Vidyamandir Classes SINCE 1986

IIT JEE | MEDICAL | FOUNDATION

Atomic structure

Pauli's exclusion Principle → It states that No two e^-s in an atom can have the same set of all four quantum numbers.

or each orbital can accomodate max. $2e^-$ (with opposite spin or antiparallel spin)

Ex. $_2He = 1s^2$

$\boxed{\uparrow\uparrow}$ or $\boxed{\uparrow\downarrow}$ or $\boxed{\downarrow\uparrow}$ or $\boxed{\downarrow\downarrow}$

✓ ✓ wrong

$n=1$	$n=1$
$l=0$	$l=0$
$m_l=0$	$m_l=0$
$m_s=+\frac{1}{2}$	$m_s=+\frac{1}{2}$

wrong

Hund's rule of max. multiplicity → It states that Pairing of e^- in degenerate orbitals doesn't take place untill each orbital has got $1e^-$ each. i.e. singly occupied.

* The orbitals which have same value of n and l but diff. value of m_l, have same energy in the absence of external electric and magnetic field, known as degenerate orbitals.

Ex.

	$2P_x$	$2P_y$	$2P_z$
$n=$	2	2	2
$l=$	1	1	1
$m_l=$	-1	$+1$	0

degenerate orbitals.

$2P_x$ and $3P_y$ are not degenerate orbitals.

$3d_{xy}$, $3d_{yz}$, $3d_{xz}$, $3d_{x^2-y^2}$, $3d_{z^2}$ are degenerate orbitals.

Ex. $2p^3$

$\boxed{\uparrow\uparrow}\boxed{\uparrow}\boxed{}$ ×

✓ $\boxed{\uparrow}\boxed{\uparrow}\boxed{\uparrow}$ $s = \pm 3/2$, $M = 4$

× $\boxed{\uparrow}\boxed{\uparrow}\boxed{\downarrow}$ $s = \pm 1/2$, $M = 2$

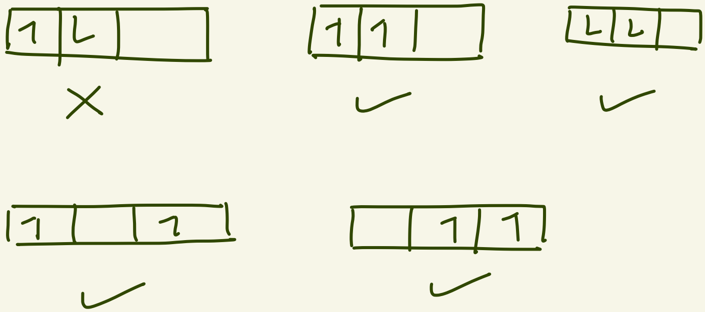
✓ $\boxed{\downarrow}\boxed{\downarrow}\boxed{\downarrow}$ $s = \pm 3/2$, $M = 4$

× $\boxed{\uparrow}\boxed{\downarrow}\boxed{\downarrow}$ $s = \pm 1/2$, $M = 2$

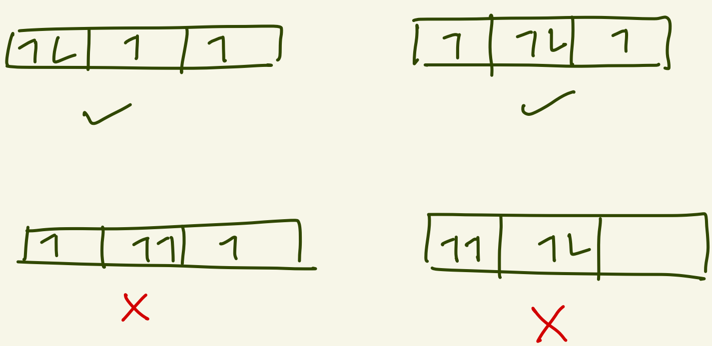
spin multiplicity $(M) = 2|s| + 1$

where s = total spin

Ex. $2p^2$



$2p^4$



Magnetic moment (spin magnetic moment), $\mu \rightarrow$

$$\mu = \sqrt{n(n+2)} \text{ Bohr magneton (B.M.)}$$

where n = No. of unpaired e^-

Q. Which of the following has max. magnetic moment? Write them in the increasing order of magnetic moment.

(i) Fe^{3+} (ii) Ni^{2+} (iii) Zn^{2+} (iv) V^{3+}

Solⁿ →

$Fe^{3+} = 1s^2, 2s^2 2p^6, 3s^2 3p^6 3d^5$

$\mu = \sqrt{5 \times 7} = \sqrt{35}$ B.M.

