Quantum Mechanical Model of Atom, Orbitals and Quantum Numbers

1. Schrodinger's wave equation is $\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} + \frac{8\pi^2 m}{h^2}(E - V)\Psi = 0$

   Where m = Mass of electron, h = Planck's constant, E = Total energy of the electron,

   V = Potential energy of electron, x, y, z are co - ordinates.

2. ψ is the wave function. It indicates amplitude of the electron wave along. X, Y, Z are co - ordinate axis. Function has certain boundary conditions they are

   1) ψ Must be continuous

   2) ψ Must be finite

   3) ψ Must be single valued

   4) The probability of finding the electron over all the space from must be equal to one.

3. ψ^2 is the probability function .It indicates the probability of finding an electron at a given point in the space around nucleus.

4. Principal, azimuthal and magnetic quantum numbers are the solutions of Schrodinger wave equation.

5. The probability of finding an electron with in a small radial space around the nucleus is called **Radial Probability or D-function.** $D = 4\pi r^2 \, d \, r \, \Psi^2$.

6. The graph showing the variation of radial probability with the radial distance of an electron from the nucleus is called radial probability distribution curve.

7. The space around the nucleus where the probability of finding the electron is zero is called node or radial node or nodal region $(\psi^2 = 0)$.

    The number of radial nodes present in an orbital $= n - l - 1$.

    The number peaks in radial probability distribution curve $= (n - l)$.

    Radial probability distribution curves for 1s, 2s, 3s, 2p, 3p & 3d, orbital are:
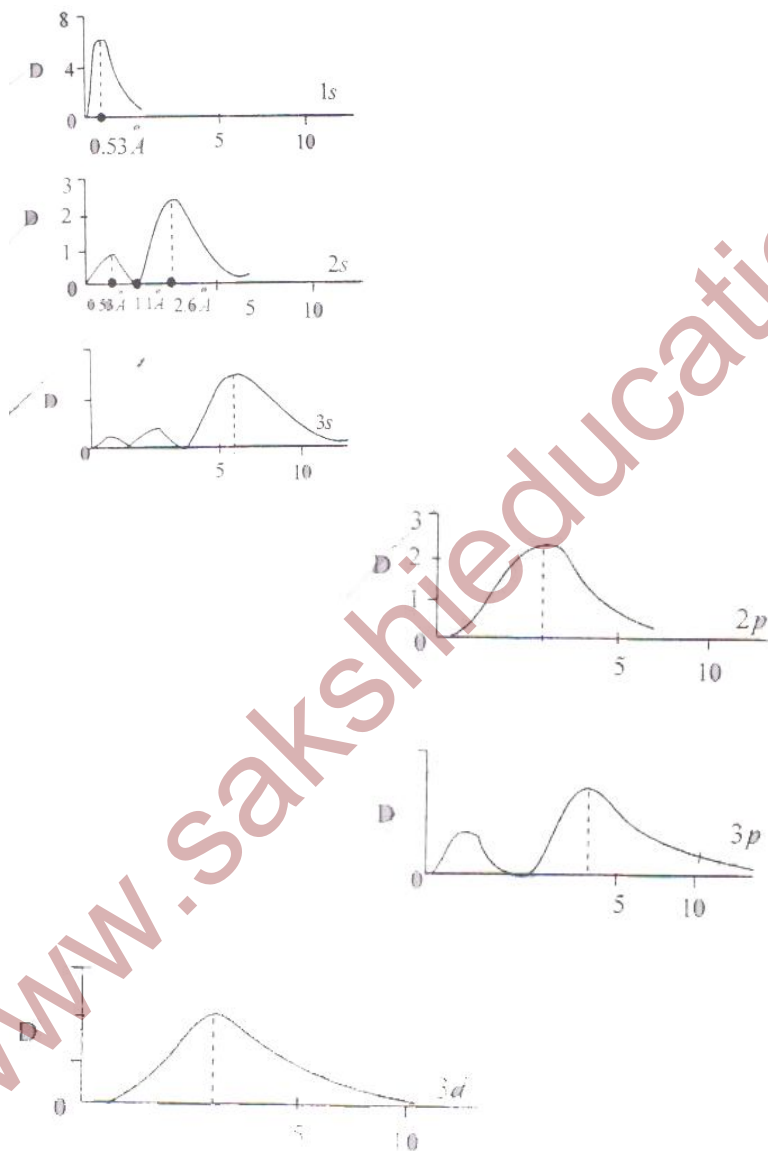
    The following points can be drawn from the above curves.

8. The space around the nucleus of an atom in which the probability of finding an electron is maximum (i.e. 95%) is called an **orbital.**

9. The shape of s orbital $(l = 0)$ is spherical and is non directional.

10. In a p - sub shell$(l=1)$, there are three degenerate orbitals which are represented as Hence a P -sublevel is Three fold degenerate .Each p - orbital is dumbbell in shape and are oriented along the axes. Thus they are directional.

11. In a d - sub shell ($l = 2$) there are five degenerate orbitals which are represented as $d_{xy}, d_{yz}, d_{zx}, d_{X^2-Y^2}$ and d_z^2. Hence a d -sublevel is Fivefold degenerate.

12. Except the remaing are double dumb bell in shape while has a large single dumbell alongZ-axis wth electron smoke ring in XY-plane.

13. d_{xy}, d_{yz} and d_{zx} Orbital's are oriented in between the axes. Orbitals are oriented along the axes.

14. The plane in which the probability of finding the electron zero is called a nodal plane. Number of nodal planes in an orbital = l.

15. S-orbital has zero, each P-orbital has one and each d-orbital has two **nodal planes.**As the number of nodal planes increases, the energy of the orbital increases.

