

Class: XI	Chapter 4- Chemical Bonding Date- 07/10/21
Subject: Chemistry	

Distinction between sigma and pi bonds

<i>Sigma (σ) Bond</i>	<i>pi (π) Bond</i>
(1) s-orbitals are involved in the formation of σ bond.	(1) s-orbitals are not involved in the bond formation.
(2) The overlap is quite large and the bond formed is strong.	(2) π bond is comparatively weak.
(3) The bond is formed by axial overlap of atomic orbitals.	(3) The bond is formed by the sidewise overlap of atomic orbitals.
(4) Only one lobe of the p-orbitals is involved	(4) Both lobes of p-orbitals are involved in the overlap.
(5) The electron cloud formed is symmetrical.	(5) The electron cloud is unsymmetrical.

Hybridisation

Hybridisation is 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.

Salient Features of Hybridisation:

- (i) Orbitals with almost equal energy take part in the hybridisation.
- (ii) Number of hybrid orbitals produced is equal to the number of atomic orbitals mixed,
- (iii) Geometry of a covalent molecule can be indicated by the type of hybridisation.
- (iv) The hybrid orbitals are more effective in forming stable bonds than the pure atomic orbitals.

Conditions necessary for hybridisation:

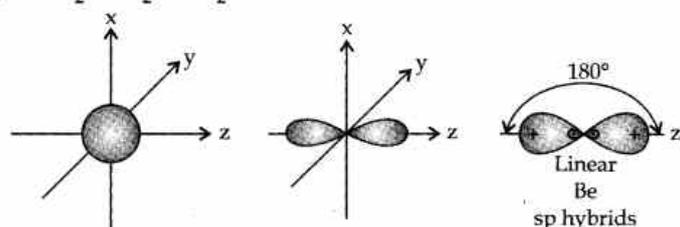
- (i) Orbitals of valence shell take part in the hybridisation.
- (ii) Orbitals involved in hybridisation should have almost equal energy.
- (iii) Promotion of electron is not necessary condition prior to hybridisation.
- (iv) In some cases filled orbitals of valence shell also take part in hybridisation.

Types of Hybridisation:

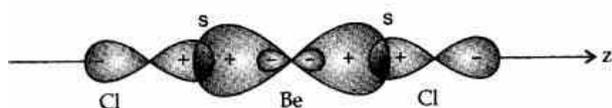
(i) sp hybridisation: When one s and one p-orbital hybridise to form two equivalent orbitals, the orbital is known as sp hybrid orbital, and the type of hybridisation is called sp hybridisation.

Each of the hybrid orbitals formed has 50% s-character and 50% p-character. This type of hybridisation is also known as diagonal hybridisation.

Examples: All compounds of carbon containing $C \equiv C$ triple bond like acetylene (C_2H_2), $BeCl_2$, BeF_2 , BeH_2 etc.



(a) Formation of sp hybrids from s and p orbitals



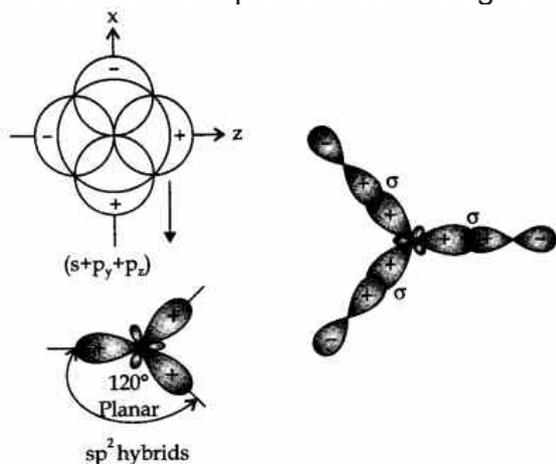
$BeCl_2$ molecule

(b) Formation of the linear $BeCl_2$ molecule

(ii) sp^2 hybridisation: In this type, one s and two p -orbitals hybridise to form three equivalent sp^2 hybridised orbitals.

