

ATOMIC MODELS

1.1 **THE PARTICLES OF MATTER & ATOMIC MODELS**

In 1807, an English school teacher, John Dalton gave the first convincing argument about the existence of atoms. He relied upon a large number of experiments and measurements to measure the masses of elements that combined together, and assembled arguments that strangely indicated the existence of atoms. Dalton picturised atoms as featureless spheres like billiard balls. Today we know that atoms have an internal structure and are built from even smaller particles. It is this knowledge that provides an insight into the difference between elements.

MODEL 1-THE PLUM PUDDING MODEL 1.2.

The earliest experimental evidence of the existence of sub-atomic particles was the discovery in 1807 by the British physicist J.J. Thompson. He was investigating "cathode rays", He said that cathode rays are emitted when a high potential difference (a high voltage) is applied between two electrodes in an evacuated glass tube. Thompson showed that cathode rays are streams of negatively charged particles. They came from inside the atoms that made up the electrode called cathode. Thomson found that the charged particles were the same regardless of the metal he used for the cathode. These particles were named electrons and denoted e⁻. Later the mass of the electrons was experimentally calculated by Robert Milkan as 9.1×10^{-28} g. Goldstein discovered the existence of protons, (positively charged particles) and neutrons (neutral charged particles) was discovered by Chadwick.

| Table 1: | | | |
|---------------|--------------------|--------------------------|------------------|
| Properties of | Electrons, Protons | & Neutrons | |
| | | ELECTRON (e) | PROTON (p) |
| | AMU | 0.000549 | 1.00727 |
| | GRAMS | 9.11 × 10 ⁻²⁸ | 1.675 × 10 |
| Mass | | 1 | 12 - 12 - 12 - 1 |

RELATIVE

RELATIVE

ESU

COULOMBS

Based on these discoveries J.J. Thompson proposed the plum pudding model. This model proposed that atoms are blobs of a positively charged jellylike material, with electrons suspended in it like raisins in a pudding.

1837

-1

 $-1.602 imes 10^{-19}$

 -4.8×10^{-10}

1.3 **MODEL 2–THE RUTHERFORD MODEL**

CHARGE

In 1908, the plum pudding model was overthrown by a simple experiment. The New Zealander Ernest Rutherford asked two students to shoot α -particles (he knew that some element like Radon emit positively charged particles, which he called alpha (α) particles) toward a

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1

+1

 1.675×10^{-24}

 $+ 1.602 \times 10^{-19}$

 $+ 4.8 \times 10^{-10}$

NEUTRON (n)

 1.675×10^{-24}

1.00866

1

Zero

Zero

Zero

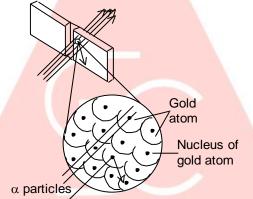


piece of gold foil only a few atoms thick. If atoms were indeed like blobs of positively charged jelly, then all the α -particles would leave similar paths as they move through the foil.

What his students observed astonished everyone around them. Although almost all the α -particles did pass through, about 1 in 20,000 was deflected through more than 90°, and a few α -particles bounced straight back in the direction from which they came. "It was almost incredible," said Rutherford, "as if you had fired a 15-inch shell at a piece of tissue paper and it can back and hit you".

The explanation was that atoms had to contain massive point like centers of positively charge surrounded by a large volume of mostly empty space. Rutherford called the point of positively charged region, the nucleus. He reasoned that closer the path of the α -particles to the nucleus of the atom, greater the deflection it experiences and the α -particles which directly hit on the molecules would rebound back.

The electrons are thinly distributed throughout the space around the nucleus. If the nucleus in a hydrogen atom were the size of a fly at the center of a cricket stadium, then the space occupied by the electron would be about the size of the entire cricket stadium.



In an atom the positive charge of the nucleus exactly cancels the negative charge of the surrounding electrons. So, for each electron outside the nucleus, there must be a matching positively charged particle inside the nucleus called the proton.

Since electrons would be attracted by the nucleus and would eventually fall into it, Rutherford assumed that electrons were not stationary and that they move in a circular path around the nucleus using the electrostatic force of attraction. This was analogues to the earth moving around the sun using the gravitational force of attraction.

