# ATOMIC STRUCTURE

① 3rd

TOPICS. ① BOHR'S THEORY & LIMITATIONS

② DIFFERENCE BETWEEN ORBIT AND ORBITALS.

③ QUANTUM NUMBERS

④ TYPES OF QUANTUM NUMBERS.

a) Principal Q.No ($n$)

b) Azimuthal " ($l$)

c) Magnetic " ($m$)

d) Spin " ($s$)

⑤ SHAPES OF ORBITALS. ($s, p, d$).

# BOHR'S THEORY

In 1913, Danish Physicist Neils Bohr proposed his revolutionary atomic model to overcome the drawbacks of Rutherford's nuclear Atomic model.

## BOHR'S POSTULATES / ASSUMPTIONS

1. The electrons revolve rapidly round the nucleus in a fixed circular path called Energy level or shells.
2. The energy levels or shells are represented in two ways – either by numbers 1, 2, 3, 4, 5 & 6 or by letters K, L, M, N, O, & P. The energy levels are counted from the centre outward.
3. Each energy level is associated with fixed amount of energy.
4. The shell nearest to the nucleus having minimum energy & the shell farthest from the nucleus having maximum energy.
5. There is no change in energy of electrons as long as they keep on revolving in the same energy level & the atom remains stable.
6. The change in energy of $e^-$ takes place when it jumps from lower energy level to higher energy level or when it comes down from higher energy level to lower energy level.
7. When an $e^-$ gains energy, it jumps from lower energy level to higher energy level & when an $e^-$ comes down from higher energy level to lower energy level, it loses energy
8. Only those orbitals are permissible for which the angular momentum of the $e^-$'s is an integral multible of $\frac{h}{2\pi}$

i.e $$mvr = \frac{nh}{2\pi}$$

Where,

$m$ = Mass of electron

$v$ = Velocity of electron

$r$ = radius of orbit

$h$ = Planck's constant

$n$ = orbit number such as 1, 2, 3, 4......,

The amount of energy absorbed or released during these jumpings can be given from Plank's Quantum theory as —

