

10/6/22

DATE _____
PAGE _____

91

Atomic Structure

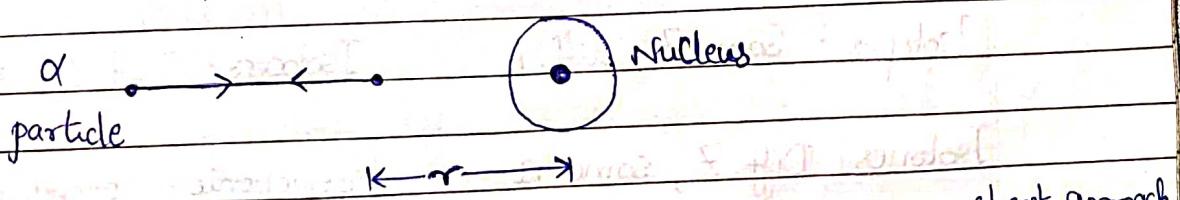
Cathode Rays : from cathode to anode. (-ve) charge.
e/m ratio const. Also called electrons.

Anode Rays : from anode to cathode. (tve) 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	$9.1 \cdot 10^{-31} \text{ kg}$	$1.67 \cdot 10^{-27} \text{ kg}$	$1.67 \cdot 10^{-27} \text{ kg}$
Charge	$-1.6 \cdot 10^{-19} \text{ C}$	$+1.6 \cdot 10^{-19} \text{ C}$	0 C

Closest Approach (Rutherford's Experiment) —



At closest dist., initial K.E. of particle = P.E. at dist. r

$$k = 9 \cdot 10^9 \text{ Nm}^2 \text{C}^{-2} \Rightarrow \text{GOOD WRITE}$$

$$\frac{1}{2} mv^2 = k \frac{(2e^-)(ze^-)}{r}$$

at no. of
element used

92

Some Imp. Terms -

DATE: ___/___/___
PAGE ___

1) At. No. (Z) : No. of protons

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

$$n = A - Z$$

$n = \# \text{ neutrons}$

$Z = \# \text{ protons}$



Atom represented by $\frac{A}{Z} X$.

$A = \text{Mass No.}$

(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 $A = 37 \Rightarrow n + p = 37 \Rightarrow n + e = 38$

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

$$\begin{aligned} n + e &= 38 \\ 10e + 9e &= 38 \\ \Rightarrow e &= 18 \\ \Rightarrow p &= 17 \end{aligned}$$

Ion : $\text{Cl}^{37}_{17} \text{Cl}^-$

Isotopes : Same Z , diff. A

Isobars : Diff Z , same A .

Isobones : Diff. Z , same n

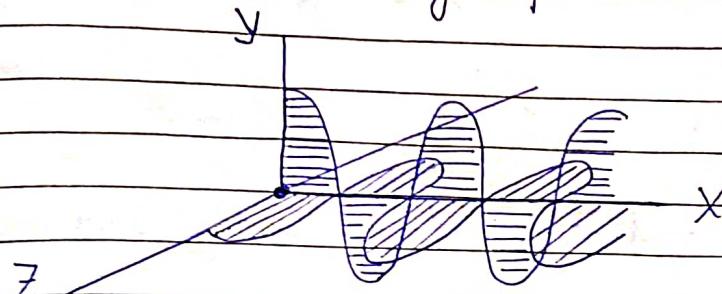
Isoelectronic : Species with same # e^-

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

Isosters : Molecules of diff. comp. with same # e^- & same # atoms

GOOD WRITE

Maxwell's Theory of E.M. radiation -



y - Electric , z - Magnetic , x - Propagation

It is form of energy which contains electric & magnetic fields oscillating 1 to each other, and both 1 to dirxn of propagation of radiation.

38)

Characteristics -

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

94

(Later proved wrong)

DATE: ___/___/___
PAGE ___

(6)

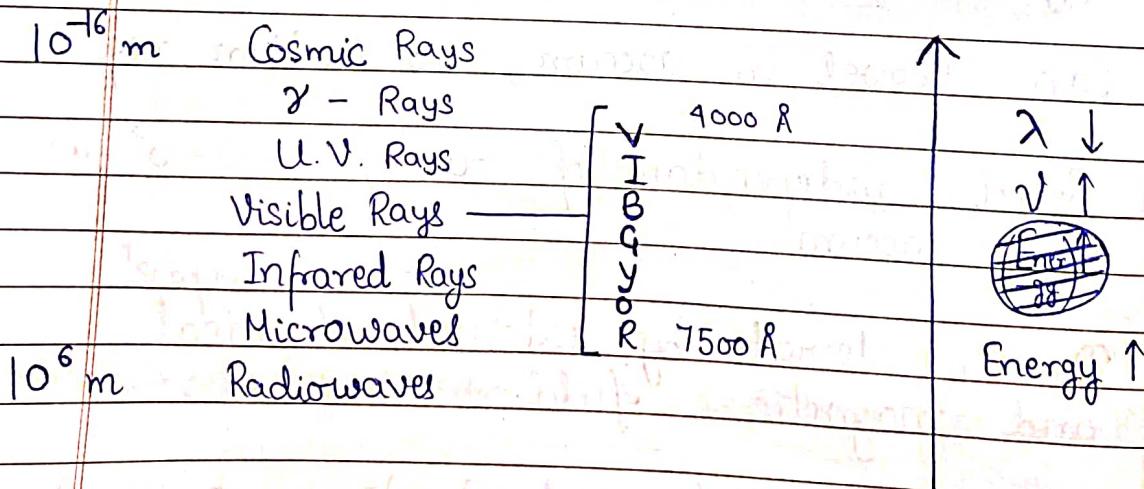
(Energy of Radiation) \propto (Intensity of light used)

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.



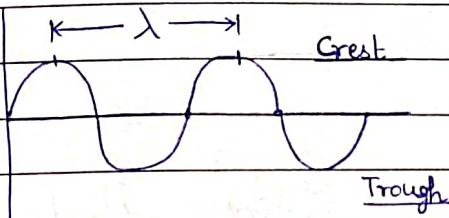
(1)

GOOD WRITE

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.



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

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

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

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

- 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.

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

GOOD WRITE

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

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

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

7) Angular freq. ω — $\omega = 2\pi\nu = \left(\frac{2\pi}{T}\right)$

Plank's Theory

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

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

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

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

$$\star \boxed{h = \hbar/2\pi}$$

GOOD WRITE

$$\boxed{E = hc\bar{\nu}}$$

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

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

no. of photons

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

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

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.

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

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

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

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

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

(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 remitted e^- .

A)

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

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

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

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

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

17/6/22

Photoelectric Effect

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

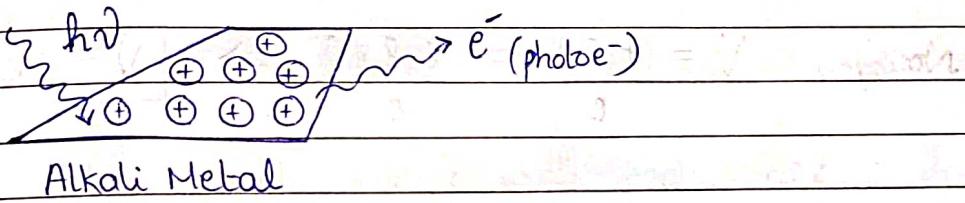


This explains particle nature of light. Only particles can transfer momentum. Hence, light acts like particle.

