Atomic Structure

Electrons → [Cathode Rays]
↳ Discovered in cathode ray tube

Protons → Discovered in anode rays discharge tube

$$\bar{\nu} \text{ (Wave No.)} = \frac{1}{\lambda}$$

Planck's Quantum Theory

$$E = nh\nu = \frac{nhc}{\lambda}$$

n = No. of photons emitted

ESTIMATE

$$hc = 20 \times 10^{-26}$$

Spectrum →

$$\bar{\nu} = R Z^2 \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

Rydberg Const

$R = 109677\ cm^{-1}$
$= 1.096 \times 10^7\ m^{-1}$

a) For α-line $\Rightarrow n_2 = n_1 + 1$ & so on
b) For β-line $\Rightarrow n_2 = n_1 + 2$

c) For limiting line $\Rightarrow n_2 = \infty$
d) Maxi. energy diff. $\Rightarrow n_2 = \infty$ (or λ_{min})
e) Mini. energy diff. $\Rightarrow n_2 = n_1 + 1$ (or λ_{max})

Ionization energy (I.E.) $= E_\infty - E_1$

For Lyman →

Radius of nth orbit

$$r_n = a_0 \frac{n^2}{Z}$$

a_0 = Bohr's Radius

$a_0 = 0.529\ \text{Å}$

$$r_n = r_H \times \frac{n^2}{Z}$$

Velocity of e^- in n^{th} orbit

$$v_n = 2.18 \times 10^6 \frac{Z}{n} \text{ m/s}$$

(v_H)

where, $v_H = \frac{c}{137} = 2.18 \times 10^6$

$$T.E. = -13.6 \frac{Z^2}{n^2} eV$$

$K.E. = -T.E.$ $\quad$ $P.E. = 2T.E.$

Angular velocity of e^- in n^{th} orbit

$$\omega_n = \frac{v_n}{r_n} \Rightarrow \omega_n \propto \frac{Z^2}{n^3}$$

frequency also $\Rightarrow \nu \propto \frac{Z^2}{n^3}$

$\nu \propto \omega$

Time Period of $e^- \Rightarrow T_n \propto \frac{n^3}{Z^2}$

$T \propto \frac{1}{\nu}$

For $e^- \Rightarrow \lambda = \frac{12.27}{\sqrt{V}}$ Å

For proton $\Rightarrow \lambda = \frac{0.286}{\sqrt{V}}$ Å

For gas molecules $\Rightarrow \lambda = \frac{h}{\sqrt{3mkT}}$ (T → Temp.)

$k = 1.38 \times 10^{-23}$ J/K (k → Boltzmann Const.)

ESTIMATE

Circumference of n^{th} orbit $= n\lambda$

★ Sommerfeld's → gives concept of subshells
- No. of subshells = No. of shell

Heisenberg's Uncertainity Principle

→ We cannot find exact position & momentum of sub-atomic particle simultaneously & accurately.

Uncertainity in position

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

→ Uncertainity in momentum

$\Delta P = m \Delta V$

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

- $\frac{h}{4\pi} \approx \frac{1}{2} \times 10^{-34}$

Also

$$\Delta E \cdot \Delta t \geq \frac{h}{4\pi}$$

→ Uncertainity in energy

→ Uncertainity in time

→ For angular motion

$$\Delta\theta \cdot \Delta\phi \geq \frac{h}{4\pi}$$

Quantum Mechanical Model of Atom

↳ Given by Erwin Schrodinger

Schrodinger wave equation is

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}+\frac{8\pi^2 m(E-V)\psi}{n^2h^2}=0$$

ψ = Orbital Wave function, m = mass of an e^-, E = Total Energy, V = Potential energy, n = shell no., h = planck's constant.

Quantum Numbers :-

a) Principal Quantum Number (n) →

represent Shell ←

n → 1 2 3 4

Shell → Ist IInd IIIrd IV ★

- No. of orbitals in shell = n^2
- Total no. of e^-s in a shell = $2n^2$

b) Azimuthal or Angular or Subsidiary

quantum no. (l) → represent subshell

Subshell → s p d f g - -

l = 0 1 2 3 4

→ l value is given by → 0 to $(n-1)$

Shape of orbitals

s - orbital → spherical
p - " → Dumbell
d " → Double dumbell

f orbital → Complicated (8-fold structure)

ESTIMATE

$l < n$ always

→ Angular momentum of an e^- in orbital →

★

$$\text{Angular momentum} = \sqrt{l(l+1)}\,\frac{h}{2\pi}$$

★

No. of orbitals in a subshell $= 2l+1$

c) Magnetic Quantum Numbers (m) →

$m \rightarrow -l$ to $+l$

It explains Zeeman effect

If $n=3$, $l=0$ → $m=0$ (s-subshell)

$n=3$, $l=1$ → $m=-1, 0, 1$ (p-subshell)

p_y p_z p_x

$n=3$, $l=2$ → $m=-2, -1, 0, +1, +2$ (d-subshell)

d_{xy} d_{yz} d_{z^2} d_{zx} $d_{x^2-y^2}$

d) Spin Quantum No. (s) → Spin of an electron

$s = +\frac{1}{2}$ or $-\frac{1}{2}$

It cannot be explained by any scientist even today

No. of e^- in an orbital = 2

No. of e^- in a subshell = $2(2l+1)$ ★

Energy of a subshell = $n+l$

- Zeeman effect → Splitting of spectral lines in magnetic field
- Stark effect → Splitting of spectral lines in electric field

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Radial Wave Function → $\psi(r)$

