

ATOMIC STRUCTURE

FUNDAMENTAL PARTICLES

Atoms are made up-essentially, of three fundamental particles, which differ in mass and electric charge as follows:

	Electron	Proton	Neutron
Symbol	e or e ⁻	p	n
Approximate relative mass	1/1836	1	1
Approximate relative charge	-1	+1	0
Mass in kg	9.109534×10^{-31}	$1.6726485 \times 10^{-27}$	$1.6749543 \times 10^{-27}$
Mass in amu	5.4858026×10^{-4}	1.007276471	1.008665012
Actual charge/C	$1.6021892 \times 10^{-19}$	$1.6021892 \times 10^{-19}$	0

ATOMIC TERMS :

Nuclide : Various species of atoms in general.

Nucleons : Sub-atomic particles in the nucleus of an atom, i.e., protons and neutrons.

Isotopes : Atoms of an element with the same atomic number but different mass number.

Mass number (A) : Sum of the number of protons and neutrons, i.e., the total number of nucleons,

Atomic number (Z) : The number of protons in the nucleus of an atom. This, when subtracted from A, gives the number of neutrons.

Isobars : Atoms, having the same mass numbers but different atomic numbers, e.g., ${}_{15}\text{P}^{32}$ and ${}_{16}\text{S}^{32}$.

Isotones : Atoms having the same number of neutrons but different number of protons or mass number, e.g., ${}_{6}\text{C}^{14}$, ${}_{8}\text{O}^{16}$, ${}_{7}\text{N}^{15}$.

Isoelectronic species : Atoms molecules or ions having the same number of electrons, e.g., N₂, CO, CN

Nuclear isomers : Atoms with the same atomic and mass numbers but different radioactive properties, e.g., uranium X (half life 1.4 min) and uranium Z (half life 6.7 hours).

Atomic mass unit : Exactly equal to 1/12th of the mass of ${}_{6}\text{C}^{12}$ atom.
(a.m.u.): 1 a.m.u. = 1.66×10^{-24} g \approx 931.5 MeV

Example 1 : How many protons, electrons and neutrons are present in 0.18 g ${}_{15}\text{P}^{30}$?

Solution : No. of neutrons in one atom = (30 - 15) = 15

$$0.18 \text{ g } {}_{15}\text{P}^{30} = \frac{0.18}{30} = 0.006 \text{ mole}$$

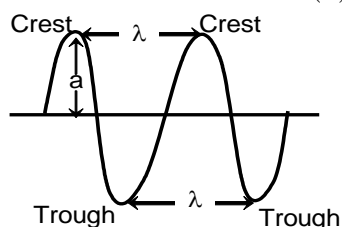
$$\text{Now, number of } {}_{15}\text{P}^{30} \text{ atoms in 0.006 mole} = 0.006 \times 6.02 \times 10^{23}$$

$$\text{Number of electrons in 0.006 mole of } {}_{15}\text{P}^{30} = \text{Number of protons in 0.006 mole } {}_{15}\text{P}^{30}$$

$$= 15 \times 0.006 \times 6.02 \times 10^{23} = 5.418 \times 10^{22} \text{ and number of neutrons} = 5.418 \times 10^{22}$$

SOME IMPORTANT CHARACTERISTICS OF A WAVE

A wave is a sort of disturbance which originates from some vibrating source and travels outward as a continuous sequence of alternating crests and troughs. Every wave has five important characteristics, namely, wavelength (λ), frequency (ν), velocity (c), wave number ($\bar{\nu}$) and amplitude (a).



Electronic Magnetic Radiation:

Ordinary light rays, X-rays, γ -rays, etc. are called electromagnetic radiations because similar waves can be produced by moving a charged body in a magnetic field or a magnet in an electric field. These radiations have wave characteristics and do not require any medium for their propagation.

- **Wavelength (λ):** The distance between two neighbouring troughs or crests is known as wavelength. It is denoted by λ and is expressed in cm, m, nanometers ($1 \text{ nm} = 10^{-9} \text{ m}$) or Angstrom ($1 \text{ \AA} = 10^{-10} \text{ m}$).
- **Frequency (ν):** The frequency of a wave is the number of times a wave passes through a given point in a medium in one second. It is denoted by ν (nu) and is expressed in cycles per second (cps) or hertz (Hz) $1 \text{ Hz} = 1 \text{ cps}$.

