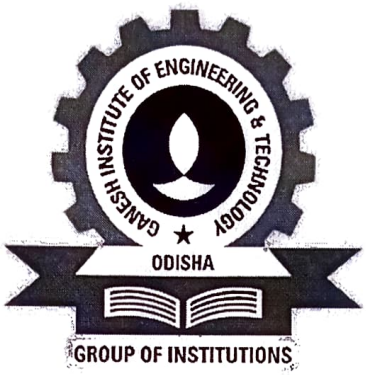
Ganesh Institute of Engineering and Technology



SCTE &VT, BHUBANESWAR, ODISHA

By

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Unit -1

Atomic structure Chemical Bonding Solution

- An atom is the smallest unit of a Matter that retains its properties and may or may not have an independent existance.
- The word Atom is derived From the ancient greek adjective "Atomos" meaning uncutable or indivisible..

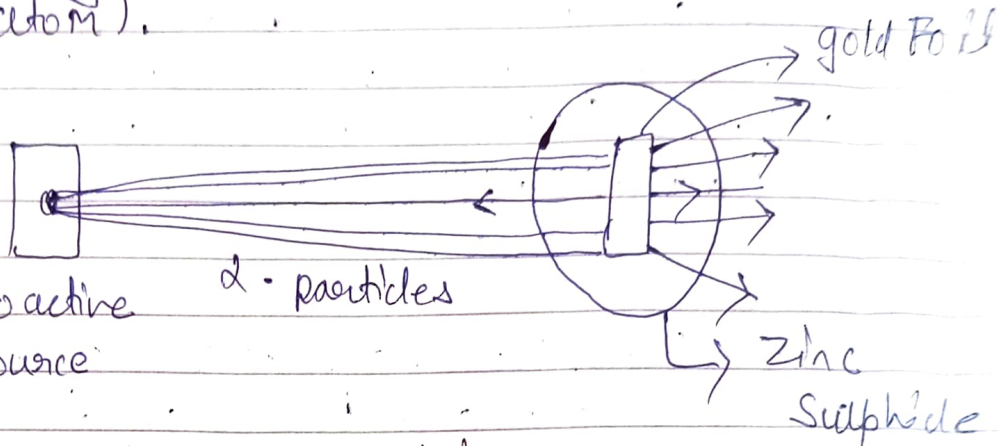
→ Rutherford Model of ATOM :-

1) Ernest Rutherford, a British scientist conducted an experiment and based on the observation of this experient he explained the atomic structure of an element.
2) Rutherford directed high energy strings of alpha particles From a radioactive source at a thin sheet of gold then studied the trajectory of these particles after their interaction with the gold Foil.
3) In order to study the deflection caused to these particles. He pleased a Flourescent zinc sulphide screen around the thin gold Foil.

→ Observation of Alpha Scattering experiment

- An major Fraction of the alpha particles passed through the shields without any deflection. (Most part of the atom is empty)
- Some of the particles were deflected by a small angle (Positive charge is not
- uniformly distributed and occupy a very small volume.

- A very few of the alpha particles were deflected back (Volume of the true charge is very small compare to total volume of the atom).



→ Rutherford atomic Model

- The true charge and most of the mass of an atom is concentrated in an extremly small volume this region is called the nucleus.
- Negatively charged electrons revolve around the nucleus with very high speed in circular paths called orbits.
- Electrons are positively charged particles are held together by strong electrostatic force of attraction.

→ Limitations

- According to Maxwell accerlated charged particles emit electromagnetic radiation so, electron revolving around the nucleus should emit electromagnetic radiation. As a result an atom should lose energy and shrink electrons should collapse into the nucleus. In less than 10^{-8} sec.

→ Bohr's theory :-

Bohr proposed his atomic model to overcome the drawbacks of Rutherford's nuclear model. Bohr atomic model is based on the following postulates.