Conclusion:

- 1) e⁻ emit only if $\nu > \nu_0$ ← Threshold freq.
- 2) K.E. $\propto (\nu - \nu_0)$ (Light used)
(of photoelectron)
- 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

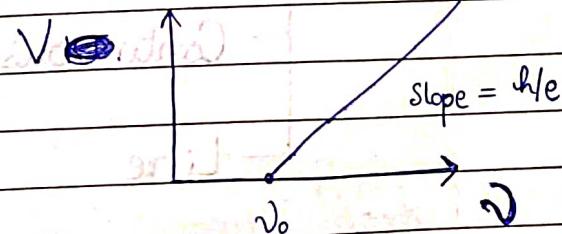
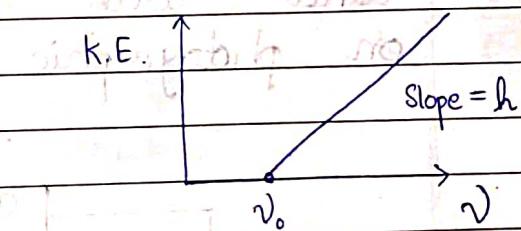
★ Threshold freq. It Energy depend on nature of metal.

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

Stopping Energy: Energy req. to stop photoe⁻.

Stopping Potential

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



100

DATE: ___/___/___
PAGE _____

Q) Calc. K.E. of photo e^- (in eV) emitted by a sodium metal when light of wavelength 100 nm strikes on it. The work f_x^n of sodium metal is 2.3 eV. Also calc. stopping potential.

A)

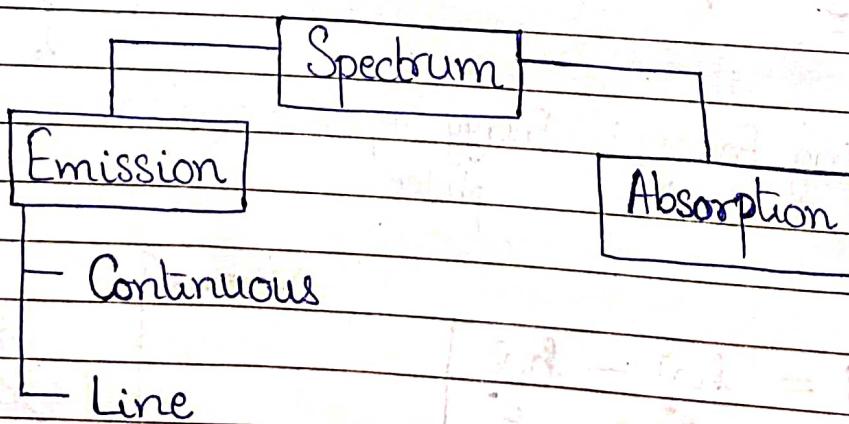
$$\text{K.E.} = h\nu - h\nu_0 = \left(\frac{12400}{1000}\right) - 2.3 \text{ eV}$$

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

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

Spectrum —

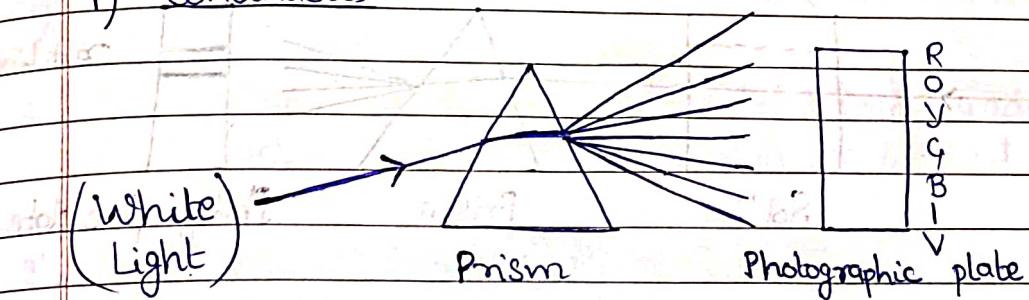
Series of radiations having diff. color bands with diff. wavelength obtained on photographic plate.



Emission Spectrum :

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

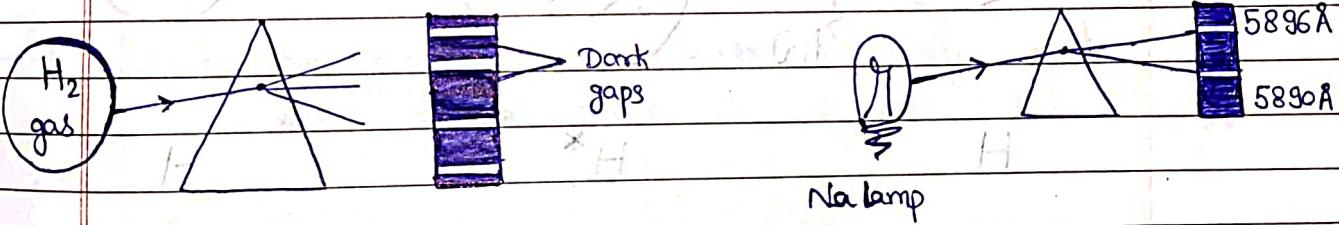
1) Continuous:



All color bands merge with each other.

No line of division b/w 2 colors; no gaps.

2) Line : (Fingerprint of element)

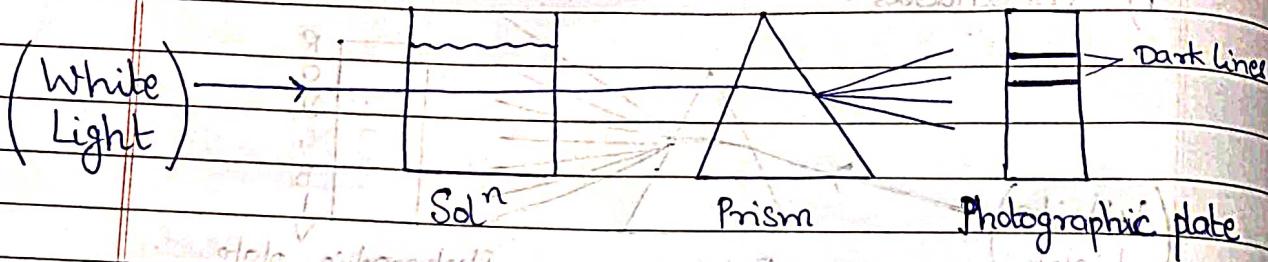


When radiation produced by passing electric discharge thru H₂ gas at low pressure, it is passed thru prism and received on photographic plate.

