ATOMIC STRUCTURE

K = °C + 273.15

1 mole = 6.023×10^{23} particles

1 amu = 1.662×10^{-24} g

n = $\frac{m}{M}$; where n = number of moles of an element

m = mass of the element

M = gram atomic mass of the element

Atomic Number (Z) = No. of protons in the nucleus

= no. of electrons in neutral atom.

Mass Number (A) = No. of neutrons + No. of protons, i.e.

$A = n + p$

No. of neutrons = $A - Z$.

Maximum no. of electrons in an orbit = $2n^2$

where n = orbit no. or principal quantum number

Maximum no. of electrons in a Sub-shell

$= 4n - 2$

$= 2(2l + 1)$

$= 4l + 2$

where l = azimuthal quantum number.

- For any value of n, there are n values of l and the value ranges from 0 to $n - 1$.
- For any value of l, there are $2l + 1$ values of m and the value ranges from $-l$ to $+l$ including zero.

  where, m = magnetic quantum number
- For each value of n, there are n^2 values of m.
- For a particular value of n, there are $2n^2$ sets of quantum numbers.

Electron

The cathode ray particles having negative charge and a specific charge to mass ratio remains constant irrespective of the nature of gas in discharge tube are known as electrons.

$\frac{e}{m}$ ratio of an electron is given by,

$$\frac{e}{m} = \frac{E}{B^2 R}$$

Where B = applied magnetic field
R = readius of circular path of electron
E = applied electric field

The value of $\frac{e}{m}$ was calculated as 1.77×10^{11} C kg^{-1}

Charge of electron
$= -1.59 \times 10^{-19}$ C $= -1.6 \times 10^{-19}$ C
So that, mass of electron $= 9.107 \times 10^{-31}$ kg

Proton

The fundamental particle of the anode ray particles having positive charge and also which is an integral multiple of electronic charge and a specific charge to mass ratio, both depending on the nature of the gas in discharge tube are known as protons.

The value of $\frac{e}{m}$ of proton was found to be 9.58×10^{7} C kg^{-1}
Charge on proton $= +1.6 \times 10^{-19}$ C
So that, mass of proton $= 1.67 \times 10^{-27}$ kg

Neutron

A neutral particle having nearly the same mass as that of the proton, discovered by Sir James Chadwick is known as the neutron.

Thomson's model of atom

An atom is a sphere of positive charges with negative charges embedded in it, such that the atom as a whole remains neutral.
This model is also known as *water-melon model of atom*. But this model could not explain the Rutherford's gold-foil scattering experiment.

Rutherford's model of atom

I. An atom consists of a positively charged heavy central core, called as *nucleus*.

II. The size of the nucleus is very small as compared to the total size of the atom.

III. The electrons revolve round the nucleus and their total negative charge is equal to the positive charge of the nucleus, so that the atom as a whole is electrically netural so they form the extra-nuclear region of the atom.

Limitations of Rutherford's theory:

I. If the electrons were at rest round the nucleus, they will be attracted by it and will finally fall into it.

II. If the electrons were revolving round the nucleus in circular orbits, they will radiate out energy continuously and hence spirally fall into the nucleus.

Isotopes

Atoms of same element are said to be isotopes of that element if they have same atomic number but different mass numbers or in other words, same number of protons and electrons but different neutron number.

such as $^{1}_{1}H$, $^{2}_{1}H$, $^{3}_{1}H$; $^{12}_{6}C$, $^{13}_{6}C$, $^{14}_{6}C$; $^{16}_{8}O$, $^{17}_{8}O$, $^{18}_{8}O$,

Isobars

Atoms of different elements are said to be isobars if they have same mass numbers though their atomic numbers are different. i.e., inspite of different number of neutrons and protons, the sum of $n + p$ is the same.

such as $^{40}_{18}Ar$, $^{40}_{19}K$, $^{40}_{20}Ca$.

Isotones

Atoms of different elements are said to be isotones if they have the same number of neutrons even though the atomic numbers and mass numbers are different.

Bohr's model of atom

Postulates of Bohr's theory

(*i*) The electrons revolve round the nucleus in closed circular orbits. Necessary centripetal forces for rotation is provided by the electrostatic force between the nucleus and the electon.

(*ii*) An electon can revolve only in certain discrete, non-radiating orbits, called stationary orbits. For these orbits, the total angular momentum of the moving electron is an integral multiple of $\frac{h}{2\pi}$.

(*iii*) The energy is radiated only when an electron jumps from one stationary orbit to another.

Atomic quantum numbers

1. **Principal quantum number (*n*):** The principal quantum number n corresponds to the principal energy level of the elctrons.

It has integral positive values excluding zero.

2. **Angular quantum number or azimuthal quantum number (l):** Having the same principal energy level, there are different orbitals having different energy and different angular momentum. These orbitals are called *subshells* and are characterized by their orbital quantum number l, l can have all integral values from 0 to $(n - 1)$. If $l = 0, 1, 2, 3$ ... the sub-shells are called as *s, p, d, f* ..... respectively.

