

E-Content Study Material

B. Sc. Chemistry (H)

1st Year

Paper I B

Inorganic Chemistry

Chapter III: Chemical Bonding

Topic: Hybridisation

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Hybridisation

According to valence bond theory, a covalent bond is formed by the overlap of half filled atomic orbitals. The direction of overlap gives the direction of the bond. However in applying this theory, a difficulty was faced in a number of cases as explained below.

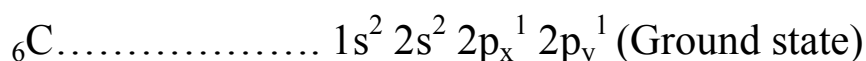
As a covalent bond is formed by the overlap of half-filled atomic orbitals, therefore, the covalency of the element should be equal to the number of half-filled orbitals present in an atom of that element. However, on the basis of this concept, the formation of many compounds such as those of Be, B and C could not be explained.

The electronic configuration of Be, B and C in the ground state are as follows.

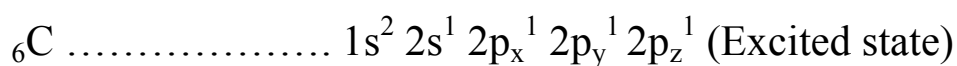
Element	Atomic Number	Electronic Configuration
Be	4	$1s^2 2s^2$
B	5	$1s^2 2s^2 2p_x^1$
C	6	$1s^2 2s^2 2p_x^1 2p_y^1$

On the basis of these configurations, we may conclude that Be, B and C should possess zero, one and two covalencies respectively because beryllium has a covalency of two as in the case of BeF_2 , boron has a covalency of three as in BF_3 whereas carbon has a covalency of four, e.g., in CH_4 , CCl_4 , CO_2 etc.

To overcome the above problem, it was suggested that one paired electron becomes unpaired and jumps to an empty orbital without consuming excessive energy. Let us, for example, consider the case of carbon. Its atomic number is 6 and so its configuration in the ground state is,



Thus, it has two unpaired electrons in the ground state. So it should form two bonds only. But actually carbon shows a covalency of 4. To explain this, it is suggested that an electron from 2s orbital jumps to 2p orbital and so the configuration of carbon in the excited state is,



Thus, now carbon has four unpaired electrons thereby explaining tetravalent nature of carbon. Its one s and three p orbitals can overlap with the half-filled orbitals of reacting atoms, forming four covalent bonds. But covalent bond formed by 2s orbital of carbon should differ in energy from the bonds obtained by the three p orbitals. However, experimental data clearly show that all the four bonds of carbon are same in energy. Moreover, the three bonds formed by 2p orbitals should be at 90° to each other and the fourth formed from 2s orbital may have any direction. However, this is actually not so. Hence, a new concept was introduced to explain this abnormal behaviour of carbon.

According to this concept, all the four orbitals of carbon having unpaired electrons and possessing slightly different energies mix up their energies and then redistribute it in four equal quantities thus giving rise to four new orbitals each having the same amount of energy. This new concept was referred as hybridisation. Thus,

Hybridisation is defined as the mixing of the atomic orbitals belonging to the same atom but having slightly different energies so that a redistribution of energy takes place between them resulting in the formation of new orbitals of equal energies and identical shapes. The new orbitals thus formed are known as hybrid orbitals. The new orbitals thus formed are called hybrid orbitals. The bonds formed by such orbitals are called hybrid bonds. The process of mixing of orbitals itself requires some energy. Thus, some additional energy, over, and above the energy required for the promotion of the required number of electrons to the higher energy orbitals, is needed for the hybridisation (mixing) of atomic orbitals.

Important Note: The energy required for excitation of electrons becomes available when the combining atoms approach each other because energy is released when combining atoms approach each other. That is why hybridisation never takes place in isolated atoms but occurs only at the time of bond formation.

The shape of hybrid orbitals (made from s and p orbitals (either p_x , p_y , p_z) is shown pictorially in Fig.

