO_4.10H_2O$), potash alum [$K_2SO_4.Al_2(SO_4)_3.24H_2O$], etc.

Malleability :

This property is shown by metals. When metallic solid is being beaten, it does not break but is converted into thin sheet. It is said to possess the property of malleability. Copper, gold, silver, aluminium, lead, etc., can be easily hammered into sheets. Gold is the most malleable metal.

Ductility :

The property of metal to be drawn into wires is termed ductility. Copper, silver, gold, aluminium, iron, etc., are ductile in nature. Platinum is the most ductile metal.

Brittleness :

The solid materials which break into small pieces on hammering are called brittle. The solids of non-metals are generally brittle in nature.

Ex: Ice, Diamond etc.

Dalton's Atomic Theory:

Ancient Indian and Greek philosophers have always wondered about the unknown and unseen form of matter. The idea of divisibility of matter was considered long back in India, around 500 BC. An Indian philosopher ***Maharishi Kanad***, postulated that if we go on dividing matter (padarth), we shall get smaller and smaller particles. Ultimately, a time will come when we shall come across the smallest particle beyond which further division will not be possible. He named these particles Parmanu. Another Indian philosopher, Pakudha Katyayama, elaborated this doctrine and said that these particles normally exist in a combined form which gives us various forms of matter. Around the same era, the Greek philosopher Democritus expressed the belief that all matter consists of very small, indivisible particles, which he named ***atomos*** (meaning uncuttable or indivisible).

John Dalton (1766 - 1844)

An Englishman, began teaching at a Quaker school when he was 12. His fascination with science included an intense interest in meteorology (he kept careful daily weather records for 46 years), which led to an interest in the gases of the air and their ultimate components, atom. Dalton is best known for his atomic theory, in which he postulated that the fundamental differences among atoms are their masses. He was the first to prepare a table of relative atomic weight.

Although Democritus' ideal was not accepted by many of his contemporaries (notably Plato and Aristotle), somehow it endured. Experimental evidence from early scientific investigations provided support for the notion of "atomism" and gradually gave rise to the modern definitions of elements and compounds. It was in ***1808, John Dalton***, formulated a precise definition of the indivisible building blocks of matter that we call atoms. Dalton's work marked the beginning of the modern era of chemistry. The hypothesis about the nature of matter on which Dalton's atomic theory is based can be summarized as follows :

(i) Elements are composed of extremely small particles called atoms.

(ii) All atoms of a given element are identical, having the same size, mass and chemical properties. The atoms of one element are different from the atoms of all other elements.

(iii) Compounds are composed of atoms of more than one element. In any compound, the ratio of the numbers of atoms of any two of the elements present is either an integer or a simple fraction.

(iv) A chemical reaction involves only the separation, combination or rearrangement of atoms ; it does not result in their creation or destruction.

Limitations of Dalton’s Atomic Theory:

According to Dalton’s atomic theory, an atom is the ultimate, discrete and indivisible particle of matter. Later researches proved that Dalton’s atomic theory was not wholly correct.

Dalton’s atomic theory suffered from the following drawbacks:

(i) Atoms of the same or different types have a strong tendency to combine together to form a new ‘group of atoms’. For example, hydrogen, nitrogen, oxygen gases exist in nature as ‘group of two atoms’. This indicates that the smallest unit capable of independent existence is not an atom, but a ‘group of atoms’.

(ii) With the discovery of sub-atomic particles, e.g., electrons, neutrons and protons, the atom can no longer be considered indivisible.

(iii) Discovery of isotopes indicated that all atoms of the same element are not perfectly identical. At least, they differ in their masses. Atoms of the same element having different masses are called isotopes.

Dalton’s atomic theory could not explain why certain substances, all containing atoms of the same element, should differ in their properties. For example, charcoal, graphite and diamond all are made up of only Carbon-atoms, but still their properties are quite different.

Some Basic Concepts:

At the center of each atom is a "***nucleus***" that consists of two types of particles called "***protons***" and "***neutrons***" (and known collectively as "nucleons"). The number of protons is called the "***atomic number***". The total number of protons and neutrons in the nucleus of the atom is called the "***mass number***" and is determined by the type of atom (i.e. which element it is) and also by the number of neutrons present in that particular atom. In many cases, different atoms of the same element can have different numbers of neutrons in their nuclei ("nuclei" is the plural word for "nucleus"; one nucleus - many nuclei). The number of neutrons in an atom of a specific element therefore determines its "mass number".

For example, most atoms of the element phosphorus have a mass number of 31 and so may be referred to as phosphorus-31, however, some atoms of phosphorus have an extra neutron and therefore a mass number of 32. They are therefore atoms of the isotope phosphorus-32.

Although there are three types of particles that form atoms (protons, neutrons and electrons), electrons have very low mass compared with protons and neutrons so the mass of atoms is mainly due to the numbers of protons and neutrons that make-up the atom, i.e. the "mass number" of the atom.

The atomic number of an atom is the same as the atomic number of the element of which that atom is a particle because the atomic number of an atom determines which element it is an atom of.

However, the mass number of an atom is not the same as the mass number of an element because atoms of the same element can have different masses due to having different numbers of neutrons (i.e. exist in the form of different isotopes, which therefore have slightly different physical properties e.g. boiling points).

That is why Atomic Number of an element is meaningful, but the Mass Number "of an element" is not so meaningful.

When dealing with elements (macroscopic scale) rather than atoms (individual particles), chemists use Relative Atomic Mass because "mass number" only applies to specific atoms of one particular isotope of the element.

Atom is actually made of 3 fundamental particles:

1. Electron **2.** Proton **3.** Neutron

Fundamental particle	**Discovered By**	**Charge**	**Mass**	$\left(\frac{\text{charge}}{\text{mass}}\right)$ **(Specific Charge)**
Electron ($e^{\ominus}$ **or** β)	J. J. Thomson	-1.6×10^{-19} coloumb -4.8×10^{-10} esu -1 Unit	9.1×10^{-31}kg 9.1×10^{-28}g 0.000544 a.m.u.	1.76×10^{8} C/g
Proton (P) **(Ionized H atom,** $H^{\oplus}$**)**	Rutherford	$+1.6 \times 10^{-19}$ coloumb $+4.8 \times 10^{-10}$esu 9.58×10^{4} C/g +1 Unit	1.672×10^{-27}kg 1.672×10^{-24}g 1.00727 a.m.u.	9.58×10^{4}C/g
Neutron (${}_0n^1$)	James Chadwick	0	1.675×10^{-27}kg 1.675×10^{-24}g 1.00867 a.m.u.	0

Representation of atom : $_ZX^A$

A $\longrightarrow$ Mass number : (total number of protons + total number of neutrons present in an atom.)

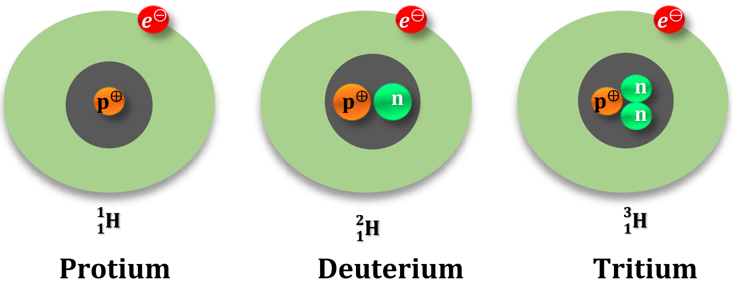
Z $\longrightarrow$ Atomic number : (total number of protons present in an atom.)

$\Rightarrow$ ***Isotope :*** Atoms of given element which have same atomic number but different mass number are called isotope :

e.g. $_1H^1$, $_1H^2$, $_1H^3$,

e.g. , $_8O^{16}$, $_8O^{18}$

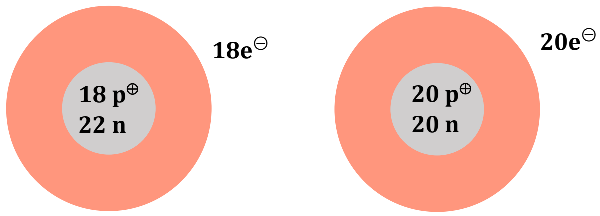
e.g. , $_{17}Cl^{35}$, $_{17}Cl^{37}$



$\Rightarrow$ ***Isobar :*** Atoms of different elements with the same mass number but different atomic number .

e.g. $_{18}Ar^{40}$, $_{19}K^{40}$ and $_{20}Ca^{40}$

e.g. $_6C^{14}$, $_7N^{14}$

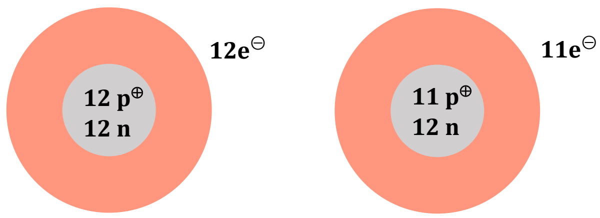


$\Rightarrow$ ***Isotones :*** Isotones are atoms that have the same number of neutrons but different number of protons.

e.g $_{12}Mg^{24}$, $_{11}Na^{23}$

e.g. $_9F^{19}$, $_8O^{18}$

$_{15}P^{31}$, $_{16}S^{32}$



⇒ ***Iso-electronic species :*** Species (atom, molecules or ions) having same number of electrons are called iso-electronic e.g $O^{2\ominus}$, $F^{\ominus}$, $Na^{\oplus}$, $Mg^{2\oplus}$

Note : Now a days this concept is extended to consider the same valence shell electron also.

eg. $SO_4^{2\ominus}, SeO_4^{2\ominus}, TeO_4^{2\ominus}$

eg. $ClO_4^{\ominus}, BrO_4^{\ominus}, IO_4^{\ominus}$

⇒ ***Iso-sters :*** Species having same number of electrons & same number of atoms. eg. N_2O, CO_2

$NO_3^{\ominus}, CO_3^{2}, BO_3^{3\ominus}$

eg. Number of atoms = 4

Number of electrons in $NO_3^{\ominus}$ = 7 + 8 + 8 + 1 =32

Number of electrons in $CO_3^{2\ominus}$ = 6 + 8 + 8 + 8 + 2 = 32

Number of electrons in $BO_3^{3\ominus}$ = 5 + 8 + 8 + 8 + 3 = 32

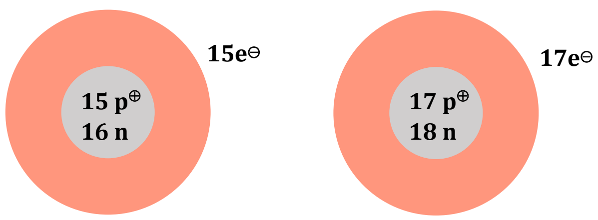
eg. $CH_4, NH_4^{\oplus}$

eg. $PO_4^{3\ominus}, SO_4^{2\ominus}, ClO_4^{\ominus}$

⇒ ***Iso-diaphers :*** Species having same difference in number of neutrons and protons or same number of excess of neutron. eg. $^{19}{}_{9}F^{23}$, $_{11}Na$

eg. $_{15}P^{31}$, $_{17}Cl^{35}$

eg. $_{17}Cl^{37}$, $_{21}Si^{45}$



Neutron – Proton = (n – p) = (A – 2Z). It is also known as neutron excess.

