Structure of Atom

1. **Sub-atomic Particles**
2. **Atomic Models and Their Limitations**
3. **Quantum Mechanical Model of Atom**

Atoms are the building blocks of elements. They are the smallest parts of an element that chemically react. The first atomic theory, proposed by John Dalton in 1808, regarded atom as the ultimate indivisible particle of matter. Towards the end of the nineteenth century it was proved experimentally that atoms are divisible and consist of three fundamental particles: electrons, protons and neutrons.

Michael Faraday discovered electrons using cathode ray discharge tube experiment. Modified cathode ray tube experiment was carried out which led to the discovery of protons.

Neutrons were discovered by James Chadwick by bombarding a thin sheet of beryllium by α- particles. They are electrically neutral particles having a mass slightly greater than that of the protons.

The discovery of sub-atomic particles led to the proposal of various atomic models to explain the structure of atom.**Thomson** in 1898 proposed that an atom consists of uniform sphere of positive electricity with electrons embedded into it. This model in which mass of the atom is considered to be evenly spread over the atom was proved wrong by **Rutherford's** famous alpha-particle scattering experiment in 1909. Rutherford concluded that atom is made of a tiny positively charged **nucleus**, at its centre with electrons revolving around it in circular orbits.

Rutherford model, which resembles the solar system, was no doubt an improvement over **Thomson model** but it could not account for the stability of the atom i.e., why the electron does not fall into the nucleus. Further, it was also silent about the electronic structure of atoms i.e., about the distribution and relative energies of electrons around the nucleus.

Planck's quantum theory: Max Planck proposed that atoms and molecules could emit or absorb energy only in discrete quantities and not in a continuous manner. Planck gave the name quantum, meaning 'fixed amount' to the smallest quantity of energy that can be emitted or absorbed in the form of electromagnetic radiation.

$$E \alpha \mathrm{V}$$

$$E = hv$$

$$= \frac{hc}{\lambda}$$

Where:
E is the energy of a single quantum
h is Planck's constant
λ is the frequency of the radiation
h= 6.626 X 10^{-34} Js

Photoelectric effect: The phenomenon of ejection of electrons from the surface of metal when light of suitable frequency strikes it is called photoelectric effect. The ejected electrons are called photoelectrons.

The difficulties of the Rutherford model were overcome by **Niels Bohr** in 1913 in his model of the hydrogen atom. Bohr postulated that electron moves around the nucleus in circular orbits. Only certain orbits can exist and each orbit corresponds to a specific energy. Bohr calculated the energy of electron in various orbits and for each orbit predicted the distance between the electron and nucleus.

Bohr model, though offering a satisfactory model for explaining the spectra of the hydrogen atom, could not explain the spectra of multi-electron atoms.

The reason for this was soon discovered. In Bohr model, an electron is regarded as a charged particle moving in a well defined circular orbit about the nucleus. The wave character of the electron is ignored in Bohr's theory.

Dual behavior of matter: de Broglie proposed that matter exhibits dual behavior. This means matter shows both particle and wave nature. de Broglie's relation:

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

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

Where:

λ- Wavelength

h – Planck's constant

p - Momentum

v - Velocity

An orbit is a clearly defined path and this path can completely be defined only if both the exact position and the exact velocity of the electron at the same time are known. This is not possible according to the **Heisenberg's un**certainty principle which states that it is impossible to determine simultaneously, the exact position and exact momentum (or velocity) of an electron. Bohr model of the hydrogen atom, therefore, not only ignores the dual behaviour of electron but also contradicts Heisenberg uncertainty principle.

Erwin Schrödinger, in 1926, proposed an equation called Schrödinger equation to describe the electron distributions in space and the allowed energy levels in atoms. This equation incorporates de Broglie's concept of wave-particle duality and is consistent with Heisenbergun uncertainty principle. When Schrödinger equation is solved for the electron in a hydrogen atom, the solution gives the possible energy states the electron can occupy [and the corresponding wave function(s) (ψ) (which in fact are the mathematical functions) of the electron associated with each energy state].

These quantized energy states and corresponding wave functions which are characterized by a set of three quantum numbers (principal quantum number n, azimuthal quantum number l and magnetic quantum number ml) arise as a natural consequence in the solution of the Schrödinger equation. The restrictions on the values of these three quantum numbers also come naturally from this solution. The quantum mechanical model of the hydrogen atom successfully predicts all aspects of the hydrogen atom spectrum including some phenomena that could not be explained by the Bohr model.

According to the **quantum mechanical model** of the atom, the electron distribution of an atom containing a number of electrons is divided into **shells.** The shells, in turn, are thought to consist of one or more **sub-shells** and sub-shells are assumed to be composed of one or more orbitals, which the electrons occupy. While for hydrogen and hydrogen like systems(such as $\left(He^{+},\ Li^{2+}etc.\right)$ all the orbitals within a given shell have same energy, the energy of the orbitals in a multi-electron atom depends upon the values of n and l: The lower the value of $(n + l)$ for an orbital, the lower is its energy. If two orbitals have the same $(n + l)$ value, the orbital with lower value of n has the lower energy.

In an atom many such orbitals are possible and electrons are filled in those orbitals in order of increasing energy in accordance with **Pauli exclusion principle** (no two electrons in an atom can have the same set of four quantum numbers) and **Hund's rule of maximum multiplicity** (pairing of electrons in the orbitals belonging to the same sub shell does not take place until each orbital belonging to that sub shell has got one electron each, i.e., is singly occupied). This forms the basis of the electronic structure of atoms.

Electronic configuration of atoms: The electronic configuration of different atoms can be represented in two ways.

a. $s^a\ p^b\ d^c$..... notation: In the first notation, the sub-shell is represented by the respective letter symbol and the number of electrons present in the sub-shell is depicted in the form of super script, like a, b, c, ... etc. The similar sub-shell for different shells is differentiated by writing the principal quantum number before the respective sub-shell.

b. Orbital diagram: In the second notation, each orbital of the sub-shell is represented by a box and the electron is represented by an arrow ($\uparrow$) a positive spin or an arrow ({tex}\downarrow{/tex}) a negative spin.