- An atom consist of a dense positively charged central part known as the nucleus which is at rest.
- The nucleus contains protons and neutrons combinly called nucleus.
- The fixed circular path in which electrons revolve around the nucleus is known as orbits or shells.
- Stationary orbits or non radiating orbits are those orbits in which electrons do not radiate energy.
- Permitted shells or orbits are those for which the angular momentum of an electron is an integral multiple of $h/2\pi$

$m \cdot v \cdot r = n\left(\frac{h}{2\pi}\right)$ where n = principle quantum no.

h = Plank's constant = 6.62×10^{-34} JS

- The shape of orbit is circular orbits are designated by K, L, M, N.... or denoted as 1, 2, 3, 4.... From the nucleus.
- The maximum capacity to accomodate electrons is given by the formula $2n^2$ where n = orbit number.
- The electrostatic force of attraction between the nucleus and electron is exactly balanced

by the Centrifugal Force that is why the electrons do not Fall into the nucleus and remain stable.

Spectra of hydrogen atom

When an electron jumps From higher energy level to lower energy level it radiates energy $e = h\nu$

h = plank's constant 6.62×10^{-34} JS

ν = Frequency of radiation

The transition Frequency emitted in the Form of Photon is given by $\bar{\nu} = \frac{1}{\lambda} = R_H \left[\frac{1}{n_F^2} - \frac{1}{n_i^2} \right]$

$\bar{\nu}$ = Wave number

λ = wavelength

R_H = Rydberg constant

n_F = Final shell

The transition Frequency emitted in the Form of Photon is given by

A.

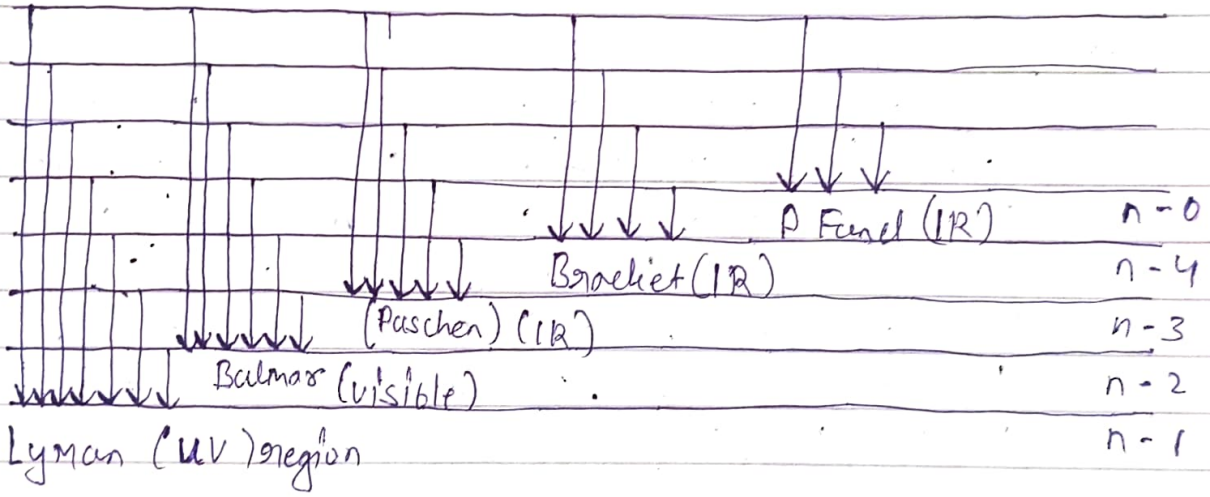
When electron jump From higher energy level to the First shell in hydrogen atom the series obtained is called lyman series.

When electrons Jump From higher energy level to Second shell of hydrogen atom the series obtained is called Balmar series.

- When electron Jump From higher energy level to third shell the series obtained Paschen series.

- When electron Jump From higher energy level to Fourth shell the series obtained Brachet series.

- When electron Jump From higher energy level to Fifth shell the series obtained P Fund series.



→ Heinsenberg Uncertainity Principle

The principle states that It is impossible to simultaneously determine the position and momentum of an electron.

Mathe.... $\Delta x \cdot \Delta P > \frac{h}{4\pi}$

Here,

Δx = Change in position

ΔP = Change in momentum

h = Plank's constant

- **Orbital concept and shapes of S, P, D, F orbital.**
An atomic orbital represents a region in 3D space around the nucleus where there is maximum probability of finding an electron of specific energy.

→ **S Orbital**
These orbitals are spherical and non directional. Each S orbital can accomodate a maximum of 2 electrons of opposite spin.

