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Atomic Structure

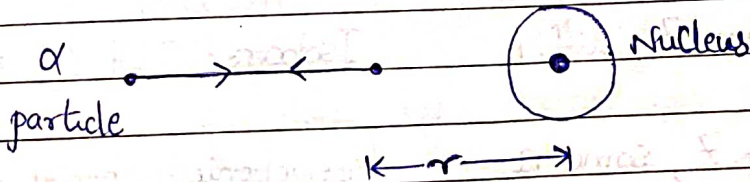
Cathode Rays : from cathode to anode. (-ve) charge.
e/m ratio Const. Also called electrons.

Anode Rays : from anode to cathode. (+ve) charge
e/m ratio varies. Due to ionisation of gas.

Specific Charge : Charge per mass. q/m or e/m

	Electron (e ⁻)	Proton (p)	Neutron (n)
Mass	$9.1 \cdot 10^{-31}$ kg	$1.67 \cdot 10^{-27}$ kg	$1.67 \cdot 10^{-27}$ kg
Charge	$-1.6 \cdot 10^{-19}$ C	$+1.6 \cdot 10^{-19}$ C	0 C

Closest Approach (Rutherford's Experiment) —



At closest dist., intial K.E. of particle = P.E. at dist. \wedge closest approach

$k = 9 \cdot 10^9 \text{ Nm}^2\text{C}^{-2}$	\Rightarrow	$\frac{1}{2} mv^2 = k \frac{(2e^-)(Ze^-)}{r}$	at. no. of element used
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Some Imp. Terms -DATE: / /
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1) At. No. (Z): No. of protons

2) Mass No. (A): No. of protons + No. of neutrons

$$n = A - Z$$

n = # neutrons

Z = # protons

A = Mass No.

★ Atom represented by ${}^A_Z X$.

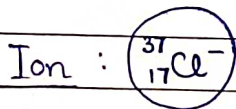
(Q) An ion with mass no. 37 posses unit of (-ve) charge. If ion contains 11.1% more neutron than electron, find ion.

A) We have $A = 37 \Rightarrow n + p = 37 \Rightarrow n + e = 38$

$$\text{Now, } \left(\frac{n-e}{e}\right) = \left(\frac{11.1}{100}\right) = \left(\frac{1}{9}\right) \Rightarrow 9n = 10e$$

$$n + e = 38 \Rightarrow 10e + 9e = 342 \Rightarrow e = 18$$

$$\Rightarrow p = 17$$



Isotopes: Same Z, diff. A

Isobars: Diff Z, same A.

Isotones: Diff. Z, same n

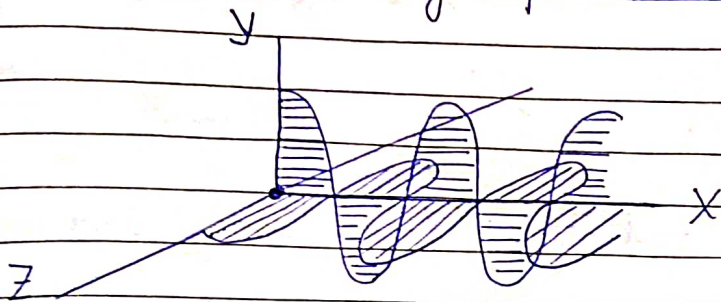
Isoelectronic: Species with same # e⁻

Isodiaphers: Diff. Z, same |n-p| or |A-2p|

Isosters: Molecules of diff. comp. with same # e⁻.
 & Same # atoms

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Maxwell's Theory of E.M. radiation -



Y - Electric , Z - Magnetic , X - Propagation

It is form of energy which contains electric & magnetic fields oscillating \perp to each other, and both \perp to dirⁿ of propagation of radiation.

Characteristics -

- 1) Rays are uncharged, carry no charge.
- 2) Can travel in vacuum, no medium req.
- 3) Speed independent of source, $= 3 \cdot 10^8 \text{ ms}^{-1}$ in vacuum.
- 4) Doesn't deviate by external electrical and magnetic field.
- 5) Every blackbody (perfect absorber or emitter) only emits radiations of only one wavelength.

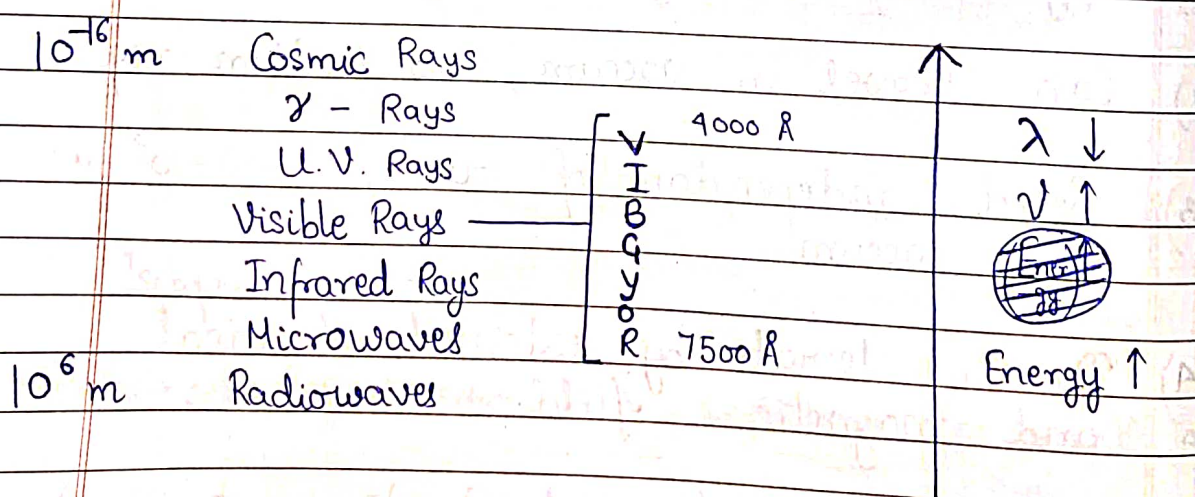
$$(6) \quad (\text{Energy of Radiation}) \propto (\text{Intensity of light used})$$

Failure -

- 1) Blackbody radiation (Proven wrong experimentally)
- 2) Photoelectric effect
- 3) Plank's Quantisation Theory

Electromagnetic Spectrum -

If E.M. rays are arranged in inc. order of their wavelength/freq. then a series of spectrum is formed, called E.M. spectrum.

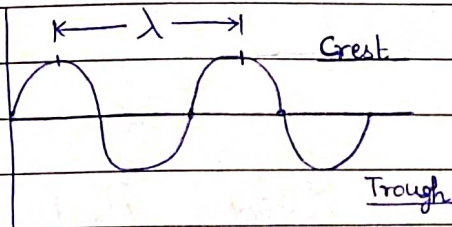


(λ)

Characteristics of Wave —

Wave: Mode of energy transmission from one place to another, w/o disp. of matter.

- 1) Wavelength (λ) — Dist. b/w successive crests or troughs.



$1 \text{ \AA} = 10^{-10} \text{ m}$
 $1 \text{ nm} = 10^{-9} \text{ m}$
 $1 \text{ pm} = 10^{-12} \text{ m}$

- 2) Frequency (ν) — No. of waves passing thru a pt. in 1 s.

$\star \boxed{\nu \lambda = c}$ Hertz (Hz) \leftrightarrow s^{-1}

- 3) Velocity (c) — Dist. travelled by wave in 1 s. Unit — ms^{-1}

- 4) Wave No. ($\bar{\nu}$) — No. of waves passing thru unit length.

$\star \boxed{\bar{\nu} = \left(\frac{1}{\lambda}\right)}$

Unit — m^{-1}

5) Amplitude (A) - Max. height of crest or trough. Unit - m

6) Time Period (T) - Time req. for 1 wave cycle to complete.

$$\star T = \left(\frac{1}{\nu}\right)$$

7) Angular ~~f~~ (w) - $\omega = 2\pi\nu = \left(\frac{2\pi}{T}\right)$

Plank's Theory

Any body can emit or absorb energy in discrete qty. (integral multiple of some smallest qty.)

Quantum/Photon: Small packets/bundles of energy, which are emitted or absorbed by a body.

Energy of photon directly proportional to freq. of radiation used.

(Energy of 1 photon) $E = h\nu$ Plank's Constant

$$E = \left(\frac{hc}{\lambda}\right)$$

$$\star h = 6.626 \cdot 10^{-34} \text{ Js}$$

$$\star \hbar = h/2\pi$$

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$$E = hc\nu$$

Since any body will emit energy in integral multiple of photon.

$$E_{\text{Total}} = N h \nu$$

no. of photons

★

$$E \text{ (in eV)} = \left(\frac{12400}{\lambda \text{ (in \AA)}} \right)$$

$$1 \text{ eV} = 1.6 \cdot 10^{-19} \text{ J}$$

Energy of 1 photon

Q) A bulb emits light of wavelength 4500 Å. Bulb is rated as 150 W, and 8% of energy is emitted as light. How many photons emitted by bulb per sec.

$$A) E = Pt = (150 \frac{\text{J}}{\text{s}})(1 \text{ s}) \Rightarrow E = 150 \text{ J}$$

$$\Rightarrow E_{\text{photons}} = \left(\frac{150}{1.6 \cdot 10^{-19}} \right) \left(\frac{8}{100} \right) \cdot \text{eV}$$

$$\text{Also, } E = N h \nu \Rightarrow E \text{ (eV)} = \left(\frac{12400}{\lambda \text{ (\AA)}} \right) N$$

$$\Rightarrow \left(\frac{150}{1.6 \cdot 10^{-19}} \right) \left(\frac{8}{100} \right) = \left(\frac{12400}{4500} \right) N$$

$$\Rightarrow N \approx 2 \cdot 10^{19}$$

Q) A photon of 300 nm wavelength is absorbed by a body which then re-emits $2e^-$. One re-emitted e^- has wavelength of 400 nm. Calc. energy of (re-emitted e^- other

A) $E_{\text{absorbed}} = E_{\text{released}}$

$$E_{\text{absorbed}} = \left(\frac{12400}{3000} \right) = 4.13 \text{ eV}$$

$$E_{\text{released}} = \left(\frac{12400}{4000} \right) + \left(\frac{12400}{10\lambda} \right) \text{ eV} = 3.1 \text{ eV} + \frac{1240}{\lambda}$$

(in nm)

$$\Rightarrow \left(\frac{1240}{\lambda} \right) = 1.03 \Rightarrow \lambda = 1200 \text{ nm}$$

$$E_{\text{photon}} = \left(\frac{12400}{10 \cdot 1200} \right) \Rightarrow E_{\text{photon}} = 1.03 \text{ eV}$$

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Photoelectric Effect —

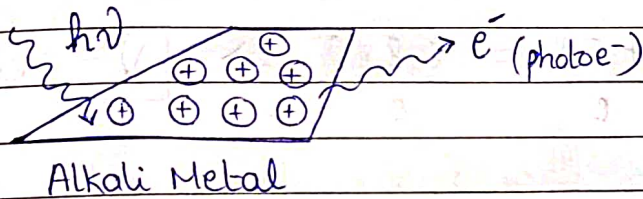
Phenomenon of emission of e^- takes place when light of suitable freq. falls on metal surface.