1.4 MODEL 3: THE BOHR'S MODEL:

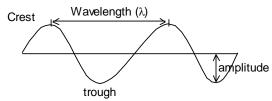
As a prelude to Bohr's theory, we should have an introduction to (i) nature of radiations (ii) atomic spectra and (iii) quantum theory.

(a) Radiations: Ordinary light, X–rays, γ –rays etc. are called electromagnetic radiations and they have wave characteristics. These radiations are called electromagnetic because when they pass through a point in space, they produce oscillating electric and magnetic fields at that point. In 1873 a Scottish physicist, James Clark Maxwell showed that a static charge or a charge with uniform velocity sets up electric and magnetic fields which gives rise to an energy density in space associated with the electric and magnetic fields, but the energy density remains constant. On the other hand, if we were to change the velocity of the charged particle, the energy density varies and then gives rise to electromagnetic waves.

There are three fundamental characteristics associated with wave motion. They are (i) wavelength (λ) (ii) frequency (v) and (iii) velocity (c).







(i) Wavelength: Consider a wave profile as shown in the above figure. The distance between two successive crests or troughs is known as wavelength (λ). It is measured in cm or Angstrom unit (Å)

 $1\text{\AA} = 10^{-8} \text{ cm} = 10^{-10} \text{ m}$

Some times nanometer, $(1nm = 10^{-9} m)$ is also used.

- (ii) Frequency: The number of waves that pass through a given point in one second is called its frequency (no. of waves per sec.). Frequency (v) is expressed in cycles per sec (cps) or Hertz (Hz).
- (iii)The distance traveled by a wave in one second is its velocity.

velocity =
$$\frac{\text{wavelength}}{T} = \frac{\text{Distance travelled in a wavelength}}{\text{Time taken to travel one wavelength}}$$

Time

 $\frac{\lambda \times 1s}{\nu \lambda} = \frac{1}{\nu}s.$

1s

If the frequency is v, it means that to travel v waves, it takes one second, then to travel one wavelength, the time taken is:

No. of wavelength

νλ

λ

 $\therefore T = \frac{1}{v}$

So, it follows that

$$\mathbf{c} = \frac{\lambda}{\mathsf{T}} = \lambda \times \mathbf{v}$$

The velocity 'c' of all types of electromagnetic radiations including light is established experimentally. It is a constant in vacuum, equal to 3×10^8 ms⁻¹. Since all electromagnetic radiations travel with the same velocity, they differ from are another in their wavelengths and consequently their frequencies.

| 9 | WAVE NATURE | λinÅ | | |
|---|---------------|--|--|--|
| | Radio waves | $3 \times 10^{7} - 3 \times 10^{14}$ | ner: | |
| | Infrared (IR) | <mark>7600</mark> −3 × 10 ⁷ | Wavelengt Frequency Energy inc | |
| | Visible | <mark>3800 -</mark> 7600 | | |
| | Ultraviolet | 1 - 3800 | ngth decreases ncy increases increases | |
| | (UV) | | l s ase | |
| | X–rays | $10^{-2} - 10$ | | |
| | γ–rays | 10 ⁻⁴ to 10 ⁻¹ | V | |

(b) Atomic Spectra: When white light is passed through a prism, it is separated into light of seven colours (VIBGYOR) or radiations of different wavelengths. The pattern obtained by splitting or sorting out of radiations into its component wavelengths is called a spectrum. The spectrum of white light when analyzed by spectrometer (an instrument that indicates the wavelengths/frequencies of individual components of a radiation) is a continuous spectrum,

suggesting that white light is made up of all possible wavelengths or frequencies of radiations.



If a gas is heated, it emits light. When this emitted light is analysed in a spectrometer, the spectra obtained consists of a series of well–defined sharp lines, each line corresponding to a definite wavelength or frequency. These line spectra are characteristic of atoms. In spectroscopic work, a term called wave number is often used. It is defined as the number of wavelengths per cm. It is given as:

