HYBRIDISATION

In order to explain the characteristic geometrical shapes of polyatomic molecules like CH4, NH3 and H2O etc., Pauling introduced the concept of hybridisation. According to him the atomic orbitals combine to form new set of equivalent orbitals known as hybrid orbitals. Unlike pure orbitals, the hybrid orbitals are used in bond formation. The phenomenon is known as hybridisation which can be defined as the process of intermixing of the orbitals of slightly different energies so as to redistribute

their energies, resulting in the formation of new set of orbitals of equivalent energies and shape. For example when one 2*s* and three 2*p*-orbitals of carbon hybridise, there is the formation of four new *sp*3 hybrid orbitals.

*Salient features of hybridization*

The main features of hybridisation are as under :

1. The number of hybrid orbitals is equal to the number of the atomic orbitals that get hybridised.

2. The hybridised orbitals are always equivalent in energy and shape.

3. The hybrid orbitals are more effective in forming stable bonds than the pure atomic orbitals.

4. These hybrid orbitals are directed in space in some preferred direction to have minimum repulsion between electron pairs and thus a stable arrangement.

Therefore, the type of hybridization indicates the geometry of the molecules.

Important conditions for hybridisation

(i) The orbitals present in the valence shell of the atom are hybridised.

(ii) The orbitals undergoing hybridisationshould have almost equal energy.

(iii) Promotion of electron is not essential condition prior to hybridisation.

(iv) It is not necessary that only half filled orbitals participate in hybridisation. In some cases, even filled orbitals of valence shell take part in hybridisation.

4.6.1 Types of Hybridisation

There are various types of hybridization involving *s*, *p* and *d* orbitals. The different types of hybridisation are as under:

(I) *sp hybridisation:* This type of hybridisation involves the mixing of one *s* and one *p* orbital resulting in the formation of two equivalent *sp* hybrid orbitals. The suitable orbitals for *sp* hybridisation are *s* and *p*z, if the hybrid orbitals are to lie along the z-axis.

Each *sp* hybrid orbitals has 50% *s*-character and 50% *p*-character. Such a molecule in which the central atom is *sp*-hybridised and linked directly to two other central atoms possesses linear geometry. This type of hybridisation is also known as diagonal hybridisation. The two *sp* hybrids point in the opposite direction along the z-axis with projecting positive lobes and very small negative lobes, which provides more effective overlapping resulting in the formation of stronger bonds.

Example of molecule having *sp* hybridisation

BeCl2: The ground state electronic configuration of Be is 1*s*22*s*2. In the excited state one of the 2*s*-electrons is promoted to vacant 2*p* orbital to account for its bivalency.

One 2*s* and one 2*p*-orbital gets hybridised to form two *sp* hybridised orbitals. These two *sp* hybrid orbitals are oriented in opposite direction forming an angle of 180°. Each of the *sp* hybridised orbital overlaps with the 2*p*-orbital of chlorine axially and form two Be-Cl sigma bonds.

(ii) sp2 hybridisation: In this hybridization there is involvement of one *s* and two *p*-orbitals in order to form three equivalent *sp*2 hybridised orbitals. For example, in BCl3 molecule, the ground state electronic configuration of central boron atom is 1*s*22*s*22*p*1. In the excited state, one of the 2*s* electrons is promoted to vacant 2*p* orbital as a result boron has three unpaired electrons.

These three orbitals (one 2*s* and two 2*p*) hybridise to form three *sp*2 hybrid orbitals. The three hybrid orbitals so formed are oriented in a trigonal planar arrangement and overlap with 2*p* orbitals of chlorine to form three B-Cl bonds. Therefore, in BCl3 , the geometry is trigonal planar with ClBCl bond angle of 120°.

(III) *sp*3 *hybridisation:* This type of hybridisation can be explained by taking the example of CH4 molecule in which there is mixing of one *s*-orbital and three *p*-orbitals of the valence shell to form four *sp*3 hybrid orbital of equivalent energies and shape. There is 25% *s*-character and 75% *p*-character in each *sp*3 hybrid orbital. The four *sp*3 hybrid orbitals so formed are directed towards the four corners of the tetrahedron. The angle between *sp*3 hybrid orbital is 109.5°. The ground state is 2*s*221*x p* 2 1*y p* 2 1*z p* having three unpaired electrons in the *sp*3 hybrid orbitals and a lone pair of electrons is present in the fourth one. These three hybrid orbitals overlap with 1*s* orbitals of hydrogen atoms to form three N–H sigma bonds. We know that the force of repulsion between a lone pair and a bond pair is more than the force of repulsion between two bond pairs of electrons. The molecule thus gets distorted and the bond angle is reduced to 107° from 109.5°. The geometry of such a molecule will be pyramidal.

Types of Overlapping and Nature of Covalent Bonds

The covalent bond may be classified into two types depending upon the types of

overlapping:

(i) Sigma(σ) bond, and (ii) pi(π) bond

(i) Sigma(σ) bond : This type of covalent bond is formed by the end to end (head-on) overlap of bonding orbitals along the internuclear axis. This is called as head on overlap or axial overlap. This can be formed by any one of the following types of combinations of atomic orbitals.

* *s-s* overlapping : In this case, there is overlap of two half filled *s*-orbitals along the internuclear axis
* *s-p* overlapping: This type of overlap occurs between half filled *s*-orbitals of one atom and half filled *p*-orbitals of another atom.
* *p–p* overlapping : This type of overlap takes place between half filled *p*-orbitals of the two approaching atoms

(ii) Pi (π) bond: In the formation of π bond the atomic orbitals overlap in such a way that their axes remain parallel to each other and perpendicular to the internuclear axis. The orbitals formed due to sidewise overlapping consists of two saucer type charged clouds above and below the plane of the participating atoms.

Strength of Sigma and pi Bonds

Basically the strength of a bond depends upon the extent of overlapping. In case of sigma bond,

the overlapping of orbitals takes place to a larger extent. Hence, it is stronger as compared to the pi bond where the extent of overlapping occurs to a smaller extent. Further, it is important to note that in the formation of multiple bonds between two atoms of a molecule, pi bond(s) is formed in addition to a sigma bond.