Structure of Atom

➤ Atom is the fundamental particle of the matter.
➤ 'Atom' is derived from the Greek word **a-tomio** which means not divisible further.
➤ In 1808 the atomic theory was propounded by John Dalton, which described law of conservation of mass, law of multiple proportions and law of constant composition very well but failed to explain some points.

Discovery of sub atomic particles

1. **Discovery of electron**
    ➤ It was discovered by M. Faraday in 1830.
    ➤ When the electricity was passed through an electrolyte, a chemical reaction takes place at the electrode. The liberation and deposition of matter at electrodes were observed. These results proposed the particle nature of electricity.
    ➤ Faraday experimented further using the electrical discharge in an evacuated tube which is known as cathode ray discharge tubes.
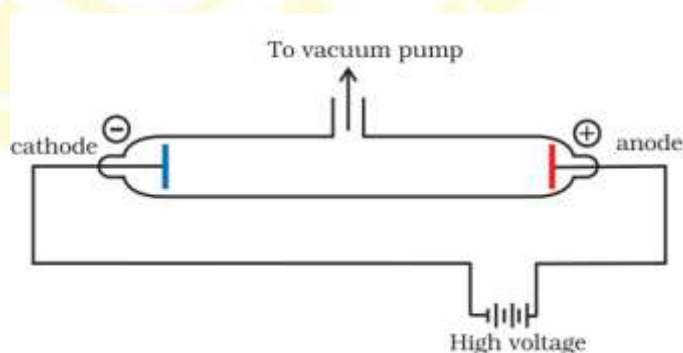

Figure: A cathode ray discharge tube

    ➤ Cathode ray tube is a sealed glass tube in which two thin metal electrodes are present. Electric discharge in gases can be seen at very low pressures and at very high voltages.
    ➤ Current flows in the form of a stream of particles which moves from cathode to anode, which is known as cathode rays.

    Results of this experiment-

1. The cathode rays start from cathode and move towards the anode.
2. These rays are not visible but can be observed by the fluorescent or phosphorescent material.
3. These rays travel in straight line.
4. In presence of magnetic or electric field cathode rays behave like charged particles.
5. This experiment suggested that cathode rays are made of negatively charged particles i.e. electrons.
6. Theses rays do not depend upon the material of electrodes, and the nature of gas present in the tube.

Charge to mass ratio of Electron

➢ J. J. Thomson measured the ratio of charge to mass of electron by using cathode ray tube in 1897.
➢ He applied the magnetic field perpendicular to the electrical field as well as to the path of electrons.
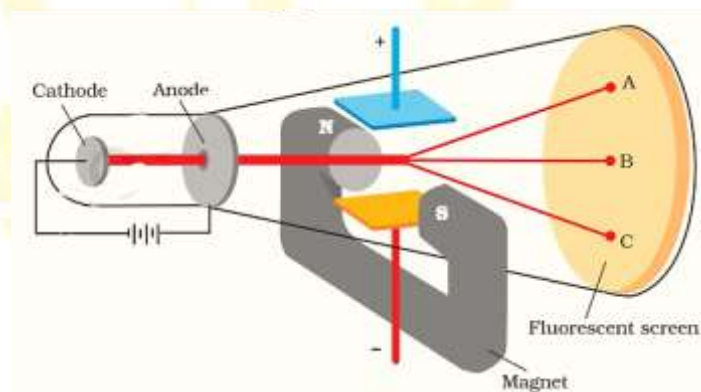

Figure: The apparatus to determine the change to the mass ratio of electron

➢ On applying only the electric field the electrons deviate from their path and hit the cathode ray tube at point A.
➢ On applying only the magnetic field, the electrons hit the tube at point C.
➢ By balancing both the fields, the electrons hit at point B, which is also obtained in the absence of both the fields.

➢ He explained the deviation of electrons in the presence of electrical and magnetic field-

> 1) The magnitude of charge on particle is directly proportional to the interaction with electrical or magnetic field.
>
> 2) Mass of the particle is inversely proportional to deflection
>
> 3) The deflection of electron is directly proportional to the voltage of electrical field or strength of magnetic field.

➢ Thomson determined the value of e/m_e :

$$\frac{e}{m_e} = 1.758820 \times 10^{11} \text{ C kg}^{-1}$$

Here e = magnitude of the charge on electron in coulomb

m_e = mass of the electron in kg.

Charge on the Electron

➢ Millikan propounded a method to calculate the charge on electron by oil drop experiment.

➢ He found the charge of an electron to be $- 1.6 \times 10^{-19}$C.

➢ The present accepted value of charge on electron is $- 1.602176 \times 10^{-19}$C.

➢ The mass of electron was determined by this formula:

$$m_e = \frac{e}{e/m_e} = \frac{1.602176 \times 10^{-19}\text{C}}{1.758820 \times 10^{-11}\text{C kg}^{-1}} = 9.1094 \times 10^{-31} \text{ kg}$$

Discovery of Protons and Neutrons

➢ The electric discharge experiment was carried out in modified cathode ray tube to discover the canal rays. Canal rays are made of positively charged particles.

➢ The characteristics of these positively charged particles are -

i) These particles depend upon the nature of gas in the cathode ray tube.

ii) The charge to mass ratio depends upon the gas from which these particles originated.

iii) They behave in opposite manner as compare to electrons in presence of electrical or magnetic field.

➢ The smallest and lightest positive ion obtained from hydrogen is known as proton. Rutherford discovered the protons.

➢ When thin sheet of beryllium was bombarded by alpha particles, electrically neutral particles were obtained which are called neutrons. They were discovered by Chadwick in 1932.

Table: properties of fundamental particles

Name	Discoverer	Symbol	Absolute charge (C)	Relative charge	Mass (Kg)	Mass (u)	Approximate mass (u)
Electron	J.J. Thompson	e	-1.602×10^{-19}	-1	9.109×10^{-31}	0.00054	0
Proton	Rutherford	p	$+1.602 \times 10^{-19}$	+1	1.6726×10^{-27}	1.00727	1
Neutron	Chadwick	n	0	0	1.6726×10^{-27}	1.00867	1

Atomic models

1. Thomson model of atom

➢ In 1898 J.J. Thomson gave plum pudding model of an atom.

➢ According to him an atom is a sphere which radius is 10^{-10} meter. In this sphere positive charge is distributed uniformly.

➢ Electrons are embedded into this sphere in electrostatically stable arrangement, like seeds in watermelon.