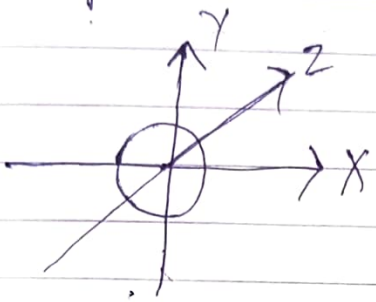
→ **P Orbital**
These orbitals are dumble shape and divided into three sub-shells, or sub orbitals. Each sub orbitals can accomodate a maximum of 2 electrons making a total of 6 electrons. These orbitals are directional and along the axis orbital. The sub orbitals are... P_x, P_y, P_z

→ **D-orbital**
These are Double Dumbell shape or have a four loop planner structure. These are divided into five sub orbitals. These are directional along axis orbitals as well as between the axis orbital. These are $d_{xy}, d_{yz}, d_{zx}, d_{x^2-y^2}$ d_{z^2}

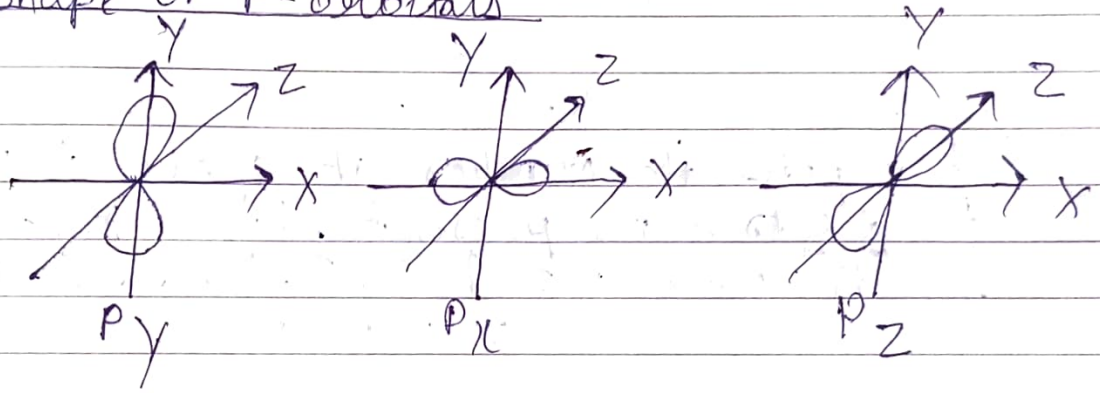
→ **F orbital**
The F orbital are divided into seven sub orbitals that is i.e. $F_{x(x^2-3y^2)}$ $f_{y(3x^2-y^2)}$ $f_{z(x^2-y^2)}$, F_{xz^2}, F_{yz^2}, F_{z^3}, F_{xyz}

The Sub orbitals have complecated structure.