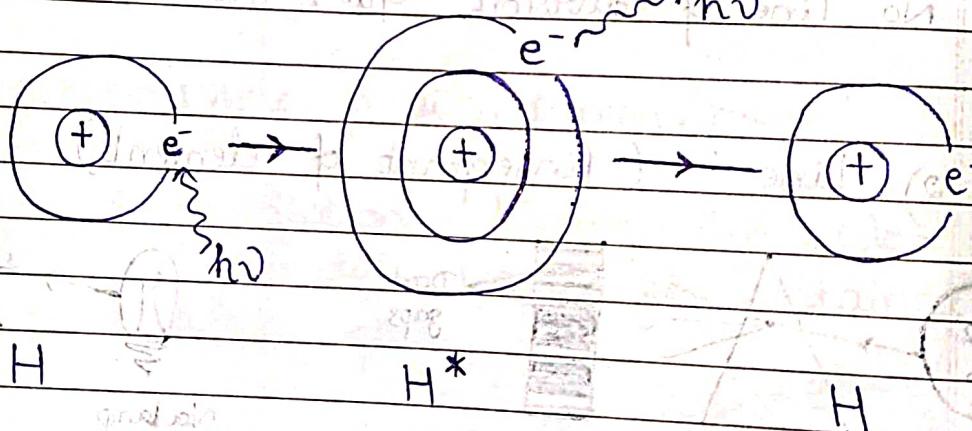
The line spectrum consists of sharp well defined lines which contain dark gaps b/w them.

Absorption Spectrum:

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



At atomic level,



GOOD WRITE

Bohr Model for Hydrogen like Species

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

Postulates :

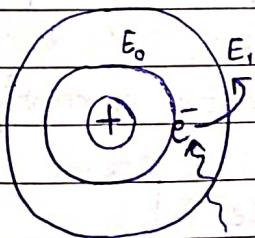
- 1) Atom consists nucleus, whose size is negligible compared to atom.
- 2) e^- revolve in fixed orbits of fixed radius and fixed vel. and fixed energy, around nucleus.
- 3) (Practically) Angular Momentum of e^- in orbit is an integral multiple of $\frac{h}{2\pi}$.

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

2nd orbit, $mvr = 2 \cdot \frac{h}{2\pi}$

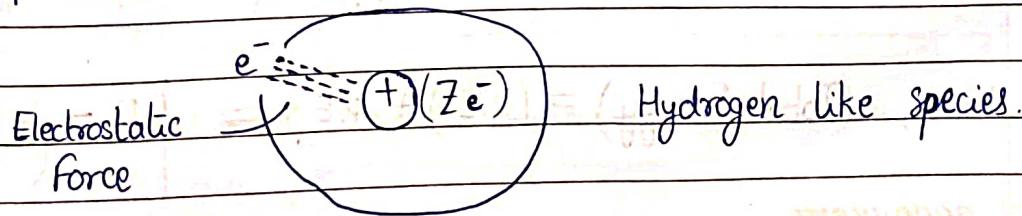
: nth orbit, $mvr = nh$

- 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



104
Since, electrostatic force acts as centripetal force.

$$Kq_1q_2 = m v_{n,z}^2 \Rightarrow K \cdot (e)(ze) = m v_{n,z}^2 / r_{n,z}$$

$$\Rightarrow Kze^2 = mv_{n,z}^2 r_{n,z} \quad \text{By Bohr's model,}$$

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

$$\Rightarrow v_{n,z} = \left(\frac{Ke^2}{h} \right) \left(\frac{z}{n} \right) \quad (\text{Vel.})$$

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

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

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

$$\Rightarrow T_{n,z} \propto \left(\frac{n^3}{z^2} \right) \Rightarrow \omega_{n,z} \propto \left(\frac{z^2}{n^3} \right) \quad (\text{Time Period}) \quad (\text{Freq.})$$

$$\text{Now, } K.E. = \frac{1}{2} m v_{n,z}^2 \quad \text{and} \quad Kze^2 = mv_{n,z}^2 r_{n,z}$$

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

$$\text{Now, } P.E. = \left(\frac{Kq_1q_2}{r_0} \right) = \frac{K(-e)(ze)}{r_{n,z}} \Rightarrow P.E. = \left(-\frac{Kze^2}{r_{n,z}} \right)$$

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



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

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

$$\Rightarrow E_{n,z} = \frac{(-K^2 e^4 m)}{h^2} \left(\frac{2\pi^2}{n^2} \right) \left(\frac{z^2}{n^2} \right) \quad E_{n,z} = \left(-m \right) \left(\frac{ke^2}{2} \right)^2 \left(\frac{z^2}{n^2} \right)$$

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

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

23/6/22

For H atom,

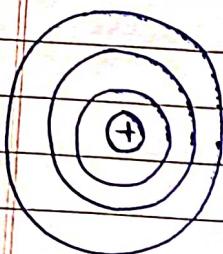
Orbit	Radius (\AA)	Velocity (m/s)	Total Energy (ev)	K.E.(ev)	P.E.(ev)
1st	0.529	$2.18 \cdot 10^6$	-13.6	13.6	-27.2
2nd	$(0.529)(2^2)$	$(2.18 \cdot 10^6)/2$	$(-13.6)/2^2$	$(13.6)/2^2$	$(-27.2)/2^2$
3rd	$(0.529)(3^2)$	$(2.18 \cdot 10^6)/3$	$(-13.6)/3^2$	$(13.6)/3^2$	$(-27.2)/3^2$
4th	$(0.529)(4^2)$	$(2.18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



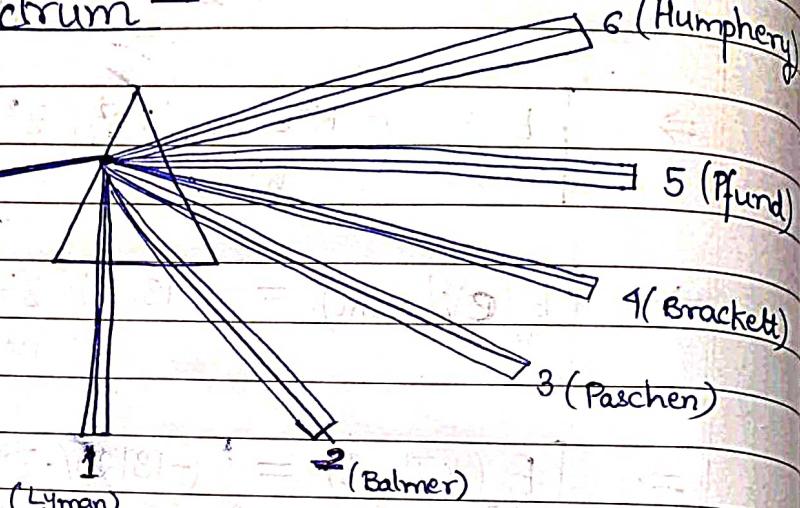
For H atom, it can also be written as

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

Hydrogen Spectrum



H atom

 $n = \infty$

Energy

U.V

(Lyman)

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)

A 8 Rays obtained from n^{th} series.