★ This explains particle nature of light. Only particles can transfer momentum. Hence, light acts like particle.

Conclusion:

- 1) e^- emit only if $\nu > \nu_0$ ← Threshold freq.
- 2) (K.E. of photoelectron) \propto (ν light used).
- 3) Intensity of light used independent of ν light used.

★ (K.E. of photoelectron) = $h\nu - h\nu_0$ (Work fxⁿ/Binding Energy / Ionisation/Critical Energy)

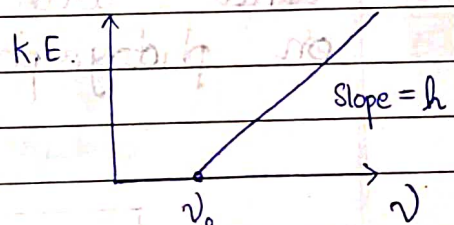


Threshold freq. : Min. freq. req. to observe this effect

★ Threshold freq. & Energy depend on nature of metal.

Stopping Potential:

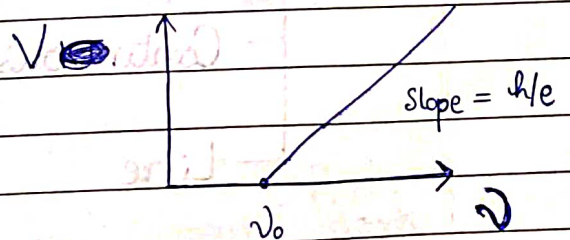
Potential ~~Energy~~ req. to stop photoe⁻.



Stopping Energy : Energy req. to stop photoe⁻.

Stopping Potential

$$V = \frac{h\nu}{e} - \frac{h\nu_0}{e}$$



Q) Calc. K.E. of photoe⁻ (in eV) emitted by a sodium metal when light of wavelength 400 nm strikes on it. The work fxⁿ of sodium metal is 2.3 eV. Also calc. stopping potential.

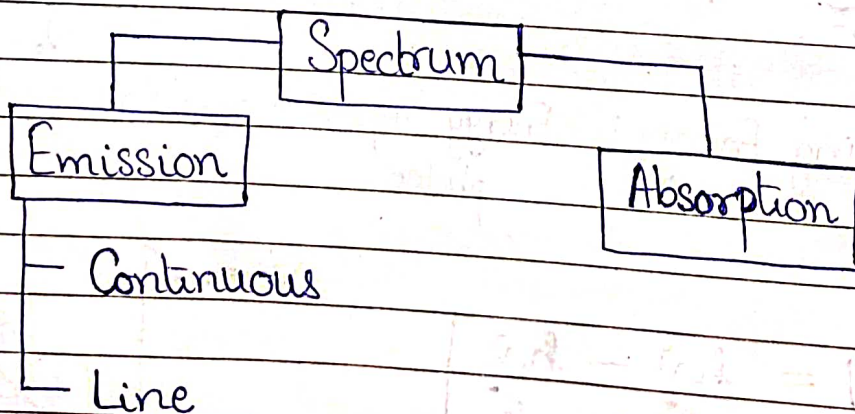
A)
$$\text{K.E.} = h\nu - h\nu_0 = \left(\frac{12400}{4000} \right) - 2.3 \text{ eV}$$

$$\Rightarrow \boxed{\text{K.E.} = 0.8 \text{ eV}}$$

Now,
$$V = \frac{\text{K.E.}}{e} = \frac{0.8 \text{ eV}}{e} \Rightarrow \boxed{V = 0.8 \text{ V}}$$

Spectrum -

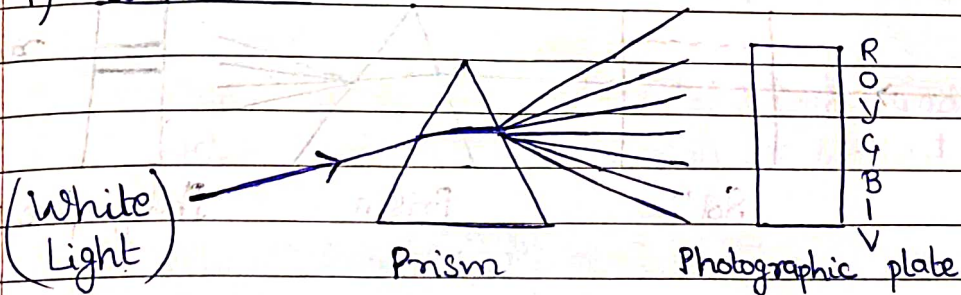
Series of radiations having diff. color bands with diff. wavelength obtained on photographic plate.



Emission Spectrum :

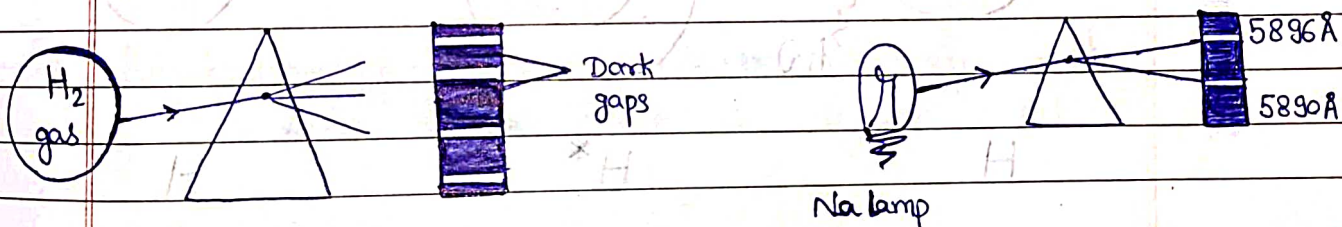
Spectrum obtained on photographic plate after passing radiation from glowing body through a prism.

1) Continuous :



All color bands merge with each other. No line of division b/w 2 colors ; no gaps.

2) Line : (Characteristic of atoms) (fingerprint of element)

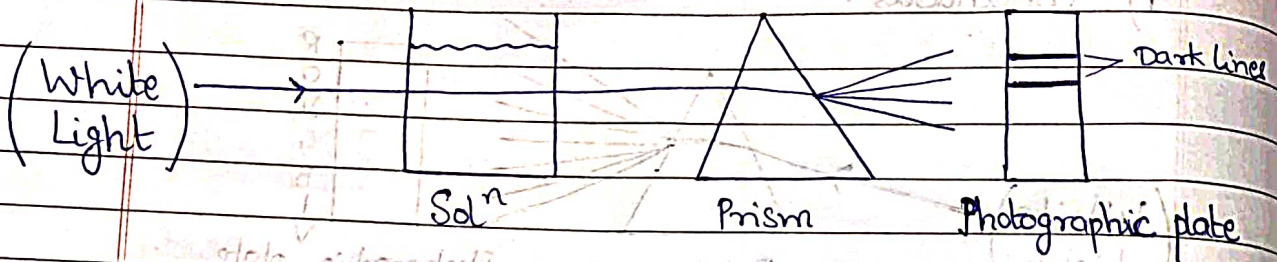


When radiation produced by passing electric discharge thru H_2 gas at low pressure, it is passed thru prism and received on photographic plate.

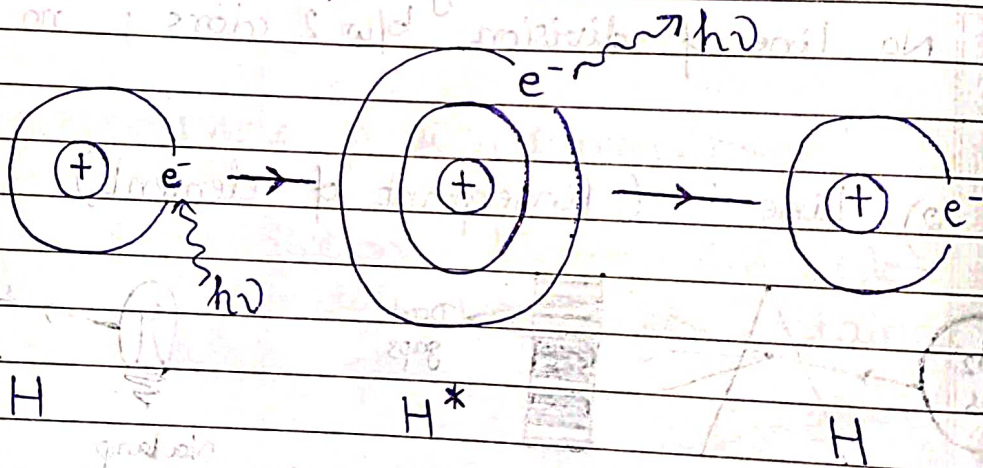
The line spectrum consists of sharp well defined lines which contain dark gaps in b/w them.

Absorption Spectrum:

White light from any source is first passed thru a solⁿ, then analysed by spectroscop it is observed that some dark lines are obtained in otherwise continuous spectrum.



At atomic level,



Bohr Model for Hydrogen like Species -

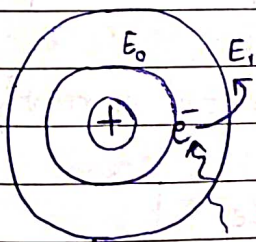
Hydrogen like Species = $1e^-$ species.

Postulates:

- 1) Atom consists nucleus, whose size is negligible compared to atom
- 2) e^- revolve in fixed orbits of fixed radius and fixed vel. and fixed energy, around nucleus.
- 3) (Practically) Angular Momentum of e^- is an integral multiple of $(\frac{h}{2\pi})$ in orbit.