➢ The mass of atom is uniformly distributed.
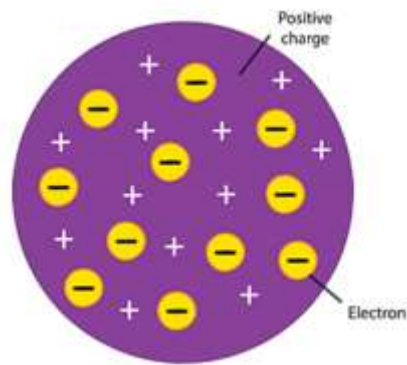
➢ According to this model atom is overall neutral.

Figure: plum pudding model

2. Rutherford's Nuclear Model of Atom

- Rutherford with some of his students bombarded some alpha particles on a thin gold foil.
- A ray of highly energised alpha particles was focused on a thin gold foil. There is a circular photographic screen of zinc sulphide around the foil. When the alpha particle hit the screen a flash light is produced at that point.
- According to Thomson, the mass of each gold atom should have been spread uniformly into the atom and alpha particle should pass directly through it.
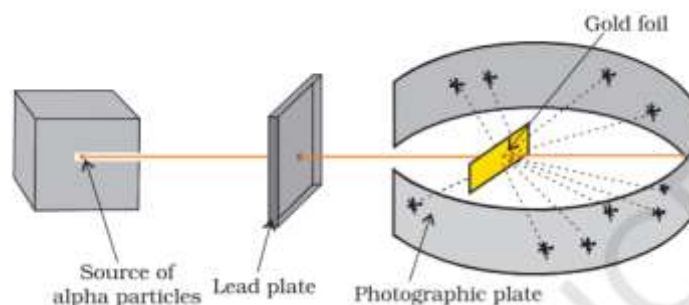

Figure: Rutherford's scattering experiment

- He changed the direction of ray containing alpha particles by small angles and observed that:
  a. Most of the space in the atom is empty, as alpha particles passed through the foil undeflected.
  b. Some alpha particles were deflected due to repulsion of positive charge present in the atom. He assumed that this

positive charge must be accumulated in the centre in very small volume.

 c. A few particles bounced back, by nearly 180 degree.

 d. According to Rutherford radius of atom is about 10^{-10}m and radius of nucleus is 10^{-15} m.

➢ Based on the observations, Rutherford propounded the nuclear model of atom. According to him:

 1. Rutherford nuclear model of an atom is similar to small scale solar system in which nucleus is playing the central role of sun and electrons are like other planets.

 2. The positive charge is concentrated in the small region which is called nucleus.

 3. The nucleus is surrounded by electrons which move around nucleus in circular path called orbit.

 4. Electron and nucleus are held together in an atom by electrostatic forces.

Drawbacks of Rutherford model

➢ Rutherford failed to explain the electromagnetic theory according to which an object revolving around the opposite charged object loses its acceleration and eventually falls into the nucleus at centre.

➢ This model failed to explain the distribution of electrons around the nucleus and the stability of an atom.

Atomic number and mass number

➢ **Atomic number (Z)** = number of protons in nucleus of an atom = number of electrons in neutral atom.

➢ **Mass number (A) =** number of protons (Z) + number of neutrons (n)

➢ Thus an atom can be represented by -

Mass Number (no. of protons + neutrons) → A
Atomic Number (no. of protons) → Z
X ← Element symbol
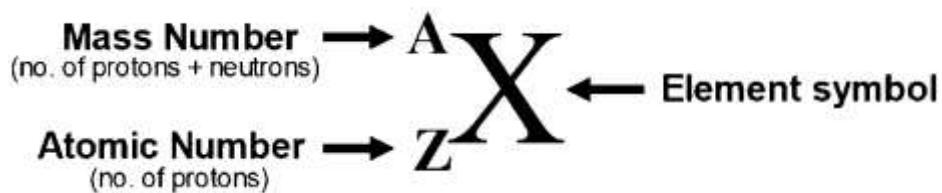
Isobars

➢ Atoms which have same mass number but different atomic number are called isobars.
➢ This means in their nucleus the number of protons is different but the sum of protons and neutrons is same.
➢ Examples- $_6C^{14}$, $_7N^{14}$.

Isotopes

➢ Atoms with identical atomic number but different atomic mass are known as Isotopes. Examples - $_1H^1$, $_1D^2$, $_1T^3$.
➢ Isotopes of an element show same chemical properties.

Isotones

➢ Atoms with same number of neutrons and differ in the number of protons are known as isotones.
➢ Examples- $_{16}S^{36}$, $_{17}Cl^{37}$, $_{18}Ar^{38}$, $_{19}K^{39}$, $_{20}Ca^{40}$ all are isotones, they all contain 20 neutrons.

Bohr's Model of Atom

➢ To overcome the objection of Rutherford's atomic model, Neil Bohr put forward his model.
➢ According to him the electromagnetic radiation has dual character, which means that radiations hold both wave like and particle like properties.

Wave nature of electromagnetic radiation

➢ James Maxwell propounded that when electrically charged particle moves under acceleration, alternating magnetic and electrical fields are produced and transmitted. These fields are transmitted in the form of waves called electromagnetic waves.
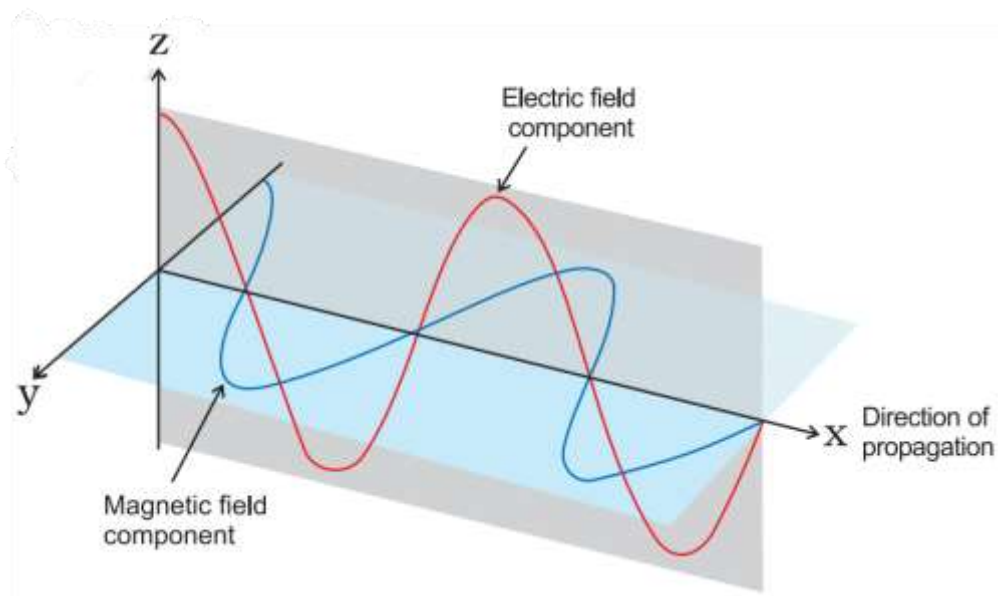

Figure: The electric and magnetic field components of an electromagnetic wave

Properties of electromagnetic waves

• The electric and magnetic fields produced by oscillating charged particles are perpendicular to each other and both are perpendicular to the direction of propagation of the wave.
• Electromagnetic waves can move in vacuum. They do not require any medium.
• There are different types of electromagnetic radiations, which have different wavelength. In the electromagnetic spectrum we can see them.
• The electromagnetic radiations are represented by different kinds of units. Examples- wavelength (λ), frequency (ν).