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

for H,

DATE: ___/___/___
PAGE: ___/107

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.	$n=5$	$n=6, 7, \dots$
Humphrey	I.R.	$n=6$	$n=7, 8, \dots$

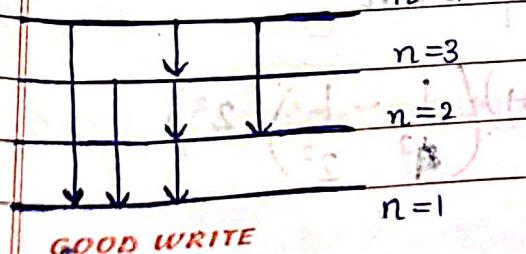
- ✓ Energy released/absorbed in transition.

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

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

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

- ✓ Max. no. of spectral lines (if ∞ atoms)



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

GOOD WRITE

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

A) For Balmer series, $n_2 = 2$

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

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

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

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

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.

$$E_{\text{photon}} = E_{n=1} - E_{n=2} = (-13.6) - (-0.85)$$

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

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

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

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

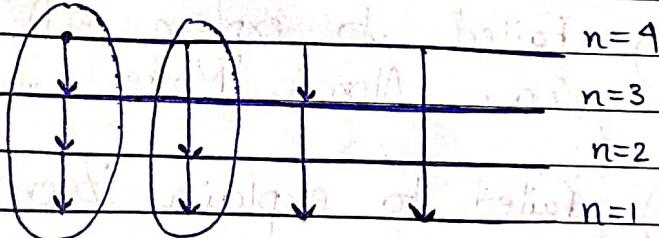
$$\Rightarrow \left(\frac{2}{n_2}\right) = 2 \text{ & } \left(\frac{2}{n_1}\right) = 1 \Rightarrow n_2 = 1, n_1 = 2$$

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.

In 2 atoms,



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

\Rightarrow (Distinct) Max. = 9
no. of lines

(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.

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

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

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

$$\Rightarrow \frac{(mv^2)}{(nh/mv)} = \frac{(3Ke^2)}{(nh/mv)^4} \Rightarrow v = \left(\frac{n^3 h^3}{24 K e^2 \pi^3 m^2} \right)^{1/2}$$

Drawbacks of Bohr's Atomic Model

- 1) Only valid for H & H-like species. It can't explain spectra of multi-electron system.
- 2) Failed to explain 3D structure of atom.
- 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
 - Heisenberg's Uncertainty Principle
 - De-Broglie Concept
 - Dual nature of matter
- 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,

$$E = h\nu \Rightarrow (E = hc) \quad (1)$$

$\nu, \lambda \rightarrow$ Wave Nature

Acc. to Einstein's theory of Relativity,

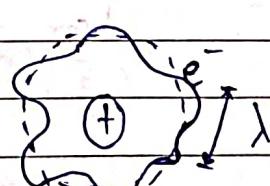
$$(E^2 = mc^2) - (2) \quad \text{Wavelength}$$

$$\lambda = \frac{h}{mc} \Rightarrow \lambda = \frac{h}{P}$$

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



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

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

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



In n th orbit, e^- makes n waves.
 $\Rightarrow (2\pi r = nh)$

24/6/22

E.M. WaveMatter Wave

Associated with Electric
et Magnetic field.

NOT associated with
Electric et Magnetic field.

Vel. $= c$ (in Vacuum)

Vel. $< c$

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

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

De-Broglie wavelength.

Significance of De-Broglie Eqn:

Although it is valid for whole material particle, it is significant 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. Reln's:

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

$$\sqrt{2m(K.E.)}$$

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

$$\sqrt{2mqV}$$

potential diff.

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

(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. (λ_0 = De-Broglie wavelength of H atom in ground state)

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

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

Species : He^{2+}

(Q) Narendra Avasthi, At. Sbctr, L-2, Q-29.

A) $\lambda = \left(\frac{h}{mv}\right) \equiv \left(\frac{h}{m}\right)\left(\frac{1}{Ke^2}\right)\left(\frac{n}{z}\right) \Rightarrow \lambda = (2\pi)\left(\frac{n}{z}\right)\left(\frac{h^2}{mKe^2}\right)$

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

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

Heisenberg Uncertainty Principle -

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

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

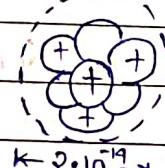
Δx = Uncertainty in Post

Δp = Uncertainty in Momentum.

Applications :

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

Proof: If e^- in nucleus $\Rightarrow \Delta x \approx 2 \cdot 10^{-19} m$



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

$$\Rightarrow \Delta v \geq 6.6 \cdot 10^{-34}$$

$$(4\pi) \cdot (2 \cdot 10^{-19}) \cdot (9.1 \cdot 10^{-31})$$

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

Since error has to be $< c$.

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

2) Proves that $(\Delta E)(\Delta t) \geq \frac{h}{4\pi}$

Proof: $(\Delta x)(\Delta p) \geq \frac{h}{4\pi} \Rightarrow (\Delta x)(\frac{\Delta p}{\Delta t})(\Delta t) \geq \frac{h}{4\pi}$

 $\Rightarrow (\Delta E)(\Delta t) \geq \frac{h}{4\pi}$ Work/Energy

3) Proves that $(\Delta x)(\Delta \lambda) \geq \frac{\lambda^2}{4\pi}$

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

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

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

$\Rightarrow (\Delta x)(\Delta \lambda) \geq \frac{\lambda^2}{4\pi}$

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

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

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

Wave Mechanical Model -

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

Schrodinger Time Independent Wave Eqn

Derivation -

$$\left(\frac{\partial^2 \psi}{\partial x^2} \right) = \left(\frac{1}{v^2} \right) \left(\frac{\partial^2 \psi}{\partial t^2} \right) \quad (\text{NOT a physical thing})$$

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

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

Now,

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

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

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

Now,

$$\omega = q\pi\nu = \left(\frac{2\pi v}{\lambda} \right) \Rightarrow$$

$$\boxed{\omega = \left(\frac{2\pi v}{h} \right) p}$$

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

Substituting,

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

Substituting,

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

Now, Total Energy = K.E. + 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, $\nabla^2 \psi = (-\psi) \left(\frac{2m(E-V)}{\hbar^2} \right)$

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

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

Schrodinger Time Dependent Wave Eqⁿ

Derivation -

$$\Psi = \Psi_0 e^{i\omega t} \Rightarrow \left(\frac{\partial \Psi}{\partial t} \right) = (-i\omega) \Psi_0 e^{i\omega t}$$

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

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

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

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

$$\text{Now, } \nabla^2 \Psi + 2m(E - V)\Psi = 0$$

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

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

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

Hamilton's Eqⁿ

Hamiltonian

Operator

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

DATE: ___/___/___
PAGE: ___

119

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

Circular region in which e^- revolves.

Shape is circular

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

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

Orbital (acc. to Schrodinger)

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

Shapes are complex.

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

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 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: if $n=1$, $l=0$

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

\star (Orbital Angular Momentum) = $\left(\frac{\hbar}{2\pi}\right)\sqrt{l(l+1)}$

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 $m = \{-1, 0, 1\}$

~~Pz~~

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

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

\star 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 (\pm) - Info. about orientation of e^-

Acc. to this, 2 e^- in an orbital always spin in opp. dir x^n .