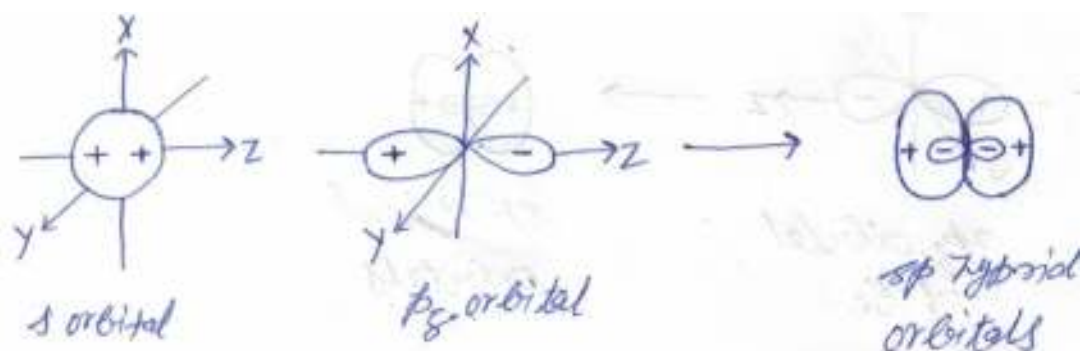


Fig. Formation of two sp hybrid orbitals. + and - are geometric signs of the curves.

A pure s and a pure p orbital (oriented in the Z direction) are shown on the left of the arrow. The two sp hybrid orbitals which result from this combination are shown on the right. Each sp hybrid orbital consists of one large lobe and one small lobe. The large lobe, it may be noted, is much more spread than the original p orbital. This is due to the incorporation of the spherical character of the s orbital into the resulting sp hybrid orbitals. The actual shape of a sp hybrid orbital is shown in Fig.

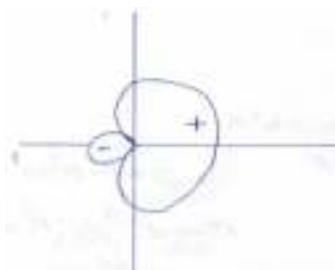


Fig. The actual shape of a sp hybrid orbital.

This clearly depicts the broader size of one of the lobes of the hybrid orbital. Wave mechanically; the shape of the sp hybrid orbital is obtained by plotting the hybrid orbital wave function in three-dimensional space. The wave function of the mixed (or hybrid) orbital is obtained by linearly combining the wave functions of pure atomic orbitals. The broader shape enables the hybrid orbital of one atom to bring about a higher degree of overlapping with the orbital of the other atom. The resulting bond is very strong since, the greater the degree of overlapping, the stronger is the bond.

Shapes of Hybrid Orbitals:

The shapes of hybrid orbitals are different from those of the parent orbitals. For example, s orbital is spherical and p orbital is dumb-bell shaped and, thus, the shape of the bigger lobe of sp hybrid orbital which results from the mixing of one s and one p orbital, is different. It has the characteristics of both the mixing orbitals, and thus has an oval shape as shown in Fig. above. The bigger lobes of sp^2 hybrid orbitals which result from the combination of one s and two p orbitals are pear-shaped because of the greater contribution of the two dumb-bell shaped p orbitals as shown in Fig.

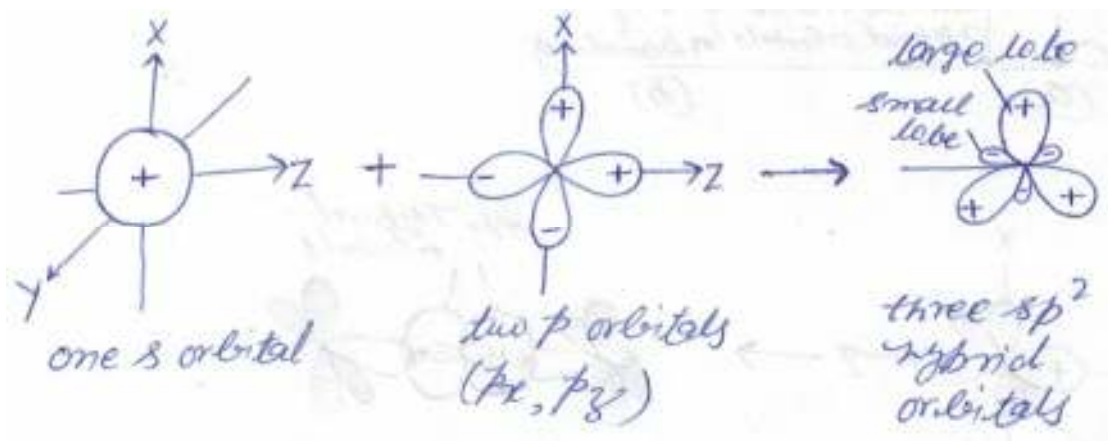


Fig. Formation of three sp^2 hybrid orbitals.