The law of chemical combination:

Atoine Lavoisier, John Dalton and other scientists formulated certain laws concerning the composition of matter and chemical reactions. These laws are known as the law of chemical combination.

I. Law of indestructibility of matter or conservation of Mass:

- This law was proposed by ***Lavosier in 1774.***
- The experimental certification was given by Landolt.
- According to this law in all chemical changes the total mass of the system remains constant or in a chemical change mass is neither created nor destroyed. Thus, in chemical change-

  Total mass of reactant = Total mass of products

  Ex. $H_2O(s) \longrightarrow H_2O(\ell)$

  Above reaction shows the physical change and the wt. of $H_2O(s)$ = wt. of $(H_2O)(\ell)$

  In case the reacting materials are not completely consumed, the relationship will be Total masses of reactants = Total masses of product + masses of unreacted reactants
- In nuclear reactions (Mass + energy) is conserved not the mass separately.

Antoine Lavosier
(1743-1794)

Antoine-Laurent de Lavosier, the "Father of modern chemistry", was a French nobleman prominent in the histories of chemistry and biology. He named both oxygen and hydrogen and predicted silicon.

Illustration 3:

When 4.2 g $NaHCO_3$ is added to a solution of CH_3COOH weighing 10.0 g, it is observed that 2.2 g CO_2 is released into atmosphere. The residue is found to weigh 12.0 g. Show that these observations are in agreement with the law of conservation of mass.

Solution:

$NaHCO_3 + CH_3COOH \longrightarrow CH_3COONa + H_2O + CO_2$

Initial mass = 4.2 + 10 = 14.2

Final mass = 12 + 2.2 = 14.2

Thus, during the course of reaction law of conservation of mass is obeyed.

II. Law of constant or definite proportion:

- This law was given by ***Joseph Louis proust. in 1799***.

Joseph Proust **(1754 - 1826)**

Proust was born the son of an apothecary at Angers in north-west France. He studied in Paris. He lived in poverty for some years before being awarded a pension by Louis XVIII

- Chemical composition of a compound remains constant whether it is obtained by any method or any source.

Example :

In water (H_2O), Hydrogen and Oxygen combine in 2 : 1 molar ratio, the ratio remains constant whether it is tap water, river water or sea water or produced by any chemical reaction.

Illustration 4:

1.80 g of a certain metal burnt in oxygen gave 3.0 g of its oxide. 1.50 g of the same metal heated in steam gave 2.50 g of its oxide. Show that these results illustrate the law of constant proportion.

Solution:

In the first sample of the oxide,

wt. of metal = 1.80 g,   wt. of oxygen = (3.0 – 1.80) g = 1.2 g

$$\therefore \quad \frac{\text{wt.of metal}}{\text{wt.of oxygen}} = \frac{1.80\text{g}}{1.2\text{g}} = 1.5$$

In the second sample of the oxide,

wt. of metal = 1.50 g,   wt. of oxygen = (2.50 – 1.50) g = 1 g

$$\therefore \quad \frac{\text{wt.of metal}}{\text{wt.of oxygen}} = \frac{1.50\text{g}}{1\text{g}} = 1.5$$

Thus, in both samples of the oxide the proportions of the weights of the metal and oxygen are fixed. Hence, the results follow the law of constant proportion.

Note :

This law is not applicable in case of isotopes.

III. The law of multiple proportion:

- This law was given by Dalton in 1804.
- If two elements combine to form more than one compound, then the different masses of one element which combine with a fixed mass of the other element, bear a simple ratio to one another.

  Ex. Nitrogen and oxygen combine to form five stable oxides –

N_2O	Nitrogen 28 parts	Oxygen 16 parts
N_2O_2	Nitrogen 28 parts	Oxygen 32 parts
N_2O_3	Nitrogen 28 parts	Oxygen 48 parts
N_2O_4	Nitrogen 28 parts	Oxygen 64 parts
N_2O_5	Nitrogen 28 parts	Oxygen 80 parts

  The masses of oxygen which combine with same mass of nitrogen in the five compounds bear a ratio 16 : 32 : 48 : 64 : 80 or 1 : 2 : 3 : 4 : 5.

Note :

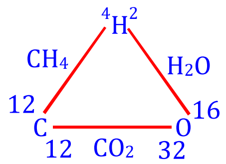
This law is not applicable in case of isotopes.

IV. Law of reciprocal proportion (or law of equivalent wt.):

This law was put forward by ***Richter in 1792***. It states as follows :

The ratio of the weights of two elements A and B which combine separately with a fixed weight of the third element C is either the same or some simple multiple of the ratio of the weights in which A and B combine directly with each other. This law may be illustrated with the help of the following example.

The elements C and O combine separately with the third element H to form CH_4 and H_2O and they combine directly with each other to form CO_2, as shown in fig.



In CH_4, 12 parts by weight of carbon combine with 4 parts by weight of hydrogen. In H_2O, 2 parts by weight of hydrogen combine with 16 parts by weights of oxygen. Thus the weight of C and O which combine with fixed weight of hydrogen (say 4 parts by weight) are 12 and 32 i.e. they are in the ratio 12 : 32 or 3 : 8.

Now in CO_2, 12 parts by weight of carbon combine directly with 32 parts by weight of oxygen i.e. they combine directly in the ratio 12 : 32 or 3 : 8 which is the same as the first ratio.

Special Note :

This law is also called as law of equivalent wt. due to each element combined in their equivalent wt. ratio.

Example based on Law of Reciprocal proportion:

Illustration 5:

Ammonia contains 82.35% of nitrogen and 17.65% of hydrogen. Water contains 88.90% of oxygen and 11.10% of hydrogen. Nitrogen trioxide contains 63.15% of oxygen and 36.85% of nitrogen. Show that these data illustrate the law of reciprocal proportions.

Solution:

In NH_3, 17.65g of H combine with N = 82.35g

$\therefore$ 1 g of H combine with N = $\frac{82.35}{17.65}$ g = 4.66 g

In H_2O, 11.10 g of H combine with O = 88.90 g

$\therefore$ 1 g of H combine with O = $\frac{88.90}{11.10}$ g = 8.00 g

$\therefore$ Ratio of the weights of N and O which combine with fixed weight (=1g) of H = 4.66 : 8.00 = 1 : 1.7

In N_2O_3, ratio of weights of N and O which combine with each other = 36.85 : 63.15 = 1 : 1.7

Thus, the two ratios are the same. Hence it illustrates the law of reciprocal proportions.

V. Law of Gaseous volumes:

- This law was given by ***Gay-Lussac.*** in 1808.

Joseph Louis Gay Lussac
(1778 - 1850)

Joseph Louis Gay-Lussac also; 6 December 1778 – 9 May1850) was a French chemist and physicist. He is known mostly for two laws related to gases, and for his work on alcohol-water mixtures, which led to the degrees Gay-Lussac used to measure alcoholic beverages in many countries.

- According to this law, gases react with each other in the simple ratio of their volumes. If products are also gases then they are also in simple ratio of volume provided that all volumes are measure at same temp. & pressure.

eg. $N_2(g) + 3H_2(g) \longrightarrow 2NH_3(g)$

1 vol. 3vol. 2vol.

Illustration 6:

For the gaseous reaction, $H_2 + Cl_2 \longrightarrow 2HCl$

If 40 ml of hydrogen completely reacts with chlorine then find out the required volume of chlorine and volume of produced HCl ?

Solution:

According to Gay Lussac's Law :

$H_2 + Cl_2 \longrightarrow 2HCl$

$\because$ 1 ml of H_2 will react will 1 ml of Cl_2 and 2 ml of HCl will produce.

$\therefore$ 40 ml of H_2 will react with 40 ml of Cl_2 and 80 ml of HCl will produce.

required vol. of Cl_2 = 40 ml, produced vol. of HCl = 80 ml

VI. Berzelious Hypothesis and Avo-Gadro's Hypothesis:

(A) Berzelious Hypothesis : Equal volumes of all gases under similar conditions of temperature and pressure contain equal number of atoms.

Berzelius
(1779 - 1848)
Jöns Jacob Berzelius was a Swedish chemist. He worked out the modern technique of chemical formula notation, and is together with John Dalton, Antoine Lavoisier, and Robert Boyle considered a father of modern chemistry.

The above statements was incorrect and later it was modified by Avo-Gadro.

(B) Avo-Gadro's Hypothesis : Equal volumes of all gases under similar conditions of temperature and pressure contain equal number of molecules.

Lorenzo Romano Amedeo Carlo Avogadro Di Quareqa edi Carreto
(1776-1856)
Italian mathematical physicist. He practiced law for many years before he became interested in science. His most famous work, now known as Avogadro's law, was largely ignored during his lifetime, although it became the basis for determining atomic masses in the late nineteenth century.