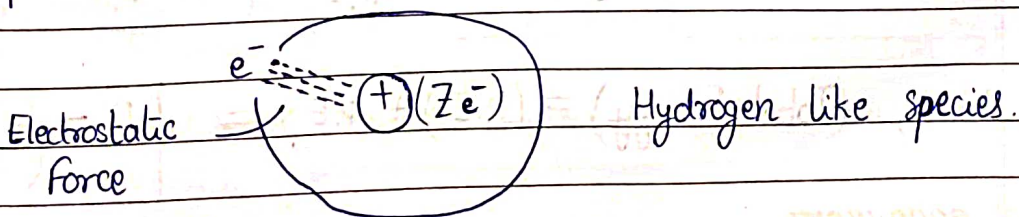
Eg: 1st orbit, $mvr = 1 \cdot \frac{h}{2\pi}$
 2nd orbit, $mvr = 2 \cdot \frac{h}{2\pi}$
 nth orbit, $mvr = \frac{nh}{2\pi}$

4) Excitation of e^- : e^- absorbs energy and jumps from lower orbit to higher orbit.




$$\Delta E = h\nu = E_1 - E_0$$

Application of Bohr Model -



Since, electrostatic force acts as centripetal force.

$$\frac{k q_1 q_2}{r_{n,z}^2} = \frac{m v_{n,z}^2}{r_{n,z}} \Rightarrow \frac{k (e)(Ze)}{r_{n,z}^2} = \frac{m v_{n,z}^2}{r_{n,z}}$$

$\Rightarrow k Z e^2 = m v_{n,z}^2 r_{n,z}$ By Bohr's  model,

$$m v_{n,z} r_{n,z} = \left(\frac{nh}{2\pi} \right)$$

$$\Rightarrow v_{n,z} = \frac{(k e^2)(2\pi)(Z)}{h(n)} \text{ (Vel.)}$$

$$\Rightarrow v_{n,z}(\text{m/s}) = (2.18 \cdot 10^6) \left(\frac{Z}{n} \right) \quad r_{n,z} = (0.529) \left(\frac{n^2}{Z} \right) \text{ (\AA)}$$

$$\Rightarrow r_{n,z} = \left(\frac{h^2}{4\pi^2 m k e^2} \right) \left(\frac{n^2}{Z} \right) \text{ (Radius)}$$

Now, $T_{n,z} = \frac{2\pi r_{n,z}}{v_{n,z}} \propto \left(\frac{r_{n,z}}{v_{n,z}} \right) \propto \frac{(n^2/Z)}{(Z/n)}$

(Time Period) (Freq.)

$$\Rightarrow T_{n,z} \propto \left(\frac{n^3}{Z^2} \right) \Rightarrow \nu_{n,z} \propto \left(\frac{Z^2}{n^3} \right)$$

Now, K.E. = $\frac{1}{2} m v_{n,z}^2$ and $k Z e^2 = m v_{n,z}^2 r_{n,z}$

$$\Rightarrow \text{K.E.} = \left(\frac{k Z e^2}{2 r_{n,z}} \right)$$

Now, P.E. = $\frac{k q_1 q_2}{r_0} = \frac{k (-e)(Ze)}{r_{n,z}} \Rightarrow \text{P.E.} = \left(\frac{-k Z e^2}{r_{n,z}} \right)$

Now, (Total Energy) = (K.E.) + (P.E.) $\Rightarrow E = \left(\frac{-k Z e^2}{r_{n,z}} \right)$

★ $E = (-K.E.) = \left(\frac{P.E.}{2}\right)$

$E_{n,z} = (-2.18 \cdot 10^{-18}) \left(\frac{z}{n}\right)^2$
(J/atom)

⇒ $E_{n,z} = \left(\frac{-k^2 e^4 m}{h^2}\right) \left(\frac{z^2}{n^2}\right)$ $E_{n,z} = \left(\frac{-m}{2}\right) \left(\frac{ke^2}{h}\right)^2 \left(\frac{z}{n}\right)^2$

⇒ $E_{n,z} \text{ (eV/atom)} = (-13.6) \left(\frac{z^2}{n^2}\right)$ $v_{n,z} = \left(\frac{ke^2}{h}\right) \left(\frac{z}{n}\right)$

⇒ $E_{n,z} \text{ (kJ/mol)} = (-1312) \left(\frac{z^2}{n^2}\right)$ $r_{n,z} = \left(\frac{h^2}{mke^2}\right) \left(\frac{n^2}{z}\right)$

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For H atom,

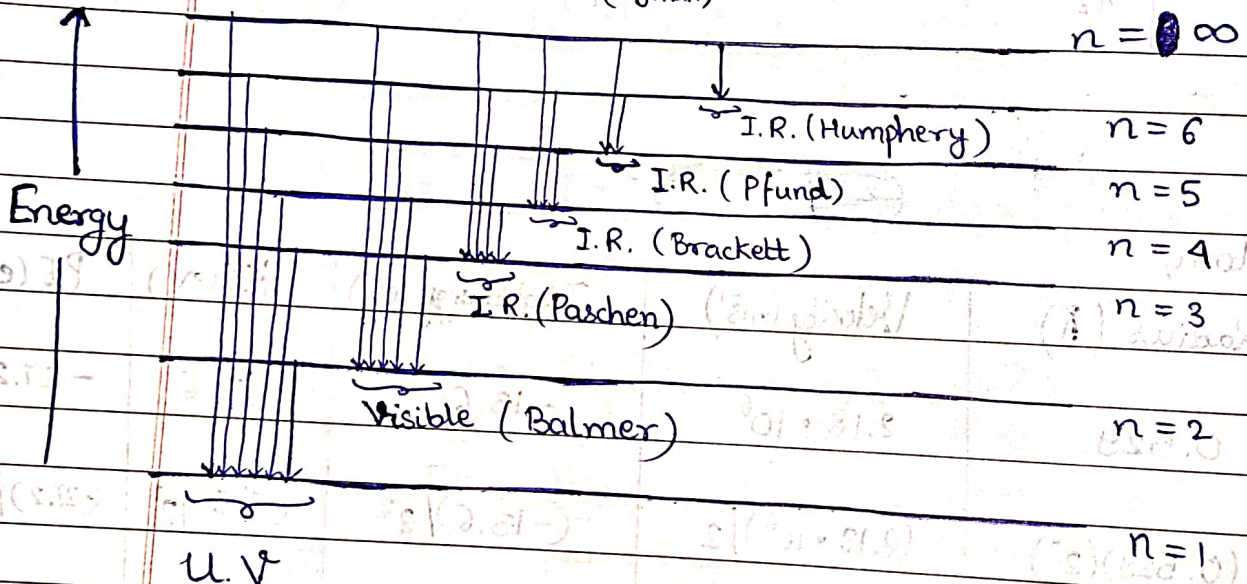
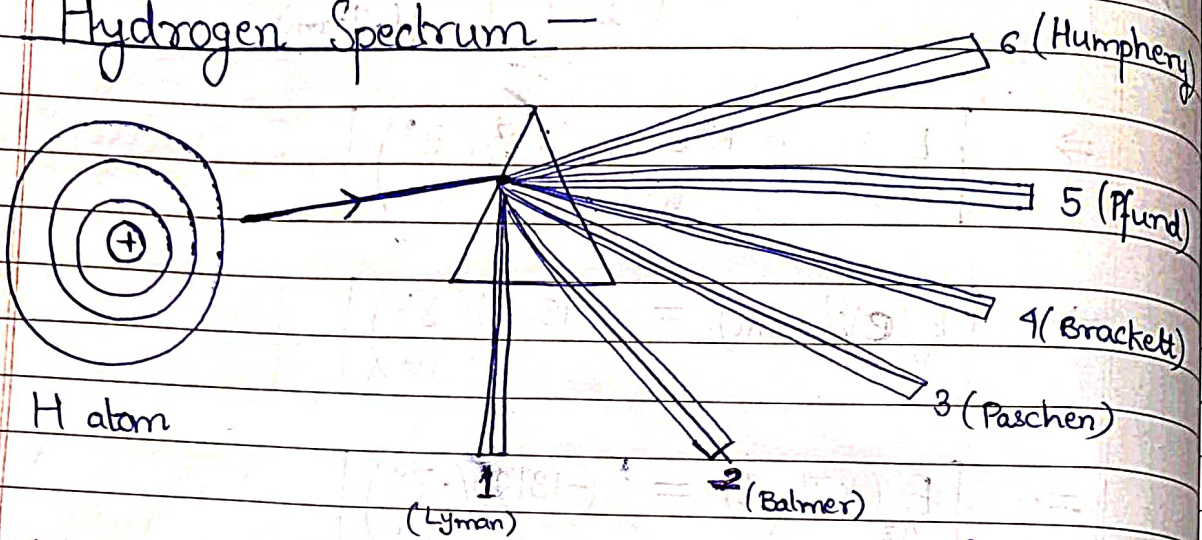
Orbit	Radius (Å)	Velocity (ms ⁻¹)	Total Energy (ev)	K.E(ev)	P.E.(ev)
1st	0.529	$2.18 \cdot 10^6$	-13.6	13.6	-27.2
2nd	$(0.529)(2^2)$	$(2.18 \cdot 10^6)/2$	$(-13.6)/2^2$	$(13.6)/2^2$	$(-27.2)/2^2$
3rd	$(0.529)(3^2)$	$(2.18 \cdot 10^6)/3$	$(-13.6)/3^2$	$(13.6)/3^2$	$(-27.2)/3^2$
4th	$(0.529)(4^2)$	$(2.18 \cdot 10^6)/4$	$(-13.6)/4^2$	$(13.6)/4^2$	$(-27.2)/4^2$

★

For H atom,

Orbit	1	2	3	4
Total Energy (ev)	-13.6	-3.4	-1.51	-0.85

Hydrogen Spectrum -



★ α ray of n^{th} series is radiation when e^- transition from $(n+1)$ orbit to (n) orbit.

✓ n^{th} Series : e^- falls from ANY orbit, to n^{th} orbit (in ANY atom). Rays obtained form n^{th} series.

★ Limiting line of n^{th} series is ray when e^- transit from ∞ orbit to n orbit

for H,

Series	Region	Lowest Energy Level	Highest Energy Level
Lyman	U.V.	$n=1$	$n=2, 3, \dots$
Balmer	Visible	$n=2$	$n=3, 4, \dots$
Paschen	I.R.	$n=3$	$n=4, 5, \dots$
Brackett	I.R.	$n=4$	$n=5, 6, \dots$
Pfund	I.R.	$n=5$	$n=6, 7, \dots$
Humphery	I.R.	$n=6$	$n=7, 8, \dots$

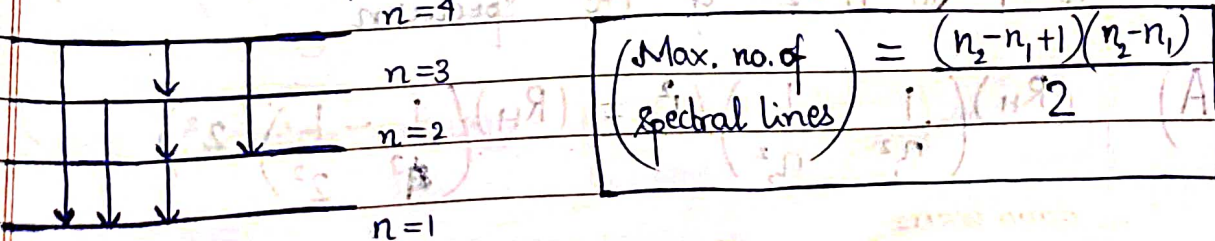
✓ Energy released/absorbed in transition.

$$\Delta E = (13.6) \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] Z^2$$

$$\Rightarrow \left(\frac{1}{\lambda} \right) = (R_H) \left[\frac{1}{n_1^2} - \frac{1}{n_2^2} \right] Z^2 \quad \left(\text{when } e^- \text{ transit from } n_1 \text{ to } n_2 \right)$$

(Rydberg Const.) $(R_H = 1.1 \cdot 10^7 \text{ m}^{-1})$

✓ Max. no. of spectral lines (if ∞ atoms) $\left[\begin{matrix} n_2 - n_1 + 1 \\ 2 \end{matrix} \right]$



$$\left(\text{Max. no. of spectral lines} \right) = \frac{(n_2 - n_1 + 1)(n_2 - n_1)}{2}$$

Q) Calc. the min. & max. λ for Balmer Series.