In the case of sp^3 hybrid orbitals which result from the mixing of one s and three p orbital, the contribution of the three p orbitals predominates over the contribution of one s orbital. The resulting shape of their bigger lobes, therefore, is practically the same as that of the parent p orbitals except for the fact that the lobes in sp^3 hybrid orbitals are somewhat more spread and is somewhat shorter in length than the pure p orbitals, as shown in Fig.

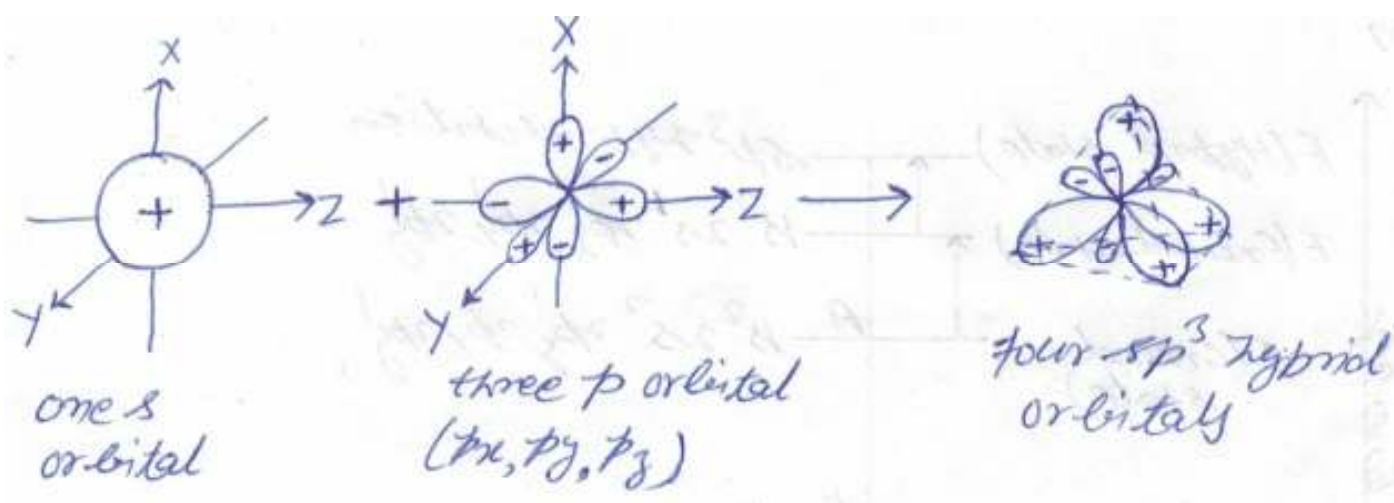
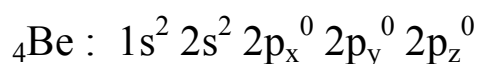
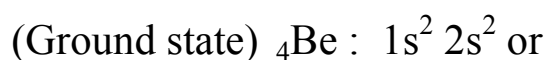


Fig. Formation of four sp^3 hybrid orbitals by overlapping of one s and three p orbitals.

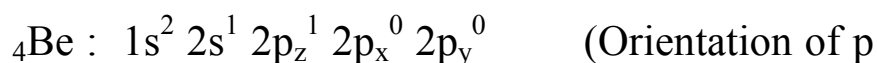
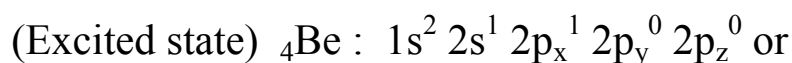
As can be seen, one lobe of the hybrid orbital in each type of hybridisation is considerably bigger in size than the other lobe. It is the bigger-sized lobe of the hybrid orbitals of an atom which overlaps with the orbital of another atom to maximise the overlap to form a stable chemical bond.

For example, formation of BeF_2 molecule.

As mentioned above, the electronic configuration of Be atom in its ground state is,



The promotion of a 2s electron to a 2p orbital results in an excited state configuration of Be which has two half-filled orbitals.



orbital in the Z-axis has been taken)

In the formation of bivalent compounds of beryllium, one s and one p orbital is involved in hybridisation, it is called sp hybridisation and the two identical orbitals which result from this process are known as sp hybrid as shown in Fig.