$Ni^{2+} = 1s^2, 2s^2 2p^6, 3s^2 3p^6 3d^8$

$\mu = \sqrt{2 \times 4} = \sqrt{8}$ B.M.

$Zn^{2+} = 1s^2, 2s^2 2p^6, 3s^2 3p^6 3d^{10}$

$\mu = 0$ (Diamagnetic)

$V^{3+} = 1s^2, 2s^2 2p^6, 3s^2 3p^6 3d^2$

$\mu = \sqrt{2 \times 4} = \sqrt{8}$ B.M.

$$Zn^{2+} < Ni^{2+} = V^{3+} < Fe^{3+}$$

129. The maximum number of electrons that can have principal quantum number, $n = 3$ and spin quantum number, $m_s = -\frac{1}{2}$ is ....

Solⁿ →

$n = 3 \Rightarrow$ 3s 3P 3d

Ans. = 9

Q. In an atom, the total number of electrons having quantum numbers $n = 4$, $|m_\ell| = 1$ and $m_s = -1/2$ is

[JEE(Advanced) 2014]

Solⁿ →

4s	4p	4d	4f
$m_\ell = 0$	$-1 \quad 0 \quad +1$	$-2 \; -1 \; 0 \; +1 \; +2$	$-3 \; -2 \; -1 \; 0 \; +1 \; +2 \; +3$

$m_s = -\frac{1}{2}$ type $= 6\ e^-$

Node → It is that zone in the space where probability of finding an e^- is zero.

Two types →

(1) Radial node or spherical node →

$$R.N. = (n - \ell - 1)$$

(2) Angular node or planar node →

$$A.N. = \ell$$

Total no. of nodes $= R.N. + A.N.$
$= n - 1$

orbital	R.N.	A.N.	T.N.
1s	0	0	0
2s	1	0	1
3s	2	0	2

2p	0	1	1
3p	1	1	2
3d	0	2	2
4d	1	2	3

Wave mechanical model of atom → The atomic model which is based on Particle and wave nature of the e^- is known as wave mechanical model of atom.

It was developed by schrodinger.

Schrodinger wave equation → According to this equation, e^- is assumed as 3-dimensional wave in the electronic field of Positively charged nucleus.

$$\frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2} + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0$$

where ψ (Psi) = wave function of e^-
or
amplitude function of e^-
or
Probablity function of e^-

x, Y, z = Cartesian coordinates

m = mass of e^-

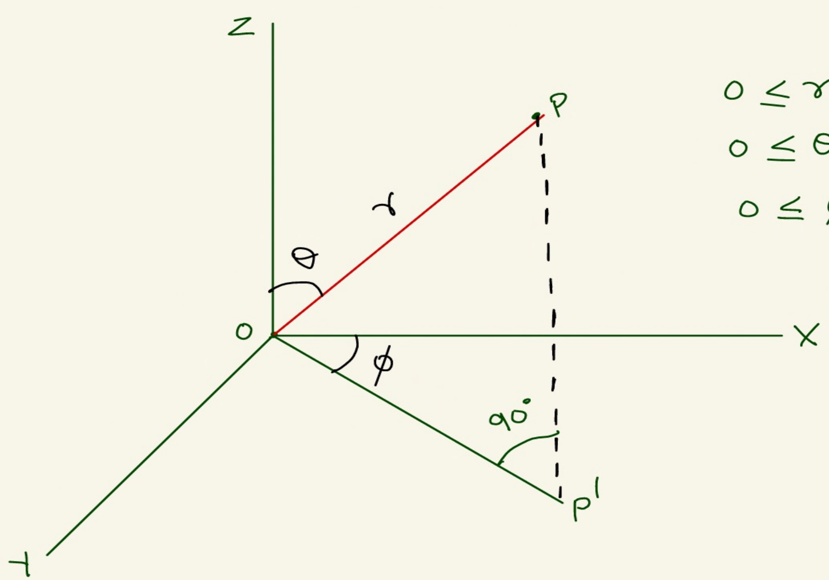
h = Planck's Const.