Application of Avogadro's hypothesis:

(a) In finding the atomicity

(b) Relation between molecular weight and vapour density

- Vapour density $= \frac{\text{density of gas}}{\text{density of } H_2}$ (constant P, T)
- Molecular weight = 2 × vapour density
- Density of H_2 = 0.000089 gm/cm^3 at 0°C & 1 atm

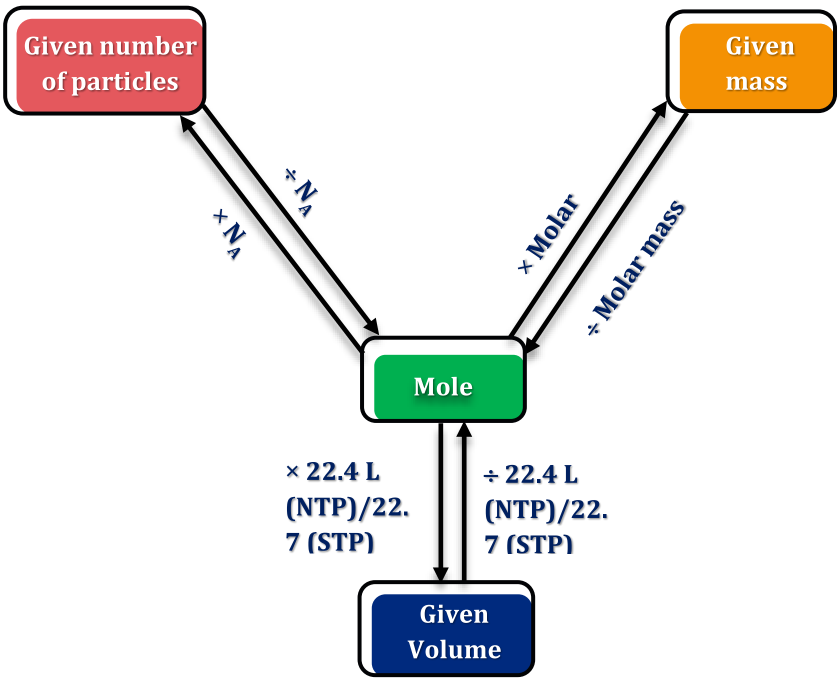
  ≈ 0.089 gm/lit.

(c) Relation between molecular weight and volume.

- 1 molecular weight = 22.4 lit. volume of gas at 0°C & 1 atm
- Weight of 1 gm mole gas = weight of 22.4 lit gas at 0°C & 1 atm
- Gram molecular volume = 22.4 lit. at 0°C & 1 atm

(d) Finding the molecular formula of gas.

Introduction to Mole:



Atoms and molecules are extremely small in size and their 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. The 14th Geneva conference on weight and measures adopted mole as a **seventh basic SI unit of the amount of a substance.** Mole concept is essential tool for the fundamental study of chemical calculations. This concept is simple but its application requires a thorough practice. There are many ways of measuring the amount of substance, weight and volume being the most common, but basic unit of chemistry is the atom or a molecule and measuring the number of molecule is more important.

Definition of mole and molar mass:

- A mole is the amount of a substance that contains as many entities (Atoms, Molecules, Ions or any other particles) as there are atoms in exactly 12 g of C-12 isotope.
- A mole of a substance contains Avogadro's number (6.022×10^{23}) of molecules (or formula units). The term mole, like a dozen or a gross, thus refers to a particular number of things. A dozen eggs equals 12 eggs, a gross of pencils equals 144 pencils, and a mole of ethanol equal 6.022×10^{23} ethanol molecules.
- The ***molar mass*** of a substance is the mass of one mole of the substance. Carbon-12 has a molar mass of exactly 12 g/mol, by definition.

Methods to calculate moles:

(i) If number of particles (molecules or atoms) is given then number of mole

$$\text{mole} = \frac{\text{Given no. of molecule / atom}}{N_A}$$

(ii) If mass is given then, number of mole = $\dfrac{\text{Given mass of substance (in gm)}}{\text{GAM / GMM}}$

(iii) If volume of gas is given then, mole = $\dfrac{\text{Volume of gas at STP (in lit.)}}{22.7\,L}$

(Standard molar volume is the volume occupies by 1 mole of any gas at STP, which is equal to 22.7 L)

- 1 gram-atom = 1 mole atoms = N_A atoms
- 1 gram-molecule = 1 mole molecules = N_A molecules
- 1 gram-ion = 1 mole ions = N_A ions

Illustration 7:

Calculate the atomic mass (average) of chlorine using the following data :

	% Natural Abundance	Molar Mass
^{35}Cl	75.77	34.9689
^{37}Cl	24.23	36.9659

Solution:

$$(\text{At. wt.})\ \text{avg} = \frac{M_1x_1 + M_2x_2}{x_1 + x_2}$$

$$= \frac{34.9689 \times 75.77 + 36.9659 \times 24.23}{100} = 35.45$$

Illustration 8:

Use the data given in the following table to calculate the molar mass of naturally occurring argon isotopes :

Isotope	Isotopic molar mass	Abundance
^{36}Ar	35.96755 g mol^{-1}	0.337%
^{38}Ar	37.96272 g mol^{-1}	0.063%
^{40}Ar	39.9624 g mol^{-1}	99.600%

Solution:

$$(\text{At wt.})\ \text{avg} = \frac{M_1x_1 + M_2x_2 + M_3x_3}{x_1 + x_2 + x_3}$$

$$= \frac{35.96755 \times 0.337 + 37.96272 \times 0.063 + 39.9624 \times 99.6}{100}$$

$$= 39.94$$

Atomic and molecular masses:

Different types of Atomic Masses:

The mass of an atom depends on the number of electrons, protons, and neutrons it contains. Knowledge of an atom's mass is important in laboratory work. But atoms are extremely small particles - even the smallest speck of dust that our unaided eyes can detect contains as many as 1×10^{16} atoms, Clearly, we cannot weigh a single atom, but it is possible to determine the mass of one atom relative to another experimentally. The first step is to assign a value to the mass of one atom of a given element so that it can be used as a standard.

Relative atomic mass:

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 ^{12}C. In this system, ^{12}C is assigned a mass of exactly 12 atomic mass unit **(a.m.u.)** and masses of all other atoms are given relative to this standard.

It is defined as the number which indicates how many times the mass of one atom of an element is heavier in comparison to $1/12^{th}$ part of the mass of one atom of C-12.

$$\textbf{Relative atomic mass (of elements)} = \frac{\textbf{mass of one atom of an element}}{\frac{1}{12}[\textbf{mass of C-12 atom}]}$$

$$= \frac{\textbf{Mass of one atom of an element}}{\textbf{1 amu}}$$

Atomic mass unit (a.m.u. or u):

The quantity $1/12^{th}$ mass of an atom of C^{12} is known as atomic mass unit.

Since mass of 1 atom of C - 12 = 1.9924×10^{-23} g

$\therefore$ $1/12^{th}$ part of the mass of 1 atom = $\frac{1.9924 \times 10^{-23}\,g}{12} = 1.67 \times 10^{-24}$ g

$$\Rightarrow 1\text{ a.m.u.} = \frac{1}{6.022 \times 10^{23}}\text{ g}$$

It may be noted that the atomic masses as obtained above are the relative atomic masses and not the actual masses of the atoms. These masses on the atomic mass scale are expressed in terms of atomic mass units (abbreviated as a.m.u.). Today, 'a.m.u.' has been replaced by 'u' which is known as unified mass.

One atomic mass unit (a.m.u.) is equal to $1/12^{th}$ of the mass of an atom of carbon - 12 isotope.

Thus, the atomic mass of hydrogen is 1.008 a.m.u. while that of oxygen is 15.9994 a.m.u. (or taken as 16 a.m.u.).

Gram atomic mass or mass of 1 gram atom:

When numerical value of atomic mass of an element is expressed in grams then the value becomes gram atomic mass or GAM.

gram atomic mass (GAM) = mass of 1 **gram atom** = mass of 1 **mole atoms**

= mass of N_A atoms = mass of 6.022×10^{23} atoms.

Ex. GAM of oxygen = mass of 1 **g atom** of oxygen = mass of 1 **mol atoms** of oxygen.

= mass of N_A atoms of oxygen.

$$= \left(\frac{16}{N_A}\,g\right) \times N_A = 16\text{ g}$$

Ex. Mass of one atom of Oxygen = 16 a.m.u. or $16 \times 1.67 \times 10^{-24}$ g

Mass of N_A atoms of Oxygen = $16 \times 1.67 \times 10^{-24} \times 6.022 \times 10^{-23}$ g = 16 g

Now see the table given below and understand the definition given before.

Element	R.A.M. (Relative Atomic Mass)	Atomic mass (mass of one atom)	Gram Atomic mass/ weight
N	14	14 a.m.u.	14 gm
He	4	4 a.m.u.	4 gm
C	12	12 a.m.u.	12 gm

Average atomic mass:

If an element exists in different isotopic forms (or allotropic forms) having relative abundance X_1%, X_2% ..... X_n%, with relative atomic masses M_1, M_2 ..... M_n respectively then,

$$\text{Avg. Atomic mass of element} = \frac{X_1}{100}(M_1) + \frac{X_2}{100}(M_2) + ... + \frac{X_n}{100}(M_n) = \sum_{i=1\text{ to }n} \frac{X_i}{100}(M_i)$$

Relative Molecular mass:

The number which indicates how many times the mass of one molecule of a substance is heavier in comparison to 1/12th part of the mass of an atom of C–12.

OR

The molecular mass of a substance 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.

Ex. molecular mass of oxygen (O_2) = 32 a.m.u.

molecular mass of (O_3) = 48 a.m.u.

molecular mass of HCl = 1 + 35.5 = 36.5 a.m.u.

molecular mass of H_2SO_4 = 2 + 32 + 64 = 98 a.m.u.

Gram molecular mass (mass of 1 gram molecule):

When numerical value of molecular mass of the substance is expressed in grams then the value becomes gram molecular mass or GMM.

gram molecular mass (GMM) = mass of 1 **gram molecule** = mass of 1 **mole molecules**

= mass of N_A molecules = mass of 6.022×10^{23} molecules

Ex. GMM of H_2SO_4 = mass of 1 **gram molecule** of H_2SO_4

= mass of 1 **mole molecules** of H_2SO_4

= mass of N_A molecules of H_2SO_4

$$= \left(\frac{98}{N_A} g\right) \times N_A = 98 \text{ g}$$

Ex. Molecular Mass of N_2 = 28 a.m.u. = $28 \times 1.67 \times 10^{-28}$ g

Mass of N_A molecules of N_2 = $28 \times 1.67 \times 10^{-24} \times 6.022 \times 10^{23}$ g = 28 g

Thus, molecular mass can be defined as the absolute mass in grams of 6.022×10^{23} molecules of a substance.

