Atomic structure

Model Before Bohr's model

Discoveries Before Bohr's model

Bohr's Model of atom

Discoveries Before Quantum mechanical model of atom

Quantum mechanical model of atom

Models Before Bohr's model of atom

Dalton's Atomic Theory

- Matter → made up of → Atoms
- Atoms → indivisible
- Atoms → same element → Identical (Shape, Size, properties)
- Atoms → Different element → Different (Shape, Size, properties)
- chemical reaction → Rearrangement of atoms.

Explan ⇒ law of Conservation of mass, Definite proportion & multiple proportion.

Thomson's Model of atom

Cathode rays

- starts from cathode.
- travels in straight line [In absence of Electrical & Magnetic field]
- Invisible but observed [with fluroscent & phosphorescent material]
- Donot depend upon → cathode material, gas present in cathode tube.

$$\boxed{\frac{e}{m} = 1.75 \times 10^{11}\ C\ kg^{-1}}$$

★ Thomson plum-pudding model explain overall neutrality of atom but not consistent with the later experiments.

Rutherford's model of atom

Gold foil → Heavy & stable nucleus

- Atoms → nucleus → Centre → small in size & Heavy
- Nucleus → All +ive charge & mass
- Nucleus → protons + neutrons ← neutrons
- $\bar{e}$ revolve → around nuclus.

Application of Rutherford Model

- Diameter of nucleus → 10^{-13} cm
- Diameter of atom → 10^{-8} cm
- Volume of atom = 10^{15} × Volume of nucleus
- Radius of nucleus = $R_0 A^{1/3}$ [$R_0 = 1.33 \times 10^{-13}$ cm, A ⇒ Mass number]
- Density of nucleus = $\frac{3}{4\pi R_0^3}$ ⇒ Constant for all atoms.
- $\frac{u_1}{u_2} = \left[\frac{\sin\frac{\theta_2}{2}}{\sin\frac{\theta_1}{2}}\right]^4$ — θ → Angle of α-particle deviation; u → no. of α-particles.

Couldnot explan stability of atom.

$_Z X^A$

no. of protons = Z

no. of electrons = Z [Neutral atom]

no. of neutrons = A − Z

$_Z A^{n+}$ → $\bar{e}$ = Z − n

$_Z A^{n-}$ → $\bar{e}$ = Z + n

Isotopes: Same atoms but different mass number

Isobar: Different atoms but same mass number

Isotones: Same number of neutrons

Isoelectronics: Same number of $\bar{e}$'s.

Discoveries Before Bohr's model of atom

- Electromagnetic waves
- Black-Body Radiation
- Planck's Quantum Theory
- photoelectric effect
- Spectrum

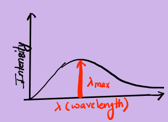
E.M Waves

- Form of energy
- travels → speed of light
- Require → No medium
- Electric field & Magnetic field ⊥ to each other.
- $\boxed{\bar{\nu} = \frac{1}{\lambda}}$ $\boxed{T = \frac{1}{\nu}}$ $\boxed{\nu\lambda = c}$

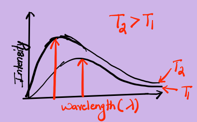
R M I L U X G

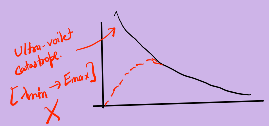
→ $\nu\uparrow$ $\lambda\downarrow$ $E\uparrow$

Black-Body Radiation

- Perfect absorber & perfect emitter.
- Radiation depend on temp. not material.
- 

- Wein's Displacement law $\left[\lambda_{max} = \frac{1}{T}\right]$





Planck's Quantum Theory

- Energy absorbed or emitted in packets ← quantum.
- Smallest packet of energy is called quanta & light → photon
- $\boxed{E = h\nu}$ ← energy of quanta
- $\boxed{E_{total} = nh\nu}$ ← total energy released or absorbed.

photoelectric effect

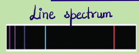
- Ejection of $\bar{e}$ → metal surface → light → suitable energy → falls on it.
- Work function → Minimum energy required to show photoelectric effect.
- Thresold frequency (ν_0) → minimum frequency to show photoelectric effect.
- *No. of ejected $\bar{e}$'s ∝ Intensity of light. (Indepent on frequency)
- *K.E/speed of ejected $\bar{e}$'s ∝ frequency of light (Independ on Intensity)
- $$\boxed{h\nu = h\nu_0 + \frac{1}{2}mv^2}$$