Wavelength (λ) – In an electromagnetic wave the distance between two successive crests of a wave is known as wavelength.
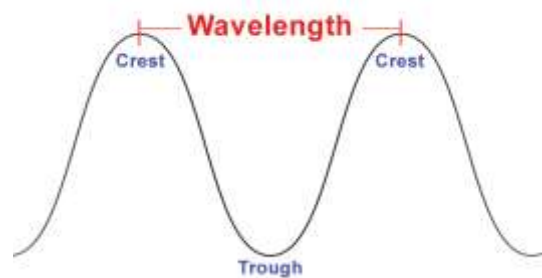

Figure: wavelength

Wavelength has the units of length. SI unit is meter (m).

Frequency (ν) – The number of waves that pass a given point in one second is known as frequency. The SI unit for frequency (ν) is Hertz (Hz, s^{-1}).
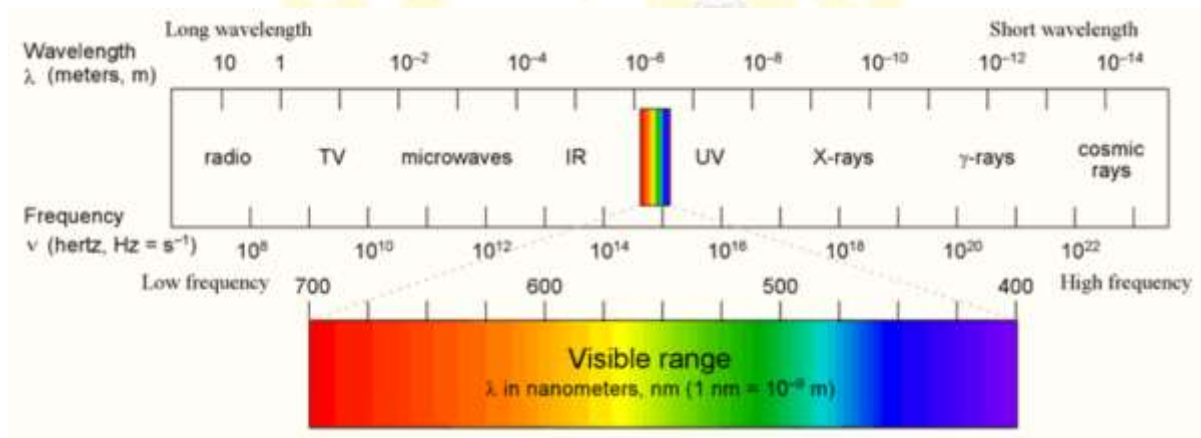

Figure: The spectrum of electromagnetic radiation

- In vacuum all electromagnetic radiations travel at the speed i.e. 3×10^8 m s^{-1}. This is called speed of light and is denoted by 'c'.
- The relation between frequency (ν), speed of light (c) and wavelength (λ) is expressed as-

$$c = \nu \, \lambda$$

- Wavenumber ($\bar{v}$) – The number of wavelengths in per unit length is known as wavenumber.
  Its unit are reciprocal of wavelength i.e. m^{-1}.

$$\bar{v} = 1/\lambda$$

Particle nature of electromagnetic radiations:

Planck's quantum theory:
➢ According to Max Planck atoms and molecules can emit or absorb energy only in discrete manner. The small quantity of energy which is released in discrete manner is known as **quantum.**
  The energy of a quantum can be expressed as-
$$E = h\nu$$
  Here ν = frequency of radiation
  h = Planck's constant. Its value is 6.626x10^{-34} J s.
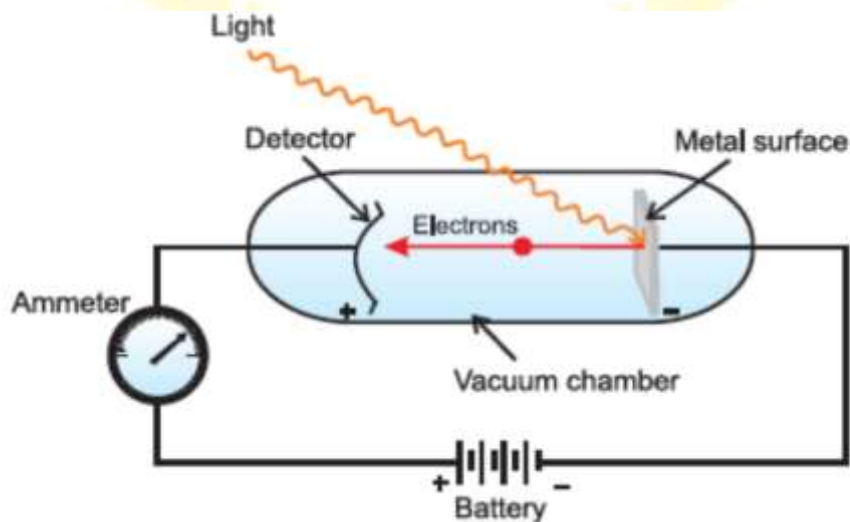
Photo electric effect:

Figure: Photo electric effect

➢ When surface of certain metals is exposed to a beam of light, electrons are ejected from the metal surface. This phenomenon is known as Photoelectric effect.

➢ The electrons are ejected from the metal surface as the beam of light hit the surface. There is no time lag in between them.

The number of ejected e⁻ $\propto$ intensity of light

➢ There is a characteristic minimum frequency for each metal below which ejection of electrons is not possible; this frequency is known as Threshold frequency. It is denoted by ν_o.
➢ The ejected electrons possess kinetic energy.

The kinetic energy of e⁻ $\propto$ the frequency of light ( )

➢ At a frequency $\nu > \nu_o$, photo electric effect is observed.
➢ According to **Einstein** the striking light is in form of photons and the energy of each photon is $h\nu$. The minimum energy required to eject an electron from metal surface is $h\nu_o$.
➢ The minimum energy required to eject an electron from metal surface is called Work function ($W_o = h\nu_o$).