A) For Balmer series, $n_2 = 2$

$$\text{For } \lambda_{\min}, E_{\max} \Rightarrow \left(\frac{1}{\lambda_{\min}} \right) = (R_H) \left(\frac{1}{\infty^2} - \frac{1}{2^2} \right)$$

$$\Rightarrow \left| \lambda_{\min} \right| = \left(\frac{4}{R_H} \right) \quad (\lambda < 0 \Rightarrow \text{Energy released})$$

$$\text{For } \lambda_{\max}, E_{\min} \Rightarrow \left(\frac{1}{\lambda_{\max}} \right) = (R_H) \left(\frac{1}{3^2} - \frac{1}{2^2} \right)$$

$$\Rightarrow \left| \lambda_{\max} \right| = \left(\frac{36}{5R_H} \right) \quad (\lambda < 0 \Rightarrow \text{Energy released})$$

Q) The energy of H in excited state is -0.85 eV . What will be energy of photon emitted, when e^- returns to ground state.

$$A) E_{\text{photon}} = E_{1,1} - E_{n,1} = (-13.6) - (-0.85)$$

$$\Rightarrow \left| E_{\text{photon}} \right| = 12.75 \text{ eV} \quad (E < 0 \Rightarrow \text{Energy released})$$

Q) What transition in H spectrum would have same wavelength as Balmer transition from $n=4$ to $n=2$ of He^+ spectrum.

$$A) (R_H) \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) (1) = (R_H) \left(\frac{1}{4^2} - \frac{1}{2^2} \right) (2^2)$$

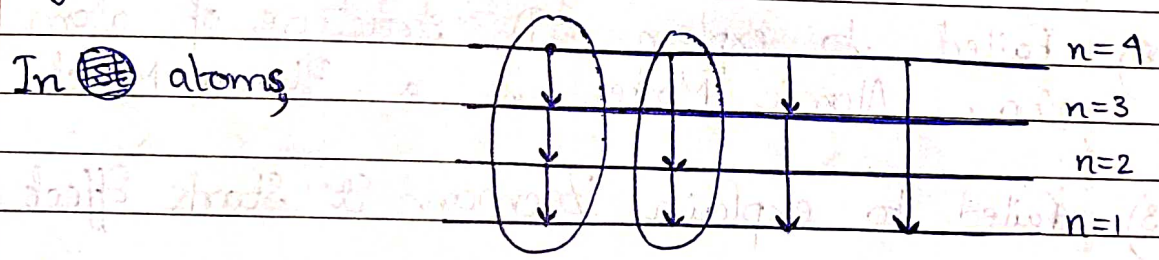
$$\Rightarrow \left(\frac{1}{n_1}\right)^2 - \left(\frac{1}{n_2}\right)^2 = \left(-\frac{3}{4}\right) \Rightarrow \left(\frac{1}{n_2}\right)^2 - \left(\frac{1}{n_1}\right)^2 = \frac{3}{4}$$

$$\Rightarrow \left(\frac{1}{n_2}\right) = \frac{2}{2} \text{ \& \ } \left(\frac{1}{n_1}\right) = \frac{1}{2} \Rightarrow n_2 = 1, n_1 = 2$$

Transition: $n=2$ to $n=1$

Q) Two hydrogen atoms present in 3rd excited state, find max. no. of possible emission lines.

A) For max. emission lines, e^- returns to ground state.



For max. no. of lines, 1st atom • 3 transitions
2nd atom 2 transitions.

$$\Rightarrow \boxed{\text{(Distinct) Max. no. of lines} = 4}$$

Q) For a hypothetical atom, potential energy $U = \left(\frac{-Ke^2}{r^3}\right)$, where r is dist. b/w particles. If Bohr's model of quantisation applies, find velocity of particle.

A) $U(r) = \left(\frac{-Ke^2}{r^3}\right) \Rightarrow \left(-\frac{dU(r)}{dr}\right) = F = \left(\frac{3Ke^2}{r^4}\right)$

Since circular motion, $\left(\frac{mv^2}{r}\right) = \left(\frac{3Ke^2}{r^4}\right)$

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We know, $mvr = nh$ (Bohr's quantisation model)

$$\Rightarrow \frac{(mv^2)}{(nh/mv)} = \frac{(3Ke^2)}{(nh/mv)^2} \Rightarrow v = \left(\frac{n^3 h^3}{24Ke^2 \pi^3 m^2} \right)$$

Drawbacks of Bohr's Atomic Model

- 1) Only valid for H & H-like species. It can't explain spectra of multi e^- system.
- 2) Failed to explain 3D structure of atom. Bohr's Atomic Model is a Planar Model.
- 3) Failed to explain Zeeman & Stark Effect.

Zeeman Effect: Splitting of spectral lines in magnetic field.

Stark Effect: Splitting of spectral lines in electric field.

- 4) Failed to account for $\left\{ \begin{array}{l} \text{Heisenberg's Uncertainty Principle} \\ \text{De-Broglie Concept} \\ \text{Dual nature of matter} \end{array} \right.$
- 5) Could only explain particle nature of e^- .
- 6) Could NOT explain size, shape & properties of molecules.

De-Broglie Concept -

for electromagnetic radiation acc. to Plank's Theory,

$$E = h\nu \Rightarrow \left(E = \frac{hc}{\lambda} \right) \quad \text{--- (1)}$$

$\nu, \lambda \rightarrow$ Wave Nature

Acc. to Einstein's theory of Relativity,

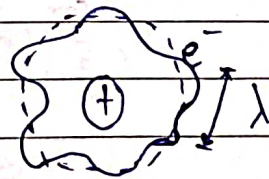
$$\left(E = mc^2 \right) \quad \text{--- (2)} \quad \text{Wavelength}$$

$$\text{(1) = (2)} \Rightarrow \frac{hc}{\lambda} = mc^2 \Rightarrow \lambda = \left(\frac{h}{mc} \right) \Rightarrow \left[\lambda = \frac{h}{p} \right]$$

Relⁿ b/w λ & $p \Rightarrow$ Dual nature of light.

Acc. to Einstein the eqⁿ of De Broglie wavelength applies to all.

Eg: If e^- wave \Rightarrow



$$n\lambda = 2\pi r \quad (\text{if } n \text{ waves})$$

$$\Rightarrow n \left(\frac{h}{p} \right) = 2\pi r \Rightarrow \left(\frac{nh}{mv} \right) = (2\pi r)$$

$$\Rightarrow \left(mvr = \frac{nh}{2\pi} \right)$$



In n th orbit, e^- makes n waves.

$$\Rightarrow 2\pi r = n\lambda$$

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E.M. Wave

Associated with Electric & Magnetic field.

Vel. = c (in Vacuum)

$$\lambda = \left(\frac{c}{\nu} \right)$$

Matter Wave

NOT associated with Electric & Magnetic field.

Vel. $< c$

$$\lambda = \left(\frac{h}{mv} \right)$$

De-Broglie wavelength.

Significance of De-Broglie Eqⁿ:

Although it is valid for whole material particle, it is sig. fig. for microscopic bodies.

Eg: λ_{car} for 4000 kg car moving at 20 ms^{-1} is $\approx 10^{-38} \text{ m}$, which is negligible.

Imp. Relⁿs:

$$\lambda = \frac{h}{\sqrt{2m(\text{K.E.})}}$$

$$\lambda = \frac{h}{\sqrt{2mqV}}$$

$$\sqrt{2mqV}$$

potential diff.

★ For e^- ,
(Starting from rest) $\lambda (\text{\AA}) = \sqrt{\frac{150}{V}}$

Q) For a Hydrogen like species, if De-Broglie wavelength in n th orbit is $\lambda_{n,z}$.
If $\lambda_{n+1,z} + \lambda_{n-1,z} = 3\lambda_0$, then find n and species.
($\lambda_0 =$ De-Broglie wavelength of H atom in ground state)

A) $\lambda_{n,z} \propto \left(\frac{1}{V_{n,z}}\right) \propto \left(\frac{n}{z}\right) \Rightarrow \left(\frac{n+1}{z}\right) + \left(\frac{n-1}{z}\right) = 3\left(\frac{1}{z}\right)$

$\Rightarrow 2n/z = 3 \Rightarrow z/n = 2/3 \Rightarrow z=2, n=3$

Species: He^{2+}

Q) Narendra Avasthi, At. Strct, L-2, Q-29.

A) $\lambda = \left(\frac{h}{mv}\right) \equiv \left(\frac{h}{m}\right) \left(\frac{h}{Ke^2}\right) \left(\frac{n}{z}\right) \Rightarrow \lambda = (2\pi) \left(\frac{n}{z}\right) \left(\frac{h^2}{mKe^2}\right)$

We are given, $3.4 = (13.6) \left(\frac{z}{n}\right)^2 \Rightarrow n/z = 2$

$\Rightarrow \lambda = (2\pi)(2)(0.529 \text{\AA}) \Rightarrow \lambda \approx 6.66 \text{\AA}$

Heisenberg Uncertainty Principle -

It is impossible to simultaneously measure exact pos. and exact momentum of a particle.

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

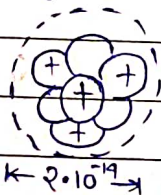
Δx = Uncertainty in Pos.

Δp = Uncertainty in Momentum.

Applications:

- 1) Proves that e^- doesn't exist in nucleus of atom.

Proof: If e^- in nucleus $\Rightarrow \Delta x \approx 2 \cdot 10^{-14} \text{ m}$



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

$$\Rightarrow \Delta v \geq \frac{6.6 \cdot 10^{-34}}{(4\pi) \cdot (2 \cdot 10^{-14}) \cdot (9.1 \cdot 10^{-31})}$$

$$\Rightarrow \Delta v \geq 3 \cdot 10^9 \text{ ms}^{-1}$$

Since error has to be $< c$.

Hence, contradiction $\Rightarrow e^-$ outside nucleus.