Wave number =
$$\bar{v} = \frac{1}{\lambda}$$

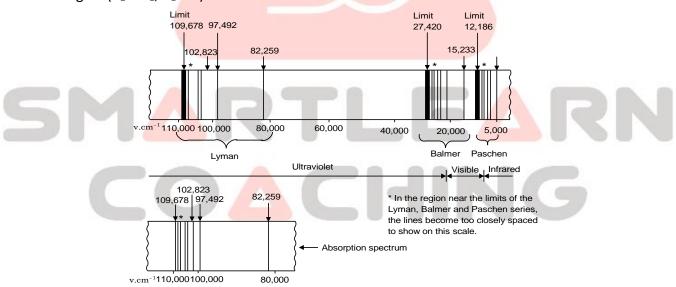
Since $c = v \times \lambda$
 $\bar{v} = \frac{v}{c}$

Spectral lines are associated with electronic transitions. Hydrogen atom contains only one electron and the spectrum is the simplest to analyze. The spectrum of atomic hydrogen consists of a number of discrete lines in the UV, visible and I.R regions. Each line corresponds to a particular frequency or wavelength. The space between two lines represents the frequency range in which no radiation is emitted by the hydrogen atom. Lines observed in the atomic spectra of hydrogen are grouped into the several series called spectral series. A group of lines appearing in the UV region is called the Lyman series; that in the visible region is called Balmer series; in the I. R region there are three – Paschen, Brackett and Pfund series.

The wave number of any line of hydrogen atom can be represented as a difference of two terms by the formula.

$$\bar{\nu} = \mathsf{R}\left[\frac{1}{n_1^2} - \frac{1}{n_2^2}\right]$$

where R is called Rydberg constant (as this was formulated by Rydberg) and n_1 and n_2 are integers ($n_2 > n_1$, $n_1 > 0$).



(c) Quantum Theory: According to this theory, a body cannot emit or absorb energy in the form of radiation of continuous energy; energy can be taken up or given out as whole number multiples of a definite amount known as a quantum. Light is imagined to consist of a stream of particles called photons. It E is the energy of a photon; its quantum for a particular radiation of frequency $v \sec^{-1}$ is given by quantum theory as

E = hv

where h is a universal constant known as planck's constant; h = 6.626×10^{-27} erg second or



 6.626×10^{-34} Joule second (Js).

$$\mathbf{E} = \mathbf{h}\mathbf{v} = \frac{\mathbf{h}\mathbf{c}}{\lambda} = \mathbf{h}\mathbf{c} \ \overline{\mathbf{v}}$$

According to quantum theory, a body can emit or absorbs either one quantum of energy (hv) or whole number multiples of this unit, 2hv, 3hv......nhv.

THE BOHR'S MODEL:

In 1913 more than a decade before quantum mechanics was established, the Danish physicist Niels Bohr proposed a model of the hydrogen atom based on a linear hybrid combination of classical and early quantum physics. Although a fully developed quantum model later replaced Bohr's model, it nevertheless served as a powerful stimulus of later developments.

Bohr retained the Rutherford model of a central positively charged nucleus containing practically all the mass surrounded by a planetary system of electrons whose number is equal to the protons. He made use of Planck's quantum theory and gave the following postulates.

In any atom electrons can rotate only in certain selected (or permissible orbits without radiating energy). Such orbits are known as stable or non-radiating orbits or stationary states. These orbits are circular with well–defined radii. These orbits are numbered 1, 2, 3,....(from the nucleus). Orbits are paths of revolution of electrons. A spherical surface around the

nucleus, which contains orbits of equal energy and radius, is called a shell. The shells are denoted as K, L, M, N,

Each stationary state or (orbit) corresponds to a certain energy level (i.e., as long as the electron is in the particular stationary state it has a definite amount of energy). The energy associated with an electron is least in the K shell and it increases as we pass to L, M, N, shells.

An electron can jump from one stationary state to another. For an electron to jump from an inner orbit of energy E₁ to an outer orbit of energy E₂, it should absorb the equivalent of a quantum of energy = $E_2 - E_1 = hv$, when v is the frequency of radiation absorbed. Similarly, when it jumps back from the outer to the inner orbit, it will emit an equal amount of energy in the form of radiation.

When an electron absorbs energy, it passes from an inner to an outer orbit; then the electron or the atom is said to be in an excited state. An exited electron has always to fall back to a lower orbit within a very short interval or time and as it does so, it releases the quantum of energy absorbed during excitation.