Sign Convention:

$$(e^-) \Rightarrow +\frac{1}{2}$$

$$(e^-) \Rightarrow -\frac{1}{2}$$

$$S = \binom{n}{2} \text{ no. of unpaired } e^-$$

$$\text{Spin Multiplicity} = 2 \binom{n}{2} + 1 \quad \text{no. of unpaired } e^-$$

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

Bohr magneton

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

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

For any shell

Subshell

Orbitals

e^-

n

n

n^2

$2n^2$

for any subshell

Orbitals
 $(2l+1)$

e^-
 $2(2l+1)$

Q) Find no. of e^- in -

- i) $n=5$
- ii) $n=4, l=2$
- iii) $n=6, l=4, m=2$
- iv) $n=3, l=0, m=0, \delta=-1/2$

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) $n=4, \delta=1/2$

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

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

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

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

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

\Rightarrow

Total $\# e^- = 8$

iii) $\ell = \{0, 1, 2\}$; $m \in [-\ell, \ell]$

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

$$\ell = 2, m = \{-2, -1, 0, 1, 2\} \Rightarrow \# e^- = 8$$

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

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

$$\Rightarrow \# e^- = \left(2 \cdot 4^2\right) \Rightarrow \boxed{\# e^- = 16}$$

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

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

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

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

Electronic Configuration

i) Aufbau's Principle —

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

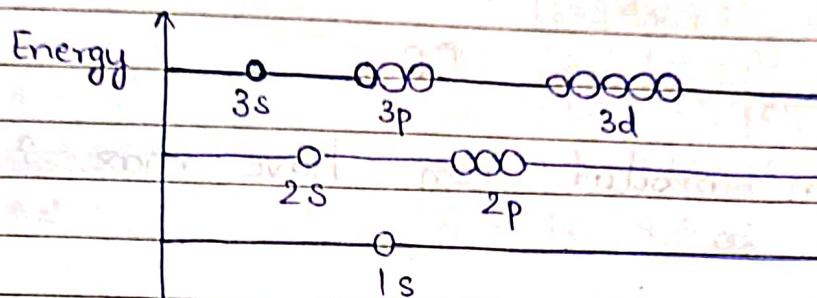
[Orbitals with same Energy \Rightarrow Degenerate]

DATE: _____
PAGE _____

125

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

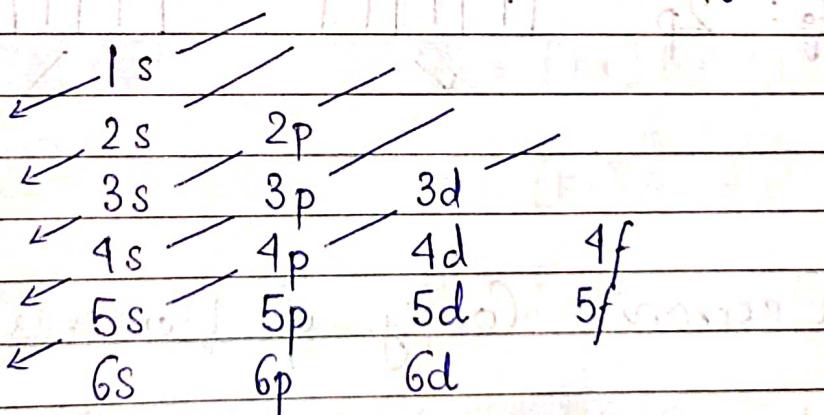
Energy depends only on 'n'.



C-2: For multi e^- system,

Energy depends only on ' $n+l$ '.

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



$$(1+0) \quad (2+0) \quad (2+1) \quad (3+0) \quad (3+1) \quad (4+0) \quad (3+2) \quad (4+1) \quad (5+0)$$

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

(S)chool (P)ublic (S)chool (P)ublic (S)chool (D)elhi (P)ublic (S)chool

(D)elhi (P)ublic (S)chool (F)ree (D)elhi (P)ublic (S)chool (F)ree (D)elhi (P)ublic

$$1s \quad 2s \quad 2p \quad 3s \quad 3p \quad 4s \quad 3d \quad 4p \quad 5s \quad 4d \quad 5p \quad 6s \quad 4f \quad 5d \quad 6p \quad 7s \quad 5f \quad 6d \quad 7p$$

2) Pauli's Exclusion Principle -

No 2 e^- can have all 4 quantum numbers same.

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.

Eg : $2p$

1	1	1
---	---	---

1	1	1
---	---	---

✓ X

Electronic Config. of Elements upto Z=30

$$H = 1s^1$$

$$He = 1s^2$$

$$Li = [He] 2s^1$$

$$Be = [He] 2s^2$$

$$B = [He] 2s^2 2p^1$$

$$C = [He] 2s^2 2p^2$$

$$N = [He] 2s^2 2p^3$$

$$O = [He] 2s^2 2p^4$$

$$F = [He] 2s^2 2p^5$$

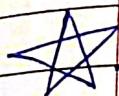
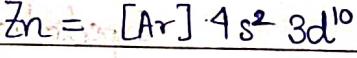
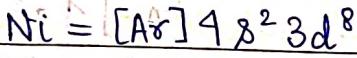
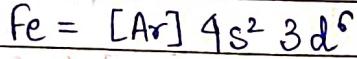
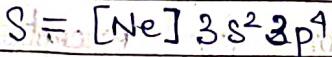
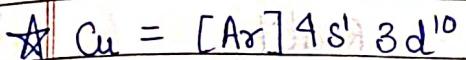
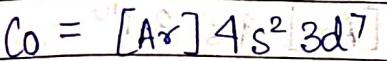
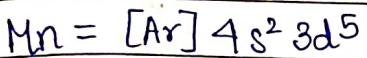
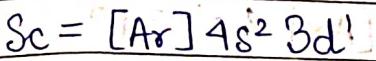
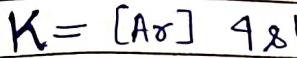
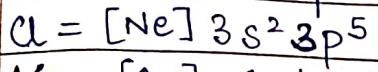
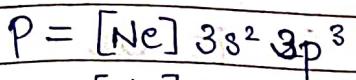
$$Ne = [He] 2s^2 2p^6$$

$$Na = [Ne] 3s^1$$

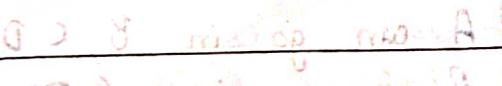
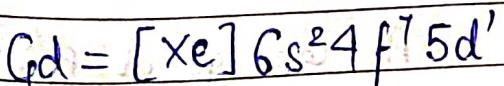
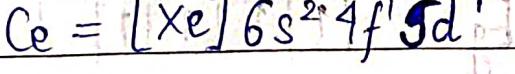
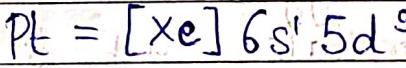
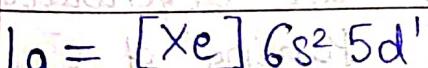
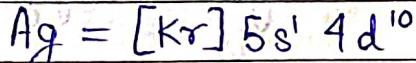
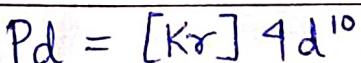
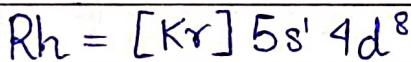
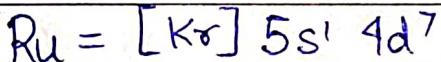
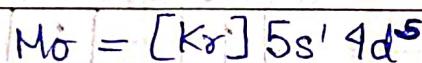
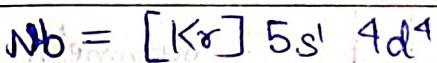
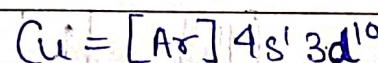
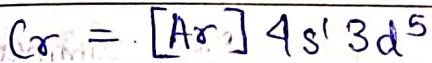
$$Mg = [Ne] 3s^2$$

