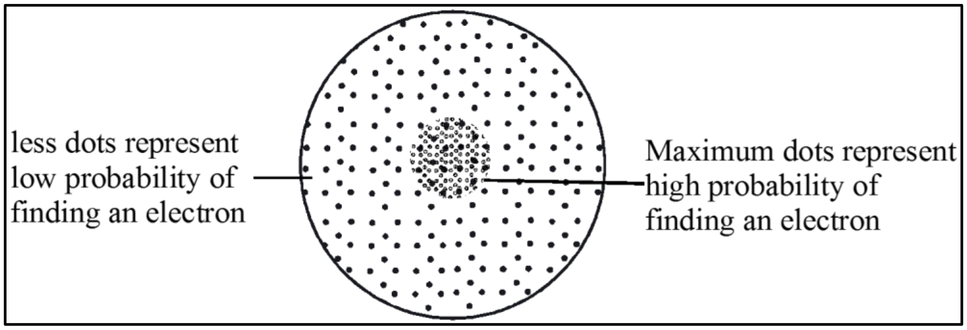
STRUCTURE OF ATOM

QUANTUM MECHANICAL MODEL OF ATOM

❖ ORBITAL

An orbital may be defined as the region of space around the nucleus where the probability of finding an electron is maximum (90% to 95%)

Orbitals do not define a definite path for the electron, rather they define only the probability of the electron being in various regions of space around the nucles.



Difference Between Orbit and Orbitals

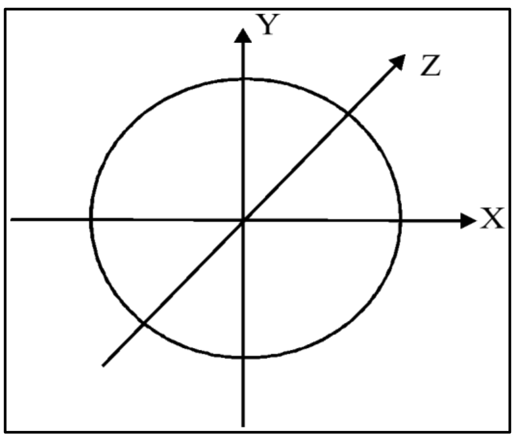
S.No.	Orbit	Orbitals
1.	It is well defined circular path followed by It is well defined circular path followed by	It is the region of space around the nucleus where electron is most likely to be found
2.	It represents planar motion of electron	It represents 3-dimensional motion of an electron around the nucleus.
3.	The maximum no. of electron in an orbit is $2n^2$ where n stands for no. of orbit.	Orbitals cannot accommodate more than 2 electrons.
4.	Orbits are circular in shape.	Orbitals have different shape e.g., s-orbital is spherical, p - orbital is dumb- bell shaped.

5.	Orbit are non-directional in character. Hence, they cannot explain shape of molecules	Orbitals (except s-orbital) have directional character. Hence, they can account for the shape of molecules.
6.	Concept of well-defined orbit is against Heisenberg's uncertainty principle.	Concept of orbitals is in accordance with Heisenberg's principle

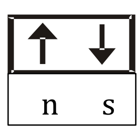
Shape of The Orbitals

Shape of the orbitals are related to the solutions of Schrodinger wave equation, and gives the space in which the probability of finding an electron is maximum.

