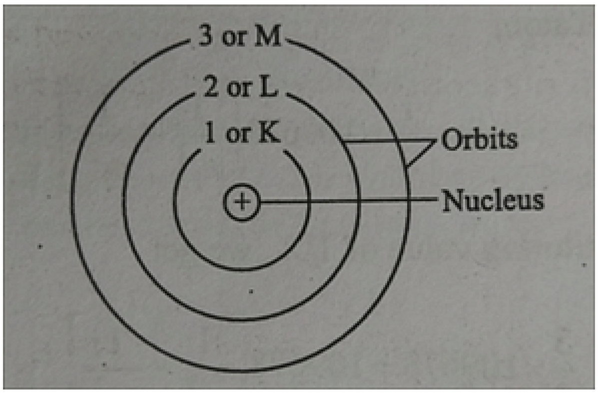
Bohr's Atomic Model

1. The **electrons** move around the nucleus in certain permitted circular paths known as orbits.
2. Each orbit is associated with a definite amount of energy and therefore, these are known as **energy levels** or energy states. The energy levels are numbered as 1,2,3,4……. etc. or designated as K, L, M, N……. etc. shells. The energy level closest to the nucleus is numbered 1 or designated as K shell.



3. While moving in a particular energy level or energy state an electron neither loses nor gains energy. The energy of an electron in a particular energy state always remains fixed or stationary. This state is called normal or ground state.
4. An **electron emits** or absorbs energy when it jumps from one orbit or energy level to another. When it jumps from a higher energy level to a lower energy level it emits energy while it absorbs energy when it jumps from a lower energy level to a higher energy level.
5. The energy absorbed or emitted is equal to the difference between the energies of the two energy levels (E_1, E_2) and is determined by **Planck's equation**.

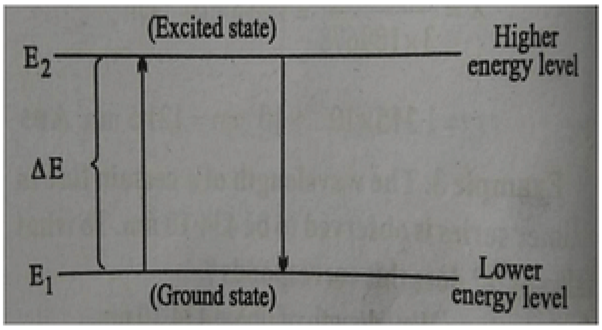
   $\Delta E = E_2 - E_1 = hv$

   Where,

   E_2 and E_1 are the energies of electrons in the higher and lower energy levels respectively

   ΔE is the difference in energies of two levels.

   V is the frequency of **electromagnetic radiation** emitted or absorbed



Transition of electrons from lower to higher and higher to lower energy levels

6. Like energy, the **angular momentum** of an electron in an atom can have certain definite or discrete values and not any values of its own. The only possible values of angular momentum are given by the expression,

   mvr =nh/2π

   i.e., h/2π will be an integral multiple of the angular momentum of the electron. Here, m= mass of electron, ν= tangential velocity of revolving electron, r= radius of the orbit, h= Planck's constant and n= integer 1,2,3………

Advantages of Bohr's theory

(i)Bohr's theory satisfactorily explains the spectra of species having one electron, *viz.* hydrogen atom, He^{+}, Li^{2+} etc.

(ii) Calculation of radius of Bohr's orbit: According to Bohr, radius of orbit in which electron moves is

$$\boxed{r=\left[\frac{h^2}{4\pi^2me^2k}\right].\frac{n^2}{Z}}$$

Where, n =Orbit number, m =Mass number $\left[9.1\times10^{-31}kg\right]$, e =Charge on the electron $\left[1.6\times10^{-19}\right]$

Z =Atomic number of element, k = Coulombic constant $\left[9\times10^{9}\ Nm^2c^{-2}\right]$

After putting the values of m,e,k,h, we get.

$$\boxed{r_n=\frac{n^2}{Z}\times0.529\ \mathring{A}\ or\ r_n=\frac{n^2}{Z}\times0.529\ nm}$$

(iii) Calculation of energy of electron in Bohr's orbit

$$E=-13.6\times\frac{Z^2}{n^2}$$

(iv) To evaluate wavelength of various H-lines Ritz introduced the following expression,

$$\upsilon=\frac{1}{\lambda}=\frac{\upsilon}{c}=R\left[1/n_1^2-1/n_2^2\right]$$

R = Rydberg's constant.