The frequency of a wave is inversely proportional to its wave length (λ)

$$\nu \propto \frac{1}{\lambda} \text{ or } \nu = \frac{c}{\lambda}$$

- **Velocity:** The distance travelled by the wave in one second is called its velocity. It is denoted by c and is expressed in cm sec^{-1} .

$$c = \nu\lambda \text{ or } \lambda = \frac{c}{\nu}$$

- **Wave number ($\bar{\nu}$):** It is defined as number of wavelengths per cm. It is denoted by $\bar{\nu}$ and is expressed in cm^{-1} .

$$\bar{\nu} = \frac{1}{\lambda} \text{ or } \bar{\nu} = \frac{\nu}{c}$$

- **Amplitude:** It is the height of the crest or depth of the trough of a wave and is denoted by a . It determines the intensity or brightness of the beam of light.
- **Electromagnetic Spectrum:** The arrangement of the various types of electromagnetic radiation in order of increasing or decreasing wavelengths or frequencies is known as electromagnetic spectrum.

ATOMIC SPECTRUM

If the atom gains energy the electron passes from a lower energy level to a higher energy level, energy is absorbed that means a specific wave length is absorbed. Consequently, a dark line will appear in the spectrum. This dark line constitutes the **absorption spectrum**.

If the atom loses energy, the electron passes from higher to a lower energy level, energy is released and a spectral line of specific wavelength is emitted. This line constitutes the **emission spectrum**.

Types of Emission Spectra:

- **Continuous spectra:** When white light from any source such as sun or bulb is analyzed by passing through a prism, it splits up into seven different wide bands of colour from violet to red (like rainbow). These colour are so continuous that each of them merges into the next. Hence the spectrum is called as continuous spectrum.
- **Line spectra:** When an electric discharge is passed through a gas at low pressure light is emitted. If this light is resolved by a spectroscope, It is found that some isolated coloured lines are obtained on a photographic plate separated from each other by dark spaces. This spectrum is called line spectrum. Each line in the spectrum corresponds to a particular wavelength. Each element gives its own characteristic spectrum.

Example 2 : The wave number of a radiation is 400 cm^{-1} . Find out its

- (a) Wavelength (b) Frequency
(c) J per photon (d) kcal per mol of photons

Solution: (a) $\bar{\nu} = \frac{1}{\lambda}$ or $\lambda = \frac{1}{\bar{\nu}} = \frac{1}{400 \text{ cm}} = 2.5 \times 10^{-3} \text{ cm}$

(b) $\nu = \frac{c}{\lambda} = c \times \bar{\nu} = 3 \times 10^{10} \text{ cm/s} \times 400 \text{ cm}^{-1} = 1.2 \times 10^7 \text{ s}^{-1}$

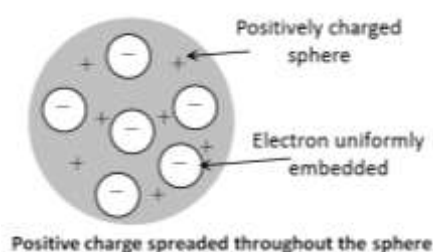
$$\begin{aligned}
 \text{(c) } E_{\text{photon}} &= hv = \frac{hc}{\lambda} = h \times c \times \bar{\nu} \\
 &= 6.626 \times 10^{-34} \text{ Js} \times 3 \times 10^8 \text{ cm/s} \times 400 \text{ cm}^{-1} = 7.95 \times 10^{-21} \text{ J} \\
 \text{(d) } E_{\text{photon}} &= 7.95 \times 10^{-21} \text{ J} \\
 \text{For 1 mol of photon energy} &= 7.95 \times 10^{-21} \text{ J} \times 6.022 \times 10^{23} \text{ mol}^{-1} \\
 &= (4.7875 \times 10^3 \text{ J mol}^{-1}) \text{ (1 kcal/4184 J)} \\
 &= 1.14 \text{ kcal mol}^{-1}
 \end{aligned}$$

ATOMIC MODELS

We know the fundamental particles of the atom. Now let us see, how these particles are arranged in an atom to suggest a model of the atom.