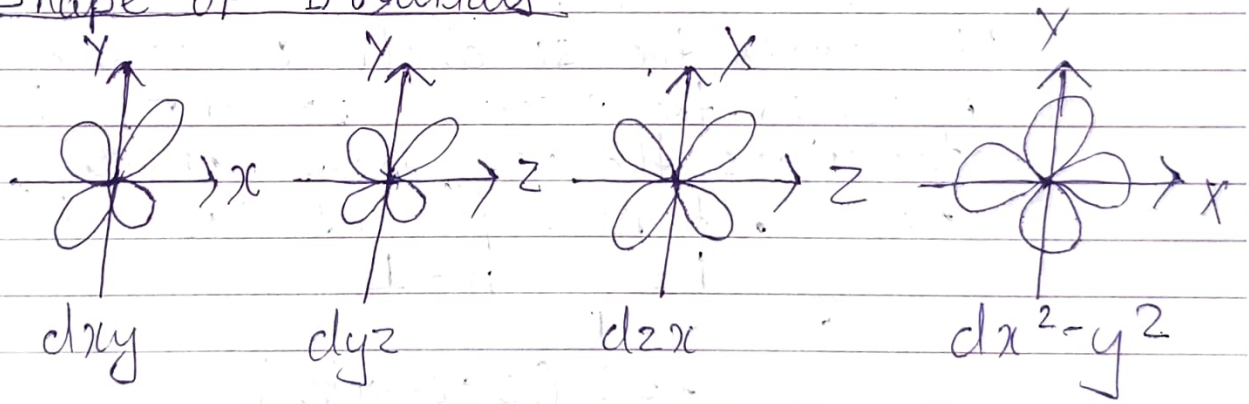
- Shape OF S-Orbital

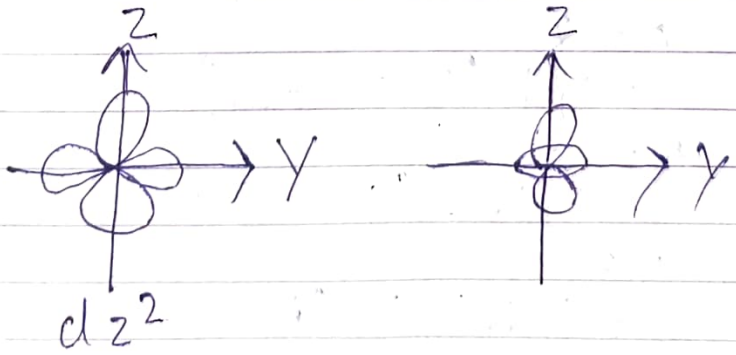


- Shape OF P-orbitals



- Shape OF D orbitals





→ Principle quantum number

- These are a set of numbers that describes the position and orientation of an electron
- quantoms number are divided into Four Categories :-

→ Principle quantum number
→ Azimuthal quantum number
→ Magnite quantum number
→ Spin quantum number

- Principle Quantum number

It denotes the number of shell in which the electron is present. It is represented by "n" where n = 1, 2, 3, 4 . . . . ∞
K L M N

- Azimuthal Quantum number

It denotes the subshell or orbital in which the electron present. It describes the orientation of an electron. It is represented as "l"

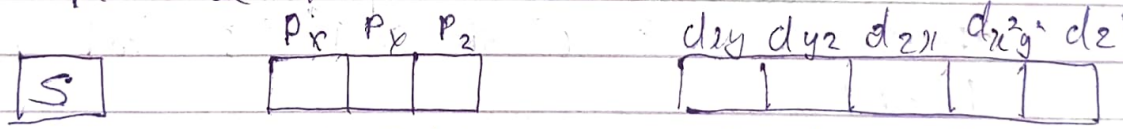
l = 0 n-1

When n = 1
l = 0 (s-orbital)
n = 2
l = 0, 1 (p-orbital)
n = 3
l = 0, 1, 2 (d-orbital)
n = 4
l = 0, 1, 2, 3 (F-orbital)

- **Magnetic quantum number**
  It describes the direction of orientation of an electron. It is represented as ('m')
  When $l = 0$ (s)
  $m = 0$
  $l = 1$ (p) $m = -1, 0, +1$
  $l = 2$ (d) $m = -2, -1, 0, +1, +2$

- **Pauli's exclusion principle. Spin quantum number** m_s
  ~~The rule~~
  It represents the spin of an electron around its own axis of rotation when the spin is clockwise it is represented by $+1/2$ and when it is anticlockwise it is represented by $-1/2$. It is denoted by (s)

- **Pauli's exclusion principle**
  The rule state that in the same orbital can have the same value for all four quantum number.



	n	l	m	s
1st - 2	1	-1	+1/2
2nd - 2	1	+1	+1/2

Aufbau's Principle

Electrons get Filled in the orbitals in the order of increasing level of energy the Orbital with lower energy gets Filled up fast The energy of the orbital is determined by adding its n and l value IF n + L value is small

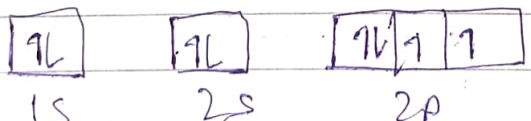
Orbital	n+l
1s	1 + 0 = 1
2s	2 + 0 = 2
2p	2 + 1 = 3
3s	3 + 0 = 3
3p	3 + 1 = 4
3d	3 + 2 = 5
4s	4 + 0 = 4

1s < 2s < 2p < 3s < 3p < 4s < 3d

Hund's Rule of Maximum multiplicity

The rules states that no pairing starts only after each orbit of the same orbital contains 1 electron

Oxygen (8)



O - $1s^2\ 2s^2\ 2p^4$

Chemical bonding

A chemical bonding is a type of force thats binds the atom in a molecule together

Types of Chemical bonding

Ionic bonding
Covalent bonding
Metallic bonding
Co-ordination bond.

