<u>Paper = 1</u>

<u>Inorganic Chemistry</u>

<u>Unit = 1</u>

<u>Atomic Structure</u>

- The Atomic structure of an element refers to the constitution of its nucleous and the arrangement of the electrons around it. Primarily, the atomic structure of matter is made up of protons, electrons and neutrons.

- Atomic structure refers to the structure of and atom comparising a nucleus (centre). In which the protons (+ive) (positivily charge) and new neutrons (neutral) are present. The negativily charge particales electrons revolve around the centre of the neucleus.

- The protons and neutrons make up the nucleus of the atom, which is surrounded by the electron belonging to the atom.

- The atomic number of an element describes the total number of proton in its neucleus.

Neutrons   Electron

Orbits

Protons
Neutrons

[The structure of an atom]
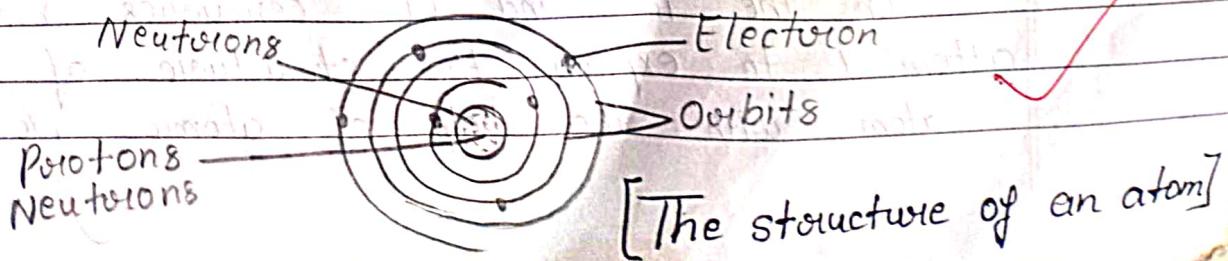
- Nutral atoms have equal numbers of protons our electrons. However, atoms may gain our loss electrons in order to increase there stability and the resulting charged entity is called an ion.

- Atoms of different elements have different atomic structure because they contain different numbers of protons and electrons. This is the reason for the unique characteristics of different elements.

Property	Protons	Electrons	Neutron
1. Symbol	p^t our p^+	e^- our e^-	n our o^n
2. Charged	$+1$ our $+1.6 \times 10^{-19} C$	-1 our $1.6 \times 10^{-19} C$	Zero
3. Mass	$1.67 \times 10^{-27} kg$	$9.1 \times 10^{-31} kg$	$1.675 \times 10^{-27} kg$
4. Location	Present in nucleus	Present around the nucleus	Present in nucleus
5. Discovery	E. Gold Stein	J.J. Thomson	Chadwick

In the 18th and 19th centuries many scientist attemted to explain the structure of the atom with the help of atomic model.

(i) John Dalton

(ii) J. J. Thomson

(iii) Ernest Rutherford

(iv) Nliels Bohr

- According to Rutherford models, most of the mass of an atom in concentrated in a small, clene nucleus.

- The electrons are revolving along the nucleus and occupy most of the volume of the atom.

- The nucleus of the hydrogen atom is of Proton.

- The nuclii of all other atoms are composed a protons and neutrons.

- To explain why the negativily charge of electron do not fall into the positivily charge nucleus.

- Nliels Bohr in 1913 proposed that the energy of electrons seems atoms are quantized, that is, they can have only certain fixed values.

- Thus, Bohr's pictured the electrons has circling along the nucleus in orbit.

- Bohri's model of atom was succesful in explaining atom sepectrum of hydrogen atom.

- However, it failed to explain the sepectrum of multielectron atom.

- Bohri's model of atom also failed to explain the spiliting of spectral lines in the megnatic field (A Henamonal called Zeeman effect).

- As well as in electricfield a Henamonal called stark effect.

- The serious of objection to Bohri's model of atom cames from the revolutionary ideas of de-Buronglie and Heisonberg, who introduced the concept of wave character of electron in addition to the particle character to the electron.

- Within a short time a redicaly different model called the Quantum mechanical model.

- The quantum machenical model of atomic structure was derived from the work of Louis de-Buronglie.

De-Bronglie ideas of Matter Wave

- According to de-Bronglie, all matarial particles in motion possess wave-characteristics. De-Bronglie showed that just as electromagnetic wave could be created of streams of particals (photons), Moving particals could also exibit wave like properties. Thus, it is important to picture electron either as particals or as wave.

- Wave associated with a matter is called matter wave.