Plum Pudding Model of Thomson

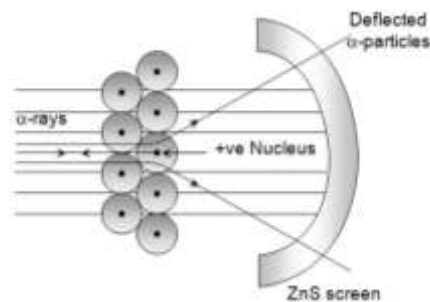
- (1) He suggested that atom is a positively charged sphere having electrons embedded uniformly giving an overall picture of plum pudding.



- (2) This model failed to explain the line spectrum of an element and the scattering experiment of Rutherford.

Rutherford's Experiment

- (a) As most of the α -particles passed undeflected, the atom must predominantly consists of empty space.
 (b) As a few α -particles carrying +ve charge are strongly deflected there must be a heavy +ve charged body present in each atom and the volume occupied by this is only a minute fraction of the total volume of an atom. He called this +vely charged body as nucleus. It is surrounded by small negatively charged particles called electrons, at relatively large distances from the nucleus.



Example 3 : An α - particle is traveling towards gold nuclei returns back through 10^{-10} m from it. What is the velocity of the α - particle. [Given 1 amu = 1.66×10^{-27} kg, atomic mass of He = 4 and gold = 79 and $\frac{1}{4\pi\epsilon_0} = 9 \times 10^9 \text{ Nm}^2\text{C}^{-2}$]

Solution: We known that $r_0 = \frac{q_1 q_2}{4\pi\epsilon_0 \left(\frac{1}{2}mv^2\right)}$ $\therefore v^2 = \frac{2q_1 q_2}{4\pi\epsilon_0 m r_0}$

Now one He atom has charge (q_1) = $2e$

One gold atom has charge (q_2) = $79e$

Putting these values we get

$$v^2 = \frac{2 \times (2 \times 1.6 \times 10^{-19}) \times (79 \times 1.6 \times 10^{-19}) \times 9 \times 10^9}{4 \times 1.66 \times 10^{-27} \times 10^{-10}}$$

$$\therefore v = 3.311 \times 10^5 \text{ m/s}$$

Planck's quantum theory

- (i) The radiant energy which is emitted or absorbed by the black body is not continuous but discontinuous in the form of small discrete packets of energy, each such packet of energy is called a 'quantum'. In case of light, the quantum of energy is called a 'photon'.
- (ii) The energy of each quantum is directly proportional to the frequency (ν) of the radiation, i.e.

$$E \propto \nu \text{ or } E = h\nu = \frac{hc}{\lambda}$$

Where, h = Planck's constant = 6.62×10^{-27} erg. sec. or 6.62×10^{-34} Joules sec.

- (iii) The total amount of energy emitted or absorbed by a body will be some whole number quanta. Hence $E = nh\nu$, where n is an integer.

Neil's Bohr Atomic Theory (1913)

Bohr's theory is applied to one electronic species. Path of electron is circular and angular momentum of electron is quantized. Bohr's has given the concept of stationary orbits i.e. while revolving in any orbit, total energy of electron remains constant.

(a) Total energy : $E = \frac{-2\pi^2 m z^2 e^4 k^2}{n^2 h^2} \text{ eV}$

On putting values of constants : $E_n = \frac{-13.6 \times z^2}{n^2} \text{ eV}$

(b) Radius of path of electron $r_n = \frac{n^2 h^2}{4\pi^2 m z e^2 k}$
 $r_n = \frac{0.529 n^2}{z} \text{ \AA}$

(c) Velocity of electron : $v_n = 2.18 \times 10^6 \frac{z}{n} \text{ cm/sec}$

(d) Energy released when electron jumps from $n_2 \longrightarrow n_1$

$$\Delta E = 13.6 Z^2 \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] \text{ eV}$$

where n_1 is lower level and n_2 is higher level

(e) Wavelength of radiation obtained : $\frac{1}{\lambda} = R z^2 \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$