Average molecular mass of gas mixture:

$$= \frac{\text{Total mass of mixture of gases}}{\text{Total mole}}$$

Ex. $M_{avg} = \dfrac{M_A n_A + M_B n_B + M_C n_C}{n_a + n_B + n_C}$

Where n_A, n_B, $n_C \rightarrow$ moles of gases A, B, C

M_A, M_B, $M_C \rightarrow$ molecular mass of gases A, B, C

$\Rightarrow M_{avg} = M_A X_A + M_B X_B + M_C X_C$

$\Rightarrow M_{avg} = \sum M_i X_i$

where X_i = mole fraction of i^{th} gas, M_i = molecular mass of i^{th} gas.

Where X_A, X_B & X_C are the mole fraction of gases A, B & C.

Illustration 9:

Find :

(i) No. of moles in 10^{20} atoms of Cu.

(ii) Mass of 200 ${}^{16}_{8}O$ atoms in a.m.u.

(iii) Mass of 100 atoms of ${}^{14}_{7}N$ in gm.

(iv) No. of molecules & atoms in 54 gm H_2O.

(v) No. of atoms in 88 gm CO_2.

Solution:

(i) $\dfrac{10^{20}}{N_A}$ moles

(ii) Mass of 1 ${}^{16}_{8}O$ atom = 16 a.m.u.

Mass of 200 ${}^{16}_{8}O$ atom = 16 × 200 = 3200 a.m.u.

(iii) Mass of 1 ${}^{14}_{7}N$ atom = 14 a.m.u. = $14 \times 1.66 \times 10^{-24}$ g

Mass of 100 ${}^{14}_{7}N$ atom = $1400 \times 1.66 \times 10^{-24}$ g

(iv) Molar mass of H_2O = 18 g mol^{-1}

Moles of H_2O molecule = $\dfrac{54}{18} = 3$

no. of molecules in H_2O = $3N_A$

no. of atoms in H_2O = $3 \times 3N_A = 9N_A$

(v) Moles of CO_2 = $\dfrac{88}{44} = 2$ (Molar mass of CO_2 = 44)

No. of atoms in CO_2 = $6N_A$

Illustration 10:

In three moles of ethane (C_2H_6). Calculate the following :

(i) Number of moles of carbon atoms.

(ii) Number of moles of hydrogen atoms.

(iii) Number of molecules of ethane.

Solution:

(i) Gram atoms of C = 3 × 2 = 6

(ii) Gram atoms of Hydrogen = 3 × 6 = 18

(iii) Number of molecules of C_2H_6 = 3 N_A.

Illustration 11:

Calculate the number of atoms in each of the following :

(i) 52 moles of Ar (ii) 52 u of He (iii) 52 g of He.

Solution:

(i) Number of atoms of Ar = $52N_A$

(ii) Wt. of He = 52 × 1.66 × 10^{-24} gm.

Moles of He = $\frac{52}{4} \times 1.66 \times 10^{-24}$

Number of atoms of He = $\frac{52 \times 1.66 \times 10^{-24}}{4} \times N_A = 13$ atoms

(iii) Moles of He = $\frac{52}{4} = 13\,\text{mol}$

Number of atoms of He = 13 N_A.

Illustration 12:

What will be the mass of one ^{12}C atom in g ?

Solution:

Wt. of 1 atom of C = 1.66 × 10^{-24} gm. × (At wt.)

= 1.66 × 10^{-24} gm × 12 = 19.92 × 10^{-24} gm

Illustration 13:

Calculate mass of O atoms in 6 gm CH_3COOH ?

Solution:

Molar mass of CH_3COOH = 60

Moles of CH_3COOH = $\frac{6}{60} = 0.1$

1 mole CH_3COOH has 2 mol O atoms

0.1 mole CH_3COOH has 0.2 mol O atoms

Mass of oxygen = moles × Atomic mass = 0.2 × 16 = 3.2 gm.

Illustration 14:

How many sucrose molecules ($C_{12}H_{22}O_{11}$) are present in 3.42 g sucrose ?

Solution:

Molar mass of sucrose = 342

Moles of sucrose = $\frac{3.42}{342}$ = 0.01

Molecules of sucrose = 0.01 N_A = 6.022 × 10^{21}

Illustration 15:

Calculate mass of water present in 499 gm $CuSO_4.5H_2O$?

(Atomic mass – Cu = 63.5, S = 32, O = 16, H = 1)

Solution:

Molar mass of $CuSO_4.5H_2O$ = 249.5

moles of $CuSO_4.5H_2O$ = $\frac{499}{249.5} = 2$

Each mole $CuSO_4$.$5H_2O$ has 5 mol H_2O

2 mole $CuSO_4$.$5H_2O$ has 10 mol H_2O

Mass of 10 mol H_2O = 10 × 18 = 180 gm.

Illustration 16:

Find mass of 12.046 × 10^{23} atoms $^{12}C_6$ sample ?

Solution:

Mass of $^{12}C_6$ atom = 12 × 1.66 × 10^{-24} g

Mass of 12.046 × 10^{23} atoms = 12 × 1.66 × 10^{-24} × 12.046 × 10^{23} = 24 gm.

Illustration 17:

What is no. of O_2 molecules in 3.2 × 10^{-15} g sample of oxygen ?

Solution:

Moles of O_2 = $\frac{3.2\times10^{-15}}{32}$ = 10^{-16}; Molecules of O_2 = 10^{-16} N_A = 6.022 × 10^7

Illustration 18:

Find no. of protons in 180 ml H_2O. Density of water = 1 gm/ml.

Solution:

Mass of water = density × volume = 180 g

Moles of water = $\frac{180}{18} = 10$

1 mol water has 10 mol protons

10 mol water has 100 mol protons

10 mol water has 100 N_A protons

10 mol water has 6.022 × 10^{25} protons

Illustration 19:

What mass of $Na_2SO_4.7H_2O$ contains exactly 6.022 × 10^{22} atoms of oxygen ?

Solution:

Molar mass of $Na_2SO_4.7H_2O$ = 275 gm.

1 mole $Na_2SO_4.7H_2O$ has 11 mol O-atoms.

$\Rightarrow$ 11 N_A O – atoms are in 275 g $Na_2SO_4.7H_2O$

$\Rightarrow$ 6.022 × 10^{22} O – atoms are in = $\frac{275}{11\times6.022\times10^{23}}\times6.022\times10^{22}$ g = 2.5 g

Illustration 20:

Oxygen exists as three isotopes $^{16}_{8}O$, $^{17}_{8}O$, $^{18}_{8}O$ with relative abundance 90%, 7% and 3% respectively. What is average atomic mass of oxygen ?

Solution:

$M_{avg.} = \sum x_i M_i$ = 0.9 × 16 + 0.07 × 17 + 0.03 × 18 = 16.13 a.m.u. or 16.13 g/mol

Illustration 21:

If an elements M has $M_{avg.}$= 51.7 find relative abundances of ^{50}M and ^{52}M isotopes in nature ?
[Assume M exists in only two allotropic forms in nature]

Solution:

Let ^{50}M isotope be x % and ^{52}M isotope be (100 – x) % in nature

$\Rightarrow$ $51.7 = M_{avg.} = \frac{x}{100}(50) + \frac{100-x}{100}(52) \Rightarrow x = 15\%$ $\Rightarrow$ 15% ^{50}M and 85% ^{52}M in nature.

Percentage Composition:

Here we are going to find out the percentage of each element in the compound by knowing the molecular formula of compound.

We know that according to law of definite proportions any sample of a pure compound always possesses constant ratio of their combining elements.

Example :

Every molecule of ammonia always has formula NH_3 irrespective of method of preparation or sources. i.e. 1 mole of ammonia always contains 1 mol of N and 3 moles of H. In other words, 17 g of NH_3 always contains 14 g of N and 3 g of H. Now find out % of each element in the compound.

Mass % of N in NH_3 = $\frac{\text{Mass of N in 1 mol } NH_3}{\text{Mass of 1 mol of } NH_3} \times 100 = \frac{14\text{g}}{17} \times 100 = 82.35\ \%$

Mass % of H in NH_3 = $\frac{\text{Mass of H is 1 mol } NH_3}{\text{Mass of 1 mol of } NH_3} \times 100 = \frac{3}{17} \times 100 = 17.65\%$

Percentage composition of a compound refers to the amount of various constituent elements present per 100 parts by mass of the compound. It can be calculated from the formula of the compound by using the following relation :

$$\text{Percentage mass of an element} = \frac{(\text{No. of atoms of element}) \times (\text{At. mass of element}) \times 100}{\text{Molecular mass of substance}}$$

In case of minerals or ores the mass percentage of a particular constituent species in a formula can also be calculated using the similar relation as follows.

$$= \frac{[\text{Total mass of constituent species in one formula unit}] \times 100}{\text{Formula mass}}$$

For example, the percentage of iron Fe and FeO can be calculated in magnetite (Fe_3O_4) as follows :

Formula mass of Fe_3O_4 = 3 × 56 + 4 × 16 = 232

Atomic mass of Iron Fe = 56

Formula mass of FeO = 56 + 16 = 72

Therefore, percentage of Fe $= \frac{3 \times 56 \times 100}{232}$ = 72.4 % and percentage of FeO $= \frac{72 \times 100}{232}$ = 31 %

Note :

- Ratio of mass of two elements in a compound is a constant (independent of amount of compound).
- Mass % of an element in a compound is a constant.

Ex.

In $KMnO_4$

with respect to K $\rightarrow \frac{M_K}{M_{KMnO_4}} = \frac{m_K}{m_{KMnO_4}}$ M $\rightarrow$ Molar mass

with respect to O $\rightarrow \frac{4M_O}{M_{KMnO_4}} = \frac{m_O}{m_{KMnO_4}}$ m $\rightarrow$ Mass or mass % of element present in compound

Illustration 22:

How many grams of $KClO_4$ contain 40 gm 'O'.

Solution:

$$\frac{40}{x} = \frac{64}{35.5+39+64} \Rightarrow x = 86.5 \text{ g}$$

Illustration 23:

Calculate mass of Cu in 3.67×10^3 g $CuFeS_2$? (Atomic mass Cu = 63.5, Fe = 56, S = 32)

Solution:

Molar mass of $CuFeS_2$ = 183.5

$$\because \frac{w_{Cu}}{w_{CuFeS_2}} = \text{constant}$$

$$\therefore \frac{63.5}{183.5} = \frac{w_{Cu}}{3.67\times10^3} \Rightarrow w_{Cu} = 1270 \text{ g.}$$

Illustration 24:

What mass of H_2SO_4 contains 32 g oxygen ?