$$Al = [Ne] 3s^2 3p^1$$

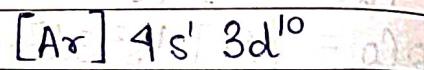
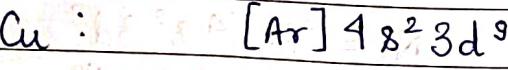
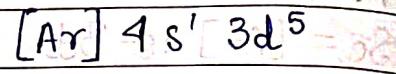
$$Si = [Ne] 3s^2 3p^2$$



Exceptional E.C. —



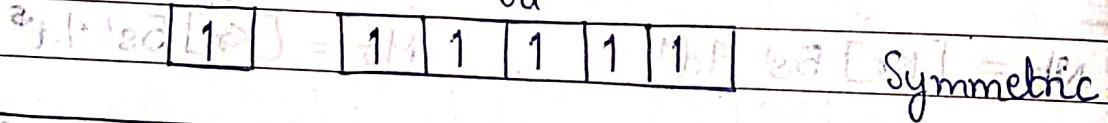
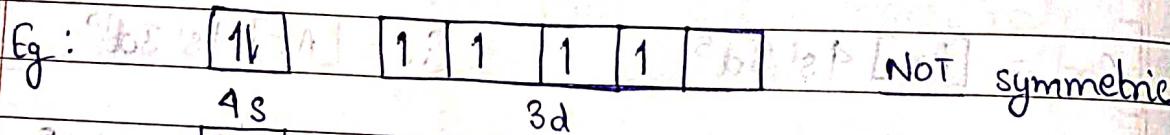
Reason for exceptional E.C. of Cr & Cu



Expectation

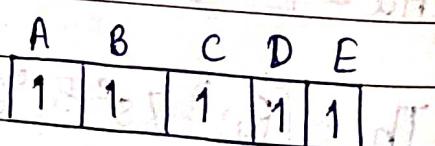
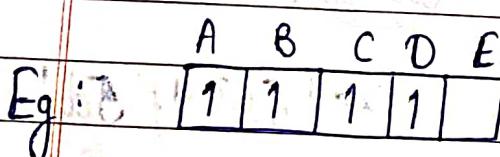
Reality

1) Symmetric E.C. -



2) Exchange Energy -

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



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

$$\# \text{ Exchanges} = 6$$

GOOD WRITE

- 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

$$\# \text{ Exchanges} = 10$$

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

156

Q) Write E.C. of the following species —

- i) Fe^{2+}
- ii) Fe^{3+}
- iii) Cr^{3+}
- iv) Cu^{2+}
- v) Zn^{2+}
- vi) H^-

A) i) $\text{Fe} = [\text{Ar}] 4s^2 3d^6$

$\text{Fe}^{2+} = [\text{Ar}] 3d^6$

✓

$\text{Fe}^{2+} = [\text{Ar}] 4s^2 3d^4$

X

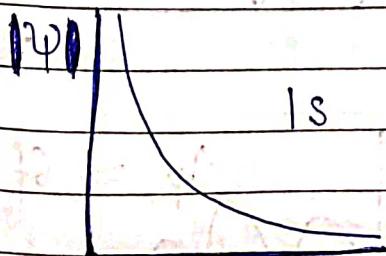
★ e^- ALWAYS removed from last shell (largest n).
 If shell same, the e^- remove from largest energy subshell.

iii) $\text{Fe} = [\text{Ar}] 4s^2 3d^6 \Rightarrow \text{Fe}^{3+} = [\text{Ar}] 3d^5$