Spectrum

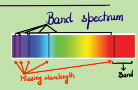
Spectrum

Continous spectrum	Discontinous spectrum
Unbroken sequence of wavelength	Broken sequence of wavelength.
e.g. rainbow	discontinous spectrum भी दो तरह के होते हैं।

Line spectrum



Band spectrum



spectrum

Emisson

- Atom/molecule
↓
absorb energy
↓
then release as light

Absorption

- Light pass through
↓
Substance.
↓
Atoms & molecule absorb

Bohr's model of atom

Postulates

- $\bar{e}$ allowed in certain orbits ← stationary orbits.
- Donot radiate energy in stationary orbits.
- Emission / absorption of light → orbit change
- $\frac{mv^2}{r} = \frac{KZe^2}{r^2}$
- $mvr = \frac{nh}{2\pi}$

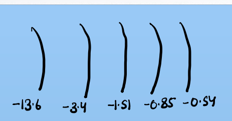
Derivation

ना हो प्यारे मुर्गी के अण्डे ज्यादा!

- $r = \frac{a_0 n^2}{Z}$ $a_0 = 0.529\ \text{Å}$ $\boxed{r = \frac{n^2h^2}{4\pi^2 mke^2 Z}}$
- $V = 2.18 \times 10^6 \frac{Z}{n}\ m/s$
- $P.E = -\frac{KZe^2}{r}$ $K.E = \frac{KZe^2}{2r}$ $T.E = -\frac{KZe^2}{2r}$

  $\boxed{T.E = -K.E}$ $\boxed{P.E = 2T.E}$

- $T.E = -13.6\frac{Z^2}{n^2}$ ev/atom , $21.7 \times 10^{-19} \frac{Z^2}{n^2}$ ev/atom , $-1312 \frac{Z^2}{n^2}$ KJ/mol , $-313\frac{Z^2}{n^2}$ kcal/mol
- $T \propto \frac{n^3}{Z^2}$ $\left[T = \frac{2\pi r_n}{V_n}\right]$



- $I.E = \Delta E = E_\infty - E_1 = -E_1$
- $E.E$ (ground state to Higher orbital (except ∞))

  1^{st} Excited state $(n=2) \Rightarrow \Delta E = E_2 - E_1$
- $S.E$ (Excited state to ∞)

  1^{st} Separtion energy → $\Delta E = E_\infty - E_2 = -E_2$

Limitations.

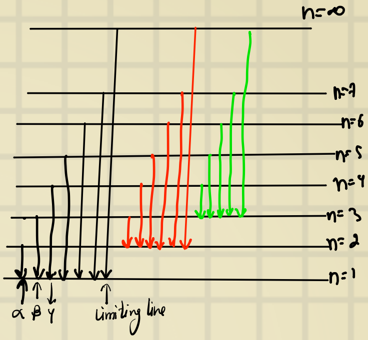
- not applicable for multielectron atom
- stark & Zeeman effect
- $mvr = \frac{nh}{2\pi}$ (why?)
- fine lines in the spectrum.

Hydrogen spectrum

★ first line of max energy = Lymen
min λ =
max ν =

★ In any series, line of max E, max ν, min λ = Last line.
Line of minimum E = first line.

(IR) Humphrey
(IR) Pfund
(IR) Brackel
(IR) Paschen
(visible) Balmer
(UV region) Lymen



Series	Region	n_2	no. of lines in spectrum
Lyman	UV	1	n_1-1
Balmer	Visible	2	n_1-2
Paschen	IR	3	n_1-3
Brackett	IR	4	n_1-4
Pfund	IR	5	n_1-5
Humfrey	IR	6	n_1-6

$$\boxed{\bar{\nu} = RZ^2\left[\frac{1}{n_f^2} - \frac{1}{n_i^2}\right]}$$

$R = 109677\ cm^{-1}$ or $10^5\ cm^{-1}$
$R = 10967700\ m^{-1}$ or $10^7\ m^{-1}$
$\frac{1}{R} = 912\ \text{Å}$

$$\text{total no. of lines} = \frac{(n_2-n_1)(n_2-n_1+1)}{2}$$
$$= \frac{n(n-1)}{2}$$