Solution:

$$\frac{w_O}{w_{H_2SO_4}} = \text{constant} \Rightarrow \frac{64}{98} = \frac{32}{w_{H_2SO_4}} \Rightarrow w_{H_2SO_4} = 49 \text{ g.}$$

Illustration 25:

A sample of $MgSO_4$ has 6.022×10^{20} O atoms. What is mass of Mg in sample ?

Solution:

$$\text{In } MgSO_4;\ \frac{\text{mass of O}}{\text{mass of Mg}} = \frac{16\times4}{24} = \frac{8}{3} = \text{constant}$$

$$\text{Mass of } 6.022 \times 10^{20} \text{ O-atoms} = \frac{6.022\times10^{20}}{6.022\times10^{23}}\times16 = 16 \times 10^{-3} \text{ g}$$

$$\Rightarrow \frac{8}{3} = \frac{16\times10^{-3}}{\text{mass of Mg}} \Rightarrow \text{Mass of Mg} = 6 \times 10^{-3} \text{ g}$$

Illustration 26:

If mass % of oxygen in monovalent metal 'M' carbonate (M_2CO_3) is 48%, find atomic mass of metal ?

Solution:

Let A be atomic mass of M

$$\text{Then } \frac{3\times16}{2A+12+3(16)} \times 100 = 48 \Rightarrow A = 20$$

Illustration 27:

Find value of X if 36.6 g $BaCl_2.XH_2O$ on strong heating loses 5.4 g moisture ?
[At. mass Ba = 137, Cl = 35.5]

Solution:

5.4 g H_2O is in 36.6 g $BaCl_2.XH_2O$

$$\frac{W_{H_2O}}{W_{BaCl_2 \times H_2O}} = \text{const.} = \frac{5.4}{36.6} = \frac{18X}{137+71+18X} \Rightarrow X = 2$$

Illustration 28:

0.492 g sample of haemoglobin has 0.34% by mass of Fe. If each molecule of haemoglobin has 4 Fe atoms find its molecular mass ?

Solution:

Let M = Molecular mass of haemoglobin $\Rightarrow \frac{0.34}{100} \times M = 4 \times 56$

M = 65882.3 a.m.u..

Empirical and Molecular Formula:

We have just seen that knowing the molecular formula of the compound we can calculate percentage composition of the elements. Conversely if we know the percentage composition of the elements initially, we can calculate the relative number of atoms of each element in the molecules of the compound. This gives us the empirical formula of the compound. Further if the molecular mass is known then the molecular formula can be easily determined.

Thus, the **empirical** formula of a compound is a chemical formula showing the relative number of atoms in the simplest ratio, the **molecular formula** gives the actual number of atoms of each element in a molecule.

i.e. **Empirical formula :** Formula depicting constituent atoms in their simplest ratio.

Molecular formula : Formula depicting actual number of atoms in one molecule of the compound.

The molecular formula is generally an integral multiple of the empirical formula.

i.e. molecular formula = empirical formula × n

where $n = \frac{\text{molecular formula mass}}{\text{empirical formula mass}}$

Example :

Molecular Formula	H_2O_2	C_6H_6	C_2H_6	$C_2H_4O_2$
	2 : 2	6 : 6	2 : 6	2 : 4 : 2
Simplest ratio	1 : 1	1 : 1	1 : 3	1 : 2 : 1
Empirical Formula	H O	C H	CH_3	CH_2O

Determination of Empirical formula:

Following steps are involved in determining the empirical formula of the compounds –

(i) First of all, find the % by wt. of each element present in the compound.

(ii) The % by wt of each element is divided by its atomic weight. It gives atomic ratio of elements present in the compounds.

(iii) Atomic ratio of each element is divided by the minimum value of atomic ratio so as to get simplest ratio of atoms.

(iv) If the value of simplest atomic ratio is fractional then raise the value to the nearest whole number or multiply with suitable coefficient to convert it into nearest whole number

(v) Write the Empirical formula as we get the simplest ratio of atoms.

Determination of molecular formula:

(i) Find out the empirical formula mass by adding the atomic masses of all the atoms present in the empirical formula of compound.

(ii) Divide the molecular mass (determined experimentally by some suitable method) by the empirical formula mass and find out the value of n.

(iii) Multiply the empirical formula of the compound with 'n' so as to find out the molecular formula of the compound.

Illustration 29:

An organic compound contains 49.3% carbon, 6.84% hydrogen and its vapour density is 73. Molecular formula of compound is :-

Solution:

V.D. = 73 $\Rightarrow$ M = 2 × 73 = 146

$$C = 146 \times \frac{49.3}{100} = 71.978 \text{ g} = \frac{71.978}{12} \simeq 6 \text{ mole}$$

$$H = 146 \times \frac{6.84}{100} = 9.9864 \text{ g} \simeq 10 \text{ mole}$$

$$O = 146 \times \frac{100-(49.3+6.84)}{100} = \frac{64.86}{16} = 64.86 \text{ g} \approx 4 \text{ mol}$$

M.F. = $C_6H_{10}O_4$

Illustration 30:

The empirical formula of an organic compound containing carbon & hydrogen is CH_2. The mass of 1 litre of organic gas is exactly equal to mass of 1 litre N_2 therefore molecular formula of organic gas is.

Solution:

Empirical Mass of CH_2 = 12 + 2 = 14

$\because$ Mass of 1 litre of organic gas = Mass of 1 litre of N_2

Since V, P, T, n is same.

Therefore, from PV = $\frac{m}{M}$RT implies that molar mass should also be same.

$\therefore$ Molecular mass of organic compound will be 28 g

$$n = \frac{\text{Molecular mass}}{\text{Empirical mass}} = \frac{28}{14} = 2$$

So molecular formula = 2 × CH_2 = C_2H_4

Illustration 31:

In which of following has same empirical formula -

C_2H_2, C_2H_4, C_2H_6, C_6H_6

Solution:

C_2H_2, C_6H_6,

Illustration 32:

Determine the empirical formula of an oxide of iron, which has 70% Fe and 30% 'O' by mass. (Fe = 56)

Solution:

Fe_2O_3

Ideal Gas Equation:

(iv) Under any condition of temperature and pressure, moles of gases may be calculated using IDEAL GAS EQUATION : PV = nRT,

where, R = Universal Gas Constant

= 0.082 L-atm/K-mol

= 8.314 J/K-mol

= 2 cal/K-mol

Units of pressure and their relation:

1 atm = 76 cm Hg

= 760 mm Hg

= 760 torr (1 torr = 1 mm Hg)

= 1.01325 10^6 dyne/cm^2

= 1.01325 10^5 N/m^2 or Pa

= 1.01325 bar (1 bar = 10^5 Pa)

1 bar = 75 cm Hg

Units of Volume and their relation:

1 ml = 1 cm^3 = 1 c.c.

1 Litre = 1000 ml = 1 dm^3

1 m^3 = 1000 L

Units of Temperature and their relation:

T = 273.15 + t

where, T = Absolute temperature (in Kelvin) and t = temperature in 0° C

(Normally, we take 273K in calculation)

(v) Sometimes gas is collected over water. In this case, the measured pressure is sum of pressure of gas and the vapour pressure of water (also called Aqueous Tension). In order to calculate moles of gas, the vapour pressure of water should be deducted from the measured pressure.

If volume of gas is given then, mole

$$= \frac{\text{Volume of gas at STP}}{22.7\,\text{L}} = \frac{\text{Volume of gas at } 0^\circ\text{C and 1 atm}}{22.4\,\text{L}}$$

(Standard molar volume is the volume occupied by 1 mole of an ideal gas at STP (Standard temperature and pressure which is 273.15 K & 1 bar respectively), which is equal to 22.7 L).

1 mole of an ideal gas occupy 22.4 L at 0° C and 1 atm.

Illustration 33:

Calculate the number of g-molecules (mole of molecules) in the following :

(i) 3.2 gm CH_4

(ii) 70 gm nitrogen

(iii) 4.5 × 10^{24} molecules of ozone

(iv) 2.4 × 10^{21} atoms of hydrogen

(v) 11.2 L ideal gas at 0° C and 1 atm

(vi) 4.54 ml SO_3 gas at STP

(vii) 8.21 L C_2H_6 gas at 400K and 2atm

(viii) 164.2 ml He gas at 27ºC and 570 torr [N_A = 6 × 10^{23}]

Solution:

(i) 3.2 gram CH_4

number of moles (CH_4) = $\frac{w}{M} = \frac{3.2}{16}$ = 0.2 moles

(ii) 70 gram N_2

Number of moles = $\frac{w}{M} = \frac{70}{28} = 2.5$

(iii) 4.5×10^{24} molecules of O_3

Number of moles = $\frac{\text{no.of molecules}}{N_A} = \frac{4.5\times10^{24}}{6\times10^{23}} = 7.5$

(iv) 2.4×10^{21} atoms of hydrogen

Number of gram molecules of H_2 = $\frac{\text{no.of molecules}}{N_A} = \frac{2.4\times10^{21}}{2\times6\times10^{23}}$ = 0.002

(v) 11.2 litre ideal gas at 0° C and 1 atm

Number of moles = $\frac{\text{Volume at } 0°C \,\&\, 1\,\text{atm}}{22.4\,\text{litre}} = \frac{11.2}{22.4}$ = 0.5

(vi) 4.54 ml SO_3 gas at STP

Number of moles = $\frac{V_{STP}(\text{ml})}{22700\text{ml}} = \frac{4.54}{22700} = 2 \times 10^{-4}$

(vii) 8.21 litre C_2H_6 at 400 K and 2 litre

$n = \frac{PV}{R.T} = \frac{2\times8.21}{0.0821\times400}$ = 0.5

(viii) 164.2 ml He gas at 27ºC and 570 torr

$n = \frac{PV}{RT} = \left(\frac{570}{760}\text{atm}\right)\times\frac{164.2\times10^{-3}\text{litre}}{0.0821\times300}$ = 0.005

Illustration 34:

What is number of atoms and molecules in 112 L of $O_3(g)$ at 0°C and 1atm ?

Solution:

Moles of molecules = $\frac{112}{22.4} = 5$

Moles of atoms = 5 × 3 = 15

No. of molecules = 5 N_A

No. of atoms = 15N_A.

Density:

It is of two types.