Unlike in Rutherford's model where an electron should constantly emit radiations (Maxwell's theory) since it gets accelerated while moving around the nucleus (with constant speed but varying direction), in Bohr's model all orbits are stable-the electron would not be radiating energy. This is because the angular momentum of an electron moving in a stable state is quantized. The angular momentum of an electron moving in a circular orbit is mvr, where m is the mass, v is the velocity and r is the radius of the orbit. According to Bohr, angular momentum is given by

mvr = n
$$\hbar$$

Where $\hbar = \frac{h}{2\pi}$
∴ mvr = $\frac{nh}{2\pi}$

where n is a positive integer 1, 2, 3, and is known as a Quantum number. The angular momentum can, therefore, be $\frac{h}{2\pi}, \frac{2h}{2\pi}, \frac{3h}{2\pi}, \dots, \frac{nh}{2\pi}$



This principle is known as quantization of angular momentum.

These postulates of Bohr lead us to:

- (i) Explain the permanence of the atom. Since electron neither loses energy nor gains energy as long as it is in its ground state, there is no question of the electron falling into the nucleus and so Bohr's theory accounts for the permanence of the atom.
- (ii) Using these postulates, Bohr calculated the energy of the electron in an orbit. In a hydrogen atom, the electron revolves around the nucleus in a circular orbit. For the system to be stable, the coulombic attraction between the electron and the nucleus must be the source of the necessary centripetal force for circular motion. i,e. coulombic force of attraction = centripetal force

$$\frac{\mathsf{K} \times (\mathsf{Z} \mathsf{e}) \times \mathsf{e}}{\mathsf{r}^2} = \frac{\mathsf{m} \mathsf{v}^2}{\mathsf{r}}$$

where,

- e = magnitude of charge on an electron (or a proton).
- Z = atomic number (e.g. for H–atom, Z = 1)
- r = radius of the orbit
- m = mass of the electron
- v = velocity of the electron
- K = coulomb's law constant = $\frac{1}{4\pi\epsilon}$

=
$$9 \times 10^9 \frac{\text{Nm}^2}{\text{C}^2}$$
 in SI system and = 1 in CGS units.

The above equation becomes,

The angular momentum of a body moving in a circular orbit is myr and as per the Bohr's theory,

$$mvr = \frac{nh}{2\pi}$$

 $v = \frac{nh}{2\pi mr}$

Substituting in equation (i)

$$\frac{\text{Kze}^2}{\text{r}} = \text{m}\left(\frac{\text{nh}}{2\pi\text{m}\text{r}}\right)^2$$

Solving for r, we get r^{2h^2}

 $r = \frac{n^2 h^2}{4\pi^2 K Z m e^2}$

This is the equation for the radius of the orbit of the electron. For hydrogen atom in the ground state, n = 1 and substituting the values of the constants in equation (iii), we get $r_1 = 0.529 \times 10^{-10}$ m = 0.529 Å

.....(iii)

.....(ii)

The radius of any other orbit in H atoms will be,

r_n = 0.529 n² Å

The total energy of the electron will be the sum of the potential and kinetic energies. Total energy, E = PE + KE

The potential energy is the energy due to coulombic attraction and so

6



$$PE = \frac{-KZe^2}{r}$$

Kinetic energy can be calculated from the velocity of the electron.

$$KE = \frac{1}{2}mv^{2}$$
Total energy, $E = \frac{-KZe^{2}}{r} + \frac{1}{2}mv^{2}$ (iv)
Substituting the value of mv^{2} from the equation (i),

$$E = \frac{-KZe^{2}}{r} + \frac{KZe^{2}}{2r}$$
(v)

$$E = \frac{-KZe^{2}}{2r}$$
(vi)
Substituting (iii) in (vi), we get

$$E = \frac{-2\pi^{2}K^{2}Z^{2}me^{4}}{n^{2}h^{2}}$$
(vii)

From equation (v), it can seen that the magnitude of the potential energy is twice that of kinetic energy.

The negative sign in the equation (vii) represents that the energy is released when the electron moves from ∞ to any orbit. Thus the energy of the electron in an atom is lower than the energy of a free electron (which is zero). As 'r' increases, the energy becomes less negative which means that energy increases.