2) Proves that $(\Delta E)(\Delta t) \geq \hbar/4\pi$

Proof: $(\Delta x)(\Delta p) \geq \frac{\hbar}{4\pi} \Rightarrow (\Delta x) \underbrace{(\frac{\Delta p}{\Delta E})}_{\text{Work/Energy}} (\Delta E) \geq \frac{\hbar}{4\pi}$

$\Rightarrow (\Delta E)(\Delta t) \geq \frac{\hbar}{4\pi}$

3) Proves that $(\Delta x)(\Delta \lambda) \geq \lambda^2/4\pi$

Proof: $\lambda = \frac{\hbar}{p} \Rightarrow \Delta \lambda = \left| \frac{-\hbar(\Delta p)}{p^2} \right|$

$\Rightarrow (\Delta \lambda) = \left(\frac{\hbar}{p^2} \right) (\Delta p)$ (we only care about magnitude)

$\Rightarrow (\Delta x)(\Delta \lambda) = \left(\frac{1}{h} \right) \left(\frac{\hbar}{p} \right)^2 (\Delta x)(\Delta p) = \left(\frac{\lambda^2}{h} \right) (\Delta x)(\Delta p) \geq \left(\frac{\lambda^2}{4\pi} \right)$

$\Rightarrow (\Delta x)(\Delta \lambda) \geq \lambda^2/4\pi$

4) Proves that $(\Delta KE)(\Delta x) \geq \frac{\hbar v}{4\pi}$

Proof: K.E. = $\left(\frac{p^2}{2m} \right) \Rightarrow (\Delta KE) = \left(\frac{2p \Delta p}{2m} \right) = (v)(\Delta p)$

$(\Delta KE)(\Delta x) = v (\Delta x)(\Delta p) \Rightarrow (\Delta KE)(\Delta x) \geq \frac{\hbar v}{4\pi}$

Wave Mechanical Model -

This model explains stability of atom by considering Heisenberg's Uncertainty Principle & De Broglie Concept.

Schrodinger Time Independent Wave Eqⁿ

Derivation -

$$\left(\frac{\partial^2 \psi}{\partial x^2}\right) = \left(\frac{1}{v^2}\right) \left(\frac{\partial^2 \psi}{\partial t^2}\right)$$

ψ - Amplitude of e^- wave
(NOT a physical thing)

ω - Angular freq.

In 3D form,

$$\left(\frac{\partial^2 \psi}{\partial x^2}\right) + \left(\frac{\partial^2 \psi}{\partial y^2}\right) + \left(\frac{\partial^2 \psi}{\partial z^2}\right) = \left(\frac{1}{v^2}\right) \left(\frac{\partial^2 \psi}{\partial t^2}\right)$$

\Rightarrow Laplacian $\left(\nabla^2 \psi\right) = \left(\frac{1}{v^2}\right) \left(\frac{\partial^2 \psi}{\partial t^2}\right)$

Now, $\psi = \psi_0 e^{-i\omega t}$ (Solⁿ of Wave)

$$\Rightarrow \left(\frac{\partial^2 \psi}{\partial t^2}\right) = (-\omega^2) (\psi_0 e^{-i\omega t})$$

$$\Rightarrow \left(\frac{\partial^2 \psi}{\partial t^2}\right) = (-\omega^2) \psi$$

Now, $\omega = 2\pi \nu = \left(\frac{2\pi v}{\lambda}\right) \Rightarrow \omega = \left(\frac{2\pi v}{h}\right) p$

$$\left\{ \lambda = h/p \right\}$$

Substituting,

$$\left(\frac{\partial^2 \psi}{\partial t^2} \right) = - \left(\frac{e \hbar v}{h} \rho \right)^2 \psi = (-\psi) \left(\frac{v \cdot mv}{h} \right)^2$$

Substituting,

$$\nabla^2 \psi = \left(\frac{1}{v^2} \right) (-\psi) \left(\frac{v \cdot mv}{h} \right)^2 = (-\psi) \left(\frac{m^2 v^2}{h^2} \right)$$

Now,

$$\text{Total Energy} = \text{K.E.} + \text{P.E.}$$

$$\Rightarrow E = \frac{1}{2} mv^2 + V$$

$$\Rightarrow E = \left(\frac{m^2 v^2}{2m} \right) + V \Rightarrow m^2 v^2 = (2m)(E - V)$$

Substituting,

$$\nabla^2 \psi = (-\psi) \left(\frac{2m(E - V)}{h^2} \right)$$

$$\Rightarrow \left(\frac{\partial^2 \psi}{\partial x^2} \right) + \left(\frac{\partial^2 \psi}{\partial y^2} \right) + \left(\frac{\partial^2 \psi}{\partial z^2} \right) + \frac{2m(E - V)\psi}{h^2} = 0$$

$$\nabla^2 \psi + \frac{2m(E - V)\psi}{h^2} = 0$$

Schrodinger Time Dependent Wave Eqⁿ

Derivation -

$$\psi = \psi_0 e^{-i\omega t} \Rightarrow \left(\frac{\partial \psi}{\partial t} \right) = (-i\omega) \psi_0 e^{-i\omega t}$$

$$\Rightarrow \left(\frac{\partial \psi}{\partial t} \right) = (-i\omega) \psi$$

Now, $E = h\nu = \frac{h\omega}{2\pi} \Rightarrow \omega = \left(\frac{E}{\hbar} \right)$

Substituting, $\left(\frac{\partial \psi}{\partial t} \right) = (-i) \left(\frac{E}{\hbar} \right) \psi$

$$\Rightarrow E\psi = \hbar i \left(\frac{\partial \psi}{\partial t} \right)$$

Now, $\nabla^2 \psi + 2m(E - V)\psi = 0$

$$\Rightarrow E\psi = V\psi - \left(\frac{\hbar^2}{2m} \right) \nabla^2 \psi$$

$$\Rightarrow \left[\hbar i \left(\frac{\partial \psi}{\partial t} \right) = V\psi - \left(\frac{\hbar^2}{2m} \right) \nabla^2 \psi \right]$$

$$\Rightarrow \left[E\psi = \hat{H}\psi \right] \quad \left(\hat{H} = V - \left(\frac{\hbar^2}{2m} \right) \nabla^2 \right)$$

Hamilton's EqⁿHamiltonian
Operator

(Ψ has no physical significance)
as it is a complex no.

Sub

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In 1927, Schrodinger described behaviour of e^- using his wave eqⁿs.

The term Ψ^2 (sq. of magnitude of Ψ) has physical significance. It gives Probability Density of finding an e^- per unit volume.

Orbital - Space where probability of finding e^- is max. (> 90%)

(Acc. to Bohr) Orbit / Shell

Orbital (acc. to Schrodinger)

Circular region in which e^- revolves.

Space where probab. of finding e^- max. (> 90%)

Shape is circular

Shapes are complex.

Max. no. of $e^- = 2n^2$

Max. no. of $e^- = 2$

Doesn't account for De Broglie Concept & Uncertainty Principle.

Accounts for De Broglie Concept & Uncertainty Principle.

By solving Schrodinger Wave eqⁿ we get 3 Quantum Nos. l, m, n .

[Bohr's Orbit = Shell in Wave Mech Model]

Quantum Nos.

⊕ 4 q'tys. which give complete info. of an e^- present in an atom.

It gives info. like Post., Energy, Angular Momentum, etc.

1) Principal (n) - Info. about shell of an e^- & Energy associated with it.

Eg:

n	1	2	3
Shell	K	L	M

2) Azimuthal (l) - Info. about subshell and Orbital Angular Momentum.

$$0 \leq l \leq n-1$$

Eg:

n=1,	l=0	1s	subshell
n=2,	l=0	2s	subshell
	l=1	2p	subshell
n=3,	l=0	3s	subshell
	l=1	3p	subshell
	l=2	3d	subshell

☆
$$\left(\begin{array}{l} \text{Orbital Angular} \\ \text{Momentum} \end{array} \right) = \left(\frac{h}{2\pi} \right) \sqrt{l(l+1)}$$

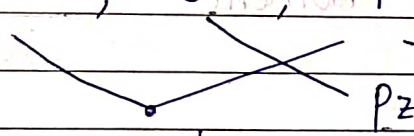
3) Magnetic (m) — Info. about orbital (Subsidiary Qntm. No.)

$$-l \leq m \leq l$$

n	l	m	(Orbital) Subshell
1	0	0	1s
2	0	0	2s
2	1	-1	2p _x
2	1	0	2p _z
2	1	1	2p _y

☆

for m = { -1, 0, 1 }



for m = { -2, 2, -1, 1, 0 }

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

☆

No. of orbitals in 'n' shell = n^2

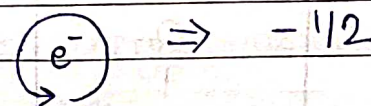
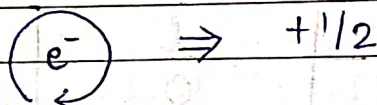
No. of orbitals in 'l' subshell = $2l+1$

No. of subshell in 'n' shell = n

4) Spin (s) - Info. about orientation of e^-

Acc. to this, $2e^-$ in an orbital always spin in opp. dirⁿ.

Sign Convention:



$S = \left(\frac{n}{2}\right)$ no. of unpaired e^-

$(\text{Spin Multiplicity}) = 2\left(\frac{n}{2}\right) + 1$ no. of unpaired e^-

$(\text{Spin magnetic Moment}) = \sqrt{4S(S+1)}$ B.M. Bohr magneton

$1 \text{ B.M.} = \left(\frac{eh}{4\pi m}\right) = 9.27 \cdot 10^{-24}$

$(\text{Magnetic Moment}) = \sqrt{n(n+2)}$ B.M.



for any shell $\opl�$

n

Subshell

n

Orbitals

n^2

e^- s

$2n^2$

for any subshell

l

Orbitals

$(2l+1)$

e^- s

$2(2l+1)$

Q) Find no. of e^- in -

i) $n=5$

ii) $n=4, l=2$

iii) $n=6, l=4, m=2$

iv) $n=3, l=0, m=0, s=-1/2$

A) i) $\# e^- = 2n^2 = 50$

ii) $\# e^- = 2(2l+1) = 10$

iii) $\# e^- = 2$

iv) $\# e^- = 1$

Q) Find no. of e^- in -

i) $n=5, m=1$

ii) $n=3, |m|=1$

iii) $n=4, s=1/2$

iv) $n=3, |m|=1, s=-1/2$

A) i) $l = \{0, 1, 2, 3, 4\}$; $m \in [-l, l]$

$l=1, m = \{-1, 0, 1\} \Rightarrow \# e^- = 3$

$l=2, m = \{-2, -1, 0, 1, 2\} \Rightarrow \# e^- = 5$

\vdots

$l=4, m = \{-4, \dots, 4\} \Rightarrow \# e^- = 9$

\Rightarrow

Total $\# e^- = 8$

$$\text{ii) } l = \{0, 1, 2\} ; m \in [-l, l]$$

$$l=1, m = \{-1, 0, 1\} \Rightarrow \#e^- = 4$$

$$l=2, m = \{-2, -1, 0, 1, 2\} \Rightarrow \#e^- = 4$$

$$\Rightarrow \boxed{\text{Total no. } e^- = 8}$$

iii) Half e^- have $s = +1/2$ & the others have $s = -1/2$

$$\Rightarrow \#e^- = \binom{2 \cdot 4^2}{2} \Rightarrow \boxed{\#e^- = 16}$$

$$\text{iv) } l = \{0, 1, 2\} ; m \in [-l, l]$$

$$l=1, m = \{-1, 0, 1\} \Rightarrow \#e^- = 2$$

$$l=2, m = \{-2, -1, 0, 1, 2\} \Rightarrow \#e^- = 2$$

$$\Rightarrow \boxed{\text{Total no. of } e^- = 4}$$

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Electronic Configuration

1) Aufbau's Principle -

e^- fill in subshell in inc. order of energy.