$$E_2 - E_1 = h\nu$$

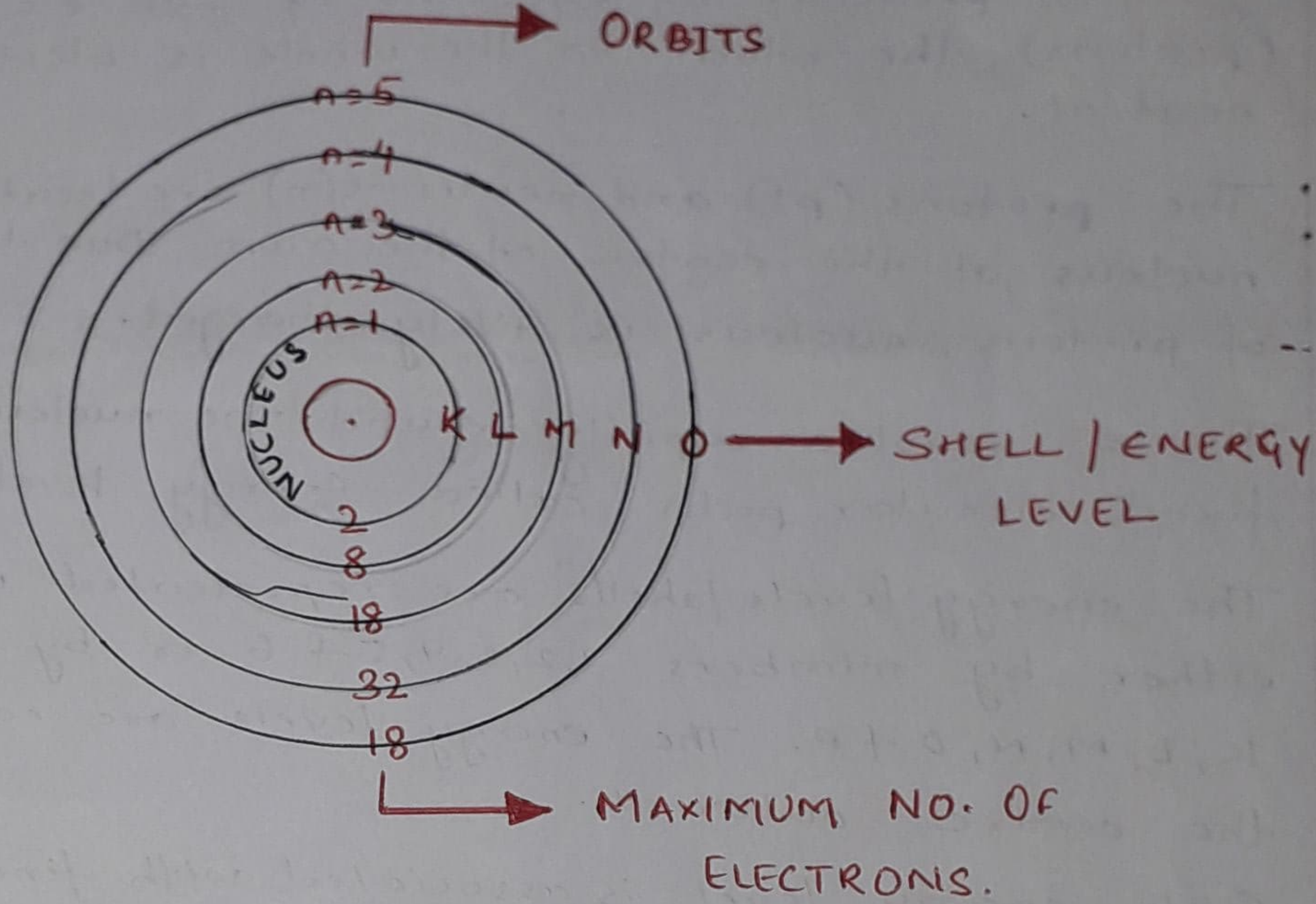
where, $E_2$ = Energy of orbit where the electron jumps.

$E_1$ = Energy of orbit from where the $e^-$ jumps.

$h$ = Planck's constant.

$\nu$ = frequency of radiation.

energy




Representation of Bohr's stationary or energy levels in an atom.