We can calculate the energy of the ground state of the electron in hydrogen atom.

$$-2 \times (3.14)^2 \times (9 \times 10^9) \times 1^2 \times 9.1 \times 10^{-31} \times (1.6 \times 10^{-19})$$

$$1^2 \times 6.626 \times 10^{-34}$$

 $E = -2.179 \times 10^{-18}$ J per atom

E = - 13.6 eV per atom (∴ 1eV = 96.368 J/mole)

$$E = -1312 \text{ kJ/mole}$$

 Z^2

From this ground state energy of hydrogen atom, we can find the energy in any other atom.

$En = EH \times n^2$

E = -

n can have only positive integral values and so the total energy of the electron is quantized. Suppose an electron jumps from n_2 to n_1 level in a hydrogen atom ($n_2 > n_1$)

$$E_{n_1} = \frac{-2\pi^2 k^2 m e^4}{n_1^2 h^2} \text{ (in C.G.S. units);}$$
$$E_{n_2} = \frac{-2\pi^2 k^2 m e^4}{n_2^2 h^2}$$

The difference in energy emitted is

$$hv = \frac{-2\pi^{2}k^{2}me^{4}}{h^{2}} \left[\frac{1}{n_{2}^{2}} - \frac{1}{n_{1}^{2}} \right]$$
$$v = \frac{2\pi^{2}k^{2}me^{4}}{h^{3}} \left[\frac{1}{n_{1}^{2}} - \frac{1}{n_{2}^{2}} \right]$$



$$\bar{v} = \frac{v}{c} = \frac{2\pi^2 k^2 m e^4}{h^3 c} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$
$$\bar{v} = R \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$
$$R = \frac{2\pi^2 k^2 m e^4}{h^3 c} = 109737 \text{ cm}^{-1}$$

This empirical value of R deduced from Balmer, Lyman and other series agreed excellently with the experimental results. This is the triumph for Bohr's theory. From the foregoing discussion, we can understand that Bohr's theory has given an expression for the energy of the electron of hydrogen atom in the nth orbit as

$$E_{n} = \frac{-21.76 \times 10^{-19} \text{ J}}{n^{2}}$$
$$E_{n} = \frac{-13.6}{n^{2}} \text{ eV}$$

It can be assumed that the electron and the nucleus revolve around their common center of mass. Therefore, instead of the mass of the electron, the reduced mass of the system was introduced and the equation becomes

$$\bar{v} = \frac{2\pi^2 k^2 \mu e^4}{h^3 c} \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right]$$

where μ is the reduced mass = $\frac{Mm}{M+m}$, whose M is the mass of the nucleus and m is the

mass of the electron.

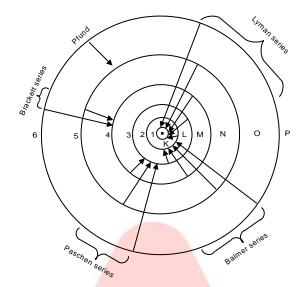
INTERPRETATION OF SPECTRAL SERIES

The hydrogen atom contains only one electron in first orbit (K shell). This is the normal orbit or ground state and represents the stationary state of the unexcited atom. Energy may be absorbed by this electron, which is then raised from its normal orbit to a higher energy level. In this new level, the electron possesses more energy and is less stable than before. It will, therefore, fall towards the nucleus until it reaches either the normal orbit or some intermediate level. In this process, energy is released as a photon of frequency E = hv.

Spectral lines are produced by radiation of photons and the position of the lines on the spectrum is determined by the frequency of photons emitted. Transition to innermost level (n = 1) from higher levels (n = 2, 3, 4 etc.) gives the first, second, third etc., line of the Lyman series. The general idea will be clear by a study of the following figure.



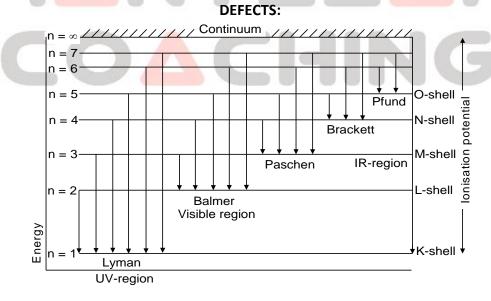




which shows the various energy changes leading to various lines in the spectrum. Thus Bohr's theory is able to account for the observed spectral lines and series in detail and with accuracy for the hydrogen atom.