Ionic bonding :-

Ionic bonding occurs due to transfer of electron from one atom to another.

Ex - NaCl Formation

$Na - 1 \longrightarrow Na^+$

$Cl + 1^- \rightarrow Cl^-$

$Na^+ + Cl^- \rightarrow NaCl$

The ion which positive charge is called Cation and the ion with negative charge is called anion. An ion is a charged species.

Hybridisation

It is a chemical phenomenon in which the atomic orbitals combine to form hybrid orbitals of equivalent shape and similar energy.

Types of hybridisation

sp hybridisation

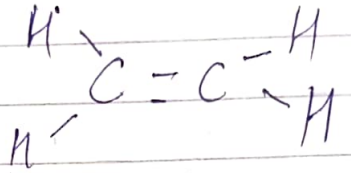
1s, 1p atomic orbital combine to form to sp hybrid orbitals the phenomenon is called sp hybridisation. sp hybridise molecules.

are linear in shape with bond angle 180°. Ex. acetelyne molecule.

H-C≡C-H Ethyne

→ SP^2 hybridisation

When 1s and 2P atomic orbitals combine to form three SP^2 hybrid orbitals. The phenomenon is called SP^2 hybridisation.



Ethene

SP^2 molecules are ~~dotagon~~ trigonal planar in shape and have a bond angle of 120°

→ SP^3 hybridisation

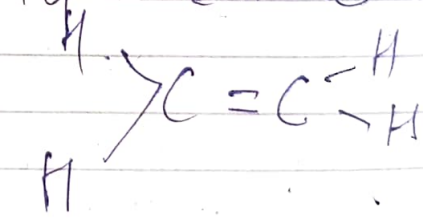
When 1s and 3P atomic orbitals combine to form $4sp^3$ hybrid orbitals. The phenomenon is called SP^3 hybridisation. SP^3 hybridised molecules are tetrahedral in structure and have a bond angle of 109°28'.

(Ethyne) C_2H_2

C: $1s^2 2s^2 2p^2$

H-C≡C-H

C_2H_4 Ethene

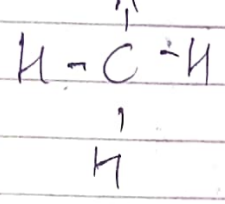


Covalent bonding

Chemical bond Formed by sharing of Valence electrons between two atoms is called Covalent bond.

- (CH_4) Methane

$C = 1s^2 2s^2 2p^2$ $H = 1s^1$

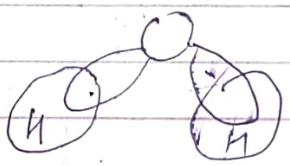


- H_2O

$O - 1s^2 2s^2 2p^4$

No of Valence $O = 6$

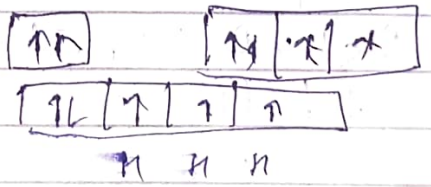
$H = 1s^1$

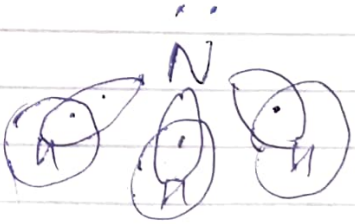


- NH_3

$1s^2 2s^2 2p^3$

No of Valence electrons 5

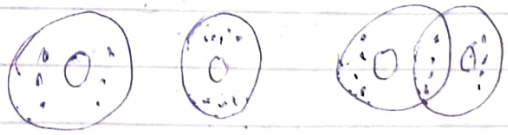




- H_2

$H - 1s^1$ $H-H$

- O_2 $O = 2s^2 2p^4$



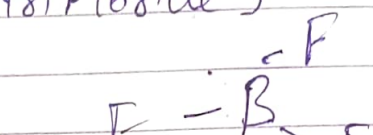
$Be = 1s^2\ 2s^2\ 2p^0$

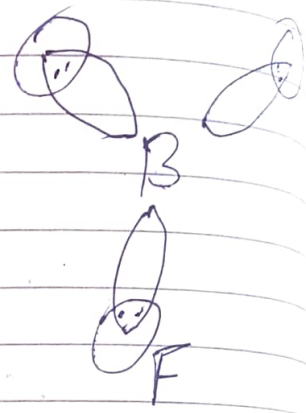
$Be = 1s^2\ \underset{\boxed{\uparrow\downarrow}}{2s^1}\ 2p^1\ 2p_y^0\ 2p_z^0$

Cl Cl

$BeCl_2$ is sp hybridised with linear shape.