Table: values of work function (W_o) for few metals

Metal	Li	Na	K	Mg	Cu	Ag
W_o (eV)	2.42	2.3	2.25	3.7	4.8	4.3

➢ The kinetic energy of photon = ($h\nu - h\nu_o$)
➢ The kinetic energy of ejected electron=
$$h\nu = h\nu_o + \frac{1}{2} m_e V^2$$

Here m_e = mass of electron
ν = velocity of ejected electron

Atomic spectra

➢ The ordinary light consists of waves of different wavelengths in the visible region. When a ray of white light is spread out into a series of coloured bands it is known as spectrum.
➢ There are two types of spectra- emission and absorption.
➢ The spectrum of radiation emitted by an excited atom/ ion/ molecule (that has absorbed the energy) is called **emission spectra**.
➢ The **absorption spectra** produced when atom/ion/ molecule absorb energy. It comprises of dark lines in the spectra. An absorption spectrum is like the photographic negative of an emission spectrum.
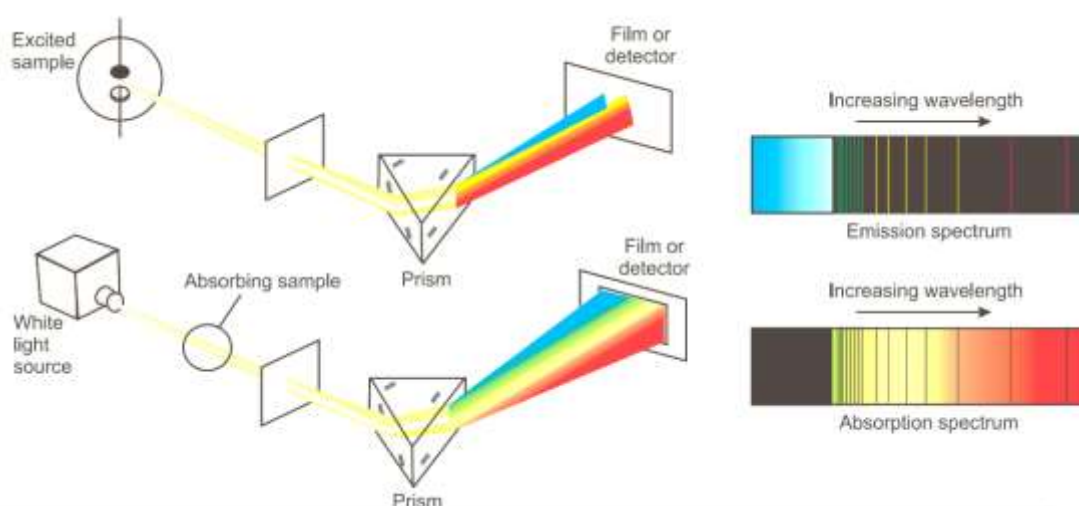➢ The study of emission or absorption spectrum is called spectroscopy.

Figure: Atomic emission and absorption spectrum

Line spectrum of Hydrogen

➢ When an electric discharge is passed through hydrogen gas, the H_2 molecules dissociate and the excited hydrogen atoms emit electronic radiation in discrete frequency.
➢ The hydrogen spectrum consists of several lines. The spectral lines are expressed as wavenumber ($\bar{v}$). In 1885 Balmer propounded a formula-

$$\bar{v} = 109,677 \left(\frac{1}{2^2} - \frac{1}{n^2} \right) \text{ cm}^{-1}$$

Here n = an integer equal to or greater than 3 (n=3,4, 5,…)

The series of lines described by this formula is known as Balmer series.

➢ Johannes Rydberg gave the following expression to find all the lines of hydrogen spectrum-

$$\bar{v} = 109{,}677 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \text{ cm}^{-1}$$

$$\bar{v} = R \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \text{ cm}^{-1}$$

Here n_1 = 1,2…..

$n_2 = n_1 + 1, n_1 + 2…..$

R = Rydberg constant for hydrogen

Table: The spectral lines for Hydrogen spectrum

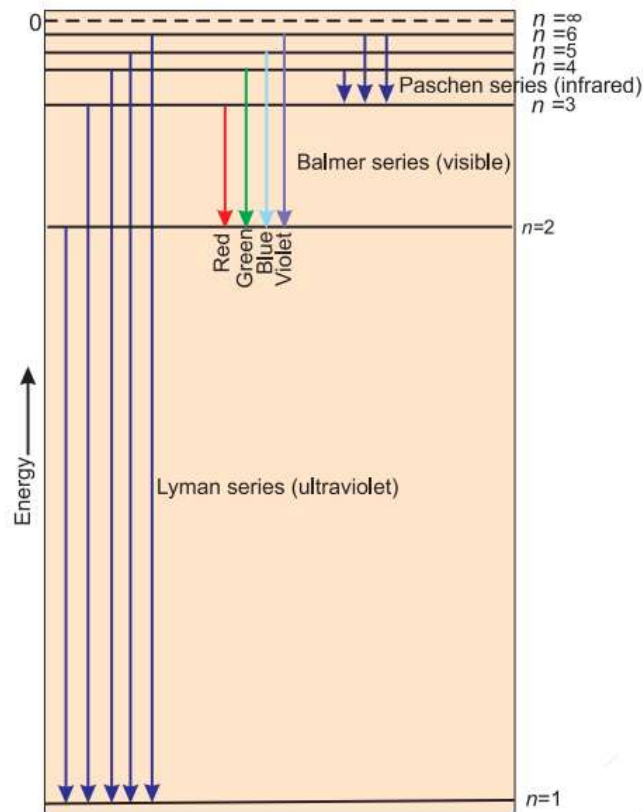| Series	n_1	n_2	Spectral Region
Lyman	1	2,3..	Ultraviolet
Balmer	2	3,4..	Visible
Paschen	3	4,5..	Infrared
Brackett	4	5,6..	Infrared
Pfund	5	6,7..	Infrared

Figure: transition of electron in hydrogen atom

Bohr's model for Hydrogen atom

➢ In 1913 Neils Bohr explained the features of structure of hydrogen atom and its spectrum.

➢ Postulates of Bohr's model for Hydrogen atom-

1. In the H-atom the electron move around the nucleus in a circular path with fixed energy and radius. Thus circular paths are known as orbits. Orbits are arranged concentrically around the nucleus.

2. The energy of an electron does not change with time in orbit. The electron move from lower to higher orbit when energy is absorbed by electron. And electron moves from higher to lower orbit when energy is emitted by the electron. Energy change does not happen continuously.