    Nodal plane for -orbital is YZ-plane, is ZX-plane and is XY-plane.

16. Four quantum numbers required for complete identification of an electron in an atom. They are:

    Principal (n), Azimuthal (l), Magnetic (m) and Spin quantum numbers

Principal Quantum Number *(n)*

a. It was proposed by Niels Bohr.It can take values n =1, 2, 3, 4..... Or K, L, M, N .... respectively.

b. It represents the size and energy of the orbit.

c. The maximum number of sublevels possible in an orbit=n.

d. The maximum number of orbitals possible in an orbit = n^2.

e. The maximum number of electrons possible in an orbit $= 2n^2$, where n is orbit number.

f. As ''n' value increases

   i) The size and energy of the orbit, potential energy and de-Brogie wavelength of electron, the gap between two successive orbits increases.

   ii) Kinetic energy and velocity of electron, the energy difference between two successive orbits decreases.

Azimuthal Quantum Number *(l)*

a. It was proposed by Sommerfeld to explain Fine spectrum of H-atom. It can take values $/= 0, 1, 2 ... (n -1)$ or s, p, d, f .... sub shells respectively.

b. It indicates the shape of orbital and orbital angular momentum of electron.

   Orbital angular momentum of the electron $= \dfrac{h}{2\pi}\sqrt{l(l+1)}$ or $\bar{h}\sqrt{l(l+1)}$

   Where $\bar{h} = \dfrac{h}{2\pi}$

c. The maximum number of orbitals possible in a sub shell = $2/+1$.

d. The maximum number of electrons possible in a sub shell = $2(2/+1)$.

Magnetic Quantum Number *(m)*

a. It was proposed by Lande to explain 'ZEEMAN'effect.The total m values are $2l + 1$ which are m = $+l$ ..... 0..... $-l$

b. The total number of m values indicates the total number of orbitals in the subshell.

c. The total number of orbitals in s, p, d and f sub shells are 1, 3, 5 and 7 respectively.

d. It indicates the orientation of orbitals in space.

e. For p_z & d_{z^2} orbitals the value of 'm' is zero.

**n, / and m are inter related.

Spin Quantum Number *(s)*

a. It was proposed by Goudsmit and Uhlenbeck to explain the duplets and the multiplets in the spectral lines and the magnetic properties of atoms. It take two values $s = +\frac{1}{2}$ in clock wise $(\uparrow)$ direction and $s = -\frac{1}{2}$ in anti clock wise $(\downarrow)$ direction spin.

b. It is independent of other three quantum numbers.

c. It indicates the direction of the spin of the electron.

d. An orbital can accommodate Maximum of 2 electrons with opposite spin.

e. The maximum capacity of s, p, d and f subshells are 2, 6, 10 and 14 electrons respectively.

Electronic configurations, Aufbau principle, Pauli principle, Hund's rule-Electronic configuration of an atom can be written by using method.

Aufbau Principle

In multi electron atoms, the energy of electron depends on both principal quantum number and azimuthal quantum number .i.e. n+l value.

a. In building up an Atom, Electrons enter in to various orbitals in the increasing order of their energy. i.e. the orbital of lowest energy is filled first.

b. The relative energy various orbitals can be obtained by using (n + *l*) rule.

c. The energy value of orbital increases as its (n + *l*) value increases.

Ex: (n + *l*) value of 1S orbital is 1+0=1 and that of 2S orbital is 2+0=2. Hence energy of 1S<2S.

d.   If two orbitals have the same value for $(n + l)$, the orbital having lower n value is first filled. Ex: $(n + l)$ value of 2p orbital is 2+1=3 and that of 3S orbital is 3+0=3. Hence energy of 2p<3S.

e.   The energy of 4f<5d<6p<7s but all are having $(n + l) = 7$.

f.   The energy of orbitals in multi electron atom is 1s<2s<2p<3s< 3p<4s< 3d< 4p< 5s.......

g.   The energy of electron in hydrogen atom is determined only by the principal quantum number (n).

     Thus the Energy of 1S<2S=2P <3S=3P=3d<4S=4P=4d=4f   etc

Pauli's Exclusion Principle

a.   No two electrons in an atom can have the same values for all the four quantum numbers.

b.   Two electrons in a given orbital have same values of n, l and m.but differ in their spin quantum number.

c.   An orbital can not accommodate more than two electrons.

d.   The capacity of S, P, d and f-sublevels are 2,6,10 and 14 respectively

     (i.e. $4l+2$)

e.   The capacity of K, L M, and N.......shells is 2, 8, 18, 32.....respectively $(i.e. 2n^2)$.

Hund's Rule

a. Orbitals of a given sub level (i.e degenerate orbitals) should be half filled before electron pairing takes place.

b. Unpaired electrons have parallel spin.

c. Half filled and completely filled degenerate orbitals give greater stability to atoms.

Ex: Chromium (Z = 24) and copper (Z = 29) have anomalous electronic configuration due to this reason.

Electronic configuration of chromium atom is $[Ar]4s^1 3d^5$ but not $[Ar]4s^2 3d^4$.

Electronic configuration of copper atom is $[Ar]4s^1 3d^{10}$ but not $[Ar]4s^2 3d^9$

d. Pairing starts in P-sublevel with 4th electron, in a d-sublevel with 6th electron and in an f-sublevel with 8th electron.

e. According to Hund's rule Nitrogen atom has 3 unpaired electrons.

f. The completely filled or half filled subshells have symmetrical distribution of electrons in them and are therefore more stable.

g. electronsof the same spin are present in a subshell then they exchange their positions release energy called exchange energy. The number of exchanges that can take place is maximum when the sub shell is either half filled or completely filled. Greater is the exchange energy, maximum will be the stablity.