Discoveries Before Quantum mechanical model

De-broglie Hypothesis

matter ⟶ Wave nature + particle nature

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

$$\lambda = \frac{h}{\sqrt{2mK.E}}$$

$$\lambda = \frac{h}{\sqrt{2mq \cdot V}}$$

$$\boxed{\lambda = \sqrt{\frac{150}{V}}\ A^\circ}$$

$$\boxed{2\pi r = n\lambda}$$

Heiserberg's uncertainity principle

Impossible ⟶ exact ⟶ position & momentum

$$\Delta x \cdot \Delta p \geq \frac{h}{4\pi}$$

$$\Delta x \cdot \Delta v \geq \frac{h}{4\pi m}$$

% error in position = $\frac{\Delta x}{x} \times 100$

Quantum mechanical Model of atom

① Quantum numbers

- $n \rightarrow$ principal Q.N. $\rightarrow$ shell
  [Energy, size]
- $l \rightarrow$ Azimuthal Q.N. $\rightarrow$ Subshell
  [shape, orbital angular momentum $= \sqrt{l(l+1)}\,\frac{h}{2\pi}$]
  $l = 0 \ldots n-1$ $[l \neq n]$ $[l = 0, 1, 2, 3]$ → s p d f
- $m \rightarrow$ Magnetic Q.N. $\rightarrow$ Orbital
  [Orientation of orbitals]
  $[m = -l \text{ to } +l]$ $[m = 2l+1]$
- $s \rightarrow$ spin Q.N. $\rightarrow$ spin
  [spin of $\bar{e}$, spin angular momentum $= \sqrt{S(S+1)}\,\frac{h}{2\pi}$ ($S \rightarrow$ sum of all s)
  $[s = +\frac{1}{2} \text{ or } -\frac{1}{2}]$

Short-Cut

Shell
- → Subshell ⇒ n
- → Orbital $= n^2$
- → $\bar{e} = 2n^2$

Sub-Shell
- → Orbital $= 2l+1$
  ध्यान रखें! Double
- → $\bar{e} = 2(2l+1)$

① Rules.

Afbau's rule: $\bar{e} \rightarrow$ filled $\rightarrow$ first $\rightarrow$ LOW ENERGY $\rightarrow$ orbitals

Multi $\bar{e}$ species
Energy $\rightarrow n+l$
if $n+l$ is same
then
low n = low Energy

Single $\bar{e}$ species
Energy $\rightarrow n$
$1s < 2s = 2p$

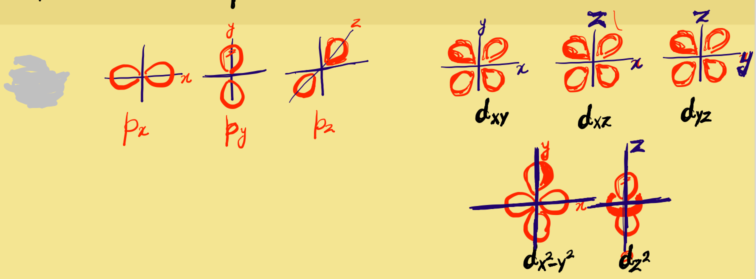
Hund's rule: DEGENRATE Orbitals → filling → Single → then pairing
↓ same spin

Pauli's rule: $\boxed{\text{Single orbital}}$ → No same spin

Half filled & fully filled orbital (Cr, Cu)
↓
Extra stable
1. symmetry
2. Exchange energy

② Shape of orbital & node

s p d



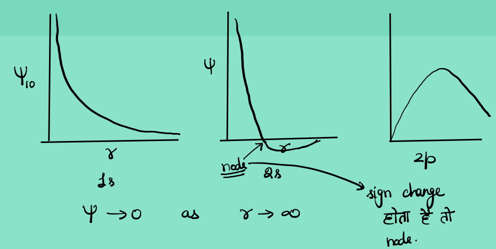
Space of No $\bar{e}$ NODE(n-1)

Planner Node
Nodal plane
Angular Node
l

Spherical Node
Radial Node
$n-l-1$

① Graph

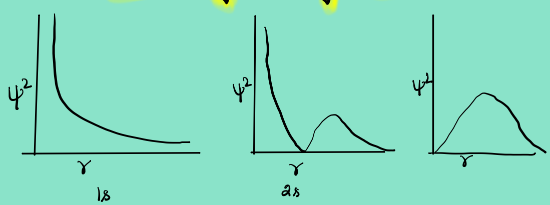
ψ v/s r



$\psi \rightarrow 0$ as $r \rightarrow \infty$

sign change होता है तो node.

Probability density (ψ^2):



Probability = $\psi^2\, 4\pi r^2 dr$

$d_{x^2-y^2}$ d_{z^2}

$d_{x^2-y^2}$ d_{z^2}