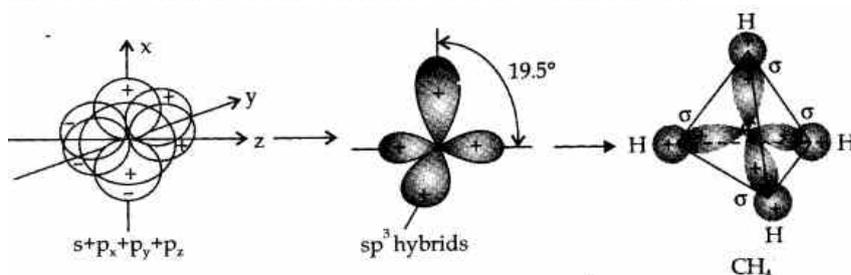
All the three hybrid orbitals remain in the same plane making an angle of 120° .

Example. A few compounds in which sp^2 hybridisation takes place are BF_3 , BH_3 , BCl_3 carbon compounds containing double bond etc.



Formation of sp^2 hybrids and the BCl_3 molecule

(iii) sp^3 hybridisation: In this type, one s and three p -orbitals in the valence shell of an atom get hybridised to form four equivalent hybrid orbitals. There is 25% s -character and 75% p -character in each sp^3 hybrid orbital. The four sp^3 orbitals are directed towards four corners of the tetrahedron.



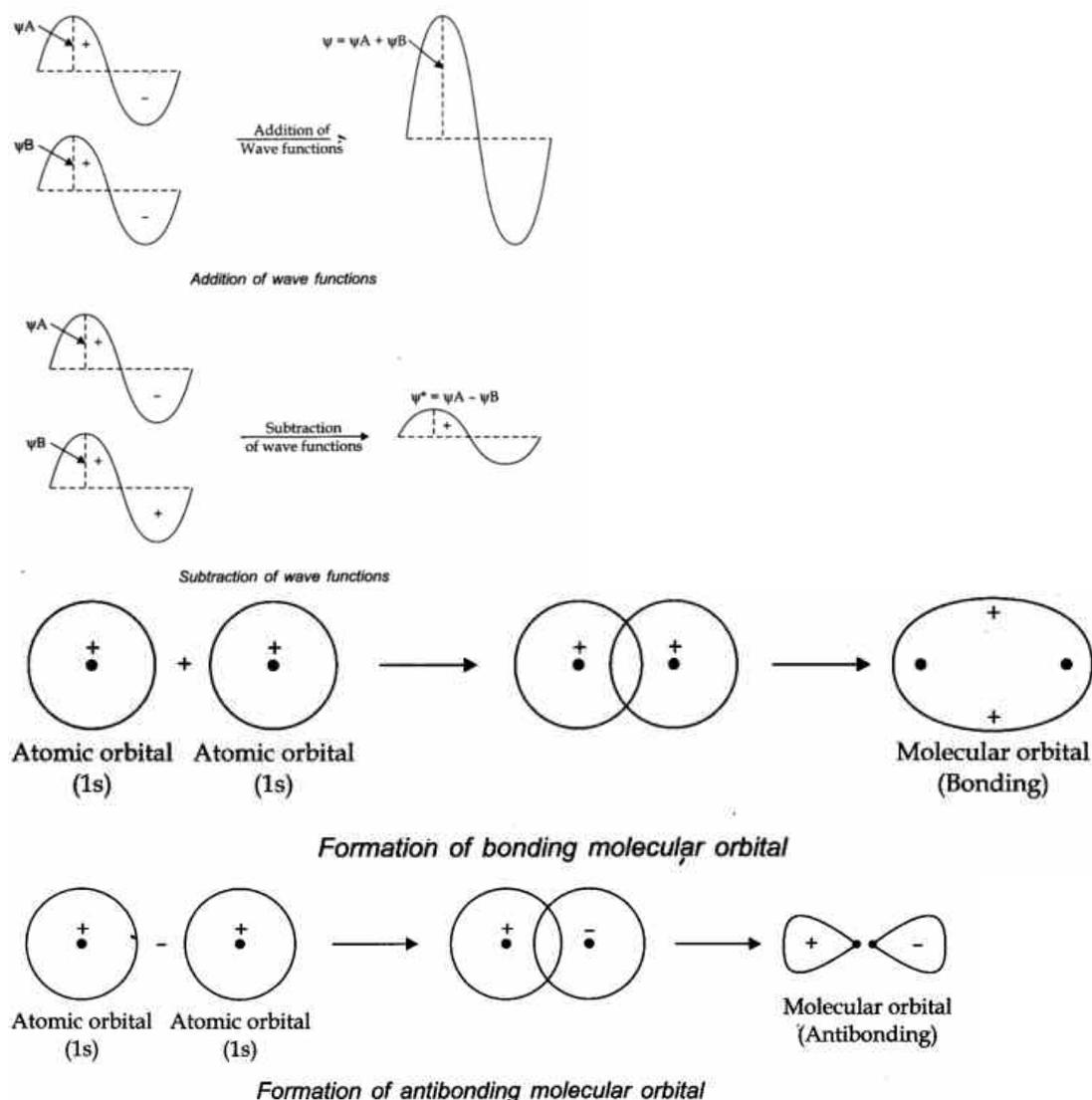
Formation of sp^3 hybrids by the combination of s , p_x , p_y and p_z atomic orbitals of carbon and the formation of CH_4 molecule.

