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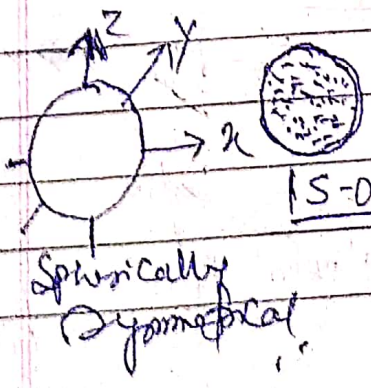
Deg-I (H/S) Inorganic (Gr-B)
Chapter - At. Structure
Topics — (a) Shapes of Atomic-orbitals
(b) Radial & angular wave function & Distribution Curve

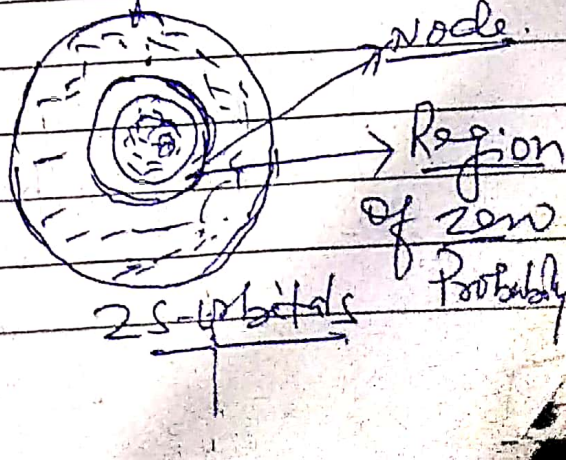
(A) Shapes of Atomic Orbitals.

We know that the probability of finding the electrons even at large distance from the nucleus is never zero. Thus it is impossible to draw a geometrical figure which encloses their probability to 100%, we draw figure in which the probability of finding electrons is maximum Called Boundary surface-diagram or Orbitals.

(1) Shapes of S-Orbitals.

S-orbitals are non-directional & Spherically Symmetrical. The probability of finding the electrons is same in all-directions at particular distance from nucleus.

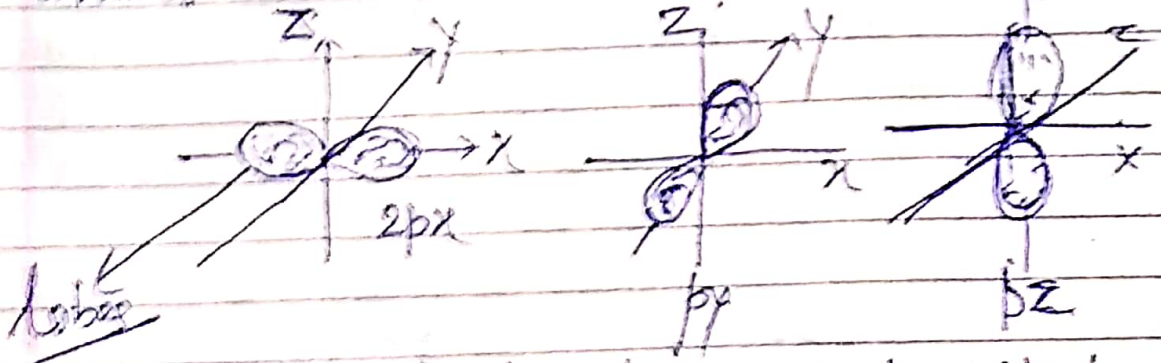




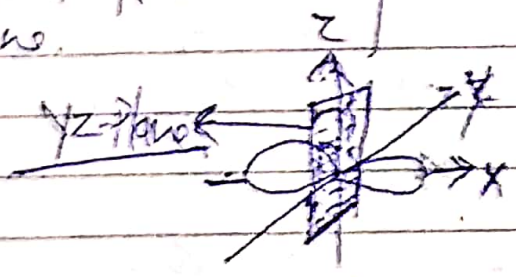
Density of charge cloud around the nucleus is maximum but decrease by increasing distance from the nucleus.

2S-orbitals differ from 1S-orbitals being larger size having nodal surface (surface having zero electron density)

(2) Shape of p-orbitals :- p-orbitals have three orientation like px, py & pz. These three orbitals are equal in energy (degenerate) but differ in their orientation. Each dumbbell shape each which have two lobes symmetrical around each axis.



Note :- The two lobes of p-orbitals are separated by a plane having zero density called nodal-plane.



Similarly for py & pz

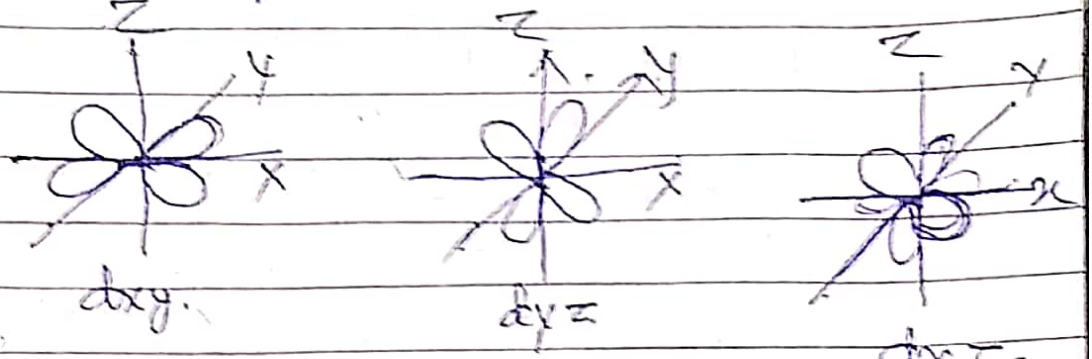
Nodal-Plane of 2px orbits.