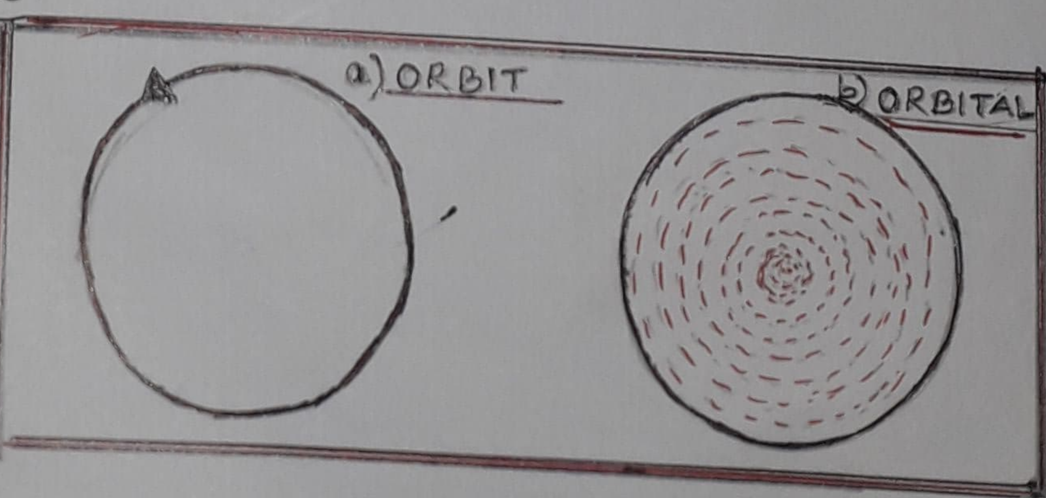
# DIFFERENCES BETWEEN ORBIT AND ORBITAL

## ORBIT :-

1. Orbit is a well-defined circular path around the nucleus in which an electron revolves.
2. It represents the planar motion of an electron.
3. It gives a definite path of an electron.
4. All orbits are circular.
5. Orbits are non- directional in character, hence they cannot explain shape of molecules.
6. The maximum number of an electron in an orbit is equal to $2n^2$ where 'n' represents the principal quantum number (number of orbit).

## ORBITAL:-

1. It represents the region in space around the nucleus of an atom where the probability of finding the electron is maximum.
2. It represents three-dimensional motion of an electron.
3. An orbital cannot have more than two electrons.
4. Orbital does not specify definite path and according to this concept, electron may be anywhere in the region.
5. Orbitals (except s-orbital) have directional character.
6. ~~and~~ Orbitals have different shapes. for example :- s-orbital is spherical, while p-orbital is dumb bell shaped.



# QUANTUM NUMBERS

## INTRODUCTION :-

An atom consist of large no. of orbitals which are distinguished from each other on the basis of their shape, size, orientation (direction) in space.

The characteristics of an orbital are expressed in terms of 4 no.s called principal, Azimuthal, magnetic & spin (rotation) Quantum No.s.

## DEFINITION :-

" Quantum numbers may be defined as a set of 4- no.s (n, l, m, s) with the help of which we get complete information about all the electrons in an atom ie, location, energy, the type of orbital occupied, shape & orientation of that orbitals etc "

## ① PRINCIPAL QUANTUM NUMBER (n)

This is the most important quantum no. as it was used to described Bohr's stationary states in the atom.

**Significance**. ① It determines the main energy level or shell in which the $e^-$ is present.

② It is denoted by 'n'. & can have positive integral values 1, 2, 3, 4 etc corresponding to K, L, M, N etc. shells.

③ It represents the size of electron orbital. Higher the value of 'n', larger is the size of orbital, and also ~~the~~ higher is the energy of the shell.

Energies of various principal shells :-

K < L < M < N or 1 < 2 < 3 < 4.

4. Principal Quantum No. (n) gives the average distance of $e^-$ from the nucleus.

5. The maximum no. of e's in a shell is given by $2n^2$

| Main Energy level | Designation | Maximum No. of $e^-$ |
|---|---|---|
| 1 | K | 2 |
| 2 | L | 8 |
| 3 | M | 18 |
| 4 | N | 32 |

## (II) AZIMUTHAL / ANGULAR QUANTUM NO.

1. This Q. No. is also known as subsidiary or orbital quantum No. It is used to describe the sub-shells (sub energy levels) within a given main shell.

Significance. (1) The Azimuthal quantum No. gives the following information —

a) The no. of subshells present in the main shell.

b) It determines the angular momentum of orbital.

c) The relative energies of various sub-shells.

d) The shape of various sub-shells present within the same principal shell.

2. It is represented by 'l'. The value of 'l' depends upon the value of 'n', hence 'l' can have the values from 0 to (n−1)

3. $l = 0, 1, 2, 3 \ldots\ldots (n-1)$.

for 1st shell (K), n = 1, l = (1−1) = 0 (only 1 value).
2nd " (L), n = 2, l = (2−1) = 1 ( 0, 1 - 2 Values)
3rd " (M), n = 3, l = 0 to (n−1) = 0, 1, 2 (3 Values)
4rth " (N) n = 4. l = 0 to (n−1) = 0, 1, 2, 3 (4 Values).