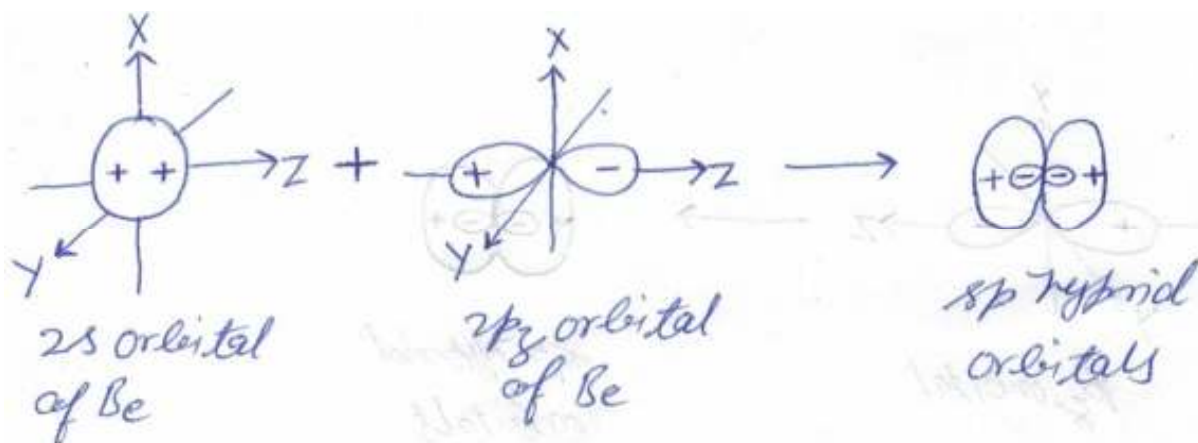


Fig. Formation of two sp hybrid orbitals of Be atom.

The amount of energy (Bond Energy) released (B. E.)₁ due to the formation of sigma bonds between Be and other atoms involving hybrid orbitals is greater than the energy released (B. E.)₂ in case the sigma bonds had involved the pure s and p orbitals. This is shown in Fig. where (B. E.)₁ and (B. E.)₂ are represented by BC and EF, respectively.

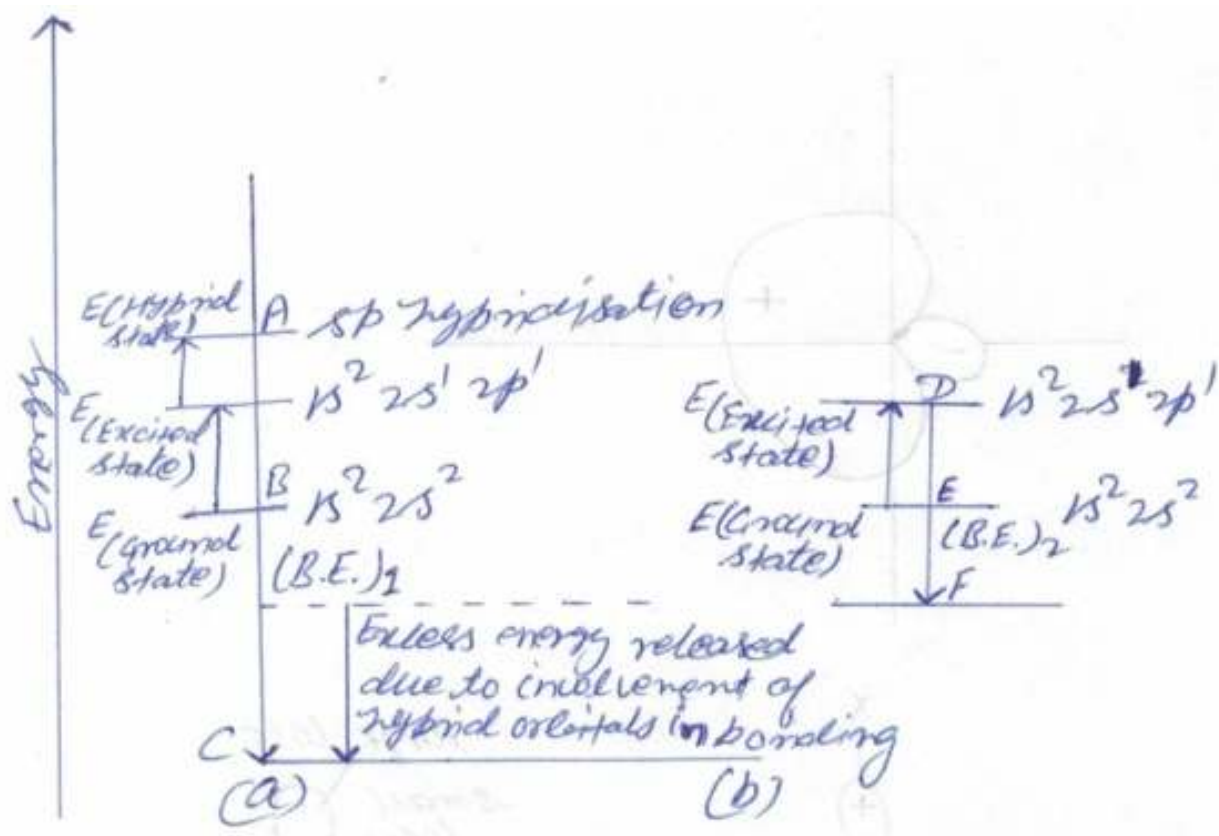
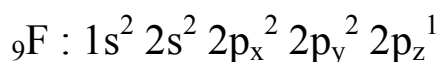