(3) Shapes of d-orbitals

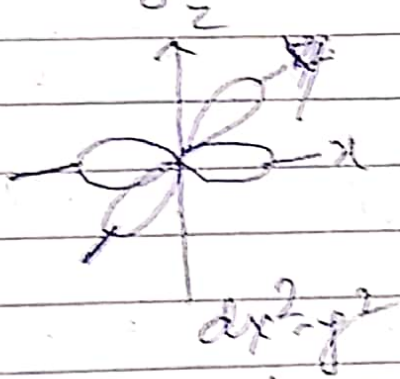
There are five orbitals in d-subshell having double-dumbell in shape. They all have equal in energy but differ in their orientation.

Shapes of various d-Orbitals

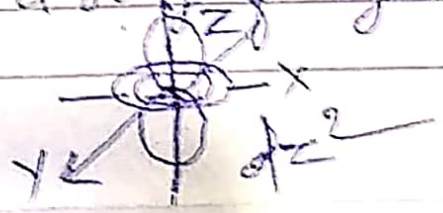
(i) The three orbitals like d_{xy}, d_{xz} & d_{yz} are similar & each have four lobes having high densities lying in xy, yz & xz plane. Their lobes lying b/w the principal axes.



(ii) The $d_{x^2-y^2}$ orbitals is exactly like d_{xy} orbitals except that it rotates through 45° around the Z-axis.



(iii) The d_{z^2} orbital consists of two lobes along Z-axis with a ring of high electron density in XY-plane.



(3) Radial & Angular wave function:

Radial wave function:- The Radial wave function gives the distribution of electron as a function of the distance (r) from the nucleus. The shape of orbitals obtained by the variation of wave function ψ as a function of distance (r) of electron upon the value of two quantum number n & l.

Radial wave function = $R_{n,l}(r)$

Angular wave function :- The product of angle θ & Φ (Schrodinger wave equation in term of polar coordinates) is called Angular wave function. It depends upon angle direction given by angles θ & Φ.

It determine the shape of electron cloud which depends upon the value of quantum numbers l & m.

Angular wave function = $\Theta(\theta).\Phi(\phi)$

Complete wave function expressed as

$\psi(r,\theta,\phi) = R(r).Y(\theta,\phi)$

The Radial part give its size & the angular part determine the shape of orbitals

Nodes & Nodal-Plane.

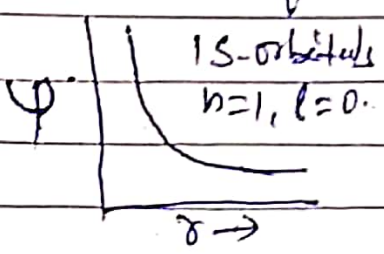
Radial Nodes $= n - l - 1$

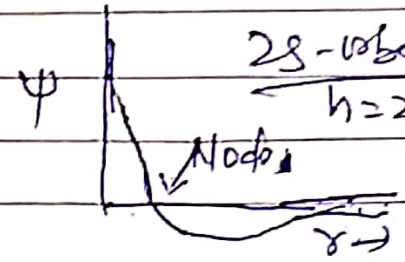
Angular Nodes $= l$

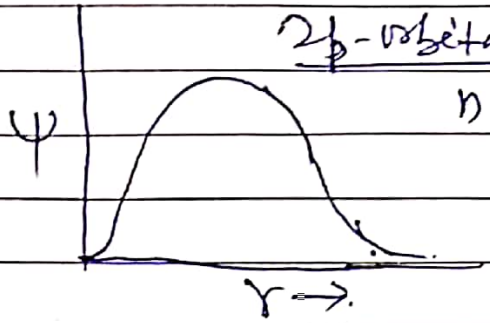
Total Nodes $= n - 1$

Distribution Curve.

ψ - wave function with r.

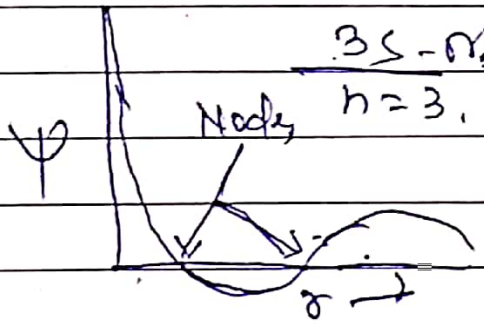




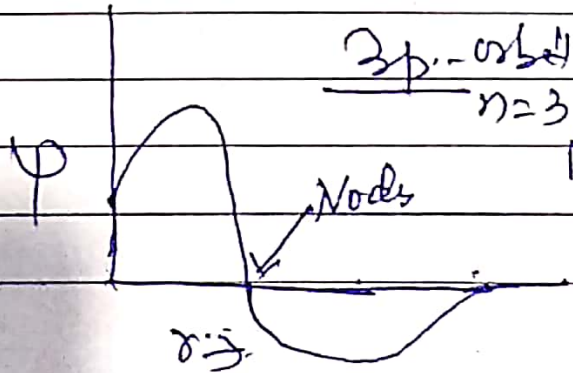


$n = 2, l = 1$

Radial Nodes $= 2 - 1 - 1 = 0$.



Radial Node. $= 3 - 0 - 1 = 2$



Radial Node. $= 3 - 1 - 1 = 1$