Hydrogen atom contains only one electron but its spectrum consists of several lines. Why? A sample of hydrogen contains a very large number of atoms. When energy is supplied, the electrons present in different atoms may be excited to different energy level. These electrons when they fall back to various lower levels emit radiations of different frequencies. Each electronic transition produces a spectral line. Energy is absorbed by an atom when an electron moves from the inner energy level to the outer energy level. The amount of energy necessary to remove an electron from its lowest level (n = 1) to infinite distance resulting in the formation of a free ion is called the ionization potential. The ionization energy of hydrogen is 2.18×10^{-18} J or 13.595 electron – volts (1 eV = 1.602×10^{-19} J).

If an electron acquires more than enough energy to permit its removal from the atom, the extra energy is carried off by the free electron as kinetic energy. Because of the very small magnitude of the quanta of translational (i.e. kinetic) energy, this energy is essentially continuously variable. The spectrum beyond the series limit thus appears continuous; from the position of continuum, we may calculate the ionization potential.





Bohr's model was quite successful in accounting for the main features of the hydrogen spectrum and also the spectrum of He⁺ ion (which has only one electron). However, it failed to predict the energy states of more complicated atoms. It is applicable only for one electron system because it does not take into account inter–electronic repulsions. Even in the case of hydrogen atom, the spectral lines under high resolution showed fine structure (a number of closely packed lines), which is not explained by Bohr's theory. Bohr's theory could not explain why an electron does not get excited if it is provided energy that will allow it to exist in between two energy levels.

Smart Notes

2 DUAL NATURE OF MATTER

2.1 DE BROGLIE WAVELENGTH

Nature abounds in symmetries of all kinds. If light can be both wave and particle, is it possible that matter can also have these properties? Can the electron, traditionally regarded as a particle since its discovery in 1898, also have a wave aspect? More specifically, can we assign a wavelength and a frequency to a moving electron?

In 1924, the French physicist Prince Louis–Victure Broglie, motivated entirely by this symmetry argument, answered yes to these questions. He proposed that an electron of energy E and linear momentum 'p' could be defined by a matter wave whose wavelength and frequency are given by

$$\lambda = \frac{h}{p}$$
; $\nu = \frac{E}{h}$

in which h is the Planck's constant. The wavelength of a moving particle calculated above is called its de Broglie wavelength. De Broglie shared the 1929 Nobel prize for his discovery of the wave nature of matter.

Objects such as marbles or cricket balls do not seem at all wave like. We can understand why this is so because the Planck's constant h is so small and the momentum p of even slowly moving macroscopic particles is so large that the calculated de Broglie wavelengths of such objects are small indeed, being many orders of magnitude smaller than the size of an atomic nucleus.

2.2 HEISENBERG'S UNCERTAINITY PRINCIPLE

First derived by the German physicist Werner Heisenberg, it states that. It is not possible to measure, simultaneously, the position and the momentum of a particle with unlimited precision. If Δx is the uncertainty in position and Δp is uncertainty in momentum then,

$$\Delta x \times \Delta p \ge \frac{h}{4\pi}$$

The message of the uncertainty principle is that there is a limit to the extent to which the concept of "particle" can be extended from the Newtonian world to the quantum world. In the quantum world, it is wrong to imagine that a particle really has a definite position and momentum but, for some reason, we are not able to measure it. It is wrong to visualize a particle as a tiny mass point moving along a path, with its position and velocity well defined at every instant. The very notion of "trajectory" belongs to the Newtonian world, not to the quantum world.

3 THE QUANTUM MODEL

Improving on the Bohr Model, Sommerfield, in order to account for the additional lines present in the spectra of atoms, assumed that each principal energy level contains a number of sub–levels, each of which possesses slightly different energy. The subsidiary orbits are designated s, p, d and f (these letters standing for the nature – sharp, principal, diffuse and fundamental – of the lines



in the spectra). The number of sub–levels in any particular energy level is fixed. The various sub–levels in K, L, M, N etc., shells and the maximum number of electrons that may be present in each of them are given below:

| Shell | К | L | | М | | | Ν | | | |
|-----------------------|----|----|----|----|----|----|----|----|----|----|
| Sublevels | 1s | 2s | 2р | 3s | Зр | 3d | 4s | 4p | 4d | 4f |
| Max. no. of electrons | 2 | 2 | 6 | 2 | 6 | 10 | 2 | 6 | 10 | 14 |