Each value of 'l' represents a different subshells. The orbitals with l= 0, 1, 2, 3 are called s-orbital, p-orbital, d-orbital & f-orbital respectively.

| L | 0 | 1 | 2 | 3 | 4 | 5 |
|---|---|---|---|---|---|---|
| Sub-shells. | s | p | d | f | g | h |

5 In a particular energy level, the energies of its orbitals are in the orders $s < p < d < f$.

| Principal Q. No. (n) | Azimuthal Q. NO (l) | Sub-shell | Designated as. |
|---|---|---|---|
| 1 | 0 | S- sub-shell | 1s |
| 2 | 0 | s - subshell | 2s |
| | 1 | p - " | 2p. |
| 3 | 0 | s - | 3s |
| | 1 | p - | 3p |
| | 2 | d - | 3d |
| 4 | 0 | s - | 4s |
| | 1 | p - | 4p |
| | 2 | d - | 4d |
| | 3 | f - | 4f. |

# MAGNETIC QUANTUM NUMBER (m).

1) Electron is a -vely charged particle. Its movement around the nucleus is like that of flow of current. Such a movement of electron creats a magnetic field. Hence it is known as Magnetic Quantum No.

**Significance.** (a) It describes the behavior of the electrons in the magnetic field.

(b) It refers to the different orientations of orbitals in space.

(c) It is designated by 'm' or '$m_l$'.

(d) The values of 'm' depends upon the value of 'l'.

(e) It can have all possible values ranging from $-l$ to $+l$ including 0.

(f) for every value of $l$, m has $(2l+1)$ values.

**Examples:-** ① $l=0$, $m = 2l+1$
(s-subshell). $= 2\times0+1 = 1$ ie, 0, $\boxed{m=0}$

It means, s-subshell has only one orientation in space. In other words, s-subshell has only one orbital called s-orbital.

② $l=1$ (p-subshell).

$m = 2l+1 = 2\times1+1 = 2+1 = 3.$

'm' can have 3 values, $\boxed{m = -1, 0, +1}$

These 3 orbitals are oriented along x-axis, y-axis, z-axis.

p-subshell has 3-orbitals - $P_x$, $P_y$, $P_z$.

$l = 2$ (d-sub-shell)

$m = 2l+1 = 2 \times 2 + 1 = 5.$

'm' can have 5 values i.e

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

5-d-orbitals, $d_{xy}, d_{yz}, d_{zx}, d_{x^2-y^2}, d_{z^2}$

$l = 3$ (f-sub shell).

$m = 2l+1 = 2 \times 3 + 1 = 7.$

$\boxed{m = -3, -2 \ -1 \ 0 \ 1 \ 2 \ 3}$

7. different orientations of f-sub-shells.

Values of m by latest orientations.

| ORBITAL | VALUE OF 'm'. |
|---|---|
| $P_z$ | $m = 0$ |
| $P_x$ | $m = +1$ |
| $P_y$ | $m = -1$ |
| $d_{z^2}$ | $m = 0$ |
| $d_{xz}$ | $m = +1$ |
| $d_{yz}$ | $m = -1$ |
| $d_{x^2-y^2}$ | $m = +2$ |
| $d_{xy}$ | $m = -2.$ |