E = Total energy of e^-

V = Potential energy of e^-

By solving this equation, Probablity of finding an e^- is determined. When this equation is solved then it is observed that for some regions of space, value of ψ is positive and for other regions, value of ψ is negative. But the Probablity can never be negative. So ψ is not favouurable to use. So ψ^2 was introduced as a Probablity factor.

Polar coordinate system (r, θ, ϕ) →



$0 \leq r \leq \infty$

$0 \leq \theta \leq \pi$

$0 \leq \phi \leq 2\pi$

OP = Radial line

r = length of radial line = Radial distance

θ = angle between radial line and Z-axis

ϕ = angle between Projection of radial line in XY plane and X-axis

$$z = r\cos\theta$$

$$x = r\sin\theta\cos\phi$$

$$y = r\sin\theta\sin\phi$$

If cartesian coordinates are repalced by Polar coordinates then ψ will be obtained in the terms of r, θ, ϕ.

$$\psi(r, \theta, \phi) = \psi(r) \cdot \psi(\theta, \phi)$$

$\psi(r)$ ⇓ Radial function ⇓ Radial nodes can be calculated

$\psi(\theta, \phi)$ ⇓ Angular function ⇓ Angular nodes can be calculated

Types of Probablity curves →

(i) Radial Probablity curve →

Curve between $\psi(r)$ V/s r.
or
$R(r)$ V/s r

(ii) Angular Probablity curve $\rightarrow$

curve between $\psi(\theta, \phi)$ and angles. $\rightarrow$ or $A(\theta, \phi)$

Types of Radial Probablity curve $\rightarrow$

(a) curve between $\psi_{(r)}$ v/s r or $R(r)$ v/s r $\Rightarrow$ Radial Probablity function curve

(b) curve between $\psi^2_{(r)}$ v/s r or $R^2_{(r)}$ v/s r

$\Rightarrow$ Radial Probablity density curve.

(c) curve between $4\pi r^2 \psi^2_{(r)}$ v/s r

or

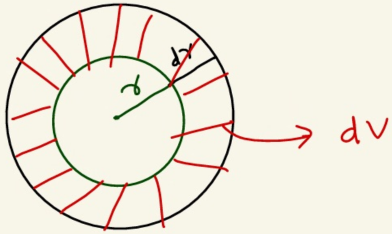
$4\pi r^2 R^2_{(r)}$ v/s r

or

P v/s r

is called Radial Probablity distribution curve.

* $\psi^2_{(r)}$ or $R^2_{(r)}$ refers to radial Probablity of finding an e^- in unit volume of an atom at distance r from the nucleus.



Total radial Probablity $= R^2_{(r)} \cdot dV$

$$dV = \frac{4}{3}\pi (r+dr)^3 - \frac{4}{3}\pi r^3$$

$$= \frac{4}{3}\pi \left(r^3 + (dr)^3 + 3r(dr)^2 + 3r^2 dr\right) - \frac{4}{3}\pi r^3$$

$\because$ dr is very small

$\therefore$ $(dr)^2, (dr)^3 \simeq 0$

$$dV = \cancel{\frac{4}{3}\pi r^3} + \left(\frac{4}{3} \times \pi \times 3r^2 dr\right) - \cancel{\frac{4}{3}\pi r^3}$$

$$dV = 4\pi r^2 dr$$

Total radial Probablity $= R^2_{(r)} \cdot 4\pi r^2 dr$

$$= 4\pi r^2 R^2_{(r)} \cdot dr = P \cdot dr$$

where P = radial Prob. distribution function

Radial wave functions of orbitals →

(1) 1s-orbital →

$$\psi_{(r)} = R_{(r)} = 2\left(\frac{Z}{a_0}\right)^{3/2} e^{-\frac{Zr}{na_0}}$$