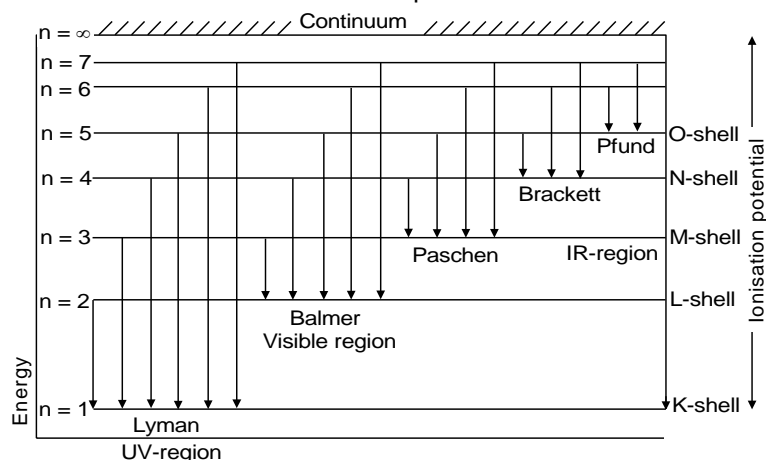
where R is Rydberg's constant $R = 109677 \text{ cm}^{-1}$

Example 4 : Find the energy released when electron jumps from 4th excited state to ground state in hydrogen atom

Solution : $\Delta E = 13.6 \times 1 \left[\frac{1}{1} - \frac{1}{25} \right] \text{ eV} = 13.6 \times \left[\frac{24}{25} \right] \text{ eV}$

Hydrogen spectrum

Hydrogen spectrum is obtained as a discontinuous line spectrum.



$$\text{Total no. of lines obtained in spectrum} = \frac{n(n-1)}{2}$$

where n = higher level

Example 5 : A hydrogen atom in ground state is supplied energy of 12.75 eV. Find how many lines are obtained in emission-spectrum ?

Solution : $\Delta E = 12.75 = 13.6 \times 1 \left[\frac{1}{1} - \frac{1}{n^2} \right]$

On solving n = 4

\therefore Total lines = $\frac{n(n-1)}{2} = \frac{4 \times 3}{2} = 6$

Quantum Mechanical Model

It is based upon wave nature of electron. Electron is moving around nucleus like a 3-D wave.

Schrodinger wave equation :
$$\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} + \frac{8\pi^2m}{h^2}(E - V)\psi = 0$$

where ψ = orbital wave function

$$\psi = R(r) \cdot A(\theta, \phi)$$

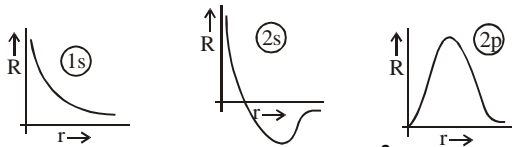
\downarrow \downarrow
 Radial wave function Angular wave function

Example 6 : Calculate radial nodes and angular nodes for the following type of orbitals.

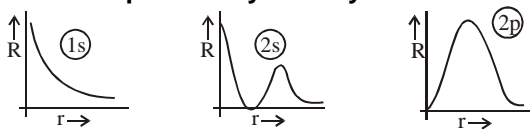
(a) 1s, (b) 2p, (c) 3p, (d) 3d, (e) 4s and (f) 4d

Solution : (a) 0, 0 (b) 0, 1 (c) 1, 1 (d) 0, 2
 (e) 3, 0 (f) 1, 2

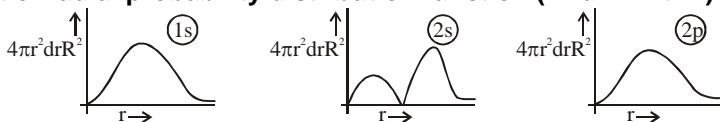
Plot of radial wave function r with r



Plot of radial probability density r² with r



Plot of radial probability distribution function (4r²drR² with r)



Total no. of radial node = (n - l - 1)

Total no. of angular node = 'l'

Example 7 : Find no. of radial and angular node in a 5p orbital?

Solution : Radial node = 5 - 1 - 1 = 3, angular node = 1

De-Broglie's relationship

Since, microscopic particles like electron have dual nature, therefore wavelength of wave created by motion of particle is given by $\lambda = \frac{h}{mv}$ is significant only when 'm' is insignificant.