The angle between sp^3 hybrid orbitals is 109.5° .

A compound in which sp^3 hybridisation occurs is, (CH_4). The structures of NH_3 and

H₂O molecules can also be explained with the help of sp³ hybridisation.

Formation of Molecular Orbitals: Linear Combination of Atomic Orbitals (LCAO)
 The formation of molecular orbitals can be explained by the linear combination of atomic orbitals. Combination takes place either by addition or by subtraction of wave function as shown below.



The molecular orbital formed by addition of atomic orbitals is called bonding molecular orbital while molecular orbital formed by subtraction of atomic orbitals is called antibonding molecular orbital.

Conditions for the combination of atomic orbitals:

- (1) The combining atomic orbitals must have almost equal energy.
- (2) The combining atomic orbitals must have same symmetry about the molecular axis.
- (3) The combining atomic orbitals must overlap to the maximum extent.

Types of Molecular Orbitals

Sigma (σ) Molecular Orbitals: They are symmetrical around the bond-axis.

pi (π) Molecular Orbitals: They are not symmetrical, because of the presence of positive lobes above and negative lobes below the molecular plane.

Electronic configuration and Molecular Behaviour

The distribution of electrons among various molecular orbitals is called electronic configuration of the molecule.

• **Stability of Molecules**

If N_b = No. of electrons occupying bonding orbitals.

N_a = No. of electrons occupying antibonding orbitals.

then

(i) If $N_b > N_a$ molecule will be stable.

(ii) $N_b < N_a$ molecule will be unstable.

Bond Order

Bond order is defined as half of the difference between the number of electrons present in bonding and antibonding molecular orbitals.

Bond order (B.O.) = $\frac{1}{2} [N_b - N_a]$

The bond order may be a whole number, a fraction or even zero.

It may also be positive or negative.

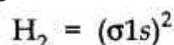
Nature of the bond: Integral bond order value for single double and triple bond will be 1, 2 and 3 respectively.

Bond-Length: Bond order is inversely proportional to bond-length. Thus, greater the bond order, smaller will be the bond-length.

Magnetic Nature: If all the molecular orbitals have paired electrons, the substance is diamagnetic. If one or more molecular orbitals have unpaired electrons, it is paramagnetic e.g., O_2 molecule.

• **Bonding in Some Homonuclear (Diatomic) Molecules**

(1) **Hydrogen molecule (H_2):** It is formed by the combination of two hydrogen atoms. Each hydrogen atom has one electron in 1s orbital, so, the electronic configuration of hydrogen molecule is



$$\text{Bond order (B.O.) of } H_2 = \frac{1}{2}(2-0) = 1$$

$$= \frac{1}{2}(N_b - N_a) = 1$$

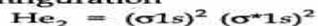
This indicates that two hydrogen atoms are bonded by a single covalent bond. Bond dissociation energy of hydrogen has been found = 438 kJ/mole. Bond-Length = 74 pm

No unpaired electron is present therefore,, it is diamagnetic.

(2) **Helium molecule (He_2):** Each helium atom contains 2 electrons, thus in He_2 molecule there would be 4 electrons.