- According to de-Bronglie, the wave length λ associated with a partical mass (m), moving with a velocity (v) is given by the relation.

$$\lambda = \frac{h}{mv} \qquad \text{①}$$

Where, h = Planck's constant

mv = momentum of the particle

λ = wave-length

m = mass

v = velocity

The waves associated with the matterial particals

are called the matter waves. The equation first is know as the de-Bronglie equation.

Derivation of de-Bronglie equation

By combining the mass-energy relationship proposed by Max Planck and Albert Einstein, the de-Bronglie relationship for can be derived.

According to Planck, a photon of light havy energy (E). is associated with the wave of fequancy (ν) has.

$$E = h\nu \quad\quad\quad \text{——— II}$$

And according to Einstein mass and energy are related as,

$$E = mc^2 \quad\quad\quad \text{——— III}$$

$$c = velocity \ of \ light$$

Equating the equation II and III

$$h\nu = mc^2$$

Since, $\nu\lambda = c$ or $\nu = \frac{c}{\lambda}$

$$\frac{hc}{\lambda} = mc^2$$

$$\frac{h}{\lambda} = mc \quad\longrightarrow\quad \lambda = \frac{h}{mc}$$

This equation is vailed for a photon. de-Bronglie suggested that an substituating the mass (m) of the

particle and its velocity (v) in place of velocity of light (c), the equation can also be used in case of the matterial partical.

Thus, the wave length of the matterial partical is

$$\lambda = \frac{h}{mv}$$

This equation is know as the de-Bronglie equation. Oer the other woerds,

$$\lambda = \frac{Planck\ constant}{mass\ of\ momentum}$$

Since, h is a constant

$$\lambda \propto \frac{1}{momentum} \qquad \qquad IV$$

It means that the wave length is inversely poroposnal to the momentum to the partical

Significance of de-Bronglie relationship

- Although the duel nature of matter is applicable to all material objects but it is signifacants foor the microscopic bodies only.
- Foor large bodies, the wave length of the associated waves core very with core very small and can not meajcor. measure, Therefoore pariacticaly all the large body have no wave length.
- Thus, the any material body can have the wave length but

Heisenberg's Uncertainty Principle

In 1927 Werner Heisenberg pointedout that one can not measure accurately both the position and velocity (momentum) of a microscopic particale. On the basis of this observation Heisenberg put fooward a principle known as Heisenberg Uncertainty principle.

According to this principle "It is not possible to determine precisely both the position and the momentum of small moving particals with accuracy".

$$(\Delta x)(\Delta p) \geqslant \frac{h}{4\pi}$$

Where,
Δx uncertainty it's position and Δp uncertainty it's momentum.

The sign $\geqslant$ means that the unsertainty can never be less that $\frac{h}{4\pi}$.

The constancty of the poroduct of unsertaintly means that -
If Δx is small that is the position of particale is measured accurately, then Δp would be looge and thus the unsertainty in momentum will

be larged.

(ii) On the other hand, if Δp is small the momentum of the particale can be measured accuratly and the unsertaity in the position that is (Δx) will be larged.

(iii) In Beaif, it is imposible to determine simultaleously the position and momentum of a microscopic particale with absoulate accuracy or certailty.

Werner Heisenberg the Greamon physicist won the physics noblel prize in 1932 by for his coantribution.

Difference between Ah. Orbit and Orbitals

Orbit	Orbitals
• An orbit is a well defined circular path around the nucleus whore electron revolves.	• An orbital represents the reigon where the probability of finding e^- is maximum.
• It represents planar po-motion of the electron.	• The electron exibit the tree dimesional motion.
• All orbits are circular in shape.	• The shapes of orbitals are different. Ex- s-orbital is sphierical shaped. p-orbital iare dumb-bell shape d-orbital are double dumb-bell shaped

• No directional character is shown by the b orbits	• An except s-orbitals, all remaining are directional in nature.
• An orbit can accomodate electrons equal to $2n^2$ where (n) represent the principle quantum number.	• An orbital can have a maximum of two electrons.

Quantum Numbers

A set of four quantum number which determine completely the position and energy of an electron in an atom are called Quantum number. These are :-

(i) Principle Quantum number (n)
(ii) Azimuthal Quantum number (l)
(iii) Magnetic Quantum number (m)
(iv) Spin Quantum number (s)

(i) **Principle Quantum Number :** It is the most important quantum number as it determines the principle energy level or shell to which the electron belongs. It is denoted by the letter small (n) and can have any integral value starting from 1 to infinity except zero (0) (i.e. $n = 1, 2, 3, 4, 5 \ldots \ldots \infty$) The various principle energy levels or shells are also designated by the letter K, L, M, N, S ...... etc.

starting from the nucleus.

(ii) __Azimuthal or Angular Quantum Number :-__ Azimuthal or Angular Quantum number refers to the sub-shell or sub level in a given principle energy shell to which the e^- belongs.