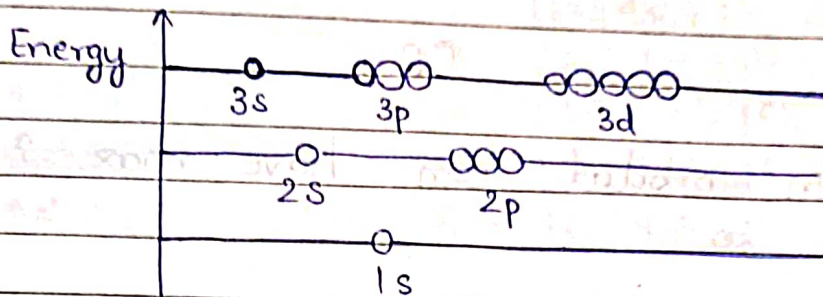
[Orbitals with same Energy \Rightarrow Degenerate]

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C-1: For H like atoms ($1e^-$ system),

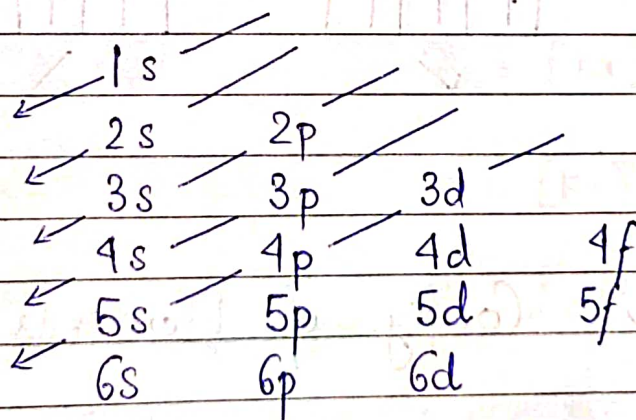
Energy depends only on 'n'.



C-2: For multi e^- system,

Energy depends only on 'n+l'.

If 'n+l' same, then $n \uparrow \Rightarrow$ Energy \uparrow



(1+0) (2+0) (2+1) (3+0) (3+1) (4+0) (3+2) (4+1) (5+0)

1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s

[School School Public School Public School Delhi Public School
Delhi Public School Free Delhi Public School Free Delhi Public]

1s 2s 2p 3s 3p 4s 3d 4p 5s 4d 5p 6s 4f 5d 6p 7s 5f 6d 7p]

2) Pauli's Exclusion Principle -

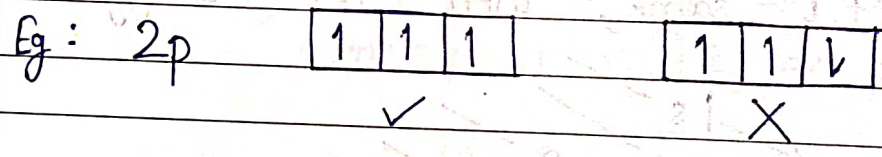
No 2 e⁻ can have all 4 quantum same nos

OR

An orbital can have max. 2 e⁻s with opp. spin

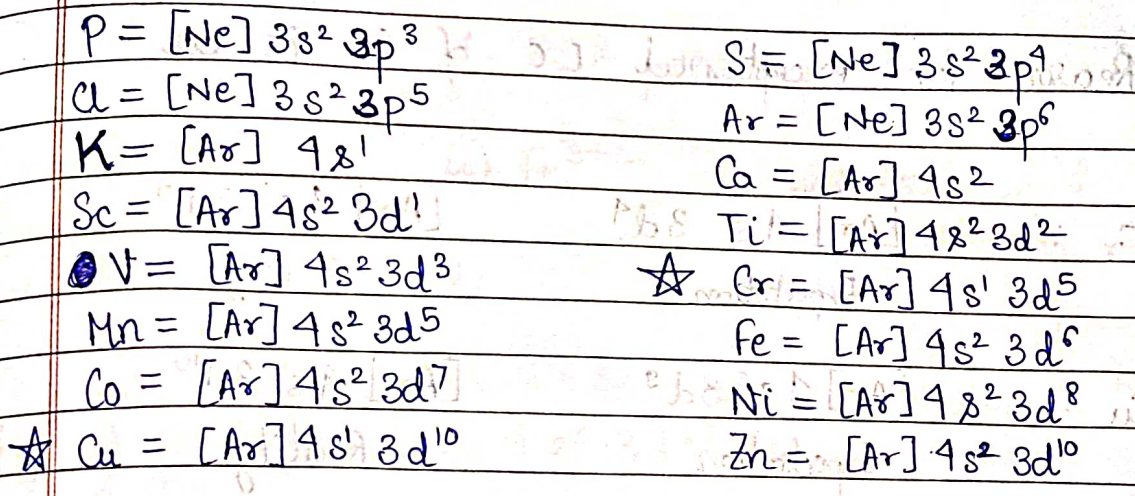
3) Hund's Rule of Max. multiplicity -

e⁻ don't pair until all degenerate orbitals are filled with e⁻ with // spin. half.

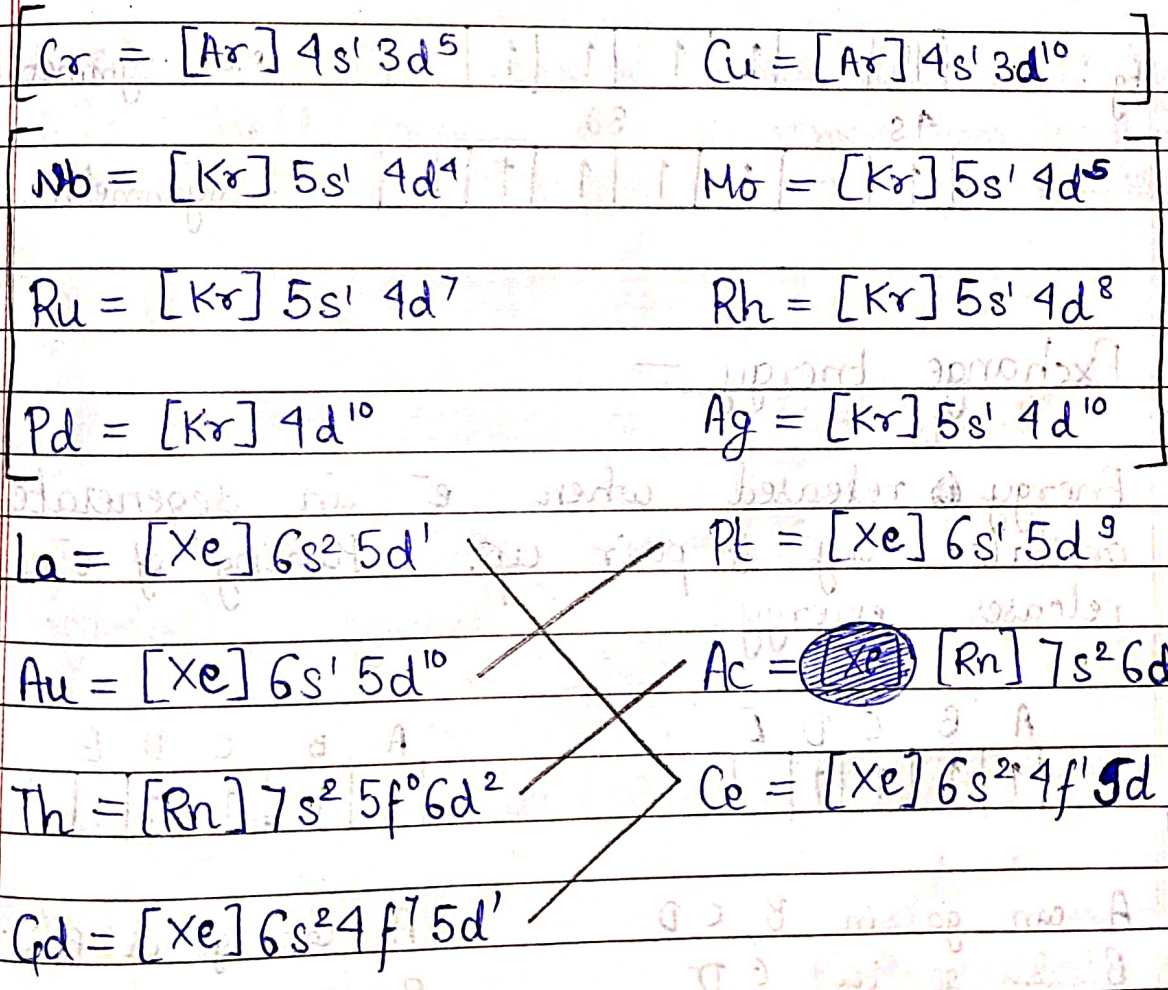


Electronic Config. of Elements upto Z=30.

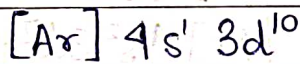
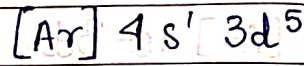
- | | |
|---|---|
| H = 1s ¹ | He = 1s ² |
| Li = [He] 2s ¹ | Be = [He] 2s ² |
| B = [He] 2s ² 2p ¹ | C = [He] 2s ² 2p ² |
| N = [He] 2s ² 2p ³ | O = [He] 2s ² 2p ⁴ |
| F = [He] 2s ² 2p ⁵ | Ne = [He] 2s ² 2p ⁶ |
| Na = [Ne] 3s ¹ | Mg = [Ne] 3s ² |
| Al = [Ne] 3s ² 3p ¹ | Si = [Ne] 3s ² 3p ² |



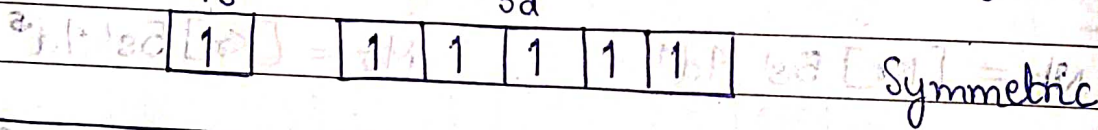
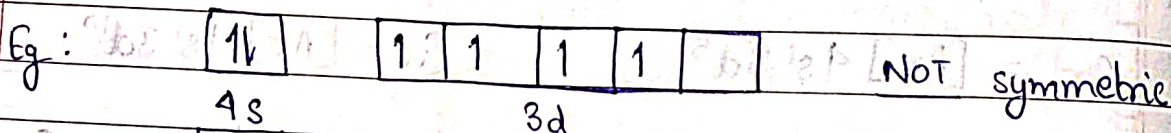
\star Exceptional E.C. —



