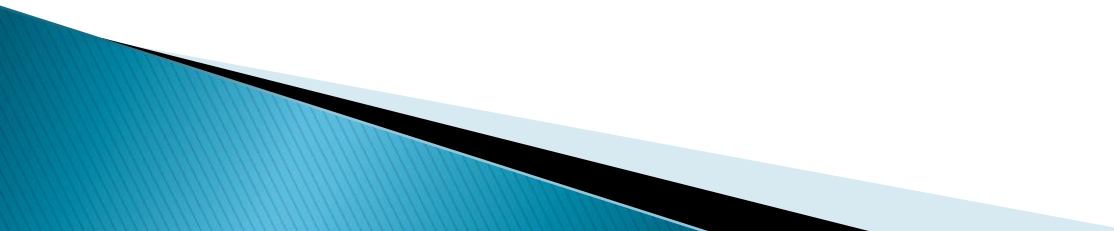


# Quantum Mechanical Model of Atom

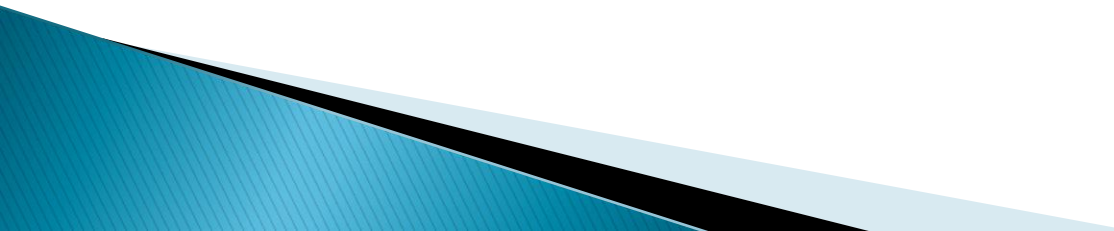
Mr.V



# Heisenberg's Uncertainty Principle

- ▶ It is impossible to measure simultaneously the position and momentum of a small particle (subatomic particle) with absolute accuracy or certainty
  - ▶ The concept of the orbital was based on the probability factor and this principle
- 

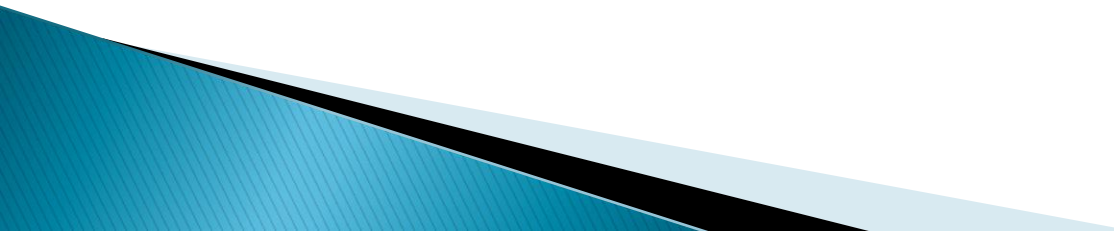
# Orbital

- ▶ It is a three dimensional space around the nucleus where there is a very high probability of locating an electron
  - ▶ Example of orbital's
    - ▶ s-orbital
    - ▶ p-orbital
    - ▶ d- orbital
    - ▶ f-orbital
- 

# Comparison between

ORBIT	ORBITAL
It is a well defined circular path around the nucleus in which the electron revolves	It is a region in three dimensional space around the nucleus where there is a very high probability of locating the electron
It is circular in shape	's', 'p' and 'd' orbitals are spherical, dumbbell and double dumbbell in shape respectively
It represents the movement of an electron around the nucleus in one plane.	It represents the movement of an electron around the nucleus in a three dimensional space.
It states with certainty the momentum and position of an electron. Violates the Heisenberg's uncertainty principle	It is a consequence of Heisenberg's uncertainty principle. .i.e. The position and momentum cannot be known with certainty
The maximum number of electrons in an orbit is $2n^2$ .	The maximum no of electrons in an orbital is 2

# Degenerate Orbitals

- ▶ Orbital's that have the same energy for the sub-shell's are called degenerate orbital's
  - ▶ The three 'p' orbitals are degenerate
  - ▶ The five 'd' orbitals are degenerate when not under the influence of a magnetic field or electric field
- 

# Orbital Wave Function $\Psi$

- ▶ It is called the orbital wave function
- ▶ When you square the value you get the electron density =  $\Psi^2$
- ▶ This is because the motion of the electron is considered to be in the form of waves.
- ▶ Look under diffraction patterns of electrons

# Schrodinger's Wave Equation

- ▶ Equation

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} + \frac{8\pi^2 m(E - V)\psi}{n^2 h^2} = 0$$

# Energy of an electron

- ▶ The equation needed for calculating the energy of an electron is given by

$$E = -\frac{2\pi^2 m e^4 z^2}{n^2 h^2}$$

# Value of energy of electron

- ▶  $E = -2.17 \times 10^{-18} \text{ J/Atom}$
- ▶ or  $-1.312 \times 10^6 \text{ J/Mole}$ .