2) BF_3 (Boron trifloride)





$B = 2s^2\ 2p_x^1\ 2p_y^0\ 2p_z^0$

$B^* = \underset{sp^2 \text{ hybridisation}}{2s^1\ 2p_x\ 2p_y^1\ 2p_z}$

$\boxed{\uparrow}\ \boxed{\uparrow}\ \boxed{\uparrow}$

F F F

BF_3 is sp hybridised and trigonal planar on shape.

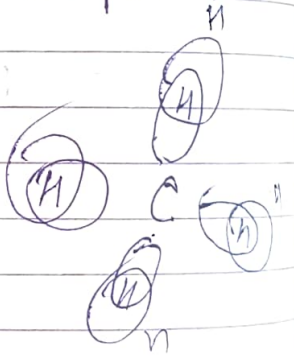
1) CH_4

$C = 2s^2\ 2p^2$

$C^* = 2s^1\ 2p_x^1\ 2p_y^1\ 2p_z$

$\boxed{\uparrow}\ \boxed{\uparrow}\ \boxed{\uparrow}\ \boxed{\uparrow}$

H H H H



CH_4 $2s^1$ sp^3 hybridised with tetrahedral structure.

2) NH_3

$N = 2s^2\ 2p_3$

$\boxed{\uparrow\downarrow}\ \boxed{\uparrow}\ \boxed{\uparrow}\ \boxed{\uparrow}$

sp^3

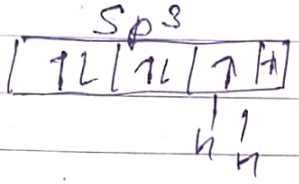
$\boxed{\uparrow\downarrow}\ \boxed{\uparrow\downarrow}\ \boxed{\uparrow}\ \boxed{\uparrow}$

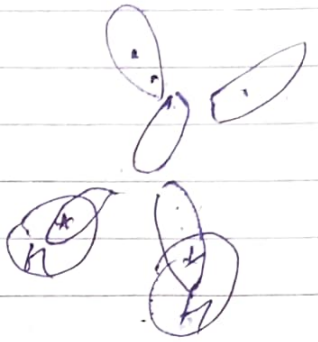
Due to lone pair bond pair repulsion NH_3 decreate From original tetrahedral structure to pyramidal geometry.

3) H_2O

$O - 2s^2\ 2p^4$

$^{+}O = 2s^2\ 2p_x^2\ 2p_y^1\ 2p_z^1$





Due to the presence of 2 lone pair of electrons H_2O molecule is V-shaped or .

Coordinate bond

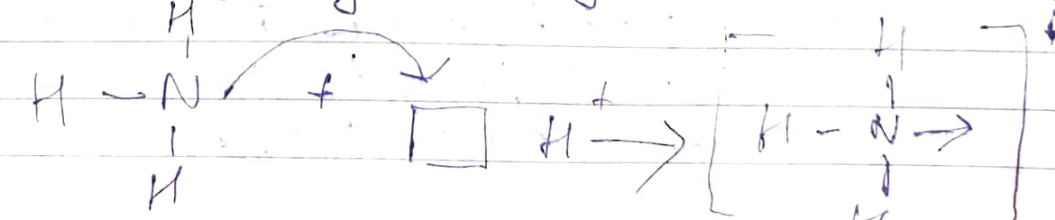
It is a special type of covalent bond in which both the share electrons are contributed by one atom only. This bond is also called a dative bond or dipolar bond.

Characteristic Feature of Coordinate Bond

i) The atom that shares electron pair From itself is known as the donner while the other atom which accepts these share pair of electrons From the donner is called the receptor or acceptor.

ii) The bond represented with an arrow pointing towards the acceptor From the donner atom.

iii) Atom gets stabilized after sharing of each electrons pairs.