3. The frequency of radiation absorbed or emitted when transition occurs between two stationary states which have an energy difference of ΔE-

Bohr's frequency rule:

$$\nu = \frac{\Delta E}{h} = \frac{E_2 - E_1}{h}$$

Here E_1 and E_2 = Energies of lower and higher energy states

4. The angular momentum is the product of moment of inertia (I) and angular velocity (ω).

   For an electron moving in a circular path of radius r round the nucleus-

$$m_e \, v \, r = n. \frac{h}{2\pi} \qquad\qquad n = 1, 2, 3...$$

Here m_e = mass of electron

v = velocity of electron

r = radius of orbit in which electron is moving

The electron can move only in those orbits for which its angular momentum is integral multiple of $h/2\pi$. That means angular momentum is quantised.

According to Bohr's theory for Hydrogen atom:

1. The stationary states for electron are numbered n = 1, 2, 3...These integral numbers are known as Principal quantum numbers.
2. The radii of the stationary states are expressed as:

$$r_n = n^2 a_o$$

Here a_o = 52.9 pm, the radius of first stationary state is called the Bohr orbit is 52.9 pm.

3. The energy of electron's stationary state-

$$E_n = - R_H \frac{(1)}{n^2} \qquad\qquad n=1, 2, 3....$$

Here R_H = Rydberg constant = 2.18×10^{-18}J.

The energy of ground state- n=1

$$E_1 = -2.18 \times 10^{-18} \frac{(1)}{1^2} = -2.18 \times 10^{-18} \text{ J}$$

The energy of the stationary state for n=2,-

$$E_2 = -2.18 \times 10^{-18} \frac{(1)}{2^2} = -0.545 \times 10^{-18} \text{ J}$$

4. Bohr's theory is applicable to ions containing only one electron. Examples- He^+, Li^{+2}, Be^{+3}, etc.
   The energy of stationary state-

   $$E_1 = -2.18 \times 10^{-18} \frac{(Z^2)}{n^2} \text{ J}$$

   Radii $r_n = \frac{52.9 \, (n^2)}{Z}$ **pm**

   Here Z = Atomic number, for He and Lithium: Z= 2.3.
5. The velocity of moving electron is possible to calculate.

   Velocity of electron $\propto$ positive charge on nucleus $\propto$ 1/ principal quantum number.

   The energy gap between the two orbits is as follows-
   $$\Delta E = E_f - E_1$$

   $$\Delta E = \left(-\frac{R_H}{n_f^2}\right) - \left(-\frac{R_H}{n_1^2}\right)$$
   Here n_1 and n_f stands for initial and final orbits.

   $$\Delta E = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_f^2}\right) = 2.18 \times 10^{-18} \text{ J} \left(\frac{1}{n_1^2} - \frac{1}{n_f^2}\right)$$

   The frequency (ν) of photon absorbed or emitted

   $$\nu = \frac{\Delta E}{h} = \frac{R_H}{h} \left(\frac{1}{n_1^2} - \frac{1}{n_f^2}\right)$$

   In terms of wavenumbers ($\bar{\nu}$)

   $$\bar{\nu} = \frac{\nu}{h} = \frac{R_H}{hc} \left(\frac{1}{n_1^2} - \frac{1}{n_f^2}\right)$$

Limitation of Bohr's Model

- Bohr's Model fails to explain the spectrum of other atoms having more than one electron.
- It was unable to explain Zeeman Effect (the splitting of spectral lines).

- This model could not explain the ability of atoms to form molecules by chemical bond.

Dual behaviour of Matter

- De Broglie in 1924 propounded that just like radiation, matter also exhibits dual behaviour means particle and wave like properties.
- De Broglie gave the following relation between wavelength and momentum (p) of a particle-

$$\lambda = \frac{h}{mv} = \frac{h}{p}$$

- Here m = mass of particle
  v = particle's velocity
  p = particle's momentum

Heisenberg's Uncertainty Principle

- In 1927 Werner Heisenberg put forward the uncertainty principle.
- According to him it is impossible to determine simultaneously the exact position and exact momentum of an electron.

$$\Delta x \times \Delta p_x \geq \frac{h}{4\pi}$$

$$\Delta x \times \Delta mv_x \geq \frac{h}{4\pi} \qquad (p=mv)$$

$$\Delta x \times \Delta v_x \geq \frac{h}{4\pi m} \qquad (p=mv)$$

Here Δx = Uncertainty in position of the particle
Δp_x = Uncertainty in momentum of the particle

- It rules out existence of definite paths or trajectories of electrons and other similar particles.

- The effect of Heisenberg uncertainty principle is significant only for motion of microscopic objects and is negligible for that of macroscopic objects.
  If uncertainty principle is applied to an object of mass, say about a milligram (10^{-6}kg) then-

$$\Delta v\,\Delta x = \frac{h}{4\pi m}$$

$$= \frac{6.626\times 10\text{-}34\ Js}{4\times 3.1416\times 10^{-6}\ kg} \sim 10^{-28}m^{-2}s^{-1}$$

- The value of $\Delta v\Delta x$ obtained is extremely small and is insignificant. In dealing with milligram- sized or heavier objects, the associated uncertainties are hardly of any real consequence.
- In the case of a microscopic object-

$$\Delta v\,\Delta x = \frac{h}{4\pi m}$$

$$= \frac{6.626\times 10\text{-}34\ Js}{4\times 3.1416\times 9.11\times 10^{-31}\ kg}$$

$$= 10^{-4}\ m^{-2}s^{-1}$$

- If one tries to find the exact location of the electron, with an uncertainty of only 10^{-8}m, then the uncertainty Δv in velocity would be

$$= \frac{10^{-4}\ m^{-2}s^{-1}}{10^{-8}m} \sim 10^{4}\ ms^{-1}$$

- The precise statements of the position and momentum of electrons have to be replaced by the statements of probability, that the electron has at a given position and momentum.

Orbitals and quantum numbers

- A large number of orbitals are possible for an atom.
- Orbitals can be distinguished by shape, size and orientation. Atomic orbitals are precisely distinguished by three quantum numbers- n, l, m_L.

Principal quantum number (n)-

- The principal quantum number determines the size and the energy of the orbital. It helps to find the shell.
- It is a positive integer with value 1, 2, 3…
- The total number of allowed orbital $=n^2$
- **Size of orbital $\propto$ principal quantum number**
- n   Shell
  1   K
  2   L
  3   M
  4   N …….and so on

Azimuthal quantum number (l)

➤ It is also known as orbital angular momentum or subsidiary quantum number.
➤ It helps to determine the shape of orbital.
➤ l have 0 to n-1 values.

n	l
1	0
2	0,1
3	0,1,2

➤ Each shell consists of subshell. The number of subshells in a principal shell is equal to the value of n.