Limitations:

(i) Bohr theory was very successful in predicting and accounting the energies of line spectra of hydrogen i.e. one electron system. It could not explain the line spectra of atoms containing more than one electron.

(ii) This theory could not explain the presence of multiple spectral lines.

(iii) This theory could not explain the splitting of spectral lines in magnetic field (Zeeman Effect) and in electric field (Stark effect). The intensity of these spectral lines was also not explained by the Bohr atomic model.

(iv) This theory was unable to explain of dual nature of matter as explained on the basis of De broglies concept.

(v) This theory could not explain Heisenberg uncertainty principle.

(vi) No conclusion was given for the concept of quantisation of energy.

de-Broglie hypothesis

In 1924 Louis de-Broglie extended the wave particle dualism of light to material particles.

“If a wave can act as a wave some time and as a particle at other time then the particles such as electron, neutron should also act as waves some times”. This is known as de-Broglie hypothesis.

De-Broglie proposed that the energy of the particle motion must be carried by some sort of waves associated with the particle, just like waves associated with photon carry energy in amount of hν. The wave associated with moving particles are called as matter waves or de-Broglie waves.

Derivation of de-Broglie equation

Very low-mass particles moving at speeds less than that of light behave like particles and waves. De Broglie derived an expression relating the mass of such smaller particles and their wavelength.

From Planck’s theory of radiation the energy of a photon is given by

$$E = h\nu = \mathrm{h}\,c/\lambda \qquad \ldots(4)$$

From Einstein mass energy relation

$$E = mc^2 \qquad \ldots(5)$$

From equation (4) and (5) , we get

$$h\frac{c}{\lambda} = mc^2 \; or \; \lambda = \frac{hc}{mc^2}$$

$$\lambda = \frac{h}{mc} = \frac{h}{p} \qquad \ldots(6)$$

where mc = p (momentum associated with photon)

This equation relating the momentum of a particle with its wavelength is the de Broglie equation, and the wavelength calculated using this relation is the de Broglie wavelength.

de Broglie wavelength in terms of K.E.

The kinetic energy of a moving particle

$$E = \frac{1}{2}mv^2 = \frac{1}{2m}m^2v^2 = \frac{p^2}{2m}$$

$$p = \sqrt{2mE}$$

Substituting the value of P in equation (6) we get

$$\lambda = \frac{h}{\sqrt{2mE}} \qquad \ldots(7)$$

Davisson and Germer experiment in 1927 gave convincing proof of the wave nature of matter.

Heisenberg's Uncertainty Principle

As a consequence of dual nature of matter, Werner Heisenberg, in 1927 stated uncertainty principle.

"It is impossible to determine simultaneously, the exact position and exact momentum (or velocity) of an electron."

or

"It is impossible to measure simultaneously the position and momentum of a small microscopic moving particle with absolute accuracy or certainty".

Mathematically, it can be given as in equation

$\Delta p . \Delta x \geq h/4\pi$.

Where h= Planck's constant

Δp = Uncertainty in momentum.

Δx = Uncertainty in position.

We know that $p = mv$

$\Delta mv. \Delta x \geq h/4\pi$.

So $\Delta v. \Delta x \geq h/4\pi m$.

If the position of the electron is known with high degree of accuracy (**Δ**x is small), then the velocity of the electron will be uncertain (**Δ**v is large). Similarly, If the velocity of the electron is known with high degree of accuracy (**Δ**v is small), then the position of the electron will be uncertain (**Δ**x is large).

It is also applicable to the relation between energy and time.

$\Delta E . \Delta t \geq h/4\pi$

where ΔE is the uncertainty in energy, Δt is the uncertainty in time

Importance of Heisenberg uncertainty principle

- It rules out the existence of definite paths of electrons and other subatomic particles
- It helps in the determination of the probability of the position of any particle at a particular time.
- Heisenberg's principle has its importance only for microscopic particles and not for macroscopic particles.

Aufbau Principle

The Aufbau Principle states that electrons fill atomic orbitals in order of increasing energy levels, meaning lower energy orbitals are filled first before higher energy orbitals.