Properties of Coordinate Compound

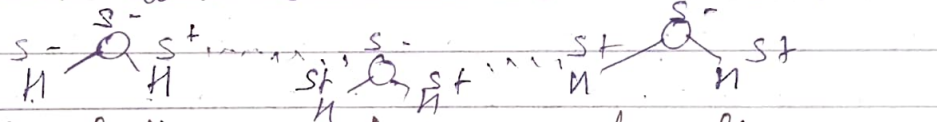
i) Coordinate compound have lower melting and boiling points than ionic compound.

iii) It is called a directional bond because sharing electrons takes place in definite direction.

iv) It is weaker than ionic bonding.

Hydrogen bonding

When a molecule with hydrogen atom is linked to a highly electronegative atom be electronegative atom attaches the share pair of electrons as result of end of the molecule become slightly -ve while the other end become slightly +ve. The -ve end of the molecule attach the +ve end of another molecule. This weak bond is formed between them."T



Condition For hydrogen bonding

i) The molecule must posses a highly electro-ve atom linked to the hydrogen atom.

ii) The size of the electro-ve atom needs to be small.

Types of hydrogen bonding

Inter molecular, Intra molecular.

i) In this two molecules of this same compound join to form aggregates this type of bonding increases solubility in water and also boiling points of the compound.

ii) In this hydrogen bonding occures between atoms of the same molecules present on different sides which leads to intra molecular ring formation called Chelation.

Consequences of hydrogen bonding

- The compounds having hydrogen bonding so abnormally high melting and boiling point because extra energy is needed to break these bonds.
- Organic compounds like alkanes, alkene, alkynes are insoluble in water due to the absence of hydrogen bonding whereas alcohols, organic acids, amines are soluble in water due to the presence of hydrogen bonding.
- The density of ice is less than water and water contracts when heated between 0 to 4°C. These two unique properties are explained on the account of the open cage structure of ices.

Covalent bonding	Hydrogen bonding
• It involves sharing of electrons between two atoms or molecules	• The dipole-dipole intermolecular attraction between hydrogen atoms and electronegative atoms leads to the formation of hydrogen bonding.
• The covalent bond is formed between two electronegative atoms belonging to the same or different elements.	• It is form between a hydrogen atom and a highly electronegative atom such as F, O, N

- The bond strength of this bond is high. It changes chemical properties of bonding molecules.
- The strength of this bond is very small. It changes the physical properties of bonding Molecules.

Anamolous Properties of H_2O and NH_3

- Water is liquid whereas H_2S, H_2Se H_2Te are all gases at ordinary temperature. In water hydrogen bonding causes linkages in water molecule which results in a higher boiling point
- Because of strong intermolecular hydrogen bonding H_2O, HF, NH_3 exist as associated molecules
- Ammonia has a higher boiling point than PH_3 because there is hydrogen bonding in ammonia

Metallic bonding

Metallic bonds are formed when a rigid definite lattice of metal cation shares delocalised valence electrons

Characteristics due to metallic bonds

1. High electrical and thermal conductivity
2. Highly malleable and ductile.
3. Metallic lustre.
4. High Melting and boiling point

Solution

i) Solution is a homogeneous mixture of solute and solvent

ii) Substances added to the solvent in small quantity is known as solute.

iii) Substance present in a large quantity to dissolve the solute is known as solvent.

Methods to express the Concentration

Molarity - A solution in which one mole of compound solute is dissolved in the solvent and diluted upto one meter is called one molar solution.

$$M = \frac{\text{No of moles of Solute}}{\text{Volume of Solvent}}$$

Parts per million - It is defined as the mass ratio of parts of solute to one million parts of gram of Sample.

$$PPM = \frac{\text{Gram of Solute}}{10^6 \text{ grams of Solution}}$$

Mass percentage

$$\frac{\text{Mass of Solute}}{\text{Mass of entire sample}} \times 100$$

$$\frac{\text{Mass of Solvent}}{\text{Mass of entire sample}} \times 100$$

Volume percentage

$$\frac{\text{Volume of Solute or solute}}{\text{Volume of entire sample}} \times 100$$