Reason for exceptional E.C. of Cr & Cu = 9

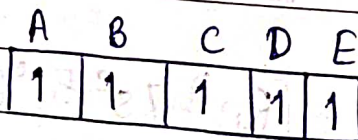
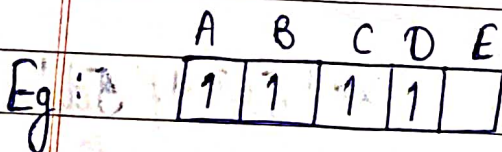


1) Symmetric E.C. —



2) Exchange Energy —

Energy released when e⁻ in degenerate orbitals try to pair up. Pairing of e⁻ releases energy. exchange exchange



- A can go in B, C, D
- B can go in C, D
- C can go in D

- A can go in B, C, D, E
- B can go in C, D, E
- C can go in D, E
- D can go in E

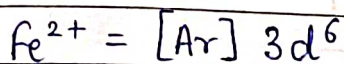
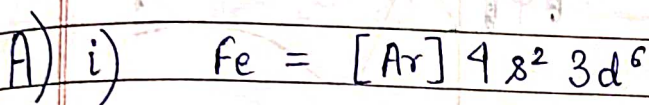
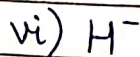
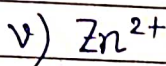
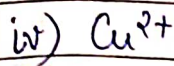
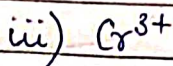
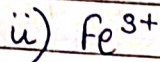
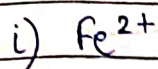
Exchanges = 6

Exchanges = 10

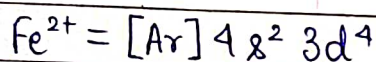
$$\left(\text{No. of Exchanges} \right) = {}^n C_2 + {}^m C_2 ; \quad n = \text{no. of } 1e^- \text{ in degenerate orbitals} \\ m = \text{no. of } 1e^- \text{ in degenerate orbitals}$$

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Q) Write E.C of the following species -

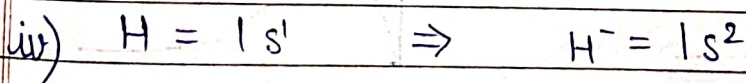
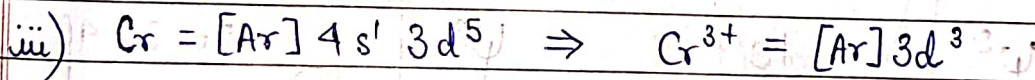
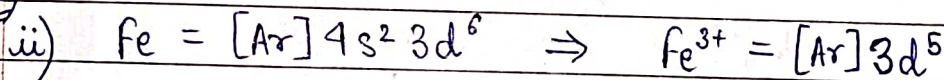


✓

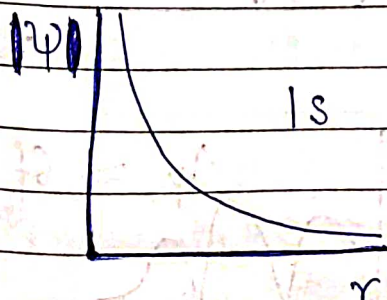


✗

★ e^- ALWAYS removed from last shell (largest n).
If shell same, the e^- remove from largest energy subshell.

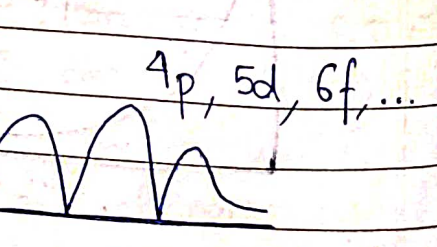
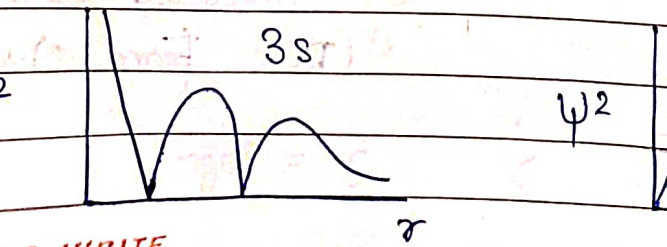
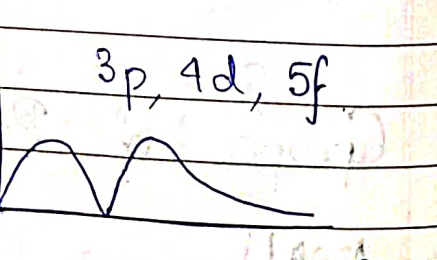
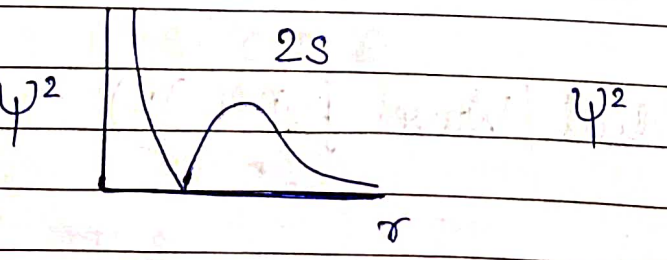
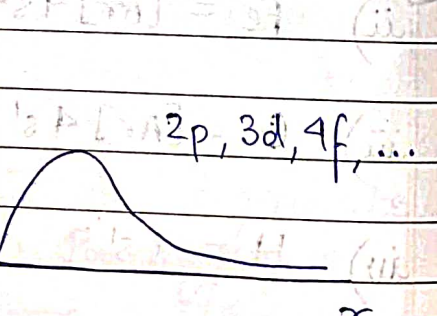
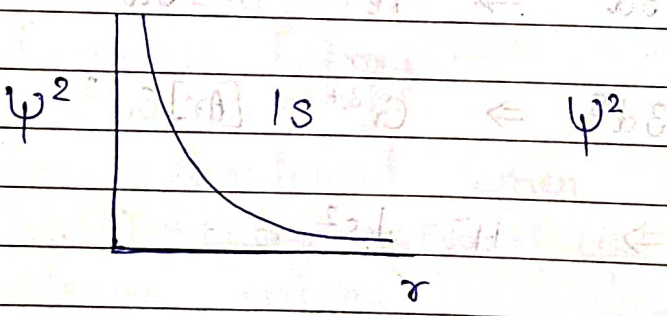
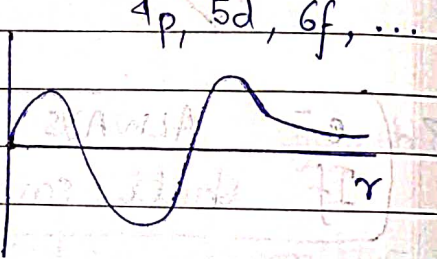
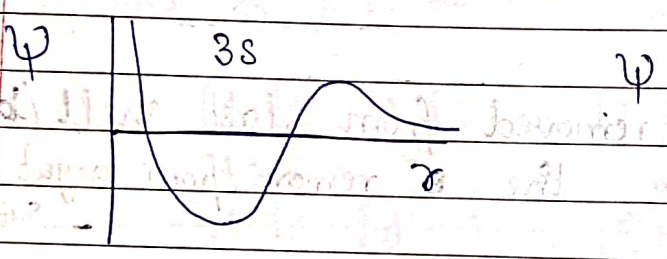
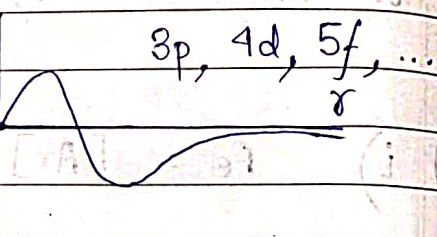
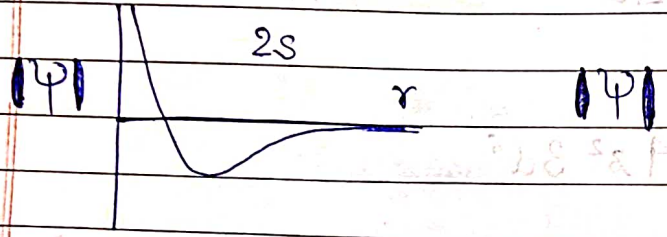
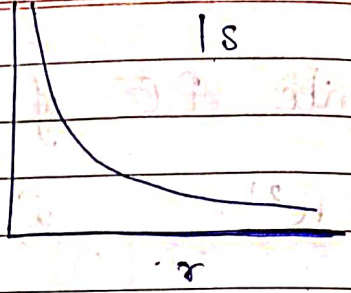
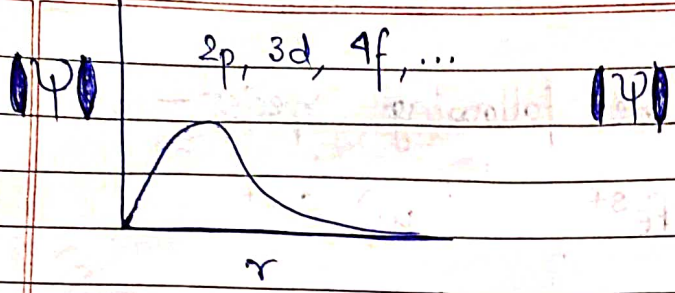


Graph of Radial/Wave $f_{x^n}(\psi)$ -

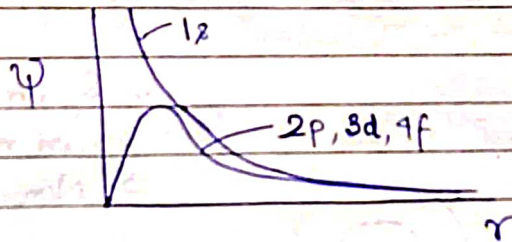


1s

$r =$ Radial dist
(Dist. from Nucleus)



Note: In all graphs portion starting from origin in p, d, f graph is BELOW s graph

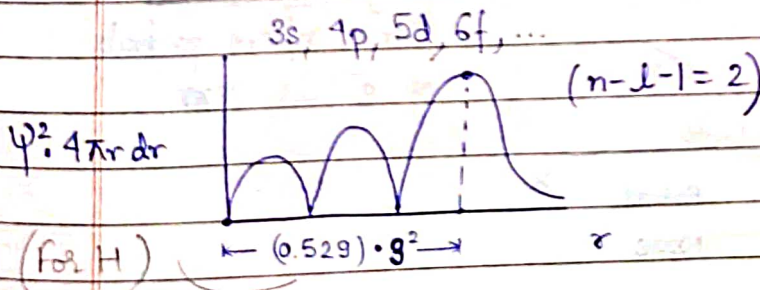
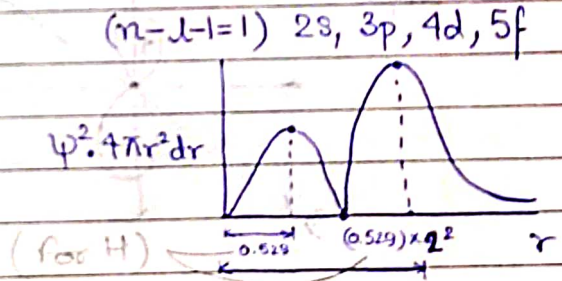
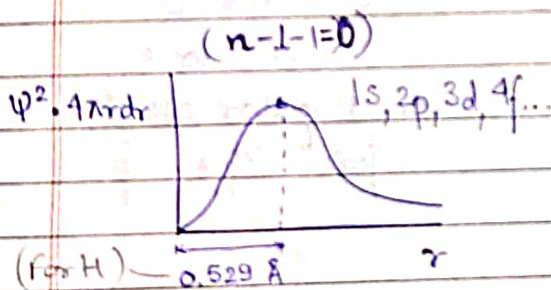


Probability = $\psi^2 \cdot 4\pi r^2$
(in small vol.)