The principle quantum number, n can have values 1, 2, 3,, and is indicative of the major energy levels of the electron in an atom in a gross way. This is similar to the quantum levels in Bohr's theory. The azimuthal quantum number, I, has values from 0 to (n-1), for each value of n. It is a

measure of the angular momentum of the electron, which is $\frac{h}{2\pi}\sqrt{l(l+1)}$ in magnitude. Values of I = 0, 1, 2, 3,, are designated by the letters s, p, d, f The magnetic quantum number m is indicative of the component of the angular momentum vector in any one chosen direction, usually the z-axis. The values of m are from -I to + I including zero for any value of I. An electron can spin either in clockwise direction or in anticlockwise direction. Spin quantum number, 's' can have two values + ½ and - ½ and also represented by arrow pointing in opposite direction i.e. 1 and 1 for any particular value of magnetic quantum number. Permissible values of the quantum numbers for various orbitals are mentioned in the table given on next page.

| Pr. Q. no. 'n' | Azimuthal Quantum no. 'l' | Magnetic Quantum no. 'm' | Spin Quantum no. 's' |
|-------------------------|--|--|----------------------------------|
| | l = 0; 1s su <mark>bshell</mark> | m = 0; s orbital | + ½ & -½ |
| 1 | | no. of orbitals in s-subshell = 1 | no. of e's in s–subshell = 2 |
| | Total no. of subshells in I shell = 1 | Total no. of orbitals in I shell = 1 | Total no. of e's in I shell = 2 |
| | | | |
| | l = 0; 2s subshell | m = 0; s orbital | + 1/2 & - 1/2 |
| | CO | no. of orbitals in s–subshell = 1 | no. of e's in s-subshell = 2 |
| | | m = -1; px / pz | + 1/2 & - 1/2 |
| 2 | l = 1; 2p subshell | m = 0; py | + ½ & – ½ |
| | | m = +1; pz / px | + 1/2 & - 1/2 |
| | | no. of orbitals in p-subshell = 3 | no. of e's in p–subshell = 6 |
| | Total no. of subshells in II shell= 2 | Total no. of orbitals in II shell = 4 | Total no. of e's in II shell = 8 |
| 3 | l = 0; 3s subshell | m = 0; s orbital | + 1/2 & - 1/2 |

Table: Permissible values of quantum numbers for atomic orbital





| | | no. of orbitals in s–subshell = 1 | no. of e's in s–subshell = 2 |
|---|--|---|---|
| | | m = –1; px / pz | + ½ & - ½ |
| | l = 1; 3p subshell | m = 0; py | + ½ & – ½ |
| | | m = +1; | + ½ & – ½ |
| | | no. of orbitals in p–subshell = 3 | no. of e's in p–subshell = 6 |
| | | m = -2 | + ½ & – ½ |
| | | m = -1 | + ½ & – ½ |
| | l = 2; 3d subshell | m = 0 | + ½ & – ½ |
| | | m = +1 | + ½ & – ½ |
| | | m = +2 | + ½ & – ½ |
| | | no. of orbital in d–subshell = 5 | no. of e's in d-subshell = 10 |
| | Total no. of subshells in III shell=3 | Total no. of orbitals in III shell = 9 | Total no. of e's in III shell = 18 |
| | | | |
| | l = 0; 4s subshell | m = 0; s orbital | + ½ & – ½ |
| | | no. of orbitals in s–subshell = 1 | no. of e's in s–subshell = 2 |
| | | m = -1; px / pz | + ½ & – ½ |
| | l = 1; 4p subs <mark>hell</mark> | m = 0; py | + ½ & – ½ |
| | | m = +1; pz / px | + ½ & – ½ |
| | | no. of orbital in p-subshell = 3 | no. of e's in p–subshell = 6 |
| | | m = -2 | $+\frac{1}{2} \& -\frac{1}{2}$ |
| | | m = -1 | + ½ & -½ |
| | l = 2; 4 <mark>d subshe</mark> ll | m = 0 | + ½ & - ½ |
| 4 | | m = +1 | + 1/2 & - 1/2 |
| | | m = +2 | + 1/2 & - 1/2 |
| | | no. of orbitals in d–subshell = | no. of e's in d-subshell = |
| | | 5 | |
| | | m = -3 | $+\frac{1}{2} & -\frac{1}{2}$ |
| | | m = -2 | $+\frac{1}{2} & -\frac{1}{2}$ |
| | l = 3; 4f subshell | m = -1 | $+\frac{1}{2} & -\frac{1}{2}$ |
| | | m = 0 | $+ \frac{1}{2} \& - \frac{1}{2}$ + $\frac{1}{2} \& - \frac{1}{2}$ |
| | | m = +1 m = +2 | $+ \frac{1}{2} & - \frac{1}{2} \\ + \frac{1}{2} & - \frac{1}{2} \\ \end{array}$ |
| | | m = +3 | $+ \frac{1}{2} \otimes - \frac{1}{2} + \frac{1}{2} \otimes - \frac{1}{2}$ |
| | | no. of orbitals in f–subshell = | |
| | | 7 | no. of e's in f–subshell = 14 |