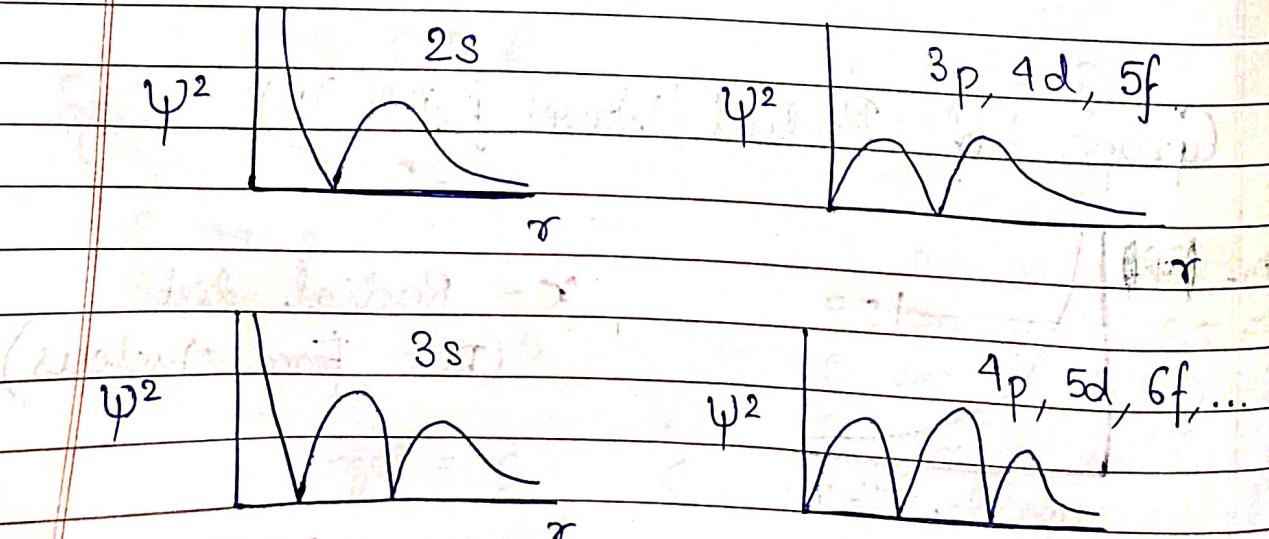
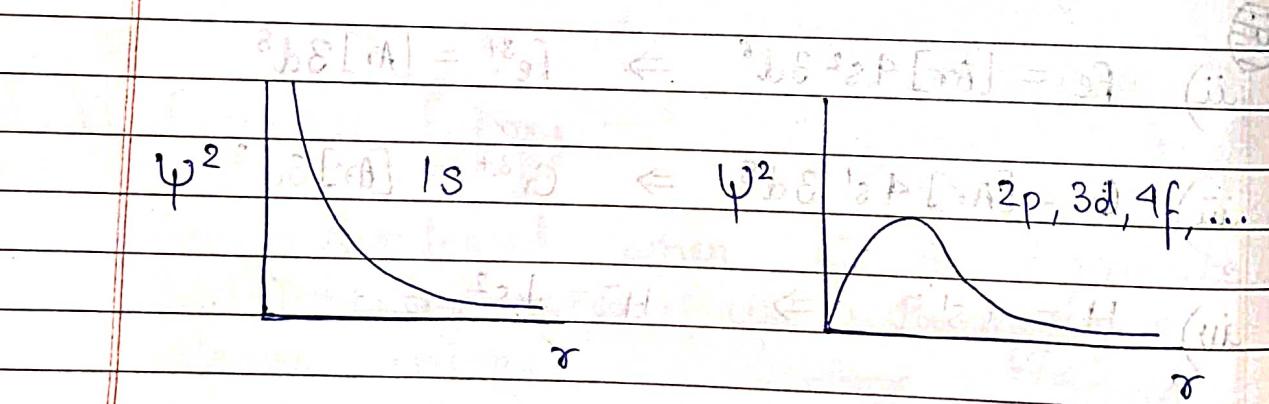
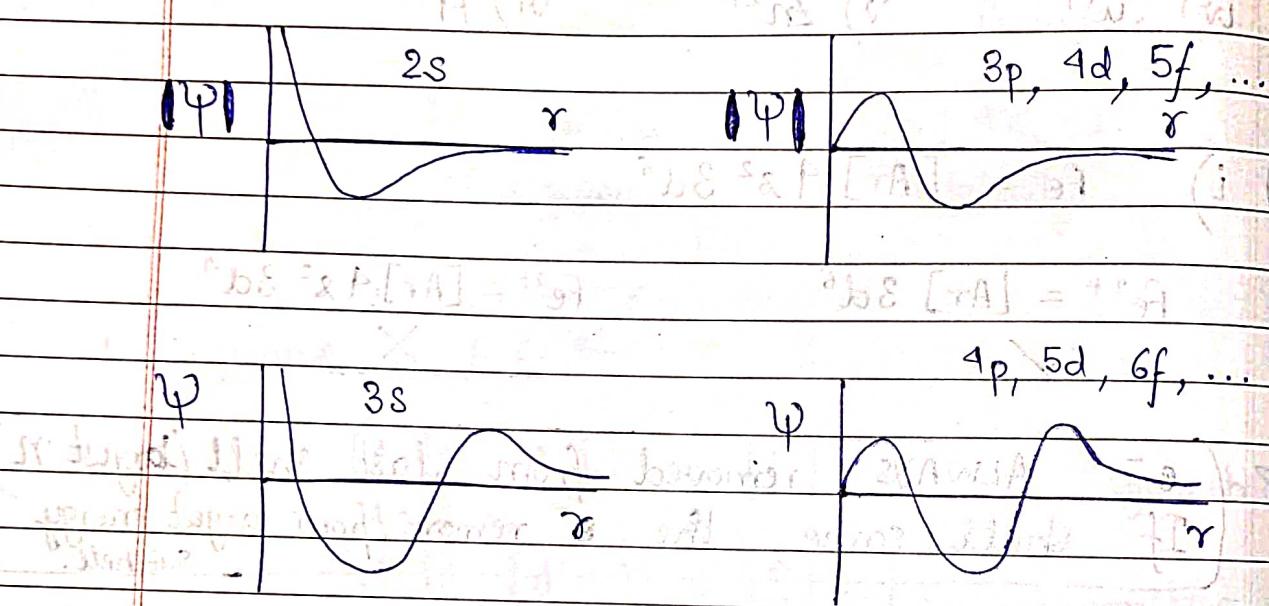
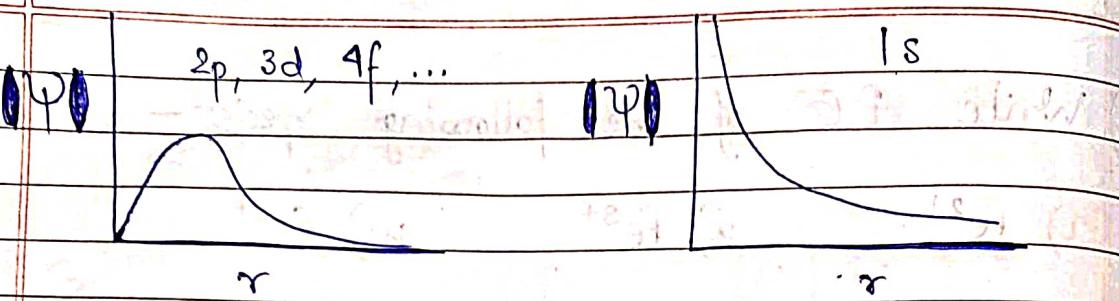
iv) $\text{Cr} = [\text{Ar}] 4s^1 3d^5 \Rightarrow \text{Cr}^{3+} = [\text{Ar}] 3d^3$

v) $\text{H} = 1s^1 \Rightarrow \text{H}^- = 1s^2$

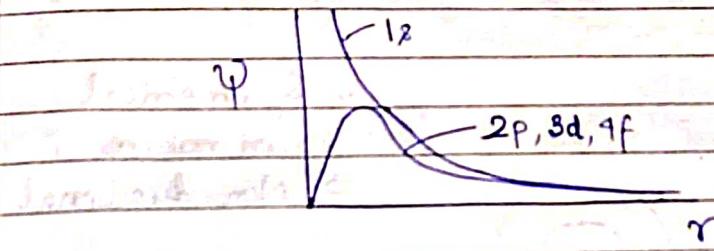
Graph of Radial/Wave $f x^n (\psi)$ —



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



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

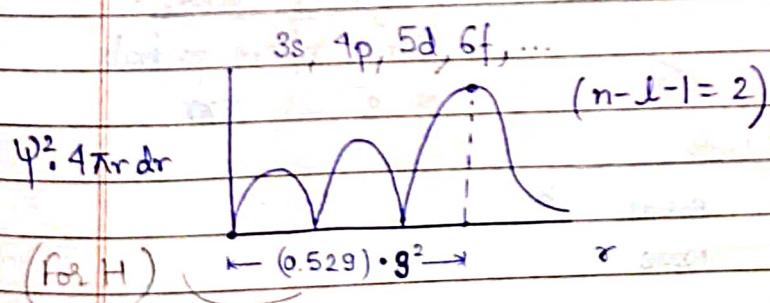
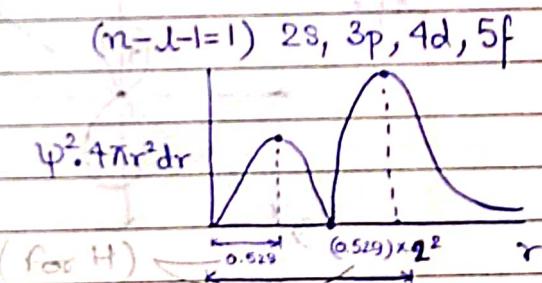
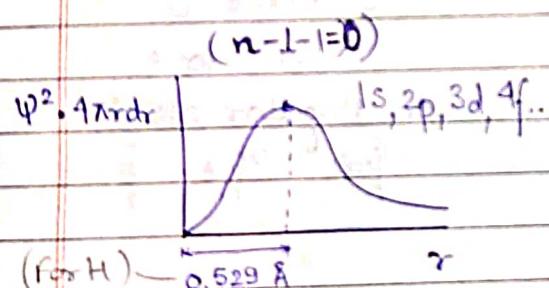