Table: subshell notation

Value of n	Value of l	Notation for subshell
1	0	1s
2	0	2s
2	1	2p
3	0	3s
3	1	3p

3	2	3d
4	0	4s
4	1	4p
4	2	4d
4	3	4f

Magnetic orbital quantum number 'm$_l$'

➤ It helps to determine the spatial orientation of orbital with respect to standard set of ordination axis.
➤ For a subshell 2l+1 values of m$_l$.
➤ m$_l$ = -l, -(l-1), -(l-2), …0,1..(l-2), (l-1), l
➤ l = 0
  m$_l$ = 0   [2(0)+1]=1
➤ l = 1
  m$_l$ = -1, 0, +1   [2(1)+1] = 3

Values of l	0	1	2	3	4	5
Subshell notation	s	p	d	f	g	h
Number of orbitals	1	3	5	7	9	11

Electron spin 's'

➤ in 1925 George Uhlenbeck and Samuel Goudsmit propounded the presence of the fourth quantum number i.e., electron spin quantum number (m$_s$).
➤ An electron spins around its own axis, so there is a spin angular momentum of electron. It is a vector quantity. It has two orientations. These orientations are denoted by spin quantum number m$_l$. the values of m$_l$ are +1/2 and -1/2.
➤ There are two spin states of the electron spin up↑ and spin down↓.

Shapes of atomic orbitals

➤ The orbital wave function (Ψ) is a mathematical function of the coordinates of the electron.

➢ Different orbitals have the plots of corresponding wave functions as a function of (r) are different.
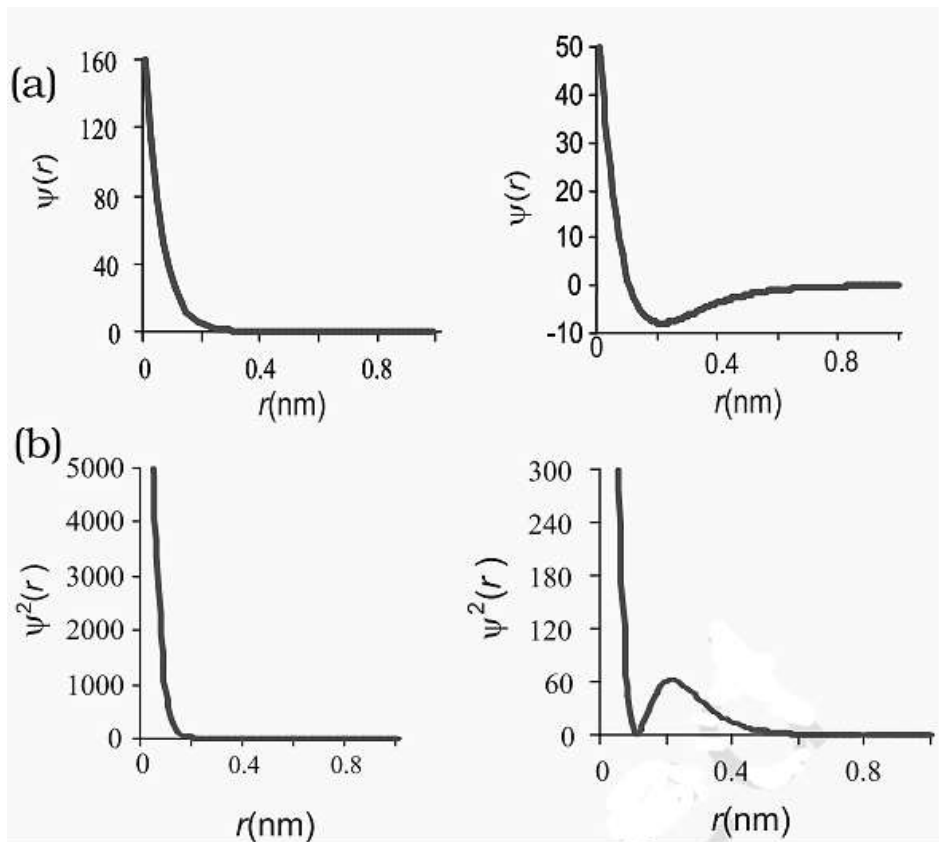
Here plots for 1s and 2s orbitals-

Figure: The plots of (a) the orbital wave function Ψ (r)
(b) The variation of probability density Ψ² (r) as a function of distance r of the electron from the nucleus for 1s and 2s orbitals.

➢ According to Max Born the square of wave function i.e., Ψ^2 is the probability density of electron at the point.
➢ For 1s orbital maximum probability of electron at the nucleus and it decreases sharply as we move away from the nucleus.
➢ For 2s maximum probability first decreases to zero and again starts increasing. After reaching a peak it decreases again to zero.
➢ The region at which probability of electron is zero is known as nodal surface or nodes.
➢ **ns**-orbital has **(n-1)** nodes.
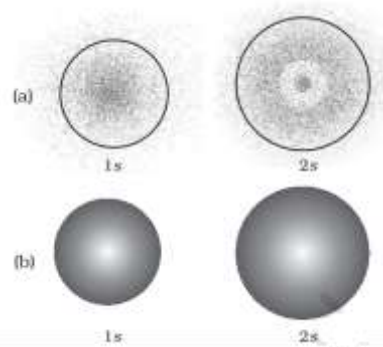
Boundary surface Diagrams

Figure: (a) Probability density plots of 1s and 2s atomic orbitals.
(b) Boundary surface diagram for 1s and 2s orbitals

➢ It is a representation of the shape of the orbitals.
➢ In this representation a boundary surface is drawn in space for an orbital on which the value of probability density I ΨI^2 is constant. In this diagram probability of finding the electron is very high.
➢ 1s and 2s orbitals are in spherical shape. The size of s orbital increases with increase in n. i.e. 4s > 3s > 2s > 1s.
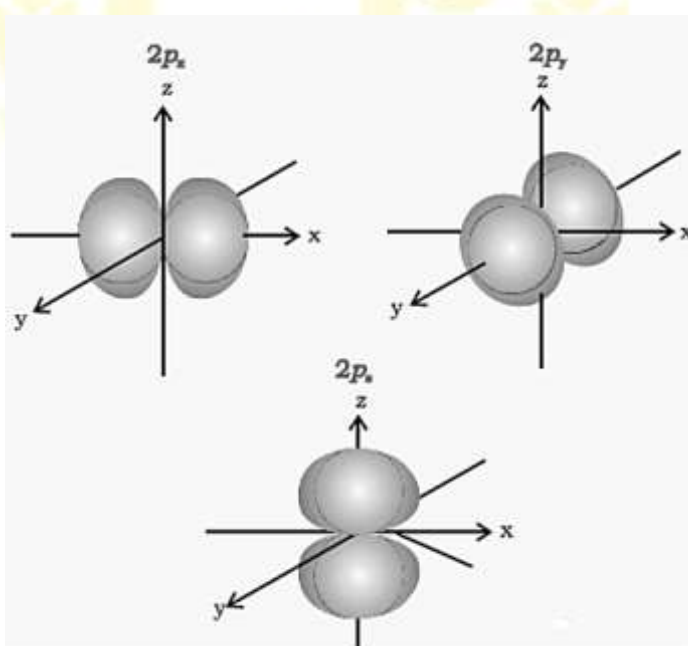

Figure: Boundary surface diagrams of the three **2p** orbitals.