| Total no. of subshells in | Total no. of orbitals in | Total no. of e's in | | |
|---------------------------|--------------------------|-------------------------|--|--|
| IV shell = 4 | IV shell = 1+3+5+7=16 | IV shell = 2+6+10+14=32 | | |

From the above table we have derived the formula, to know the number of subshells/orbitals/electrons in a shell/subshell.

- 1. Total number of subshells in a particular shell = 'n'
- 2. Total number of orbitals in a particular subshell = (2l + 1)
- 3. Total number of orbitals in a particular shell = n2
- 4. Total number of electrons in a particular subshell = 2 (2l + 1)
- 5. Total number of electrons in a particular shell = 2 n2

3.1 NODE AND NODAL PLANE

Node is defined as a region where the probability of finding an electron is zero. Nodes can be of two types.

- (a) Radial node or spherical node
- (b) Angular node or planar node
- Radial node or spherical node

They correspond to 'n' values i.e. as the distance between nucleus & outermost shell increase, the number of radial nodes increases. For example 1s, 2p, 3d & 4f orbital are closest to nucleus (:: 1p, 1d, 2d, 1f, 2f, 3f doesnot exist) so there is no radial node but for higher values of 'n', radial nodes can be defined.

Angular node or planar node

They correspond to 'l' value. It depends upon the shape of orbitals. For example,

's' orbitals are spherically symmetrical in all three planes; so in s-orbital, no angular node exists. p-orbitals are not spherically symmetrical but the electron density is concentrated in one plane either x, y or z. So they have one angular node. Similarly electron density in d-orbital is concentrated in two planes i.e. xy, yz, zx etc. So the d-orbitals have two angular nodes.

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

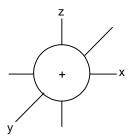
Total no. o<mark>f an</mark>gular nodes = l

Total no. of nodes = (n - l - 1) + l = n - 1

3.2 Shapes of atomic orbitals

(i) s-orbital: An electron is considered to be smeared out in the form of a cloud. The shape of the cloud is the shape of the orbital. The cloud is not uniform but denser in the region where the probability of finding the electron in maximum.

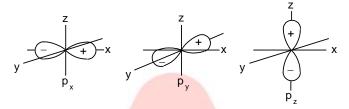
The orbital with the lowest energy is the 1s orbital. It is a sphere with its center at the nucleus of the atom. The s—orbital is said to spherically symmetrical about the nucleus, so that the electronic charge is not concentrated in any particular direction. 2s orbital is also spherically symmetrical about the nucleus, but it is larger than (i.e., away from) the 1s orbital.



Shape of s-orbital



(ii) p-orbitals: There are three p-orbitals: px, py and pz. They are dumb-bell shaped, the two levels being separated by a nodal plane, i.e., a plane where there is no likely hood of finding the electron. The p-orbitals have a marked directional character, depending on whether px, py and pz orbital is being considered. The p-orbitals consist of two lobes with the atomic nucleus lying between them. The axis of each p-orbital is perpendicular to the other two. The px, py and pz orbitals are equivalent except for their directional property. They have the same energy. Orbitals having the same energy are said to be degenerate.



Shapes of p-orbital

(iii) d–orbitals: There are five d–orbitals. The shapes of four d–orbitals resemble four leaf cloves. The fifth d–orbital loops differently. The shapes of these orbitals are given below.

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MIND MAP