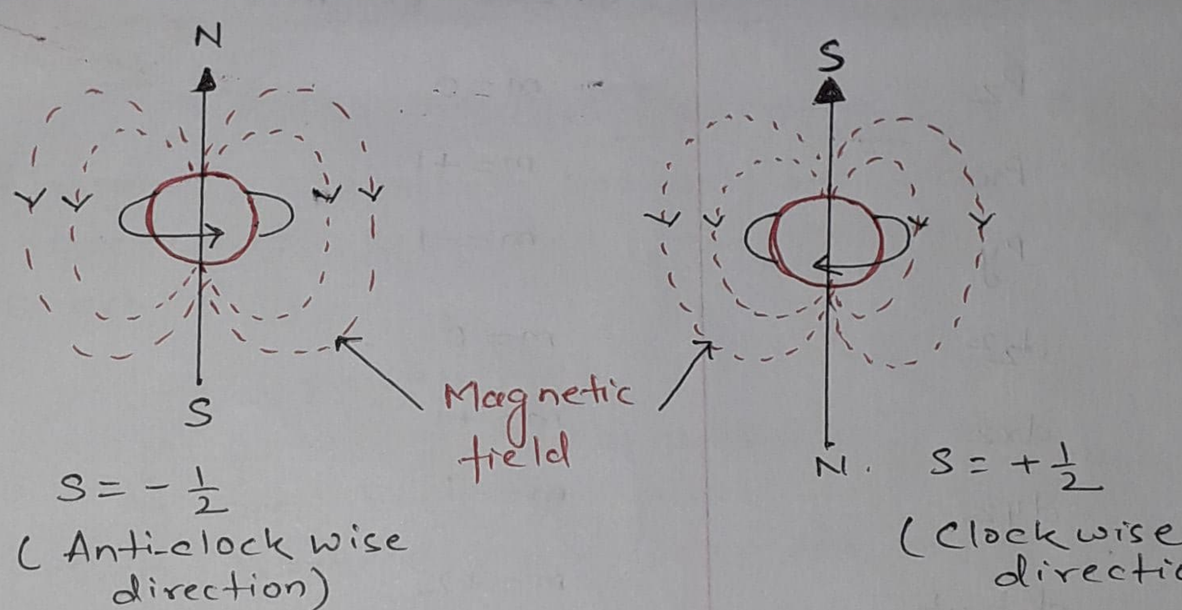
## SPIN QUANTUM NUMBER (s)

An electron in its motion around the nucleus spins on its own axis. A spinning electron behaves like a small magnet.

**Significance:-** ① It indicates the direction in which the electron is spinning about its own axis.

② The electron can spin clockwise (↑) or anticlockwise (↓).

③ Spin Quantum Number (s) can have two possible values i.e, $+\frac{1}{2}$ and $-\frac{1}{2}$. depending upon the direction of spin. Thus, only two electrons can accomodated in the orbital with opposite spins (↑↓).




$\boxed{\uparrow\downarrow}$

paired electrons with opposite sites.

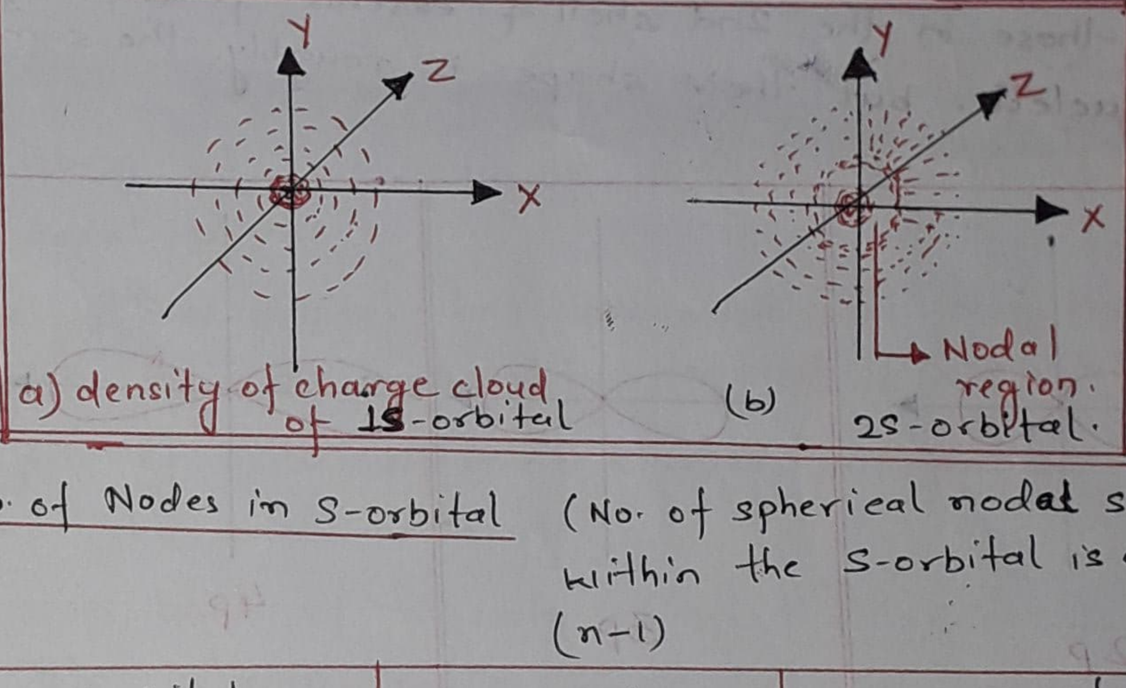
# SHAPE OF ORBITALS (s, p, d)