$$\text{Probability} = \psi^2 \cdot 4\pi r^2 dr \quad (\text{in small vol.})$$



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 $e^- = 0$

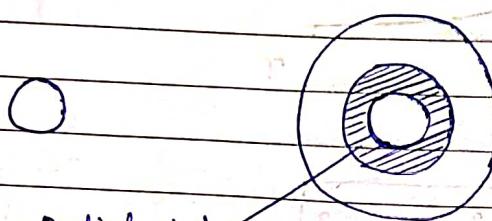
GOOD WRITE

Shapes of Atomic Orbitals

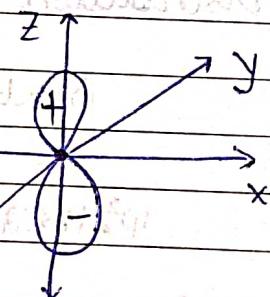
1) S orbital: (+ and - give sign of Ψ in the region)

 $1s$ $2s$

✓ Symmetrical
in nature.
⇒ Non directional

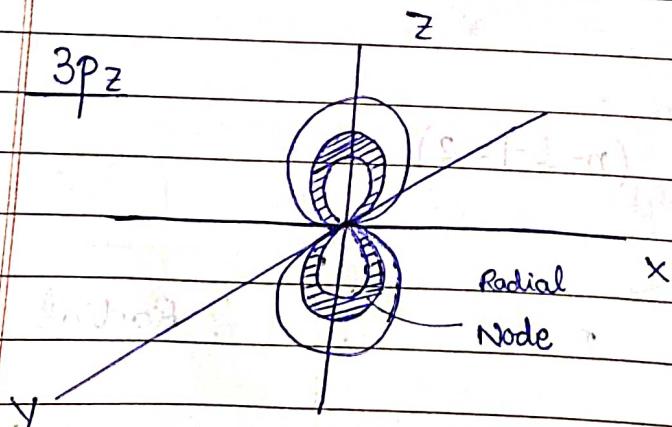


Radial Node

2) p orbital: $2p_z$ 

xy plane is
Nodal Plane

or Angular Node
for $2p_z$

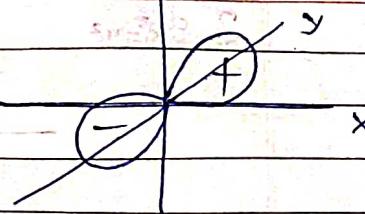
 $3p_z$ 

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



(# Angular Node)

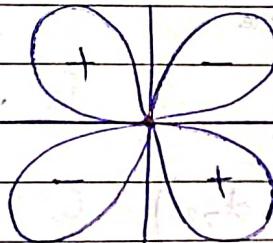
l

$2p_x$  $2p_y$  z

✓ Dumbbell shape

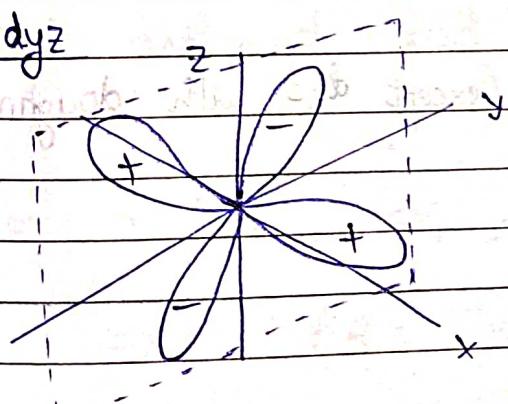
✓ Directional in nature

3) d orbital :

 $3d_{xy}$ 

✓ Angular Nodes -

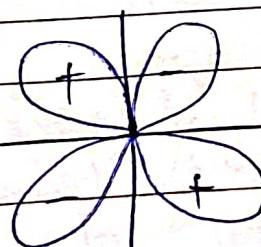
- YZ plane ($x=0$)
- XZ plane ($y=0$)

 $3d_{yz}$ 

✓ Angular

- XZ plane ($y=0$)

Nodes - XY plane ($z=0$)

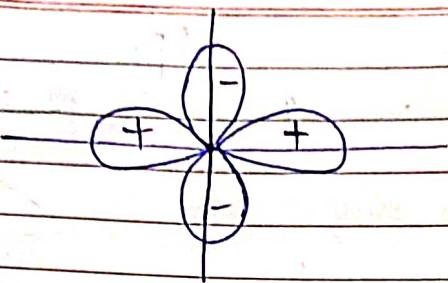
 $3d_{zx}$ 

✓ Angular Nodes -

- XY plane ($z=0$)

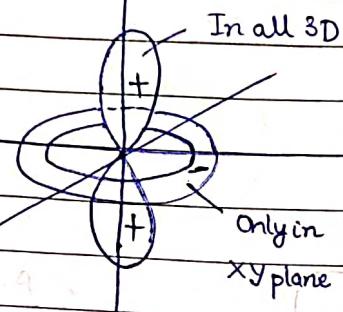
- YZ plane ($x=0$)

161

SPP DATE: ___/___/___
PAGE ___ $3d_{x^2-y^2}$ 

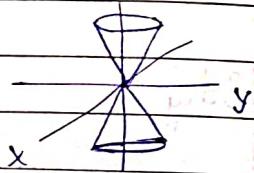
✓ Angular Nodes -

- $x = y$ plane
- $x = (-y)$ plane

 $3d_{z^2}$ only in
xy plane

✓ 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 prob. of finding e^- is max. for $1s$ orbital in He atom. Ψ for orbital given as -

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

GOOD WRITE

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

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

$$\Rightarrow \frac{dP(r)}{dr} = \left(\frac{64\pi}{a_0^3}\right) \left[2re^{-\frac{4r}{a_0}} - \left(\frac{4}{a_0}\right) r^2 e^{-\frac{4r}{a_0}} \right] = 0$$

$$r = \frac{a_0}{2}$$

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, $\Psi = 0, \Psi^2 = 0$,

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

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

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

belongs to which orbital.

- A) 1) Since ϕ is not present, it can only be z purely.
- NOT present
- 2) If ϕ is present, z is totally absent.
- 3) To find radial nodes, $\Psi = 0$ or $\Psi^2 = 0$.
- 4) Take highest common factor of r or σ out of bracket. Its power = (# Angular Nodes)

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

(# Angular) = $l = 1$ (σ^1)

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

Imp. Pts.

1) Even if 1 e⁻ unpaired \Rightarrow Paramagnetic.

If all e⁻ paired \Rightarrow Diamagnetic.