Radial Probability density → $(\psi^2)(r)$

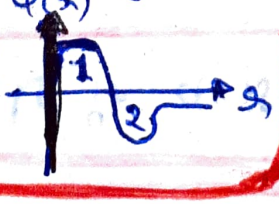
↳ tell us about the probability of finding e^- at any point along the straight line

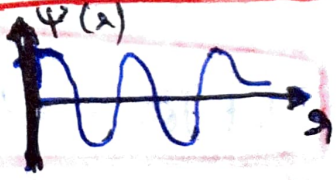
Graph of $\psi(r)$ vs distance (r)

a) For s-orbitals →

(i) Cosine Wave (ii) 1 phase = 1 orbital

(iii) last phase graph will not touch r

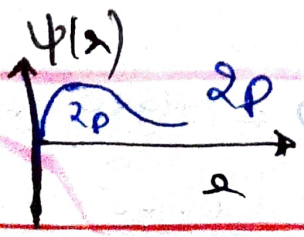
e.g. for 2s → 

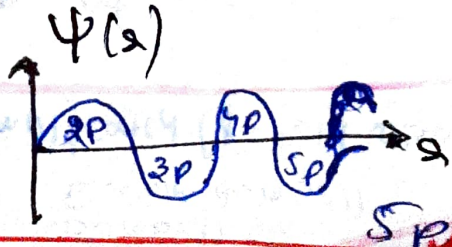
5s → 

b) For p-orbitals →

(i) Sine Wave (ii) 1 phase = 1 orbital

(iii) last phase $\psi(r)$ will not touch r.

e.g. 2p → 

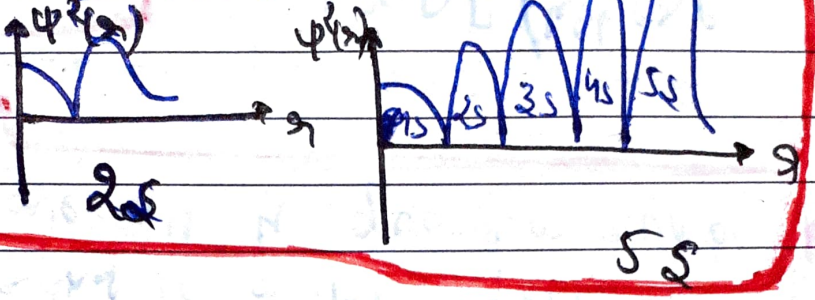


ESTIMATE

Graph of $\psi^2(x)$ vs x

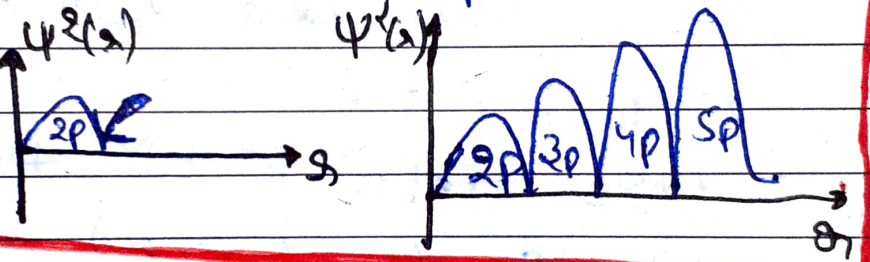
a) For s-orbitals → • Cosine • 1 phase = 1 orbital
★ last phase $\psi^2(x)$ will not touch x
★ $\psi^2(x)$ will never be negative
★ peak increases

e.g., 2s →



b) For p-orbitals → • Sine wave • never negative | • 1 phase = 1 orbital
★ Peak increases ★ Last phase will not touch x

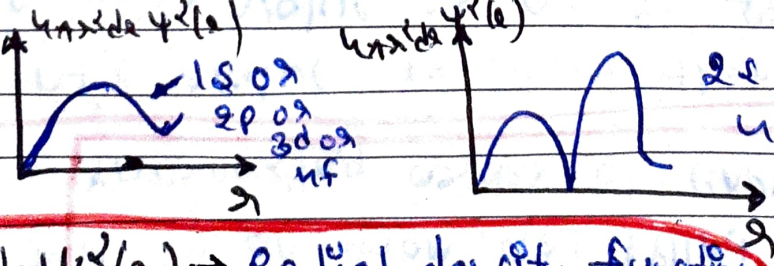
e.g., 2p



Graph of $4\pi x^2 dx\, \psi^2(x)$ vs x

Same graph for all orbitals (s or p or d or f)
↳ • 1 phase = 1 orbital
• Sine wave • never negative
• Peak increases • last phase will not touch x

e.g.,



$4\pi x^2 dx\, \psi^2(x)$ → Radial density function
↳ Probability of finding an e⁻ in a shell of thickness dx

Aufbau Principle

- Energy = n+l rule ← for multi-electron atoms
- e⁻ in an atom are filled in increasing order of energy
- * If n+l value is same than one with lower value of n is filled first

∴ For H & H-like atoms,

Energy = n

Hund's Rule of Maximum Multiplicity

Pairing of electrons in an orbital will not start unless each orbital in same subshell have electrons with same spin

Pauli's Exclusion Principle

"Two electrons in same orbital cannot have all 4 quantum numbers same"

If $\psi^2(r) = 0$ → NODE (where probability of finding an e^- is zero)

No. of radial nodes = $n - l - 1$
No. of angular nodes = l
Total no. of nodes = $n - 1$

Nodal plane → plane where prob. of finding an e^- is zero.

ESTIMATE

Exception →
d_{z^2} → 0 Nodal planes