

E-Content Study Material

B. Sc. Chemistry (H)

1st Year

Paper I B

Inorganic Chemistry

Chapter III: Chemical Bonding

Topic: Points and Examples of Hybridisation

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Some Important Points about Hybridisation.

- (i) One or more electrons from fully filled orbitals of the atom in the ground state, get promoted to the next available orbitals of higher energy (as, for example, from 2s to 2p orbitals in the case of second row elements and from ns to (n-1)d orbitals in the case of transition elements), resulting in an excited state with appropriate number of half-filled orbitals. This process requires sufficient amount of energy. The orbitals in the excited state then undergo hybridisation giving hybrid orbitals of equivalent (or sometimes even of non-equivalent) energy. The process of hybridisation, i.e., mixing of orbitals, further requires some energy. The entire input of energy is, however, more than recovered when the hybrid orbitals combine with the orbitals of other atoms to form covalent bonds.

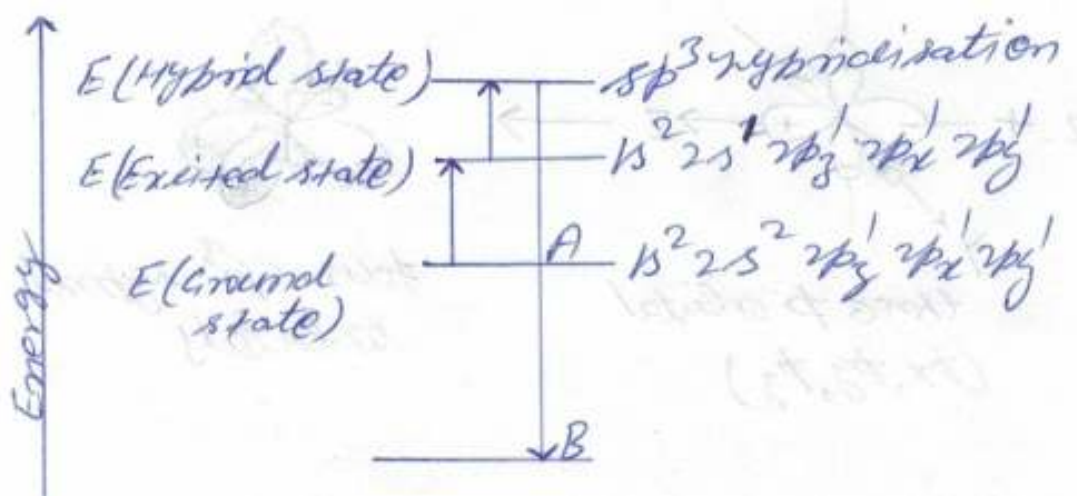


Fig. Energy required (i) for the promotion of a 2s electron to a 2p orbital (II) for the hybridisation of s and p orbitals to give sp^3 hybrid orbitals in case of carbon atom and (III) energy released (represented by AB) in the formation of covalent bonds involving sp^3 hybrid orbitals.

- (ii) Only those orbitals which have approximately equal energies and belong to the same atom or ion can undergo hybridisation.
- (iii) Number of hybrid orbitals produced is equal to the number of atomic orbitals mixed.
- (iv) It is not necessary that all the half-filled orbitals must participate in hybridisation. Similarly, it is not necessary that only half filled orbitals should participate in hybridisation. Even completely filled orbitals with slightly different energies can also participate.
- (v) Hybridisation never takes place in isolated atoms but it occurs only at the time of bond formation.
- (vi) Type of hybridisation indicates the geometry of molecules. One can tell the shape of a molecule by knowing the kind of hybridisation involved.
- (vii) The bigger lobe of the hybrid orbitals always has +ve sign while the smaller lobe on the opposite has a -ve sign.
- (viii) Hybrid orbitals generally form either a sigma bond or contain a lone pair of electrons.

- (ix) The energy released during covalent bond formation involving the hybrid orbitals is much more than the energy released if covalent bond formation involves the pure atomic orbitals. Therefore, the covalent bonds formed with hybrid orbitals are more stable than those formed with pure atomic orbitals.
- (x) The hybrid orbitals are associated with higher energy than the pure atomic orbitals from which they are formed. The greater stability of bonds formed by the hybrid orbitals is due to enhanced overlapping capacity of such orbitals.