## Shape of S-orbital:-

* S-orbital are non-directional.
* spherical symmetrical about the nucleus.
* Probability of finding the electron belonging to s-orbital of any main shell is found to be equal in all directions at a given distance from the nucleus.
* On the basis of Quantum no.s for s-orbital—

$\boxed{m = 0, \quad l = 0}$ i.e, s-orbital has only one orientation.

* The shape having one orientation is sphere. Hence, S-orbital has always spherical in shape.




a) density of charge cloud of 1s-orbital (b) 2s-orbital.

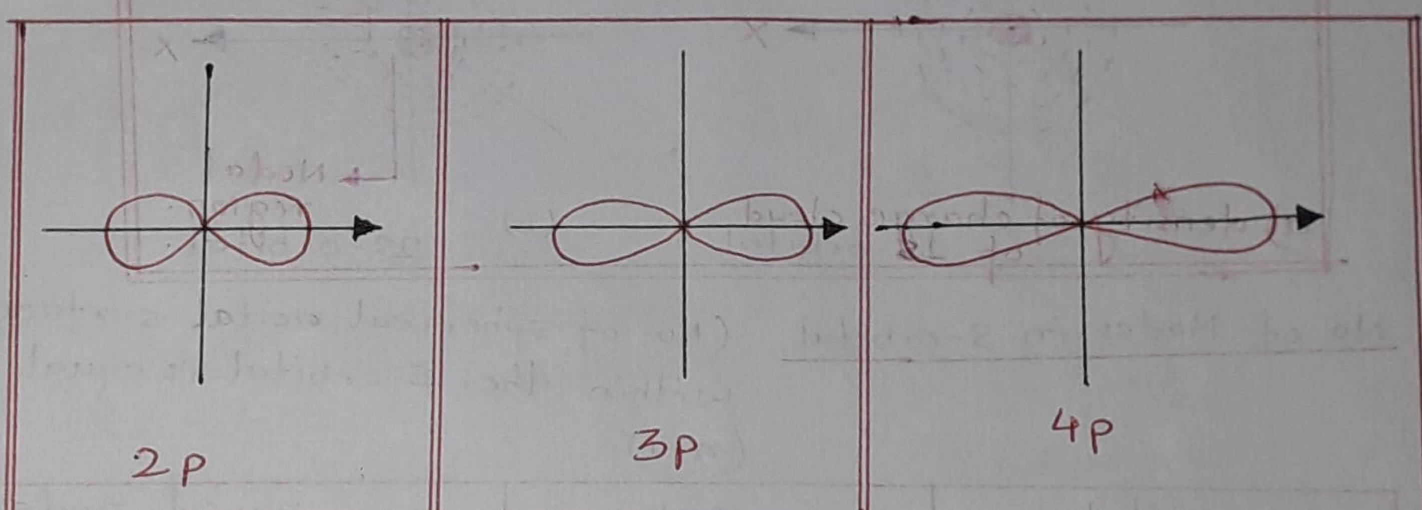
* No. of Nodes in S-orbital (No. of spherical nodal surfaces within the s-orbital is equal to $(n-1)$

| s-orbital | n-1 | no. of nodes |
|---|---|---|
| 1s | (1-1) | 0 |
| 2s | (2-1) | 1 |
| 3s | (3-1) | 2 |
| 4s | (4-1) | 3 |