I. Absolute density

II. Relative density

For liquids and solids :

Absolute density = $\frac{\text{mass}}{\text{volume}}$

Relative density or specific gravity = $\frac{\text{density of the substance}}{\text{density of water at } 4°C\ (1\,\text{gm ml}^{-1})}$

For gases :

Absolute density = $\dfrac{\text{mass}}{\text{volume}} = \dfrac{PM}{RT}$

where P is pressure of gas, M = molar mass of gas, R is the gas constant, T is absolute temperature.

Vapour Density :

Vapour density is defined as the density of the gas with respect to hydrogen gas at the same temperature and pressure.

Vapour density = $\dfrac{d_{gas}}{d_{H_2}} = \dfrac{PM_{gas}/RT}{PM_{H_2}/RT}$

V.D. = $\dfrac{M_{gas}}{M_{H_2}} = \dfrac{M_{gas}}{2} \Rightarrow \boxed{\mathbf{M_{gas} = 2 \times V.D.}}$

Illustration 35:

A gaseous mixture of H_2 and NH_3 gas contains 68 mass % of NH_3. The vapour density of the mixture is –

Solution:

No. of moles of NH_3 in 100g mixture = $\dfrac{68}{17} = 4$

No. of moles of H_2 in 100g mixture = $\dfrac{32}{2} = 16$

$M_{average} = \dfrac{\text{Total mass}}{\text{Total moles}} = \dfrac{100}{4+16} = 5$ V D = $\dfrac{5}{2}$ = 2.5

Stoichiometry:

Stoichiometry is the calculation of amounts of reactants and products involved in a reaction. Stoichiometric calculations require a balanced chemical equation of the reaction.

- Remember a balanced chemical equation is one which contains an equal number of atoms of each element on both sides of equation.

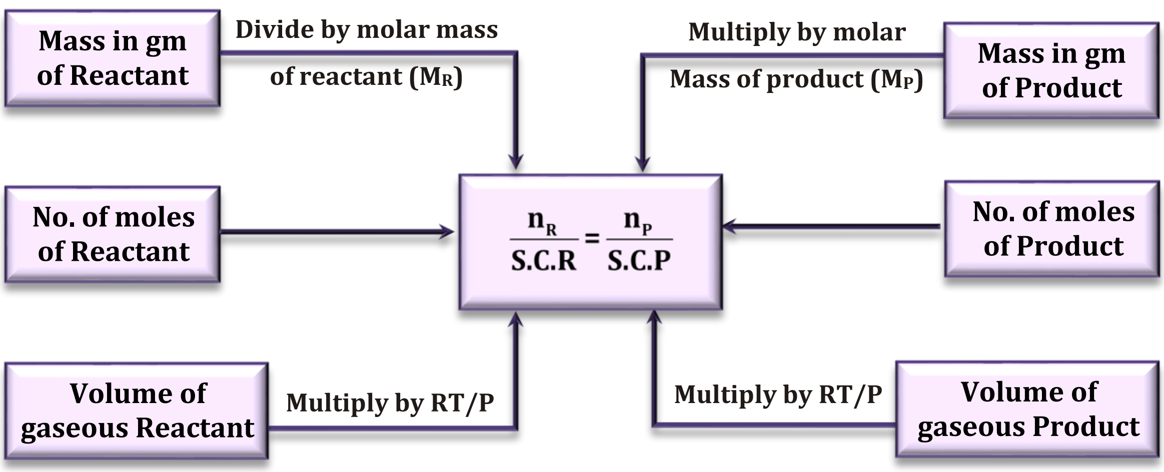
Significance of stoichiometric coefficients:

Stoichiometric coefficients of chemical equation tells us about the ratio in which moles of reactants react and moles of products form.

Ex.

	$2H_2(g)$ +	$O_2(g)$ $\longrightarrow$	$2H_2O(g)$
1st interpretation	2 moles	1 mole	2 moles
2nd interpretation	2 N_A molecules	N_A molecules	2 N_A molecules
3rd interpretation	2 molecules	1 molecules	2 molecules
4rd interpretation (at constant P & T)	2 volume	1 volume	2 volume
5th interpretation (at constant V & T)	2 atm	1 atm	2 atm
6th interpretation	4 g	32 g	36 g

SUMMARY OF STOICHIOMETRIC CALCULATION



Here : S.C.R. - Stoichiometric coefficient of reactant,

S.C.P.- Stoichiometric coefficient of product

- Consider a balanced Chemical reaction :

$$aA \quad + \quad bB \quad \longrightarrow \quad cC \quad + \quad dD$$

$$\left[\frac{\text{mole of A reacting}}{a} = \frac{\text{mole of B reacting}}{b} = \frac{\text{mole of C produced}}{c} = \frac{\text{mole of D produced}}{d}\right]$$

$\Rightarrow$ If mole of A is n_A, then -

- mole of B consumed = $n_A \times \left(\frac{b}{a}\right)$
- mole of C produced = $n_A \times \left(\frac{c}{a}\right)$
- mole of D produced = $n_A \times \left(\frac{d}{a}\right)$

I. Mass - mass analysis:

This relates the mass of a species (reactant or product) with the mass of another species (reactant or product) involved in a chemical reaction.

In general, the following steps are adopted in making necessary calculations :

(A) Write down balanced molecular equation for the chemical change.

(B) Write down the relative masses of the reactants and the products with the help of formula below the respective formula. These shall be the theoretical amounts of reactants and product.

(C) Calculate the number of moles below the formula of each of the reactant and product.

(D) By the applications of mole concept, mass co-relation through unitary method or proportionality method the unknown quantity can be determined.

Let us consider a balanced chemical reaction,

$$a\,A \quad + \quad b\,B \quad \longrightarrow \quad c\,C$$

W_A gm ?

If M_A, $M_C \rightarrow$ Molar mass of A and C respectively.

W_A = Mass of A reacted

W_C = Mass of C formed (to be found).

Method $aA \quad + \quad bB \quad \longrightarrow \quad cC$

W_A gm $\qquad\qquad W_C = \left(\frac{c}{a}\right)\frac{W_A}{M_A}M_C$ gm

$\downarrow \qquad\qquad \uparrow$

$\left(\frac{W_A}{M_A}\right)$moles $\rightarrow \qquad \left(\frac{c}{a}\right)\frac{W_A}{M_A}$ moles

Illustration 36:

What mass of CaO is formed by heating 50 g $CaCO_3$ in air ?

[molar mass : $CaCO_3$ = 100, CaO = 56].

Solution:

$CaCO_3(s) \longrightarrow CaO(s) + CO_2(g)$

50 gm

$= \frac{50}{100}$mol

$= \frac{1}{2}$mol $\quad \frac{1}{2}$mol

$= \frac{1}{2} \times 56 = 28$ gm

II. Mass-volume Analysis:

This establishes the relationship between the mass of a species (reactant or product) and the volume of a gaseous species (reactant or product) involved in a chemical reaction.

For example the volume of CO_2 at STP formed by heating 200 g $CaCO_3$:-

$CaCO_3(s) \longrightarrow CaO(s) \quad + \quad CO_2(g)$

200 gm

$= \frac{200}{100}$mol $\qquad = 2$ mol $\qquad 2$ mol

Volume of gas at STP = No. of moles × 22.7 L = 2 × 22.7 = 45.4 L.

III. Volume-volume Analysis:

This relationship deals with the volume of a gaseous species (reactant or product) with the volume of another gaseous species (reactant or product) involved in a chemical reaction.

Gay Lussac's law of combining volumes :

$aA(g) \quad + \quad b(B)(g) \quad \longrightarrow \quad cC(g)$

V_A mL $\qquad V_B$ mL $\qquad V_C$ mL

reacted $\qquad$ reacted $\qquad$ formed

$V_A : V_B : V_C = a : b : c$
At constant P, T :
Volume of gaseous species reacting or formed is in ratio of their stoichiometric coefficients.

Illustration 37:
What volume of H_2 (g) is produced by decomposition of 2.4 L NH_3 (g) ?
Solution:

$$NH_3\,(g) \longrightarrow \frac{1}{2}N_2(g) + \frac{3}{2}H_2\,(g)$$

	NH_3 (g)	N_2(g)	H_2 (g)
t = 0	2.4 L	0	0
t = ∞	0	v_1	v_2

Gay-Lussac's law, $2.4 : v_1 : v_2 = 1 : \frac{1}{2} : \frac{3}{2} \Rightarrow \frac{2.4}{v_2} = \frac{2}{3} \Rightarrow v_2 = 3.6$ L

Quantum Numbers:
Quantum numbers give complete information about an electron or orbital in an atom.

1. Principal Quantum number (n) :
(i) Permissible value of $\mathbf{n \rightarrow 1}$ **to** ∞
(ii) It represents shell number/energy level
(iii) The energy states corresponding to different principal quantum numbers are denoted by letters K, L, M, N etc.

N :	1	2	3	4	5	6
Designation of shell :	K	L	M	N	O	P

(iv) It indicates the distance of an electron from the nucleus.
(v) It also determines the energy of the electron. In general, higher the value of 'n', higher is the energy of the electron.
(vi) It gives an idea of total number of orbitals & electron (which may) present in a shell & that equal to $\mathbf{n^2}$ & $\mathbf{2n^2}$ respectively.

2. Azimuthal Quantum number (ℓ) :
(i) The values of ℓ depends upon the value of 'n' and possible values are '0' to (n –1).
(ii) It gives the name of subshells associated with the energy level and number of subshells within an energy level.
(iii) The different value of 'ℓ' indicates the shape of orbitals and designated as follows :

Value	Notation	Name	Shape
$\ell = 0$	s	Sharp	Spherical
$\ell = 1$	p	Principal	Dumbell
$\ell = 2$	d	Diffused	Double Dumbell
$\ell = 3$	f	Fundamental	Complex

(iv) It also determines the energy of orbital along with n.
For a particular energy level/shell energy of subshell is in the following order → **s < p < d < f**
(v) It gives the total number of orbitals in a subshell & that equals to $\mathbf{(2\ell + 1)}$ and number of electrons in a subshell = $\mathbf{2\,(2\ell + 1)}$

3. Magnetic Quantum number (m or m_l) :

(i) The value of m depends upon the value of ℓ and it may have integral value $-\ell$ to $+\ell$ including zero.

(ii) It gives the number of orbitals in a given subshell and orientation of different orbitals in space.

e.g. for n = 4, l = 0 to 3.