H-atom $\Rightarrow Z = 1$, 1s $\Rightarrow n = 1$

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

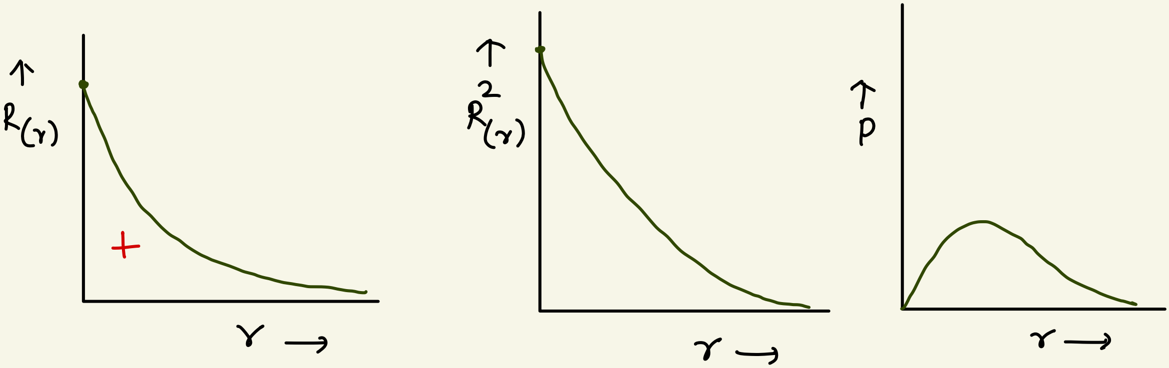
where z = atomic no

a_0 = bohr radius = 0.529 $\mathring{A}$

* Radial nodes at $r = 0$ (if present), $r = \infty$ are not counted.

$$R(r) = 0 \Rightarrow r = \infty \text{ only}$$

No. of radial node = 0



$$P = 4\pi r^2 R^2_{(r)}$$

at $r = 0 \Rightarrow P = 0$ for any orbital

(2) <u>2s orbital</u> →

$$R(r) = \frac{1}{2\sqrt{2}}\left(\frac{z}{a_0}\right)^{3/2}\left(2 - \frac{2zr}{na_0}\right)e^{-zr/na_0}$$

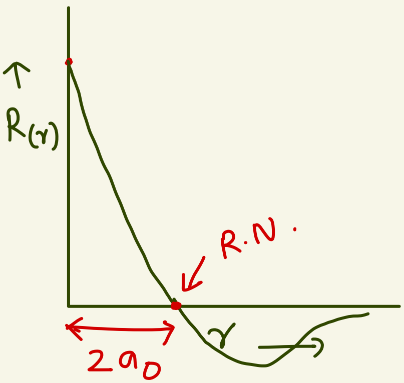
$2s \Rightarrow n = 2$, H-atom $\Rightarrow z = 1$

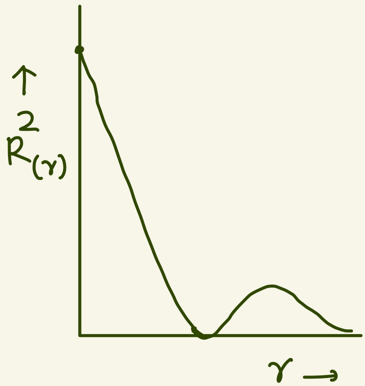
$$R(r) = \frac{1}{2\sqrt{2}}\left(\frac{1}{a_0}\right)^{3/2}\left(2-\frac{r}{a_0}\right)e^{-\frac{r}{2a_0}}$$

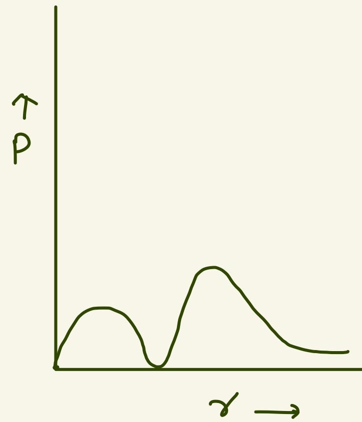
$$R(r) = 0 \Rightarrow r = \infty$$

$$2-\frac{r}{a_0} = 0 \Rightarrow r = 2a_0$$

No. of R.N. = 1







(3) 3s – orbital $\rightarrow$

$$R(r) = \frac{1}{9\sqrt{3}}\left(\frac{Z}{a_0}\right)^{3/2}\left(6-\frac{4Zr}{a_0}+\frac{4Z^2r^2}{9a_0^2}\right)e^{-\frac{Zr}{na_0}}$$