(10)

## Shapes of p- orbital

* Shape :- Dumb- bell rather than spherical.
* $e^-$ distribution concentrated in identical lobes on either side of the nucleus & separated by a nodal plane & cuts through the nucleus.
* For p- orbitals, $\boxed{l=1,\ m=(-1,0,+1)}$ ie 3 possible orientations
* For every p- orbitals, there are 3 - p- orbitals ie, $P_x, P_y, P_z$ which are oriented in space at $90°$ angles to one another along the 3- co-ordinate axis. x, y, z.
* ~~3p~~ 3 p-orbitals in the 2nd shell is designated as — $2P_x, 2P_y, 2P_z$.
* P- orbitals in the 3rd shell & higher shells are larger than those in the 2nd shell & extend farther from the nucleus. but their shape is roughly the same.

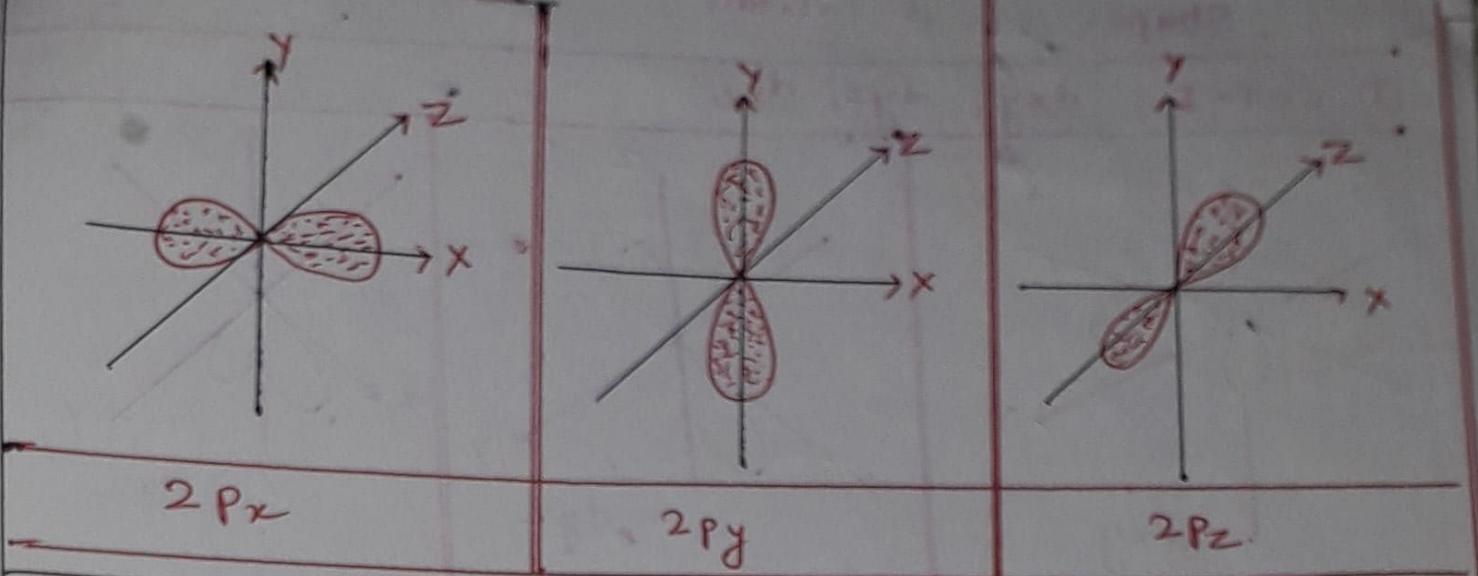



* No. of nodes in p- orbital

| P- orbital | (n-2) | no. of nodes. |
|---|---|---|
| 2 P | (2-2) | 0 |
| 3P | (3-2) | 1 |
| 4P | (4-2) | 2 |