s- Orbital : Shape spherical

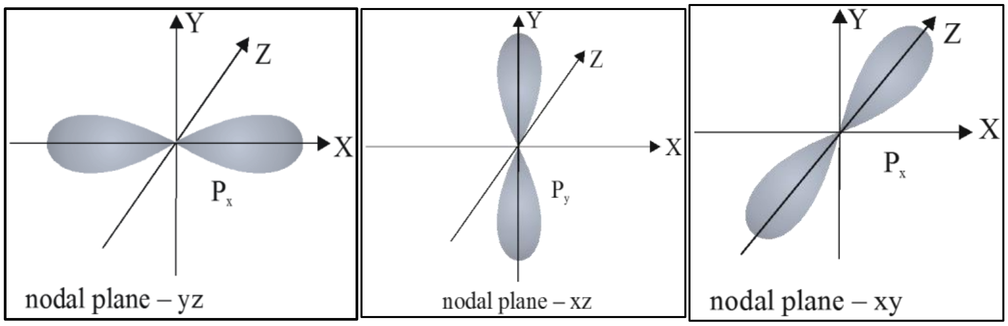


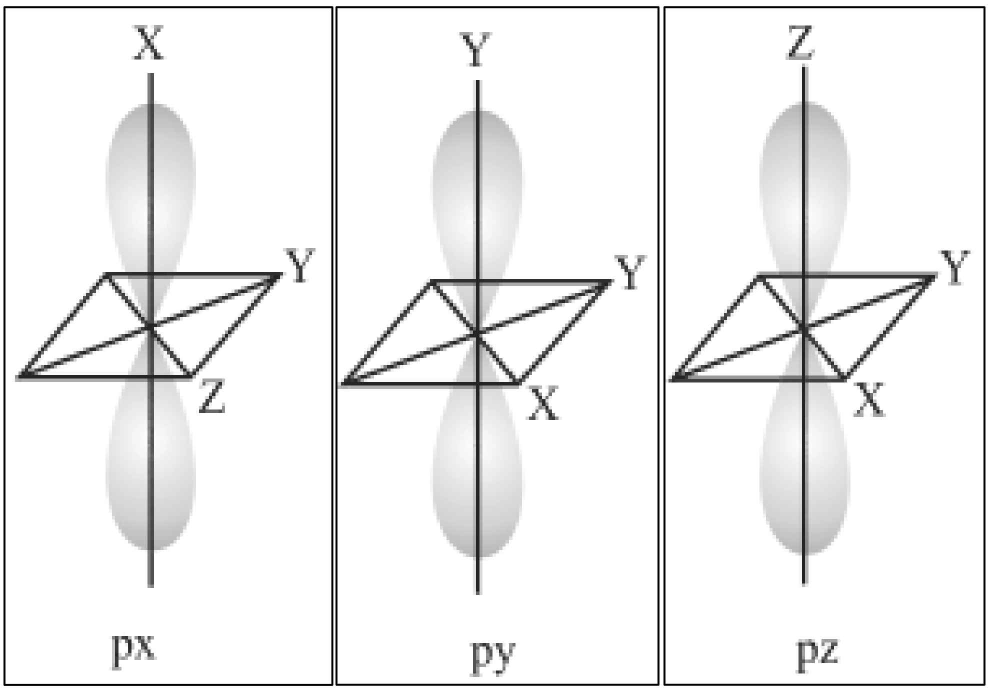
s- orbital is non-directional and it is closest to the nucleus, having lowest energy.
s-orbital can accomodate maximum no. of two electrons.



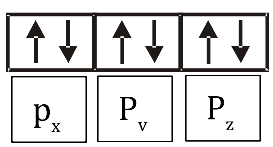
p-Orbital: Shape dumb bell Dumb bell shape consists of two lobes which are separated by a region of zero probability called node.

Nodal Plane – The imaginary plane where probability of finding an electron is zero.

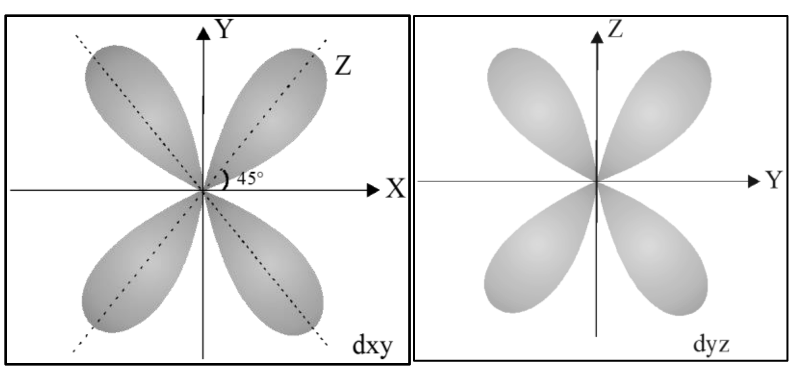


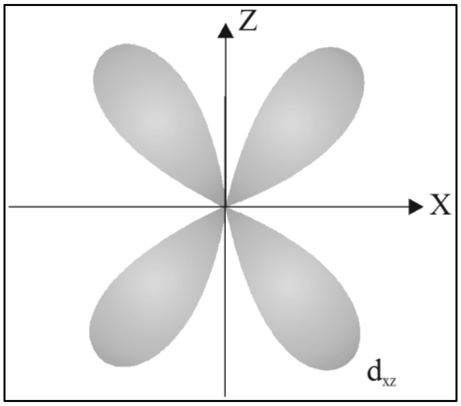


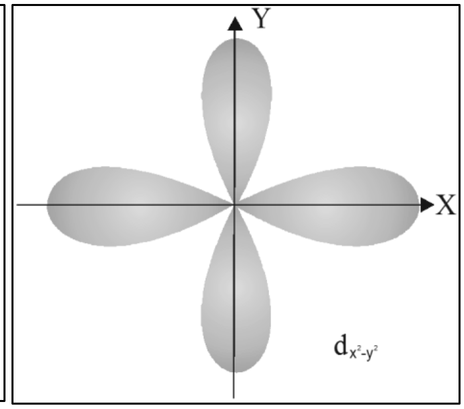
p - subshell can accomodate maximum of six electrons.