For H-atom $\Rightarrow Z = 1$, 3s orbital $\Rightarrow n = 3$

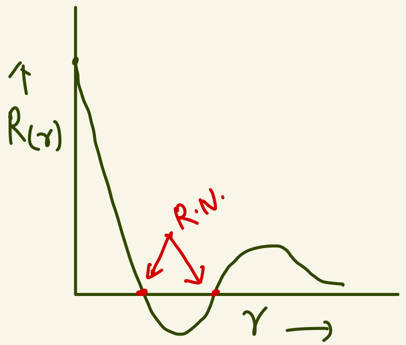
$$R(r) = \frac{1}{9\sqrt{3}}\left(\frac{1}{a_0}\right)^{3/2}\left(6-\frac{4r}{a_0}+\frac{4r^2}{9a_0^2}\right)e^{-\frac{r}{3a_0}}$$

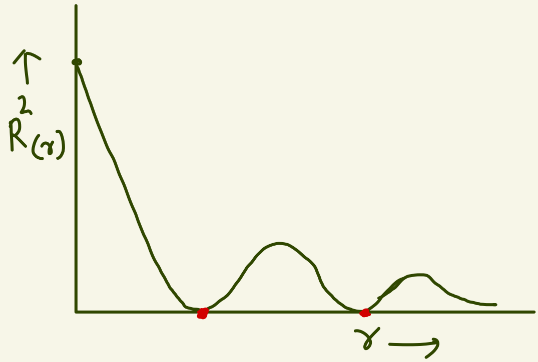
$R(r) = 0 \quad \Rightarrow \quad r = \infty$

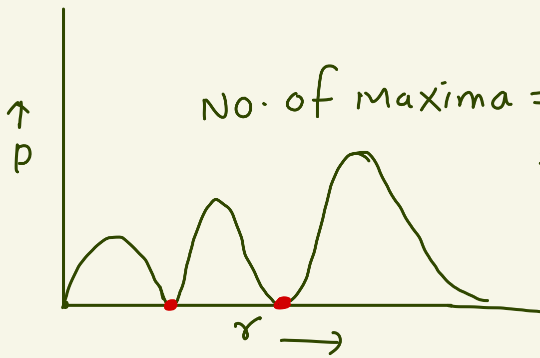
$$\Rightarrow \underbrace{6 - \frac{4r}{a_0} + \frac{4r^2}{9a_0^2} = 0}_{\Downarrow}$$

2 Roots of r

No. of R.N. = 2







No. of maxima = No. of R.N + 1

$= n - l - 1 + 1$

$= n - l$

(4) 2P-orbital $\rightarrow$

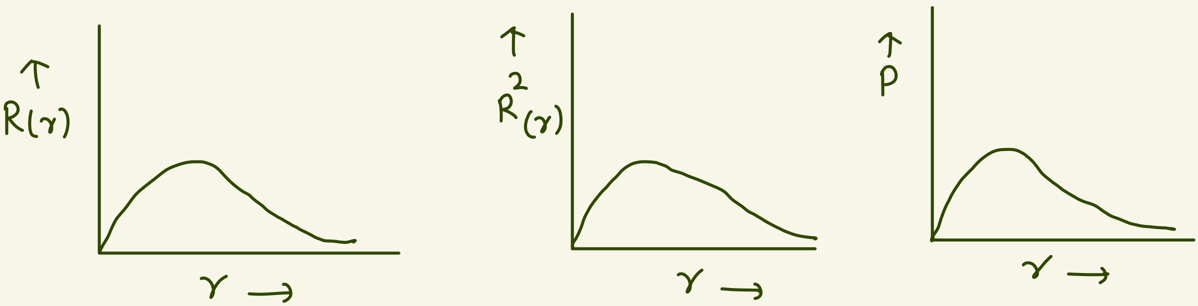
$$R(r) = \frac{1}{2\sqrt{6}} \left(\frac{Z}{a_0}\right)^{3/2} \left(\frac{2Zr}{na_0}\right) \left(e^{-Zr/na_0}\right)$$

H-atom $\Rightarrow$ $Z = 1$, $2p$ $\Rightarrow$ $n = 2$

$$R(r) = \frac{1}{2\sqrt{6}}\left(\frac{1}{a_0}\right)^{3/2}\left(\frac{r}{a_0}\right)\left(e^{-r/2a_0}\right)$$

$$R(r) = 0 \Rightarrow r = 0 , \quad r = \infty$$

No. of R.N. $= 0$



(5) 3p-orbital →

$$R(r) = \frac{1}{9\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2}\left(\frac{2Zr}{na_0}\right)\left(4 - \frac{2Zr}{na_0}\right) e^{-\frac{Zr}{na_0}}$$