➢ In case of 2p orbital the shape is not spherical, each p orbital consists of two lobes. There is a nucleus between them. The lobes are lie along x, y and z axis, there are three p orbitals. 2P$_X$, 2P$_Y$ and 2P$_Z$.
➢ The size shape and energy of three orbitals are identical.

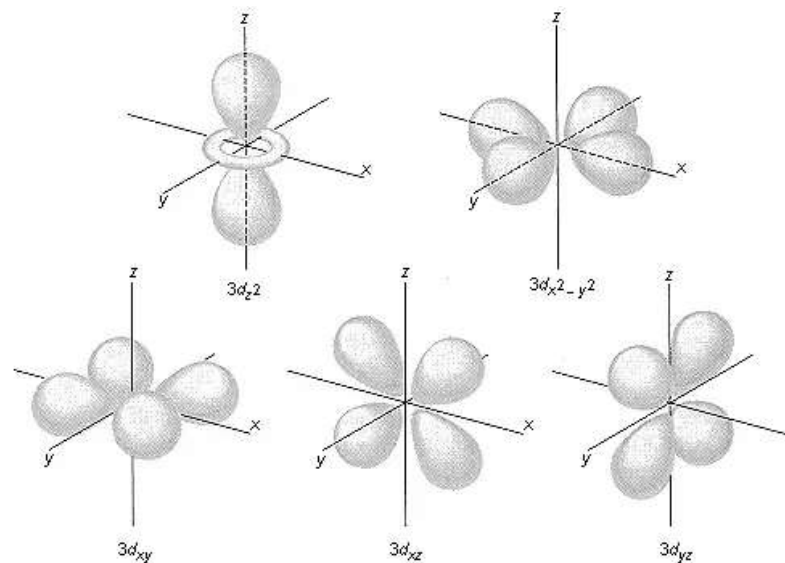➤ The order of the energy and size of various p-orbitals- 4p > 3p > 2p.

Figure: Boundary surface diagrams of the five 3d orbitals.

➤ For l =2, orbitals is d-orbital. n = 3, m_l = -2, -1, 0, +1, +2.
➤ The five d-orbitals are d_{xy}, d_{yz}, d_{xz}, $d_{x^2-y^2}$ and d_{z^2}.
   The first four orbitals are same in shape; the fifth d_{z^2} is different from others in shape.

❖ **The total number of nodes are given by (n-1), i.e. sum of 1 angular nodes and (n-l-1) radial nodes.**

Energies of orbitals

➤ Energies of the orbitals is calculated by principal quantum number.
➤ The energy of the orbitals in H-atom-
      1s < 2s = 2p < 3s = 3p = 3d < 4s = 4p = 4d = 4f <
➤ The orbitals having same energy are called degenerate.
➤ In H-atom 1s orbital is most stable and is called ground state. And electron in higher orbitals like 2s, 2p are called excited state.
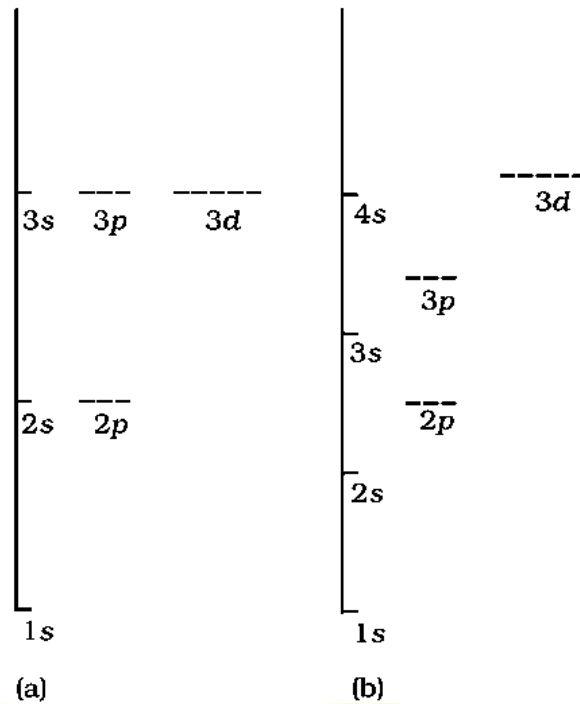
Figure: Energy level diagrams for the few electronic shells of (1) hydrogen and (b) multi electronic atoms.

➤ In case of multi electron atom, the energy of electron depends not only on principal quantum number but also on its azimuthal quantum number.
➤ Within a given principal quantum number, the order of energy of orbitals: s < p < d < f.

Effective nuclear charge (Z_{eff})

➤ The repulsive interactions of the electrons in the outer shell with the electron of inner shell are important.
➤ The attractive interactions of an electron increase with increase in the +ve charge (**Ze**) of nucleus.
➤ Due to presence of electrons in the inner shell, outer electron will not experience the full positive charge of nucleus. The shielding of outer shell electrons from the nucleus by the inner shell electrons is called shielding effect. The total positive charge experienced by outer shell electrons is known as **effective nuclear charge** (Z_{eff}).
➤ (n+l) rule- the lower the value of (n+l) for an orbital, the lower is its energy. If two orbitals have the same value of (n+l), the orbital with lower value of n will have the lower energy.

Table: Arrangement of Orbitals with Increasing Energy on the Basis of (n+l) Rule

Orbital	Value of n	Value of l	Value of (n+l)	
1s	1	0	1 + 0 = 1	
2s	2	0	2 + 0 = 2	
2p	2	1	2 + 1 = 3	2p(n=2) has lower energy than
3s	3	0	3 + 0 = 3	3s (n=3)
3p	3	1	3 + 1 =4	3p (n=3) has lower energy than
4s	4	0	4 + 0 = 4	4s (n= 4)
3d	3	2	3 + 2 = 5	3d (n=3) has lower energy than
4p	4	1	4 + 1 = 5	4p (n=4)

➢ The energies of the orbitals in the same subshell decrease with increase in atomic number.
➢ Example: 2s orbital

$$E_{2s} (H) > E_{2s} (Li) > E_{2s} (Na) > E_{2s} (K).$$

Filling of orbitals in Atom

The filing of electrons in the orbitals of atom is done according to the Aufbau principle which is based on Pauli's exclusion principle and Hund's rule of maximum multiplicity.