The electrons will be accommodated in $\sigma 1s$ and $\sigma^* 1s$ molecular orbitals:

Electronic configuration



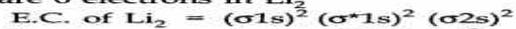
$$\text{Bond order} = \frac{1}{2}[2-2] = 0$$

He_2 molecule is therefore unstable and does not exist.

(3) **Lithium molecule (Li_2)**

E.C. of Li = $1s^2 2s^1$

There are 6 electrons in Li_2



It can also be represented as KK $[\sigma 2s]^2$

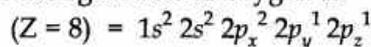
$$\text{Bond order} = \frac{1}{2}[N_b - N_a]$$

$$= \frac{1}{2}[4-2] = 1$$

Nature = Diamagnetic, since molecular orbitals are completely filled.

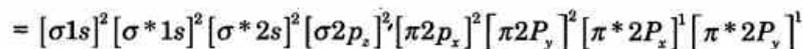
(4) Oxygen molecule (O₂)

The orbital configuration of oxygen is:

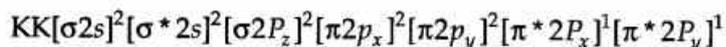


This means that sixteen electrons are to be filled in the molecular orbital of oxygen molecule (O₂).

The molecular orbital configuration



It may also be written as:

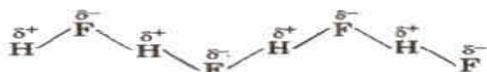


$$\text{B.O.} = \frac{1}{2}[N_b - N_a] = \frac{1}{2}[8 - 4] = 2$$

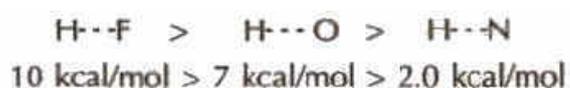
Nature: Paramagnetic due to the presence of two unpaired electrons.

Hydrogen Bond

It is defined as the force of attraction existing between hydrogen atom covalently bonded to highly electronegative atom (N, O or F) and the electronegative atom belonging to another molecule of the same or different substance. It is represented by dotted lines. The chains possess a zig – zag structure.



(Hydrogen bond is purely electrostatic and a weak bond. The strength of the strongest hydrogen bond is about 5-10 kcal per mol. The more the electronegativity of atom involved in H-bonding, the more is the bond strength, e.g.,



Types of hydrogen bonds are

- (i) **Intermolecular H-bonding** : H-bonding involving two or more molecules.
- (ii) **Intramolecular H-bonding** : H-bonding within a molecule.

Applications of Intermolecular H-bonding

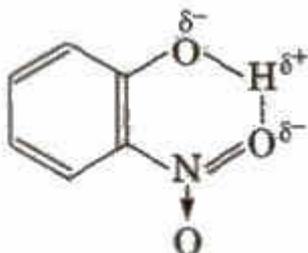
- (i) **Melting point and boiling point of water** Water has the lowest molecular weight among the hydrides of group 16 elements yet it has the highest melting and boiling points. It is due to intermolecular H-bonding in H₂ O.
- (ii) **Ice has less density than water** In crystal structure of ice every water molecule is associated with four other water molecules by H-bonding in a cage like tetrahedral structure. On melting, the ice H-bonds are broken and space between water molecules decreases and density of water increases up to 4° C Above 4°C. more H-

bonds are broken. the water molecules get apart from each other and the density again decreases. Thus, water has maximum density at 4°C.

(iii) **Melting point and boiling point of alcohols** The marked difference between the melting and boiling points of alcohols is also due to H-bonding.

Applications of Intramolecular H-bonding

Volatile character of nitrophenols o-nitrophenol is more volatile (b.p. 214°C) as compared to meta (b.p. 290°C) and para (b.p. 279°C). It is due to chelation.



In meta and para isomer chelation is not possible due to the formation of desired size of ring.

Metallic Bond

Metallic bond is the force of attraction between a metal ion to a number of electrons within its sphere of influence. Electron-sea theory of metallic bond explains number of the properties of the metal

Strength of bonds

Ionic bond > covalent bond > metallic bond > H-bond

Note-The above content has been absolutely prepared from home