Probab. of finding e^- b/w r & $r+dr$ dist.

Graph of Probability Distribution Curve:



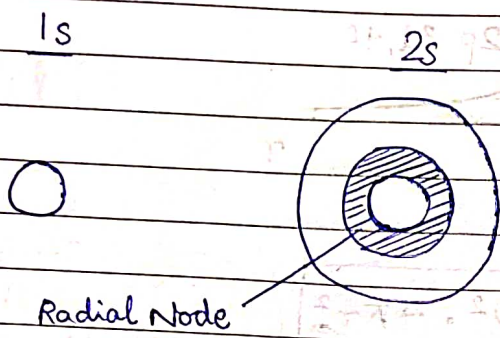
☆ (# Radial Nodes)
= $(n-l-1)$

- Probability = 0 \Rightarrow Radial node

 Region where probab. of finding $e^- = 0$

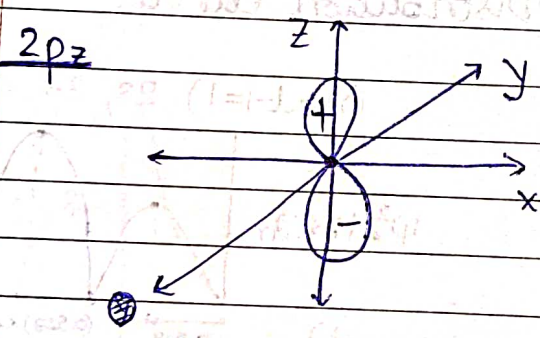
Shapes of Atomic Orbitals —

1) S orbital: (+ and - give sign of Ψ in the region)

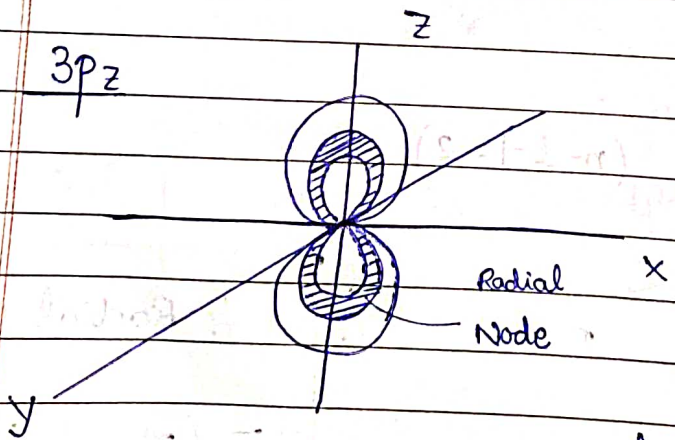


✓ Symmetrical in nature
⇒ Non directional

2) p orbital:



xy plane is Nodal Plane or Angular Node for $2p_z$

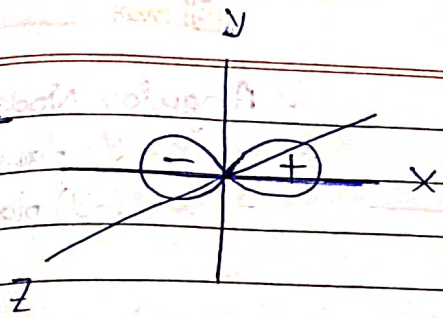


Angular Node: Plane where probab. of e^- is zero.

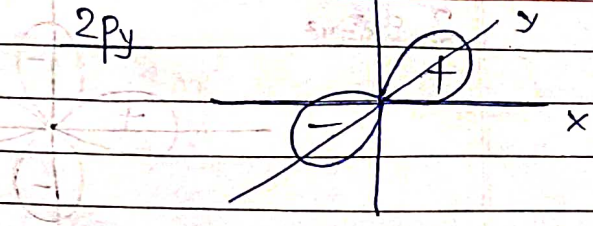


(# Angular Node)
= l

2p_x



2p_y

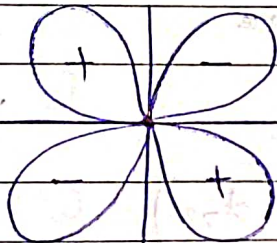


✓ Dumbbell shape

✓ Directional in nature

3) d orbital:

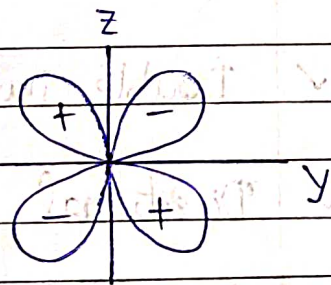
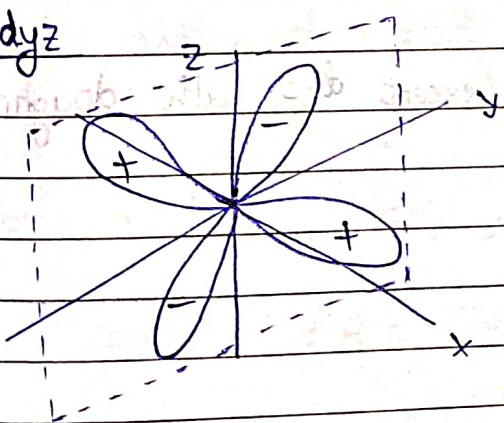
3d_{xy}



✓ Angular Nodes -

- YZ plane (x=0)
- XZ plane (y=0)

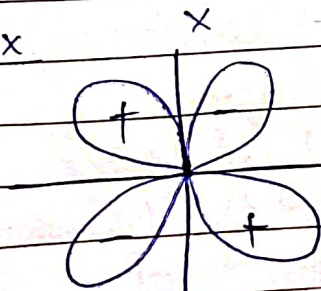
3d_{yz}



✓ Angular Nodes

- XZ plane (y=0)
- XY plane (z=0)

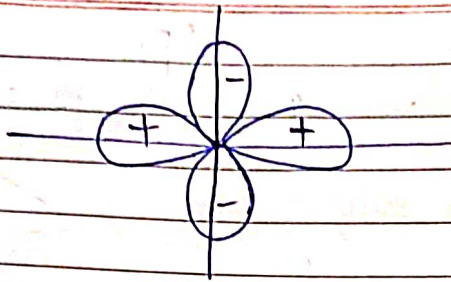
3 d_{zx}



✓ Angular Nodes -

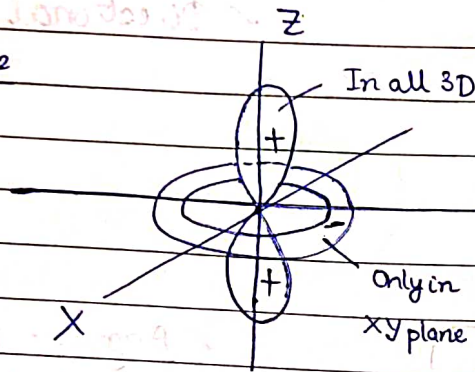
- XY plane (z=0)
- YZ plane (x=0)

3 $d_{x^2-y^2}$

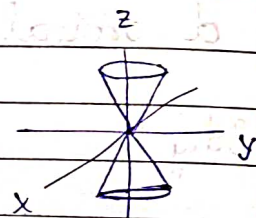


- ✓ Angular Nodes -
- $x=y$ plane
- $x=(-y)$ plane

3 d_{z^2}



- ✓ Angular Nodes -
- 2 cones.



★ No Nodal plane in d_{z^2}

- ✓ Double Dumbbell Shape (except d_{z^2} with doughnut shape)
- ✓ Directional in nature

★ Q) Find dist. at which probab. of finding e^- is max. for 1s orbital in He atom. ψ for orbital given as -

$$\psi = \left(\frac{1}{a_0^{3/2}} \right) \left(e^{-\frac{2r}{a_0}} \right)$$

$$A) \psi^2 = \left(\frac{16}{a_0^3}\right) \left(e^{-4r/a_0}\right) \Rightarrow P(r) = 4\pi r^2 \cdot \psi^2$$

$$\Rightarrow P(r) = \left(\frac{64\pi}{a_0^3}\right) r^2 e^{-4r/a_0}$$

$$\Rightarrow \left(\frac{dP(r)}{dr}\right) = \left(\frac{64\pi}{a_0^3}\right) \left[2r e^{-4r/a_0} - \left(\frac{4}{a_0}\right) r^2 e^{-4r/a_0} \right] = 0 \quad \text{for max.}$$

$$\Rightarrow \boxed{r = a_0/2}$$

★
Q) Consider ψ for 2s orbital of H atom as

$$\psi = \left(\frac{1}{4\sqrt{2\pi}}\right) \left(\frac{1}{a_0^{3/2}}\right) \left[2 - \frac{r}{a_0} \right] e^{-r/2a_0}$$

Find dist. of radial node.

A) For radial node, $\psi = 0$, $\psi^2 = 0$,

$$\Rightarrow \left(2 - r/a_0\right) = 0 \Rightarrow \boxed{r = 2a_0}$$

★
Q) If an orbital is represented by $\left\{ \sigma = \frac{2r}{a_0} \right\}$

$$\psi = \left(\frac{2}{3}\right) \left(\frac{1}{3a_0}\right)^{3/2} (\sigma - 1) (\sigma^2 - 8\sigma + 12) \sigma e^{-\sigma/2} \cos(\theta)$$

belongs to which orbital.



- A)
- 1) Since ϕ is not present, it can only be Z purely.
 - 2) If ϕ is present, Z is ^{NOT} ~~totally~~ ^{present} ~~absent~~.
 - 3) To find radial nodes, $\psi = 0$ or $\psi^2 = 0$.
no. of
 - 4) Take highest common factor of r or σ out of bracket. Its power = (# Angular Nodes)

Now, (# Radial) = $n - l - 1 = 3$ $\left((\sigma - 1)(\sigma^2 - 8\sigma + 12) \right)$
 (# Angular) = $l = 1$ $\left(\sigma^1 \right)$

$\Rightarrow n = 3, l = 1 \Rightarrow 3p_z$ orbital

Imp. Pts. — $0 = (0, 0, \pm a)$

- 1) Even if 1 e^- unpaired \Rightarrow Paramagnetic.
- If all e^- paired \Rightarrow Diamagnetic.