The word 'Aufbau' in German means 'Building up'.

Rules of the Aufbau Principle:

1. **Order of Orbital Filling:**
   Electrons occupy orbitals in the sequence of increasing energy levels. The order follows:
   1s → 2s → 2p → 3s → 3p → 4s → 3d → 4p → 5s → 4d → 5p → 6s → 4f → 5d → 6p → 7s → 5f → 6d → 7p

2. **n + l Rule:**

   The energy of an orbital is determined by the sum of its principal quantum number (**n**) and azimuthal quantum number (**l**).

   Orbitals with lower **(n + l)** values are filled first. If two orbitals have the same **(n + l)** value, the one with a lower **n** is filled first.

Examples:

3d (n = 3, l = 2) → (3+2 = 5)

4s (n = 4, l = 0) → (4+0 = 4). Since 4s has a lower (n+l) value, it is filled before 3d.

Some elements do not strictly follow the Aufbau order due to electron repulsions and stability factors.

Chromium (Cr) – [Ar] $3d^5$ $4s^1$ instead of [Ar] $3d^4$ $4s^2$

Copper (Cu) – [Ar] $3d^{10}$ $4s^1$ instead of [Ar] $3d^9$ $4s^2$

These exceptions occur because half-filled (d^5) and fully filled (d^{10}) orbitals provide extra stability.

Hund's rule

Hund's Rule is a fundamental principle in quantum mechanics that governs the arrangement of electrons in atomic orbitals. It helps predict the most stable electronic configuration of atoms.

Statement:

"Electrons occupy orbitals with the same energy singly before pairing up, and all singly occupied orbitals will have the same spin."

Key Points of Hund's Rule:

1. Maximum Multiplicity Principle: Electrons fill orbitals in such a way that the total spin is maximized, leading to greater stability.
2. Degenerate Orbitals: These are orbitals of the same energy level, such as the three *p* orbitals (px, py, pz) or five *d* orbitals.
3. Parallel Spin Preference: Electrons prefer to occupy empty orbitals first, and all unpaired electrons have the same spin (either all ↑ or all ↓).

Ex: 1. Nitrogen (N) – Atomic Number 7

Electronic Configuration: $1s^2 2s^2 2p^3$

The three electrons in the 2p orbitals are arranged as:
↑ (px) ↑ (py) ↑ (pz)

All three electrons occupy separate orbitals with parallel spins, maximizing stability.

1. Oxygen (O) – Atomic Number 8

Electronic Configuration: $1s^2 2s^2 2p^4$

The electrons in the 2p orbitals are arranged as:
↑↓ (px) ↑ (py) ↑ (pz)

Here, one electron pairs up in px after the other two p orbitals are singly occupied.

Applications of Hund's Rule

1. Used to determine the arrangement of electrons in atoms and ions.
2. Atoms with unpaired electrons (e.g., O, Fe) exhibit paramagnetism.
3. Helps explain hybridization and the behavior of transition metals.

Pauli Exclusion Principle

The Pauli Exclusion Principle is a fundamental concept in quantum mechanics proposed by Wolfgang Pauli in 1925. It explains how electrons are arranged in atoms and ensures that no two electrons in an atom have identical quantum states.

Statement

"No two electrons in an atom can have the same set of four quantum numbers (n, l, m_l, m_s)."

Ex:1. Helium (He) – Atomic Number 2

Electronic Configuration: $1s^2$

The two electrons in 1s must have opposite spins

Electron 1: ($n=1, l=0, m_l=0, m_s=+\frac{1}{2}$)

Electron 2: ($n=1, l=0, m_l=0, m_s=-\frac{1}{2}$)

2. Carbon (C) – Atomic Number 6

Electronic Configuration: $1s^2 2s^2 2p^2$

In 2p orbitals, the electrons must have unique quantum numbers.

Importance of Pauli Exclusion Principle

1. Electron Configuration: Defines how electrons are distributed in orbitals.
2. Structure of Periodic Table: Determines how elements are arranged.
3. Chemical Bonding: Explains valency and why certain elements form specific bonds.
4. Stability of Matter: Prevents all electrons from occupying the same state, leading to distinct atomic structures.