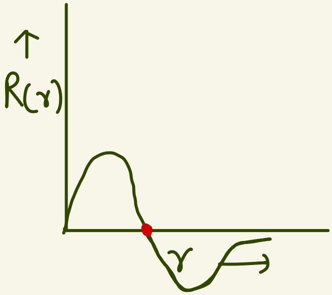
H-atom $\Rightarrow$ $Z = 1$, $3p$ $\Rightarrow$ $n = 3$

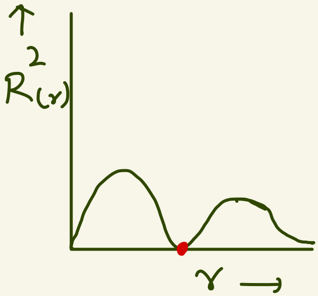
$$R(r) = \frac{1}{9\sqrt{6}}\left(\frac{1}{a_0}\right)^{3/2}\left(\frac{2r}{3a_0}\right)\left(4 - \frac{2r}{3a_0}\right) e^{-\frac{r}{3a_0}}$$

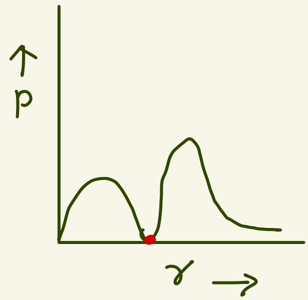
$$R(r) = 0 \Rightarrow r = 0 , \quad r = \infty$$

$$4 - \frac{2r}{3a_0} = 0 \Rightarrow r = 6a_0$$

No. of R.N. = 1







(6) 3d-orbital $\longrightarrow$

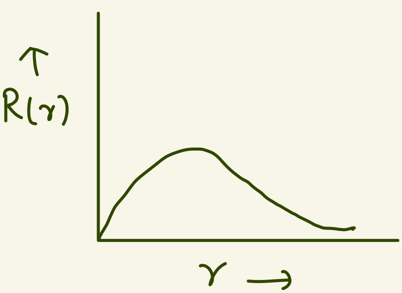
$$R(r) = \frac{1}{9\sqrt{30}}\left(\frac{Z}{a_0}\right)^{3/2}\left(\frac{2Zr}{na_0}\right)^2 e^{-\frac{Zr}{na_0}}$$

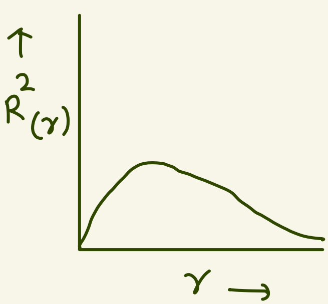
For H-atom $\Rightarrow$ $Z = 1$, 3d $\Rightarrow$ $n = 3$

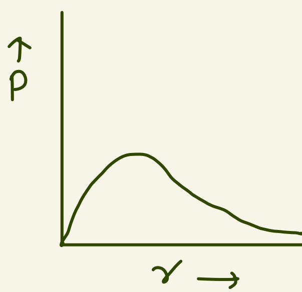
$$R(r) = \frac{1}{9\sqrt{30}}\left(\frac{1}{a_0}\right)^{3/2}\left(\frac{2r}{3a_0}\right)^2 e^{-r/3a_0}$$

$R(r) = 0 \Rightarrow r = 0,\ r = \infty$

No. of R.N. = 0







Spin Q.no. is not related with schrodinger wave eqn.

Angular wave functions of orbitals →

(1) s-orbital →

$$A(\theta, \phi) = \text{Const.} = \frac{1}{(4\pi)^{1/2}}$$

(2) p_x orbital $\Rightarrow$ $A(\theta, \phi) \propto \sin\theta \cos\phi$

p_y orbital $\Rightarrow$ $A(\theta, \phi) \propto \sin\theta \sin\phi$

p_z orbital $\Rightarrow$ $A(\theta, \phi) \propto \cos\theta$

(3) d_{xy} orbital $\Rightarrow$ $A(\theta, \phi) \propto \sin^2\theta \sin 2\phi$

d_{yz} orbital $\Rightarrow$ $A(\theta, \phi) \propto \sin\phi \sin 2\theta$

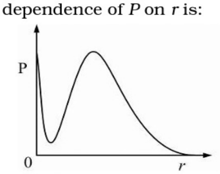
d_{zx} orbital $\Rightarrow$ $A(\theta, \phi) \propto \cos\phi \sin 2\theta$