It is also named as Secondary Quantum number and is designated by the symbol (l).

This quantum number gives the energy of the e^- due to the angular momentum of the e^-. The magnitude of the angular momentum of the e^- is related to l by the expression.

$$\text{Angular momentum} = \frac{\sqrt{l(l+1)} \cdot h}{2\pi}$$

Where $l = 0, 1, 2, 3, \ldots\ldots (n+1)$

Is value of l represent a particular sub shell or sub level

l can If $n=1$ than l can have only one value
l can $n=2$ l can have two value
$n=3$ than l can have three value
$n=4$ than l can have four value

Thus, for each value of (n), there (n) different values of (l).

The different value of (l) are coorded by the letters s, p, d, f depinding ⊙ upon the value of (l).

Value of (l)	Symbol	Designation
0	s	sharp
1	p	Poincipal
2	d	diffuse
3	f	fundamental

for all atoms (with the exception of Hydrogen) the energys of the sub shell within the increases sligtly with increasing (l) in the order.
$$s < p < d < f$$

Example: In the fourth shell (n=4), the energy of the sub shell increases as $4s < 4p < 4d < 4f$

For hydrogen atom, however all the sub-shells have equal energy. Energy have $4s = 4p = 4d = 4f$.

(iii) Magnetic Quantum Number (m).

The quantum number descoibes the preferred orieantation of the e^- in the presens of the magnetic field. An e^- is a charge particale and the movement of the e^- along the nucleus geneoiates an electonic field.

The magnetic quantum number determins the number of prefered orientation of the e⁻ present in th a sub-shell. Since each is orientation corresspondes to an orbitals. Therefore the magnetic quantum no. determins the no. the orbital present in any sub-shell.

The value of (m) depends upon the value of (l). For a given value of (l), (m) e can have integlar values starting from $-l, 0, -l$.

Thus, for any value of (l), (m) can have a total of $2l + 1$ values.

$$l = 1$$

$$m = -1, 0, +1$$

$$l = 2$$

$$m = -2, -1, 0, +1, +2$$

$$l = 3$$

$$m = -3, -2, -1, 0, +1, +2, +3$$

(iv) <u>Spin Quantum Number (s)</u>

The electron is continuously revolving around the nucleus. In addition the e⁻ is revolving around it's own axix.
The spining also produces a small magnetic field.
The e⁻ can spin in the two ways either clock-wise or anticlockwise.
Clockwise and anticlockwise spin of about it's own @ exis.
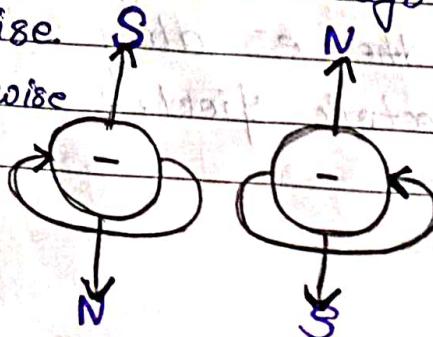
There is addtional additional quantum number that describe the ○ spin orientation of the e- and is called the *Spin Quantum Number (S)*.

For any particular value of magnetic quantum no., spin quantum number can have two values, That is either $+\frac{1}{2}$ or $-\frac{1}{2}$.

The + or - sign before $\frac{1}{2}$ indicate the direction of speed, clockwise or and anticlockwise.

Some times the spin values are represented by two arrows pointing in the oppsite direction (↑ or ↓).

The spine spinning e- behaves like the microomagnet and the mangnitude of angular momentum due to the spin.

Angular momentum due to spinning of e- $= \frac{h}{2\pi} \cdot \sqrt{S(S+1)}$

Where, s represent the spin of the electron

Shapes of s, p, d - orbitals

(i) __S - orbitals :-__ s-orbitals are spherical inshape because a spherea can be defined compeletly by the single value that is it's radius. Hence, s-orbitals are non-directional and spherically sumitrical about the nucleus.
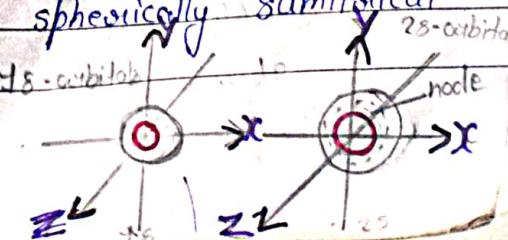
The size of orbitals dependes upon the value of principle quantum number. The larger the valure of (n) the larger is size of the orbitals. Therefore, 2s orbital is larger than the 1s orbital. Both these orbital are non-directional and sphesical in shape.