Fig. (a) Energy required for the promotion of a 2s electron to a 2p orbital as also for the hybridisation of s and p orbitals to give sp hybrid orbitals. $(B. E.)_1$ is the energy released when hybrid orbitals are involved in covalent bond formation.

(b) $(B. E.)_2$ is the energy released in the formation of covalent bonds involving pure s and p orbitals.

It is evident from the figure that some additional energy is released due to the involvement of the sp hybrid orbitals in bond formation. Because of this additional decrease of energy, the sigma bonds formed by hybrid orbitals of Be atom are stronger than the bonds formed by pure s and p orbitals.

The electronic configuration of F atom is,



In the formation of BeF_2 molecule, the half-filled p_z orbital of each fluorine atom overlaps with each of the two half-filled sp hybrid orbitals of the beryllium atom. In this electron sharing process, each orbital contains two electrons and beryllium fluoride, BeF_2 , results. This is represented in Fig.

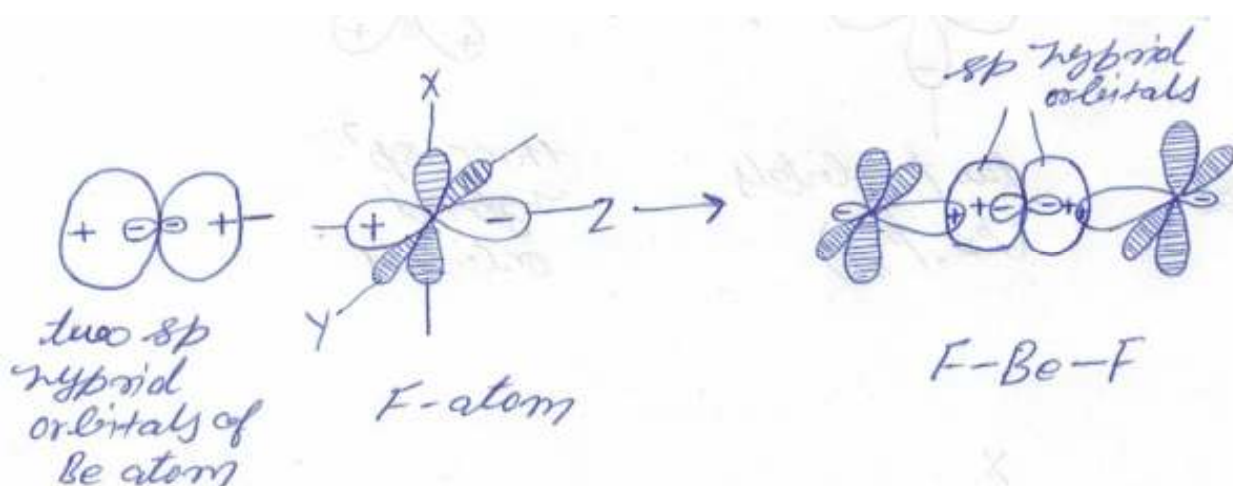


Fig. Formation of beryllium fluoride molecule by overlapping of the half-filled $2p_z$ orbitals of fluorine atoms with the two sp hybrid orbitals of beryllium atom.

The shaded orbitals of fluorine are fully occupied.

As is clear from the figure, the overlap which leads to bonding has a + sign always.