$d_{x^2-y^2}$ orbital $\Rightarrow$ $A(\theta, \phi) \propto \sin^2\theta \cos 2\phi$

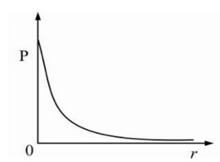
d_{z^2} orbital $\Rightarrow$ $A(\theta, \phi) \propto (3\cos^2\theta - 1)$

62. *P* is the probability of finding the 1s electron of hydrogen atom in a spherical shell of infinitesimal thickness, *dr*, at a distance *r* from the nucleus. The volume of this shell is $4\pi r^2 dr$. The qualitative sketch of the dependence of *P* on *r* is: **(2016)**

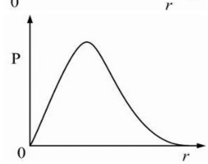
(A)



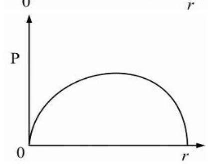
(B)



(C)



(D)



***107.** Choose the correct statements among the following:

(A) A node is a point in space where the wave-function Ψ has zero amplitude

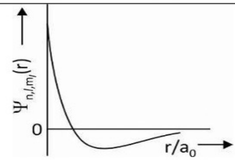
(B) The number of maxima (peaks) in radial probability distribution function is $(n - l)$

(C) Radial probability is $4\pi r^2 R_{n,l}^2(r)$

(D) Ψ^2 represents probability density of finding electron

Paragraph for Question No. 63 – 65 **(2017)**

The wave function, ψ_{n,l,m_l} is a mathematical function whose value depends upon spherical polar coordinates (r, θ, ϕ) of the electron and characterized by the quantum numbers n, l and m_l. Here r is distance from nucleus, θ is colatitude and ϕ is azimuth. In the mathematical functions given in the Table, Z is atomic number and a_0 is Bohr radius.

Column 1		**Column 2**		**Column 3**	
(I)	1s orbital	**(i)**	$\psi_{n,l,m_l} \propto \left(\frac{Z}{a_0}\right)^{3/2} e^{-\left(\frac{Zr}{a_0}\right)}$	**(P)**	
(II)	2s orbital	**(ii)**	One radial node	**(Q)**	Probability density at nucleus $\propto \frac{1}{a_0^3}$
(III)	$2p_z$ orbital	**(iii)**	$\psi_{n,l,m_l} \propto \left(\frac{Z}{a_0}\right)^{\frac{5}{2}} r e^{-\left(\frac{Zr}{2a_0}\right)} \cos\theta$	**(R)**	Probability density is maximum at nucleus
(IV)	$3d_z^2$ orbital	**(iv)**	xy-plane is a nodal plane	**(S)**	Energy needed to excite electron from n = 2 state to n = 4 state is 27/32 times the energy needed to excite electron from n = 2 state to n = 6 state

63. For He^+ ion, the only **INCORRECT** combination is:

(A) (I) (iii) (R) **(B)** (II) (ii) (Q) **(C)** (I) (i) (R) **(D)** (I) (i) (S)

64. For hydrogen atom, the only CORRECT combination is:

(A) (II) (i) (Q) **(B)** (I) (i) (P) **(C)** (I) (iv) (R) **(D)** (I) (i) (S)

65. For the given orbital in Column 1, the only CORRECT combination for any hydrogen-like species is:

(A) (I) (ii) (S) **(B)** (IV) (iv) (R) **(C)** (II) (ii) (P) **(D)** (III) (iii) (P)

$$\psi(r,\theta,\phi) = \psi_{(r)} \cdot \psi(\theta,\phi)$$

$$= (\text{const. term})\underbrace{(r^{l})}_{s/p/d}\underbrace{(\text{Polynomial of } r)}_{\text{No. of radial nodes}} e^{\frac{-Zr}{na_0}} \cdot \underbrace{\psi(\theta,\phi)}_{\text{Name of orbital}}$$

Homework

*** All questions can be solved from atomic Structure workbook and module.**

*** Self study of periodic classification from NCERT. Periodic properties will be taught in live class.**