4. CHEMICAL BONDING AND MOLECULAR STRUCTURE

1 OMQ + 2 VSAQ + 2 SAQ [1 M + 2M + 2M+ 4M + 4M = 13 M]

CONCEPTS & DEFINITIONS

1. Chemical Bonds: The forces of attraction between atoms, ions or molecules are called 'Chemical bonds'.

1.1 Atoms **combine** and form molecules, to get **more stability** and **less energy.**

1.2 Types of Chemical bonds:

(i) Ionic bond

(ii) Covalent bond (σ,π bonds)

(iii) Co-ordinate covalent bond(dative bond)

(iv) Metallic bond **(v)** Hydrogen bond

1.3 Shapes of Chemical bonds in molecules:

(i) Linear:180° (CO_2–sp)

(ii) Trigonal planar:120° (BF_3–sp^2)

(iii) Tetrahedral:109°28' (CH_4 –sp^3)

(iv) Trigonal bi pyramidal: 90°,120° (PCl_5–sp^3d)

(v) Octahedral:90° (SF_6–sp^3d^2)

1.4 Various approaches of chemical bonds:

(i) Kossel-Lewis approach

(ii) VSEPR Theory

(iii) Valence Bond Theory (VBT)

(iv) Molecular Orbital Theory (MOT)

2.0 Kossel-Lewis approach : Atoms combine to acquire nearest inert gas configuration.

This is possible in two ways.

(i) By the transfer of valence electrons from one atom to another (proposed by Kossel).

(ii) By mutual sharing of electrons (proposed by Lewis).

3.0 Ionic bond : An ionic bond is formed by the transfer of electrons from one atom of an element to the atom of another element. In this process, both atoms become oppositely charged ions.

The electrostatic force of attraction between oppositely charged ions is called **Ionic bond.**

3.1 Ionic compounds : The compounds which are formed by the transfer of electrons from one atom to the other are called ionic compounds (or) electrovalent compounds. **Ex:** NaCl, KCl

3.2 Electro Valency: The number of electrons, which an atom loses or gains, while forming an ionic bond is known as electro valency of the atom.

3.3 Steps in the formation of Ionic compounds:

(i) Formation of Cation

(ii) Formation of Anion

(iii) Formation of Crystal lattice.

3.4 Favourable factors for the formation of **cation :**

(i) Low ionisation potential

(ii) Low charge on cation

(iii) Large atomic size.

3.5 Favourable factors for the **formation of anion:**

(i) High electro negativity, electron affinity **(ii)** Low charge on anion

(iii) Small atomic size.

3.6 Characteristics that are related to Ionic compounds :

(i) Physical state

(ii) M.P, B.P

(iii) Solubility

(iv) Electrical conductivity

(v) Reactivity

(vi) Isomerism

4. VB Theory: VB Theory explains the shapes of molecules and directions of bonds.

5. VSEPR Theory: VSEPR theory is proposed to explain the deviation in the bond angles of certain molecules. The shape of the molecules is determined by the arrangement and repulsions between all electron pairs (both lone pairs and bond pairs) present in the valence shell of central atom.

6.0 COVALENT BOND: A chemical bond involving the sharing of electron pair between the atoms, is called covalent bond.

6.1 Sigma bond: A covalent bond formed by an **axial overlapping** of orbitals is called σ -bond.

6.2 Pi bond: A covalent bond formed by **lateral overlapping** of orbitals is called π -bond.

6.3 Hybridisation : The phenomenon of intermixing up of two or more dissimilar orbitals of nearly equal energy of an atom, giving rise to **same number of identical orbitals** having **same energy,** is called hybridisation.

6.3.1 sp hybridisation : The intermixing of one s-orbital and one p-orbital resulting two new orbitals is called sp- hybridisation.

The bond angle is 180° and the shape is linear. **Ex :** CO_2, $BeCl_2$, C_2H_2.

6.3.2 sp^2 hybridisation : The intermixing of one s-orbital and two p-orbitals, resulting three new orbitals, is called sp^2 hybridisation.

The bond angle is 120° and shape is trigonal planar. **Ex :** BF_3, BCl_3, C_2H_4.

6.3.3 sp^3 hybridisation : The intermixing of one s-orbital and three p-orbitals, resulting four new orbitals, is called sp^3 hybridisation.

The bond angle is 109°28' and the shape is tetrahedral. **Ex :** CH_4

6.3.4 sp^3d hybridisation: The intermixing of one s-orbital, three p-orbitals and one d-orbital is called sp^3d hybridisation.

The bond angles are 90° and 120° and the shape is trigonal bi pyramidal.**Ex :** PCl_5

6.3.5 sp^3d^2hybridisation: The intermixing of one s-orbital, three p-orbitals and two d-orbitals is called sp^3d^2 hybridisation.

The bond angle is 90° and the shape is octahedral. **Ex:** SF_6.

6.4 Fajan's rules are used to predict the nature of the bond (Ionic, covalent)

7.0 Co-ordinate covalent bond (Dative Bond): It is a special type of covalent bond, in which the shared pair of electrons are contributed by **only one of the bonded atoms**.

7.1 The atom **contributing** the pair of electrons is known as **donor**, while the atom which **does not contribute but shares** the pair of electrons is called **acceptor**.

8. Metallic Bond: The bond present between atoms of metallic elements is called metallic bond.

9.0 Hydrogen Bond: It is the 'weak electrostatic force of attraction' between a partially positively charged hydrogen atom of a molecule and high electronegative atom of the same or different molecule.

9.1 Types of Hydrogen bonds :

(i) Inter molecular Hydrogen bond **(ii)** Intra molecular Hydrogen bond

10.0 Molecular Orbital Theory (MOT): According to this theory the 'atomic orbitals' of the bonded atoms combine to form molecular orbitals and loose their identities. The electrons in the molecule reside in molecular orbitals instead of atomic orbitals.

10.1 Molecular orbital : Molecular orbitals is a region around the nuclei of the bonded atoms in a molecule, where the probability of finding electrons is maximum.

10.2 Order of energy levels of M.O's:

a) In Li_2, Be_2,B_2,C_2, N_2 molecules:

$$\sigma_{1s} < \sigma^*_{1s} < \sigma_{2s} < \sigma^*_{2s} < \pi_{2py} = < \pi_{2pz} < \sigma_{2px} < \pi^*_{2py} = \pi^*_{2pz} < \sigma^*_{2py}$$

b) In O_2, F_2, Ne_2 molecules:

$$\sigma_{1s} < \sigma^*_{1s} < \sigma_{2s} < \sigma^*_{2s} < \sigma_{2px}\ \pi_{2py} = \pi_{2pz} < \pi^*_{2py} = \pi^*_{2pz} < \sigma^*_{2px}$$

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