Shapes of 2p-orbitals






## SHAPES OF d- ORBITALS

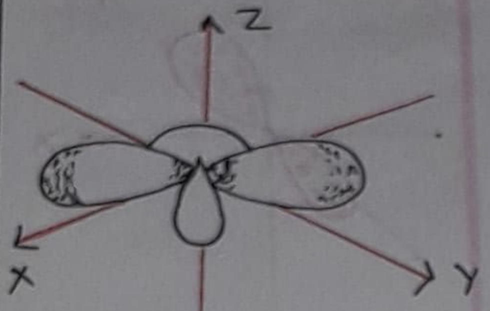
* An orbital with $L=2$ called d-orbital.
* For d-orbital, $m = -2, -1, 0, +1, +2$
  5 possible orientations.
* four of 5 d-orbitals are clover leaf shaped & have 4 lobes of maximum $e^-$ probability separated by 2 nodal planes.
* The 5th d-orbital has an additional donut shaped region of $e^-$ probability centred in the XY plane.
* Inspite of their different shapes, all the 5d-orbitals have the same energy.
* On the basis of orientation of the lobes of these orbitals w.r.to x, y, z axes, d-orbitals have been divided into 2-sets.

① $d_{xy}$, $d_{yz}$ & $d_{zx}$ orbitals.

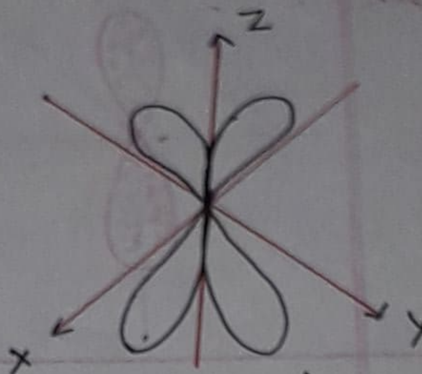
② $d_{x^2-y^2}$, $d_{z^2}$.

## Shapes of d- orbitals

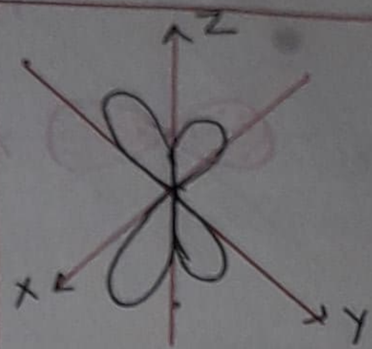
1) SET- I dxy, dyz, dxz




dxy

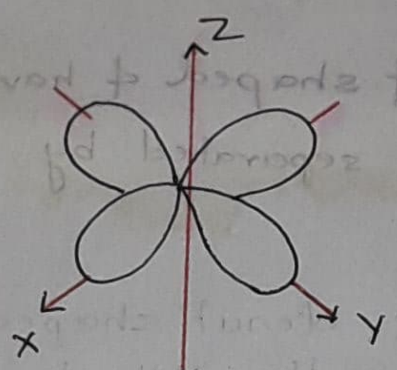



dyz

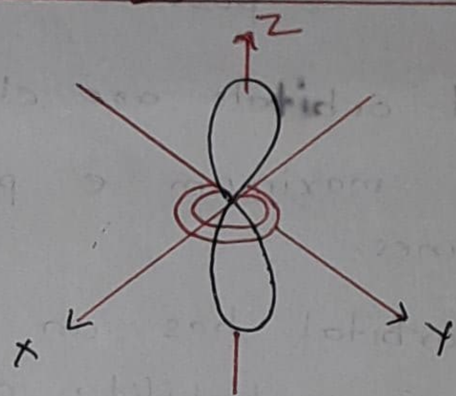



dxz

2) SET- 2 $d_{x^2-y^2}$, $d_{z^2}$




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




$d_{z^2}$