An impoortant fituores are 2s orbital is that their is the spheorical shell within this orbital Where the porobability of findling the e^- is zeuro (0). This is called the **node** oor **The nodal surface.**

Shapes of p - orbital :- (dumb-bell shape)

$$l = 1$$
$$m = -1, 0, +1$$
$$p = \boxed{1 \mkern-2mu \mid 1 \mkern-2mu \mid 1 \mkern-2mu}$$
$$P_x \quad P_y \quad P_z$$

For p-orbital ($l = 1$, there are three values of m). It means p-sub-shell can have three possible oritentation. These are orepresented by P_x, P_y, P_z.

The destoribution of e^- density foor an e^- in the 2p orbitals is not in distoributed in a sumituri symmitorical manner as in an s-orbitals.

This three orbitals are equal in enorgy. As the p-orbital consist of two loops symmitorical about a poorticuloor axis.
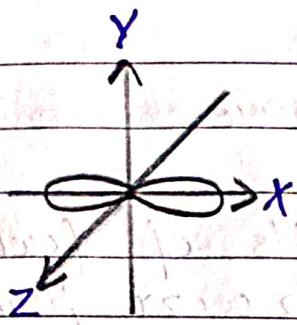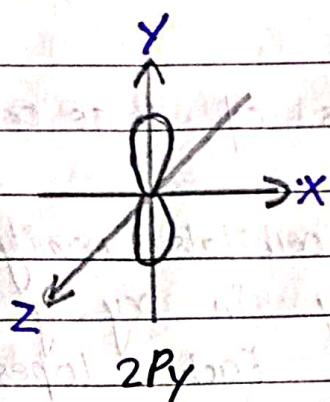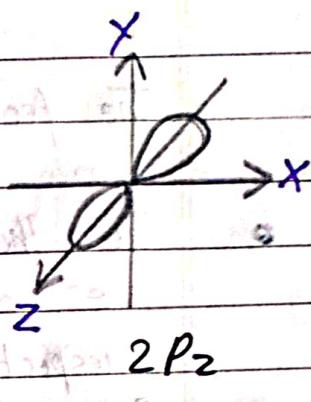
2Px   2Py   2Pz

The p-orbitals thus, is dumb-bell shaped and has a directional character.

The propability of finding the e^- is equal in both loops.

The p-orbitals of a higher energy level (3,4,5, etc) have similar shape although their sizes are bigger.

(iii)   <u>Shape of d-orbital</u>:- (double dumb-bell shape)

$$l = 2$$
$$m = -2, -1, 0, +1, +2$$
$$d = \boxed{1\!\!\downarrow\,|\,1\!\!\downarrow\,|\,1\!\!\downarrow\,|\,1\!\!\downarrow\,|\,1\!\!\downarrow}$$

3dxy, 3dyz, 3dxz, 3dx²y², 3dz²

For d-orbitals, the value of (l) is 2, their are high possible 5 orientations corresponding to allowed values (m).

For 3D subshells, these are designated as. All these orbitals are designate. That is they possess the same energy.
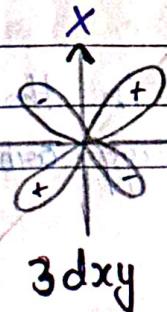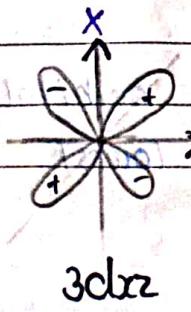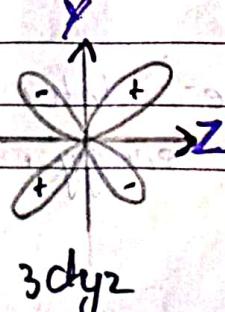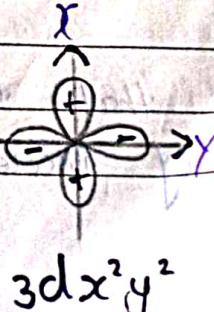

3dxy   3dxz   3dyz   3dx²y²   3dz²
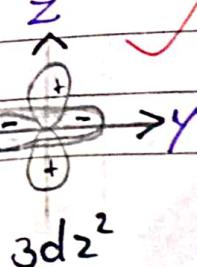
The features of these orbitals are

- The three orbitals namily consists of four lopes of e^- density in xy, yz and xz or zx planes respectivily. Each lopes bisectes the principle axis into two equal halve. These are double-bell dum-bell in shape.
- The $3dx^2y^2$ orbitals have has four lopes of high e^- density along the principle axis x and y
- The $3dz^2$ orbital has a unique shape. It has two lopes along the z axis with a ring of e^- density around the nucelus in the z,y plane. Infact dz^2 is formed by the linner combination of two orbitals $3dy^2$, $3d \cdot 3dy^2z^2$, $3dz^2x^2$ each of which has four lopes along the correspounding axis.