Shells	Values of n	Values of l	Representation of sub-shells
K	1	0	1s
L	2	0, 1	2s, 2p
M	3	0, 1, 2	3s, 3p, 3d
N	4	0, 1, 2, 3	4s, 4p, 4d, 4f

3. **Magnetic quantum number (m):** The changing the orientation of the electrons in space around the nucleus are determined by magnetic quantum numbers m. For a given value l, m can have any integral value from $-l$ to $+l$ including zero, i.e., for a given value of l, m can have of $(2l + 1)$ values.

Sub-Shells	Values of l	Values of m	Number of orbitals
s	0	0	1
p	1	–1, 0, +1	3
d	2	–2, –1, 0, +1, +2	5
f	3	–3, –2, –1, 0, +1, +2, +3	7

4. **Spin quantum number (s):** Spin quantum number determines the spining of an electron about its own axis and can have only two directions: clockwise or anti clockwise, can have either of the two values, $+\frac{1}{2}$ or $-\frac{1}{2}$.

Pauli's Exclusion Principle

It states that no two electrons in an atom can have the same values of all the four quantum numbers. In other words, no two electrons can occupy the same energy state.

$(n + l)$ rule

It states that a sub-shell having lower value of $(n + l)$ has lower energy. If the value of $(n + l)$ for two sub-shells is the same, then the one having lower value of n has lower energy.

Aufbau principle

It states that electrons enter the various orbitals of an atom according to their increasing energies, and energy of the orbitals is governed by $(n + l)$ rule. The electrons enter sub-shell of lowest energy first.

Hund's rules

Rule I. When there are several orbitals of equal energy available, first of all electrons enter these orbitals singly, pairing of electrons takes place later.

Rule II. The spins of all these electrons in orbitals of equal energies, should be parallel.

Bond order : It is a measure of the strength of the chemical bond. It is equal to the number of covalent bonds in a molecule.Now,

Bond order

$$= \frac{\begin{bmatrix} \textit{Number of electrons in} \\ \textit{bonding molecular orbitals} \end{bmatrix} - \begin{bmatrix} \textit{Number of electrons in} \\ \textit{antibonding molecular orbitals} \end{bmatrix}}{2}$$

$= (N_B - N_A)/2$

(*i*) Greater the bond order, greater is the stability of the molecule.

(*ii*) Bond length is inversely proportional to the bond order.

(*iii*) Bond dissociation energy is directly proportional to the bond order.

Hybridization

It is used to explain the shapes of molecules. *It is a process of inter mixing of orbitals of slightly different energies and redistribute their energies to give rise to new set of orbitals of same energy, size and shape.*

The new orbitals formed are called **hybrid** or **hybridized orbitals**. The number of hybridized orbitals formed is equal to the number of combining pure orbitals.

Energy of Electron in nth Orbit (E_n)

(a) In C.G.S. unit :

$$E_n = \frac{2\pi^2 m z^2 e^4}{n^2 h^2} \text{ erg / electron}$$

In another way, $E_n = -\frac{E_1}{n^2}$

where, m = mass of electron = 9.11×10^{-28} gm

e = charge of electron = -4.8×10^{-10} esu

Types of hybridization

Type of hybridization	Atomic orbitals	Bond angle	Orientation of hybridized orbitals	Examples
sp	$s + p$	180°	Linear	$BeCl_2$, $HgCl_2$, $ZnCl_2$, N_2O, C_2H_2,
sp^2	$s + 2(p)$	120°	Triangular planar	BCl_3, BF_3, $AlCl_3$, SO_2, SO_3, C_2H_4, CO_2^{-2}, NO_3^-
sp^3	$s + 3(p)$	109° 28'	Tetrahedral	$SiCl_4$, SiF_4, $SnCl_4$, CCl_4, CH_4, NH_4^+, BF_4^-
dsp^2	$d + s + 2(p)$	90°	Square planar	$[PtCl_4]^{2-}$, $[Ni(CN)_4]^{2-}$ $[Cu\ (NH_3)_4]^{2+}$
dsp^3 or sp^3d	$d + s + 3(p)$	90°, 120°	Trigonal bipyramidal	PF_5, PCl_5, SbF_5
d^2sp^3, or sp^3d^2	$2(d) + s + 3(p)$	90°	Octahedral	SF_6, $[SiF_6]^{2-}$, CrF_6^{3-}, $[Co(CN)_6]^{3-}$, $[Co(NH_3)_6]^{3+}$
d^3sp^3 or sp^3d^3	$3\ (d) + s + 3(p)$	90°, 72° bipyramidal	Pentagonal	IF_7

z = atomic number

h = Planck's constant = 6.625×10^{-27} erg-sec

E_n and E_1 represents the energies of electron in nth and 1st orbit respectively.