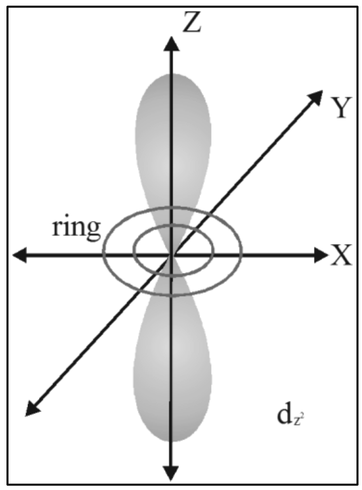


d - Orbital: Shape double dumb bell

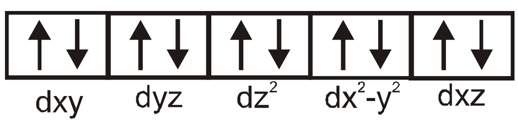




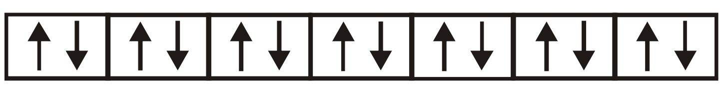




d - subshell can accomodate maximum of 10 electrons.



f - Orbital: Shape leaf like or Complex



f - orbital can accomodate maximum no. of 14 electrons.

Quantum Numbers

The set of four numbers required to define the possible location of an electron in an atom are called quantum numbers. The first three have been derived from Schrodinger wave equation.

(i) Principal Quantum Number (n) : (Proposed by Bohr)

It describes the size of the electron wave and the total energy of the electron. It has integral values 1, 2, 3, 4 ...., etc., and is denoted by K, L, M, N. ..., etc.

- Number of subshells present in n^{th} shell = n

n	**subshell**
1	s
2	s, p
3	s, p, d
4	s, p, d, f

- Number of orbitals present in n^{th} shell = n^2 .
- The maximum number of electrons which can be present in a principal energy shell is equal to $2n^2$.

  No energy shell in the atoms of known elements possesses more than 32 electrons.
- Angular momentum of any orbit $= \frac{nh}{2\pi}$

(ii) Azimuthal Quantum Number (λ) : (Proposed by Sommerfield)

It describes the shape of electron cloud and the number of subshells in a shell.

It can have values from 0 to (n – 1). Each value of λ represents a subshell.

value of λ	**subshell**
0	s
1	p
2	d
3	f

Number of orbitals in a subshell = $2\lambda + 1$

Maximum number of electrons in particular subshell = $2 \times (2\lambda + 1)$

Orbital angular momentum $L = \frac{h}{2\pi}\sqrt{\ell(\ell+1)} = \eta\sqrt{\ell(\ell+1)}[h = \frac{h}{2\pi}]$

i.e. Orbital angular momentum of s orbital = 0, Orbital angular momentum of p orbital

$= \sqrt{2}\frac{h}{2\pi}$,

Orbital angular momentum of d orbital $= \sqrt{3}\frac{h}{2\pi}$

(iii) Magnetic Quantum Number (m) : (Proposed by Linde)

It describes the orientations of the subshells. It can have values from $-\lambda$ to $+\lambda$ including zero, i.e., total $(2\lambda + 1)$ values. Each value corresponds to an orbital. s-subshell has one orbital, p-subshell three orbitals (p_x, p_y and p_z),

d-subshell five orbitals(d_{xy}, d_{yz}, d_{zx}, $d_{x^2-y^2}$, d_{z^2}) and f-subshell has seven orbitals.

The total number of orbitals present in a main energy level is 'n^2'.

(iv) Spin Quantum Number (s) : (Proposed by Samuel Goudsmit & Uhlenbeck)

It describes the spin of the electron. It has values +1/2 and −1/2. signifies clockwise spinning and anticlockwise spinning.

(i) Spin magnetic moment $\mu_s = \frac{eh}{2\pi mc}\sqrt{s(s+1)}$ or $\mu = \sqrt{n(n+2)}$ B.M.

(n = no. of unpaired electrons)

(ii) It represents the value of spin angular momentum which is equal to $\frac{h}{2\pi}\sqrt{s(s+1)}$

(iii) Maximum spin of atom $= \frac{1}{2}$ x No. of unpaired electron.