ℓ	0	1	2	3
m	0	–1, 0, +1	–2, –1, 0, +1, +2	–3,–2,–1,0+1,+2,+3
Possible Orientation	1	3	5	7
Orbitals	s	p_x, p_y, p_z	d_{z^2}, $d_{x^2-y^2}$ d_{xy}, d_{yz}, d_{xz}	Diffused *** Not in syllabus

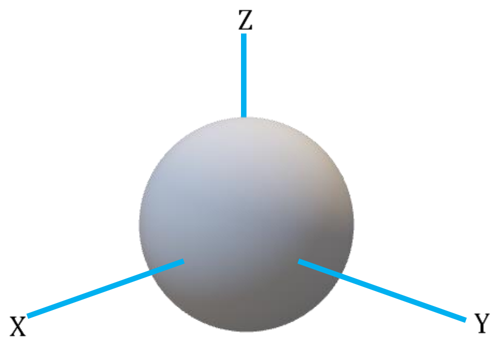
(iii) The orbitals having same value of n and ℓ but different value of m, have same energy in absence of external electric & magnetic field. These orbitals having same energy of a particular subshell is known as Degenerate orbitals.

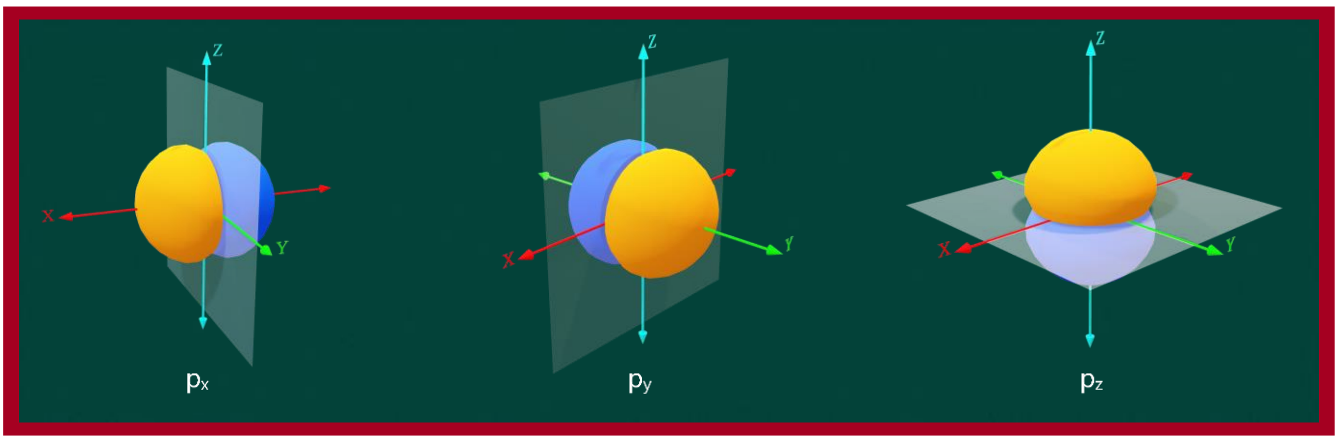
4. Spin Quantum number (s) OR Magnetic spin quantum number (m_s) :

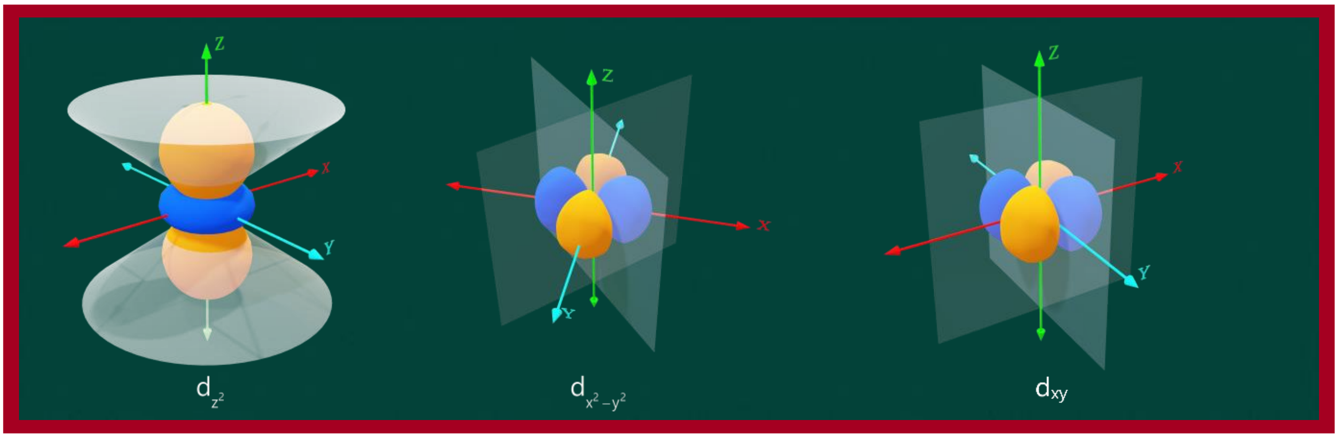
(i) While moving around the nucleus, the electron always spins about its own axis either clockwise or anticlockwise. The magnetic spin quantum number represents the direction of electron spin (rotation) around its own axis (clockwise or anticlockwise).

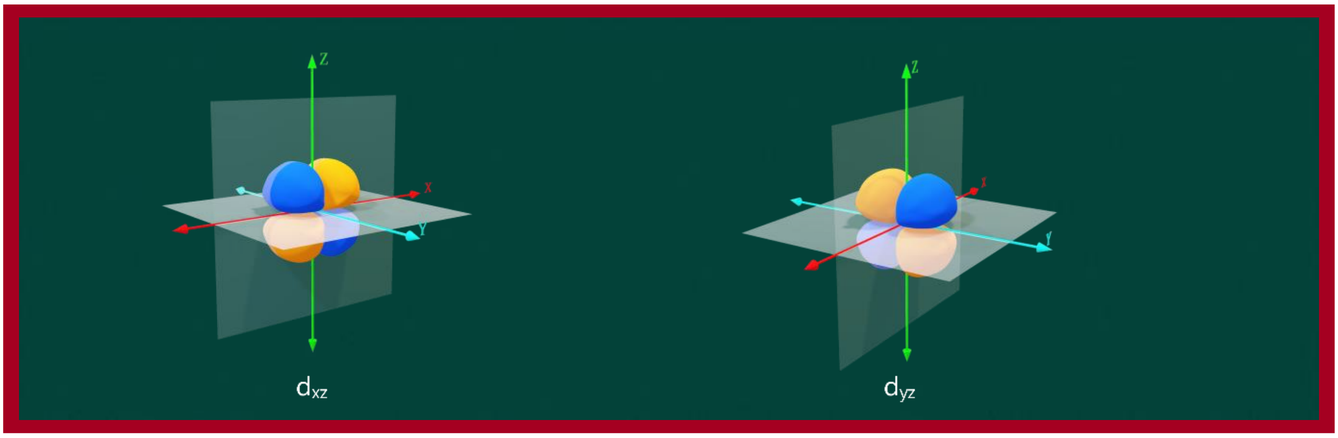
(ii) There are two possible values of m_s are $+\frac{1}{2}$ & $-\frac{1}{2}$ and represented by the two arrows (spin up) and $\downarrow$ (spin down).

Shapes of Atomic Orbitals:









Rules for filling Electrons:

1. Pauli's exclusion principle

'No two electrons in an atom can have same values of all the four quantum numbers.

An orbital accommodates two electrons with opposite spin. These two electrons have same values of principal, azimuthal and magnetic quantum number but the fourth, i.e. magnetic spin quantum number will be different. i.e.

For K, shell (n = 1)

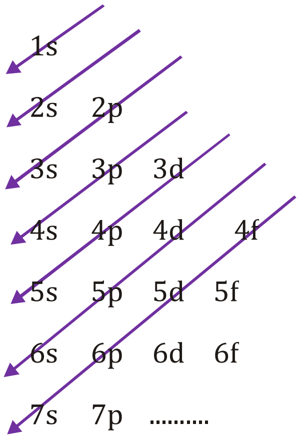
l = 0, m = 0

For 1st Electron $n = 1, l = 0, m = 0, m_s = +\frac{1}{2}$

For 2nd Electron $n = 1, l = 0, m = 0, m_s = -\frac{1}{2}$

2. Aufbau Principle (Means Building up) :

The electrons are added progressively to the various orbitals in the order of increasing energies starting with the orbital of the lowest energy



1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 6s < 4f < 5d < 6p < 7s < 5f < 6d < 7p

Alternatively, the order of increase of energy of orbitals can be calculated from $(n + \ell)$ rule.

(i) Lower the value of $(n + \ell)$ for an orbital, the lower will be its energy.

(ii) If two orbitals have the same $(n + \ell)$ value, then orbital with lower value of n has the lower energy.

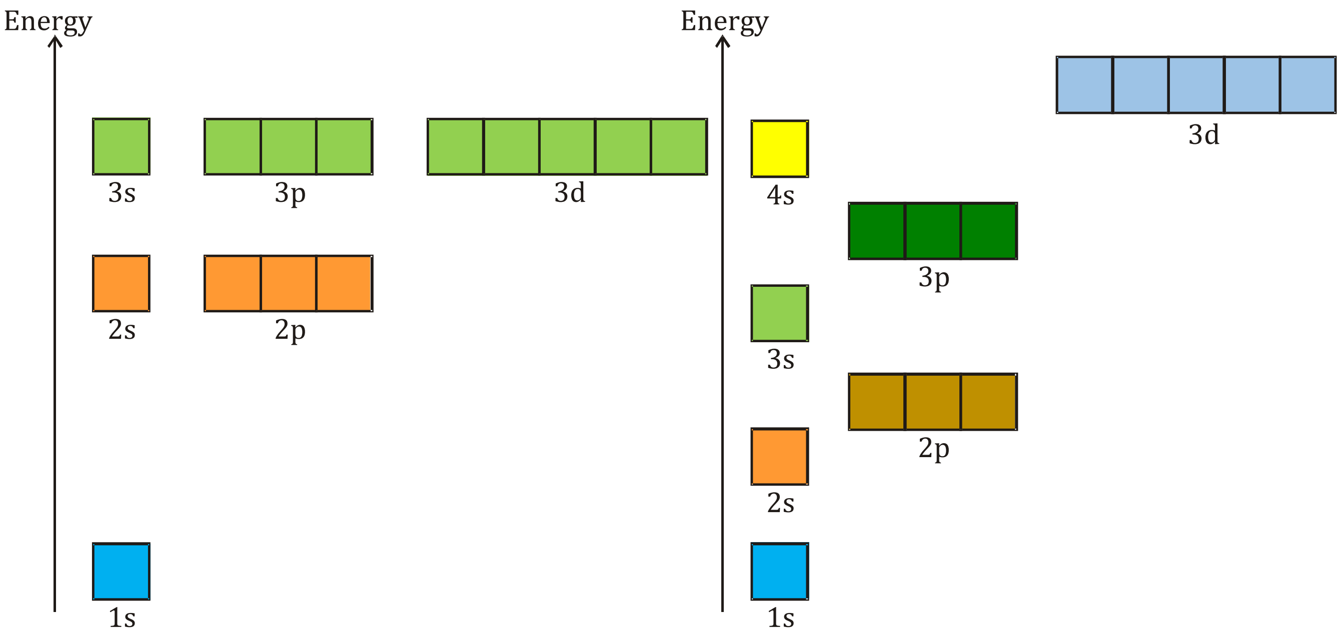
e.g. 2p & 3s

For 2p, $n = 2$, $\ell = 1$, $(n + \ell) = 2 + 1 = 3$

For 3s, $n = 3$, $\ell = 0$, $(n + \ell) = 3 + 0 = 3$

Then for 2p, n is lesser than for 3s, so 2p has lower energy than 3s.