Heisenberg's uncertainty principle

$$\Delta x \cdot \Delta p \geq h / 4\pi \text{ or } \Delta E \times \Delta t \geq \frac{h}{4\pi}$$

Example 8 : Calculate the de Broglie wavelength of a ball of mass 0.1 kg moving with a speed of 60ms^{-1} .

Solution : $\lambda = \frac{h}{mv} = \frac{6.6 \times 10^{-34}}{0.1 \times 60}$; $\lambda = 1.1 \times 10^{-34}$ m.

This is apparent that this wavelength is too small for ordinary observation.

Although the de Broglie equation is applicable to all material objects but it has significance only in case of microscopic particles.

Since, we come across macroscopic objects in our everyday life, de Broglie relationship has no significance in everyday life.

RULES FOR FILLING OF ELECTRONS IN THE ORBITAL(S): ELECTRONIC CONFIGURATION

The Aufbau Principle

According to it an electron enters the orbital that has the minimum energy.

or

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

This is correct for multi electron atoms.

Hund's Rule

It states that electron pairing in any s, p, d or f-orbital is not possible until all the available orbitals of the same orbital contain one electron each.

Pauli Exclusion Principle

It states that no two electrons in an atom can have all the four quantum number identical. In other words, maximum number of electrons in an orbital can be two with opposite spin.

Example 9 : Write down the electronic configuration of $\text{Cr}^{(24)}$ and $\text{Cu}^{(29)}$?

Solution : Cr : $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^5$

Cu : $1s^2 2s^2 2p^6 3s^2 3p^6 4s^1 3d^{10}$

QUANTUM NUMBERS

(a) **Principal quantum no. 'n' :** It represents the distance between electron and nucleus, the energy of electron in the orbit and the angular momentum

(b) **Azimuthal or secondary or subsidiary quantum number 'l' :** It represents the no. of subshells. Can have the values 0 to (n - 1). It gives the shape of the subshell.

The volume of space where probability of finding an electron is maximum, is called orbital.

NODE :

Node is the 3-D region where probability of finding electron is zero and the plane passing through node is called as Nodal plane.

	s	p	d	f
shape	Spherical	Dumb-bell	Double dumb-bell	Complicated

$$\text{Orbital angular momentum} = \sqrt{l(l+1)} \frac{h}{2\pi}$$

(c) **Magnetic quantum no. 'm' :** This gives the no. of orbitals in a subshell (under the influence of magnetic field). It takes only integral values from -l to +l through zero, $m = 2l + 1$ for any value of l,

$$m = n^2 \quad (\text{no. of orbital in a shell})$$

Also explains the orientation of orbital.

(d) **Spin quantum no. 's'** : When an electron rotates around a nucleus, it spins around its axis. Spin of clockwise it is written as $+1/2$ or \uparrow .

If anticlockwise then it is $-1/2$ \downarrow (even no. e).

$$mvr = \frac{h\sqrt{s(s+1)}}{2\pi}$$

Example 10 : Write all the quantum numbers for the following orbitals (i) d_{z^2} (ii) $3s$ (iii) $4p_x$

Solution: (i) $n = 3, \ell = 2, m = 0, s = \pm 1/2$
(ii) $n = 3, \ell = 0, m = 0, s = \pm 1/2$
(iii) $n = 4, \ell = 1, m = -1$ or $+1, s = \pm 1/2$

PHOTOELECTRIC EFFECT

The emission of electron from the metal surface when a radiation of certain minimum frequency strike on it is called photoelectric effect.

$$E = h\nu_0 + \frac{1}{2}mv^2$$

1. Frequency of incident radiation is directly proportional to kinetic energy of emitted electron.
2. Intensity of radiation is proportional to no. of ejected electron but independent of kinetic energy of emitted electron.

Example 11 : What is the wavelength of the electron emitted from a metal surface of work function 1.5×10^{-12} J due to incidence of a photon of energy 2.5×10^{-12} J.

Solution : Kinetic energy of ejected electron
 $= 2.5 \times 10^{-12} - 1.5 \times 10^{-12}$
 $= 1.0 \times 10^{-12}$ Joule

$$\text{Wavelength; } \lambda = \frac{h}{\sqrt{2m(\text{KE})}} = \frac{6.6 \times 10^{-34}}{\sqrt{2 \times 9 \times 10^{-31} \times 10^{-12}}} = 4.8 \times 10^{-13} \text{ m.}$$