(b) In S.I. unit :

$$E_n = -\frac{2\pi^2 m z^2 e^4}{(4\pi \in_0)^2 n^2 h^2}$$

$$= -\frac{m z^2 e^4}{8 \in_0^2 n^2 h^2} \text{ joule / electron}$$

where, m = mass of electron = 9.11×10^{-31} kg

e = charge of an electron

= -1.6×10^{-19} coulomb

z = atomic number

h = Planck's constant = 6.625×10^{-34} joule-sec

$4\pi\in_0$ is called permittivity factor and is equal to

$$\frac{1}{9 \times 10^9} \frac{(\text{Coulomb})^2}{\text{Newton} \times (\text{metre})^2} = \frac{1}{9 \times 10^9} \frac{C^2}{N \times m^2};$$

$\in_0$ is called permittivity of free space and is equal to

$$\frac{1}{36\pi \times 10^{9}} \frac{C^2}{N \times m^2} = 8.85 \times 10^{-12} \frac{C^2}{N \times m^2}$$

Speed of the nth Stationary Orbit (v_n)

(a) In C.G.S. unit

$$v_n = \frac{2\pi ze^2}{nh} \text{ cm / sec}$$

In another way

$$v_n = \frac{v_1}{n}$$

where v_n and v_1 represent the velocities of electron in nth and 1st orbit respectively.

(b) In S.I. unit

$$v_n = \frac{ze^2}{2 \epsilon_0 nh} \text{ m / sec}$$

Angular momentum of electron in nth orbit :

$$I\omega_n = mv_n r_n = \frac{nh}{2\pi}$$

- Radius of atom $\approx 10^{-8}$ cm = 1 Angstrom unit (1 Å)
- Radius of nucleus $\simeq 10^{-13}$cm = 1 Fermi
E = h.ν, where E = energy; ν = Frequency of radiation
- Wt. of a single particle (atom, molecule, ion, etc.) $= \dfrac{\text{gram formula wt.}}{N}$
- Molar volume of gas = 22.4 litres at S.T.P. or N.T.P.
- Normal temperature = 0°C or 273°K
- Normal pressure = 1 atmosphere or 700 mm of Hg

- Vapour density (V.D.) $= \dfrac{W}{V} \times 11.2$
- Molecular Wt. (M) $= \dfrac{W}{V} \times 22.4$; where V is the volume in litres at S.T.P. or N.T.P.
- M = 2 × V.D.
- No. of moles after decomposition or dissociation

$= 1 + (n - 1) \times \alpha$; where α is degree of dissociation and n = no. of particles after dissociation

- $\frac{M_c}{M_o} = \frac{D_c}{D_o} = 1 + (n - 1) \times \alpha$ in case of dissociation
- $\frac{M_c}{M_o} = \frac{D_c}{D_o} = 1 - \alpha\left(\frac{n-1}{n}\right)$ in case of association

  where α = degree of association, c stands for calculated or normal value and o stands for observed or abnormal value.
- Equivalent weight of an element

  $= \frac{\text{At. wt.}}{\text{Valency}}$
- 1 gm eq. wt. = eq. wt. in gram.

  No. of gram equivalent

  $= \frac{\text{Wt. in gram}}{\text{gram equivalent wt.}}$
- Equivalent wt. of an acid

  $= \frac{\text{Molecular wt.}}{\text{Basicity of an acid}}$

- Equivalent wt. of base

$$= \frac{\text{Molecular wt.}}{\text{Acidity of a base}}$$

- If no redox reaction, then equivalent wt. of a radical

$$= \frac{\text{Formula wt.}}{\text{Charge on ions (radicals) or valency}}$$

- Eq. wt. of a compound

$$= \frac{\text{Molecular wt.}}{\text{Total charge of its cation or anion}}$$

= sum of equal wt. elements and radicals

= Eq. wt. of cation + Eq. wt. of anion

- For reaction with H_2 : $E = \frac{W_1}{W_2(H)}$

$$= \frac{\text{wt. of metal}}{\text{wt. of } H_2}$$

$$= \frac{W_1}{V} \times 11{,}200$$

- For reaction with chlorine :

$$E = \frac{W_1}{W_2(Cl)} \times 35.5$$

$$= \frac{W}{V} \times 11{,}200$$

$$= \frac{\text{wt. of element}}{\text{wt. of chlorine}} \times 35.5$$

- For reaction with oxygen :

$$E = \frac{W_1}{W_2(O_2)} \times 8$$

$$= \frac{\text{wt. of substance}}{\text{wt. of Oxygen}} \times 8$$

$$= \frac{W_1}{V} \times 5{,}600$$

In general reaction : $\frac{W_1}{W_2} = \frac{E_1}{E_2}$

In redox reaction : Equivalent wt. of a substance $= \frac{\text{Formula wt.}}{\text{No. of electrons lost or gained per molecule}}$

$$= \frac{\text{Formula wt.}}{\text{Total change in oxidation number per molecule}}$$

For an isomorphous AX, BX

$$\frac{\text{wt. of A that combines with x gm. of X}}{\text{wt. of B that combines with x gm. of X}}$$

$$= \frac{\text{At. wt. of A}}{\text{At. wt. of B}}$$