# Quantum Numbers

- ▶ These are a set of 4 integers necessary to specify the energy , position, shape , size and orientation of orbital's to which electrons belong.

# Principal Quantum Number 'n'

- ▶ It specifies the location and *energy* of an electron,
- ▶ It is a measure of the effective volume or *size* of the electron cloud
- ▶ The letter 'n' is used to indicate it
- ▶ 'n' can have values 1,2,3,4..... $\infty$

# Azimuthal or Angular momentum quantum number = $l$

- ▶ It determines the *shape* of the orbital.
- ▶ It takes integral values from  $0 \rightarrow (n-1)$  where 'n' is the principal quantum number.
- ▶ When ' $l$ ' = 0, 1, 2, the shapes of the orbitals are 's' Spherically symmetrical, 'p' dumbbell, and 'd' double dumbbell.

# Shape of orbital's and 'l' values

l value	0	1	2	3	4
Orbital	s	p	d	f	g
Shape	Spherically Symmetrical	Dumbbell	Double Dumbbell		

# Hybridization – Shapes of molecules

- ▶ [Flash File](#)

Hybr18.swf

# Magnetic Moment q.n 'm'

- ▶ It gives the *orientation* of the orbital's in space. (how many sub shells)
- ▶ It takes integral values ranging from
- ▶  $-l \dots 0 \dots +l$
- ▶ 's' orbital has got one orientation,
- ▶ 'p' orbital has got 3 orientations,
- ▶ 'd' orbital has got '5' orientations
- ▶ 'f' orbital has got 7 orientations.

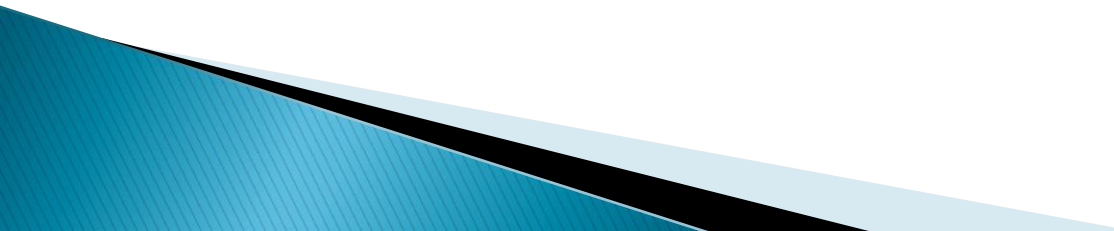
# Spin quantum number 's'

- ▶ It indicates the direction in which the electron *spins* on its own axis or the magnetic property that is associated with it .
- ▶ This value is quantised the two values that are permitted
- ▶ They are  $+ \frac{1}{2}$  and  $- \frac{1}{2}$

# Electronic Configuration

- ▶ Aufbau Order or principle
- ▶ According to the principle the electrons are filled in the various sub-shells in the order of their increasing energies.

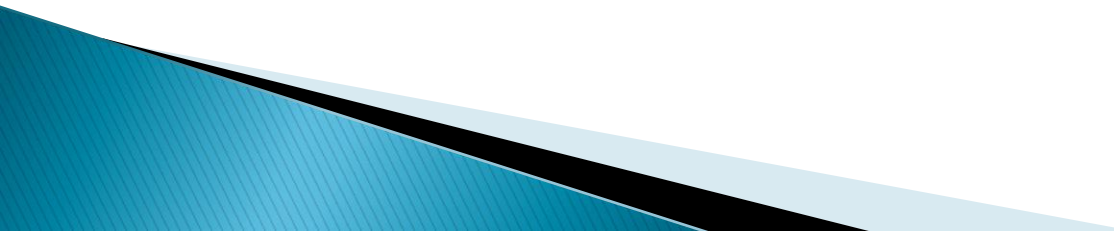
# $n+l$ rule

- ▶  $(n + l)$  Rule: The subshell with lower  $n+l$  value will possess lower energy and will be filled first.
  - ▶ This information can be used instead of Aufbau order.
  - ▶ Or you can verify the order of the orbitals written.
- 

# Aufbau order

- ▶  $1s < 2s < 2p < 3s < 3p < 4s < 3d < 4p < 5s < 4d < 5p < 4f \dots\dots$

# Hund's Rule

- ▶ Electron pairing will not take place in degenerate orbitals (same energy subshell) until each orbital is first singly filled with electrons having parallel spins. Or
  - ▶ Electron pairing will take place only after each sub shell has one electron each.
- 

# Exceptional Configurations

- ▶ Half Filled 'd' orbital configurations are preferred as there is extra stability because of the symmetrical distribution of the electrons in the orbitals.
- ▶ The Exchange energy is High for Cr, Mo & W. and Cu, Ag and Au
- ▶ Exchange energy can be calculated using the following equation Where 'n' is the number of electrons having parallel spins. In the equation given below 'n' stands for the number of unpaired electrons in the d orbital.

▶

▶

$$\text{Exchange Energy} = \frac{n!}{n(n-2)!}$$