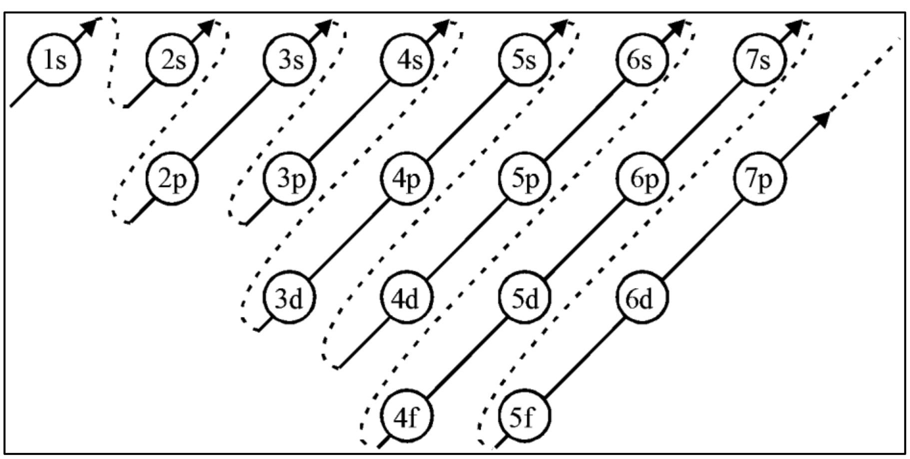
Rules for Filling of Orbitals

1. **Aufbau Principle**

Aufbau is a German word and its meaning 'Building up'

Aufbau principle gives a sequence in which various subshell are filled up depending on the relative order of the Energies of various subshell.

- **Principle:** The subshell with minimum energy is filled up first and when this subshell obtained maximum quota of electrons then the next subshell of higher energy starts filling.
- The sequence in which various subshell are filled is the following.



$1s^2, 2s^2, 2p^6, 3s^2, 3p^6, 4s^2, 3d^{10}, 4p^6, 5s^2, 4d^{10}, 5p^6, 6s^2, 4f^{14}, 5d^{10}, 6p^6, 7s^2, 5f^{14}, 6d^{10}, 7p^6$

2. $(n + \lambda)$ Rule

According to it the sequence in which various subshell are filled up can also be determined with the help of
$(n + \lambda)$ value for a given subshell.

PRINCIPLE OF $(n + \lambda)$ RULE

The subshell with lowest$(n + \lambda)$ value is filled up first, when two or more subshell have same $(n+\lambda)$ value then the subshell with lowest value of n is filled up first.

Sub Shell	n	λ	$n+\lambda$	
1s	1	0	1	
2s	2	0	2	
2p	2	1	3	(1)
3s	3	0	3	(2)
3p	3	1	4	(1)
4s	4	0	4	(2)
3d	3	2	5	(1)
4p	4	1	5	(2)
5s	5	0	5	(3)
4d	4	2	6	(1)
5p	5	1	6	(2)
6s	6	0	6	(3)

For H atom the energy of orbital depends only on the value of n.

i.e., $1s < 2s = 2p < 3s = 3p = 3d < 4s = 4p = 4d = 4f$.................

3. Pauli's Exclusion Principle

In 1925 Pauli stated that no two electron in an atom can have same values of all four quantum numbers.

λ An orbital can accomodates maximum 2 electrons with opposite spin.

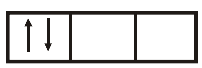
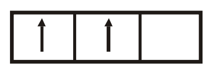
4. Hund's Maximum Multiplicity Rule

(Multiplicity: Many of the same kind)

According to Hund's rule electrons are distributed among the orbitals of subshell in such a way as to give maximum number of unpaired electron with parallel spin. i.e., in a subshell pairing of electrons will not start until and unless all the orbitals of that subshell will get one electron each with same spin.

SPIN MULTIPLICITY

It is given by 2S + 1 where S is the total spin.

(a)  (b) 

For (a), $S = +\frac{1}{2} - \frac{1}{2} = 0$

Spin multiplicity = $2S + 1 = 0 + 1 = 1$ (singlet)

For (b), $S = +\frac{1}{2} + \frac{1}{2} = 1$

Spin multiplicity = $2S + 1 = 2 \times 1 + 1 = 3$ (triplet)

Ex. Find out the angular momentum of an electron in

(a) 4s orbital (b) 3p orbital (c) 4^{th} orbital

Sol. Angular momentum in an orbital = $\frac{h}{2\pi}\sqrt{\ell(\ell+1)}$

(a) λ = 0 for 4s orbital, hence orbital angular momentum = 0

(b) λ = 1 for 3p orbital

∴ Angular momentum = $\frac{h}{2\pi}\sqrt{(1+1)\times 1}$

$$= \frac{h}{\sqrt{2}\pi}$$

(c) Angular momentum in 4^{th} orbit

$$= \frac{nh}{2\pi} = \frac{4\ h}{2\pi} = \frac{2\ h}{\pi}$$

Ex. Given below are the sets of quantum numbers for given orbitals. Name these orbitals.

(i) $n = 4, \lambda = 2, m = 0$ (ii) $n = 3, \lambda = 1, m = \pm 1$

(iii) $n = 4, \lambda = 0, m = 0$ (iv) $n = 3, \lambda = 2, m = \pm 2$

Sol. (i) $4dz^2$ (ii) $3p_x$ or $3p_y$

(iii) 4s (iv) or $3d_{xy}$