(iii) 1s < 2s = 2p < 3s = 3p = 3d < 4s = 4p = 4d = 4f .... energy order of different orbitals for single electron system like H, $He^{\oplus}$, $Li^{2\oplus}$ etc. (used in Bohr model)



(A) For single electron or hydrogenic atom (B) Multi electronic atoms

Energy level diagram for few electronic shells

Illustration 38:

Write the increasing order of energies of 4s, 3p, 4p and 3d.

Solution:

For 4s, n = 4, l = 0, (n + l) = 4

For 3p, n = 3, l = 1, (n + l) = 4

For 4p, n = 4, l = 1, (n + l) = 5

For 3d, n = 3, l = 2, (n + l) = 5

$\Rightarrow$ 3p < 4s < 3d < 4p increasing order

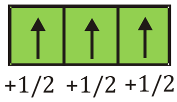
3. Hund's rule of maximum multiplicity :

This rule deals with the filling of electrons into the orbitals belonging to the same subshell i.e. orbitals of equal energy, called degenerate orbitals.

"Electrons are distributed among the orbitals of a subshell in such a way so as to give the maximum number of unpaired electrons with parallel spins."

"Pairing of electrons in the orbitals belonging to the same subshell (p, d, f) does not take place until each orbital belonging to that subshell has got one electron each i.e. singly occupied. Moreover, the singly occupied orbitals must have the electrons with the parallel spin multiplicity"

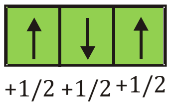
Multiplicity = 2|S| + 1, where S = Total spin.

i.e. 

Find total spin & multiplicity

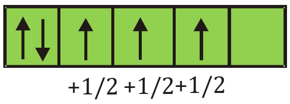
Total spin S = $\frac{1}{2}+\frac{1}{2}+\frac{1}{2}=\frac{3}{2}$

Multiplicity = $2\times\frac{3}{2}+1=4$

i.e. 

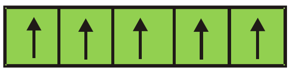
Total spin S = $\frac{1}{2}-\frac{1}{2}+\frac{1}{2}=\frac{1}{2}$

Multiplicity = $2\times\frac{1}{2}+1=2$

i.e. 

Total spin S = $\frac{1}{2}+\frac{1}{2}+\frac{1}{2}=\frac{3}{2}$

Multiplicity = $2\times\frac{3}{2}+1=4$

i.e. 

Total spin = $5\times\frac{1}{2}=\frac{5}{2}$

Multiplicity = $2\times\frac{5}{2}+1=6$

Electronic Configuration of Atoms:

The distribution of electrons in various shells, subshells and orbitals, in an atom of an element, is called its electronic configuration.

$n l^{x}$ ← no. of electrons in subshell

n (represents shell); l ← represents subshell

$2p^5$ ← no. of electrons in p-subshell

2 → Second shell; p ← p subshell

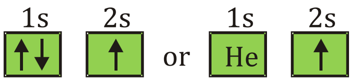
$_3Li$; $1s^2, 2s^1$ or [He] $2s^1$ or 

Illustration 39:

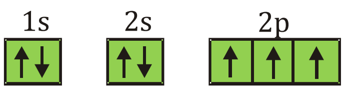
Write electronic configuration of Nitrogen.

Solution:

$_7N$: $1s^2, 2s^2\ 2p^3$ [Orbital notation method]

$1s^2, 2s^2\ 2p_x^1\ 2p_y^1 2p_z^1$

or



[Orbital diagram method]

or

[He] $2s^2\ 2p^3$ [Condensed form]

Extra stability of Half-filled and fully-filled orbitals.

The electronic configuration of most of the atoms follows the Aufbau's rule. However, in certain elements such as Cr, Cu etc. Where the two subshells (4s and3d) differ slightly in their energies (4s < 3d), an electron shifts from a subshell of lower energy (4s) to a subshell of higher energy (3d), provided such a shift results in all orbitals of the subshell of higher energy getting either completely filled or half-filled.

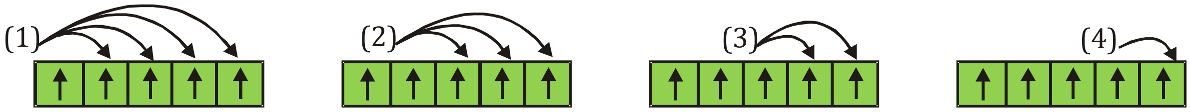
$_{24}Cr \rightarrow$ [Ar] $3d^5, 4s^1$ and not [Ar] $3d^4\ 4s^2$

$_{29}Cu \rightarrow$ [Ar] $3d^{10}, 4s^1$ and not [Ar] $3d^9\ 4s^2$

It has been found that there is extra stability associated with these electronic configuration. This stabilization is due to the following two factors.

(i) Symmetrical distribution of electron : It is well known that symmetry leads to stability. The completely filled or half-filled subshell have symmetrical distribution of electron in them and are therefore more stable. This effect is more dominant in d and f-orbitals. This means three or six electrons in p-subshell, 5 or 10 electrons in d-subshell and 7 or 14 in f-subshell forms a stable arrangement.

(ii) Exchange energy : This stabilizing effect arises whenever two or more electrons with the same spin are present in the degenerate orbitals of a subshell. these electrons tend to exchange their positions and the energy released due to this exchange is called exchange energy. The number of exchanges that can take place is maximum when the subshell is either half-filled or fully filled. As result the exchange energy is maximum and so is the stability.



4-exchanges by electron 1 | 3-exchanges by electron 2 | 2-exchanges by electron 3 | 1-exchanges by electron 4

Total exchange pairs = 10

$\frac{n(n-1)}{2} \rightarrow$ Number of exchange pairs

$n \rightarrow$ Number of electron with parallel spins.

e.g. 

Only 6 total exchange possible

Exceptional electronic configuration

S.No.	**Element**	**Z**	**Configuration**
1	Cr	24	**$[Ar]4s^1 3d^5$**
2.	Cu	29	**$[Ar]4s^1 3d^{10}$**
3.	Nb	41	**$[Kr]5s^1 4d^4$**
4.	Mo	42	**$[Kr]5s^1 4d^5$**
5.	Ru	44	**$[Kr]5s^1 4d^7$**
6.	Rh	45	**$[Kr]5s^1 4d^8$**
7.	Pd	46	**$[Kr]4d^{10}$**
8.	Ag	47	**$[Kr]5s^1 4d^{10}$**
9.	La	57	**$[Xe]6s^2 5d^1$**
10.	Pt	78	**$[Xe]6s^1 4f^{14} 5d^9$**
11.	Au	79	**$[Xe]6s^1 4f^{14} 5d^{10}$**
12.	Ac	89	**$[Rn]7s^2 6d^1$**
13.	**Th**	**90**	**$[Rn]7s^2 6d^2$**

Magnetic Properties:

Para magnetism :

(i) The substances which are weakly attracted by magnetic field are paramagnetic and this phenomenon is known as para magnetism.

(ii) Their magnetic character is retained till they are in magnetic field and lose their magnetism when removed from magnetic field.

Diamagnetism :

(i) The substances which are weakly repelled by magnetic field are diamagnetic and this phenomenon is known as diamagnetism.

(ii) Diamagnetic substances lack unpaired electrons and their spin magnetic moment is zero e.g., NaCl, N_2O_4 etc.

Spin magnetic moment :

The spin magnetic moment of electron (excluding orbit magnetic moment) is given by :

$$\mu = \sqrt{n(n+2)}\ \textbf{B.M.}$$

Where n is number of unpaired electrons in species.

The magnetic moment is expressed in Bohr magneton (B.M.)

Illustration 40:

A compound of vanadium has magnetic moment of 1.73 BM. Work out the electronic configuration of vanadium ion in the compound.

Solution:

Vanadium belongs to 3d series with Z = 23. The magnetic moment of 3d series metal is given by spin only formula.

$\mu = \sqrt{n(n+2)}$ BM (BM = Bohr's magneton)

$\because \quad 1.73 = \sqrt{3}$

$\Rightarrow$ n(n+2) = 3 $\Rightarrow$ n = 1

$\Rightarrow$ Magnetic moment corresponds to one unpaired electron.

$\Rightarrow$ Electronic configuration of vanadium atom $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^3$.

For one unpaired electron 4 electron must be removed in which first 2 electron are lost from 4s orbital (outermost).

Electronic configuration of $V^{4\oplus}$

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^0\ 3d^1$

Nodal Planes of different orbitals :

Nodal plane is a plane at which the probability of finding an electron becomes zero.

e.g.

Orbital	Nodal plane	Orbital	Nodal plane
s	None	d_{xy}	XZ & YZ planes
p_x	YZ plane	d_{yz}	XZ & XY planes
p_y	XZ plane	d_{xz}	XY & YZ planes
p_z	XY plane	$d_{x^2-y^2}$	Planes perpendicular to XY plane, passing through origin (nucleus) and inclined at 45° to X & Y axis.
		d_{z^2}	None (two nodal cones are available)