Aufbau Principle- In the ground state of the atoms, the orbitals are filled in order of their increasing energies.
In this order orbitals are filled:
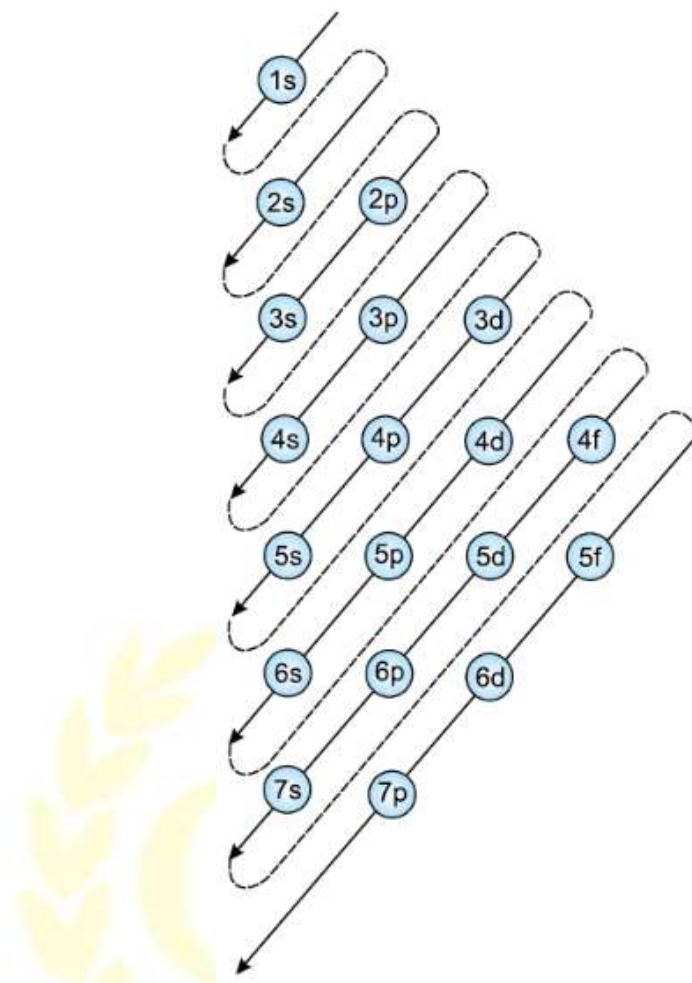
1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 4f, 5d, 6p, 7s…

Figure: Order of filling of orbitals

Pauli Exclusion Principle- No two electrons in an atom can have the same set of all four quantum numbers.

- ➢ **Only two electrons may exist in the same orbital and these electrons must have opposite spin.**
- ➢ The maximum number of electrons in the shell with principal quantum number n is equal to $2n^2$.

Hund's Rule of maximum multiplicity- Pairing of electrons in the orbitals belonging to the same subshell (p, d or f) does not take place until each orbital belonging to that subshell has got one electron each i.e., it singly occupied.

Electronic configuration- The distribution of electrons into orbitals of an atom is called its electronic configuration.

- ➢ It can be represented in two ways:
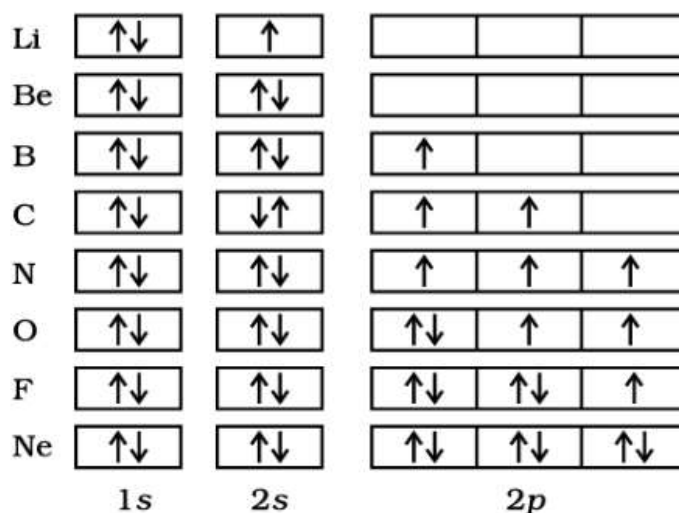 1. $s^a \, p^b \, d^c$

2. Orbital diagram

s p d

➤ The electronic configuration of H-atom is $1s^1$. In case of Helium second electron occupies 1s orbital.

H   ↑   He   ↑↓
     $1s$ $1s$

➤ The orbital picture of other atoms-

	1s	2s	2p		
Li	↑↓	↑			
Be	↑↓	↑↓			
B	↑↓	↑↓	↑		
C	↑↓	↓↑	↑	↑	
N	↑↓	↑↓	↑	↑	↑
O	↑↓	↑↓	↑↓	↑	↑
F	↑↓	↑↓	↑↓	↑↓	↑
Ne	↑↓	↑↓	↑↓	↑↓	↑↓

➤ In an atom the electron filled in the shell with highest principal quantum number are called valence electrons.

Stability of completely filled and Half-filled subshells

➤ Symmetrical distribution of electrons- The symmetry leads to stability. The completely filled and half-filled subshells have symmetrical distribution of electrons, thus are more stable.
➤ Exchange energy- When two or more electrons with the same spin are present in a degenerate orbital of subshell, stabilizing effect arises. The electrons tend to change their position and energy released. The energy released due to this exchange is known as exchange energy.
➤ The maximum exchanges take place when subshell is half or fully filled. Thus exchange energy is maximum so is the stability.
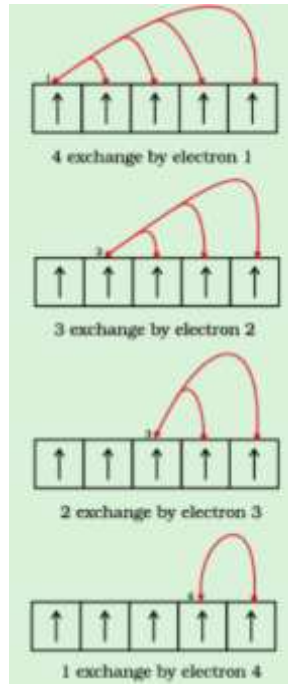
Figure: possible exchange for a d^5 configuration