Types of hybridisation:

There are various types of hybridisation. Some common types of hybridisation with shapes and examples are as follows.

Type of molecules	No. of bond pairs of electrons	No. of lone pairs of electrons	Total number of electron pairs	Type of hybridisation involved	Atomic orbitals involved	Geometry of molecules	Examples
AB ₂	2	0	2	sp	One s + one p (p _x or p _y or p _z)	Linear	BeF ₂ , BeCl ₂ , BeH ₂ , C ₂ H ₂ , HgCl ₂ , [Ag(NH ₃) ₂] ⁺
AB ₃	3	0	3	sp ²	One s + two p (any two p _x , p _y or p _z)	Trigonal or Traingular planar	BF ₃ , BCl ₃ , BH ₃ , C ₂ H ₄ , NO ₃ ⁻ , CO ₃ ²⁻
AB ₂ L	2	1	3	sp ²	''	Bent (V-shaped)	SnCl ₂ , PbCl ₂
AB ₄	4	0	4	sp ³	One s +	Tetrahadal	CH ₄ , CCl ₄ ,

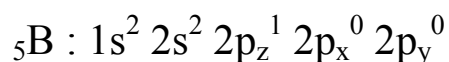
					three p (p_x, p_y, p_z)		$\text{SnCl}_4, \text{NH}_4^+$
AB_3L	3	1	4	sp^3	''	Trigonal pyramidal	$\text{NH}_3, \text{NCl}_3, \text{PCl}_3,$ $\text{PH}_3, \text{H}_3\text{O}^+$
AB_2L_2	2	2	4	sp^3	''	Bent	$\text{H}_2\text{O}, \text{H}_2\text{S}, \text{SeCl}_2,$ NH_2^-
AB_4	4	0	4	sp^2d or dsp^2	One d ($d_x^2 - y^2$) + one s + two p	Square planar	$[\text{Ni}(\text{CN})_4]^{2-},$ $[\text{PtCl}_4]^{2-}$
AB_5	5	0	5	sp^3d	One s + three p + one d (d_z^2)	Trigonal bipyramid al	$\text{PF}_5, \text{PCl}_5,$ $\text{Fe}(\text{CO})_5, \text{SbCl}_5,$ AsF_5
AB_4L	4	1	5	sp^3d	''	Irregular tetrahedral	$\text{SF}_4, \text{TeBr}_4,$
AB_3L_2	3	2	5	sp^3d	''	T-shaped	ClF_3
AB_2L_3	2	3	5	sp^3d	''	Linear	$\text{XeF}_2, \text{ICl}_2^-$
AB_6	6	0	6	sp^3d^2 or d^2sp^3	One s + three p + two d ($d_x^2 -$ y^2 and d_z^2)	Octahedral	$\text{SF}_6, [\text{SbF}_6]^-,$ $[\text{CrF}_6]^{3-},$ $[\text{Co}(\text{NH}_3)_6]^{3+}$
AB_5L	5	1	6	sp^3d^2	''	Square pyramidal	$\text{IF}_5, \text{ClF}_5, \text{BrF}_5,$ $[\text{SbF}_5]^{2-},$
AB_4L_2	4	2	6	sp^3d^2	''	Square planar	$\text{XeF}_4, \text{ICl}_4,$
AB_7	7	0	7	sp^3d^3	One s + three p + three d ($d_{xy},$ d_{yz}, d_{xz})	Pentagona l bipyramid al	IF_7

Note: $d_x^2 - y^2$ and d_z^2 orbitals are involved in sp^3d^2 hybridisation obviously because lobes of $d_x^2 - y^2$ lie along the X and Y-axis and those of d_z^2 lie along the Z-axis. The four hybrid orbitals lie along the X and Y-axis where the remaining two lie along the Z-axis.

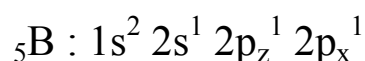
Example.

Formation of BF_3 molecule (sp^2 hybridisation of orbitals of boron atom).

The outer electronic configuration of boron atom in its ground state is,



Promotion of one of the 2s electrons into one of the vacant 2p orbitals gives rise to an excited state configuration,



There are, thus, three half-filled orbitals which account for tri-covalency of boron. The three orbitals, one 2s and two 2p hybridise to give three hybrid orbitals of equivalent energy. The formation of sp^2 hybrid orbitals is shown in Fig.

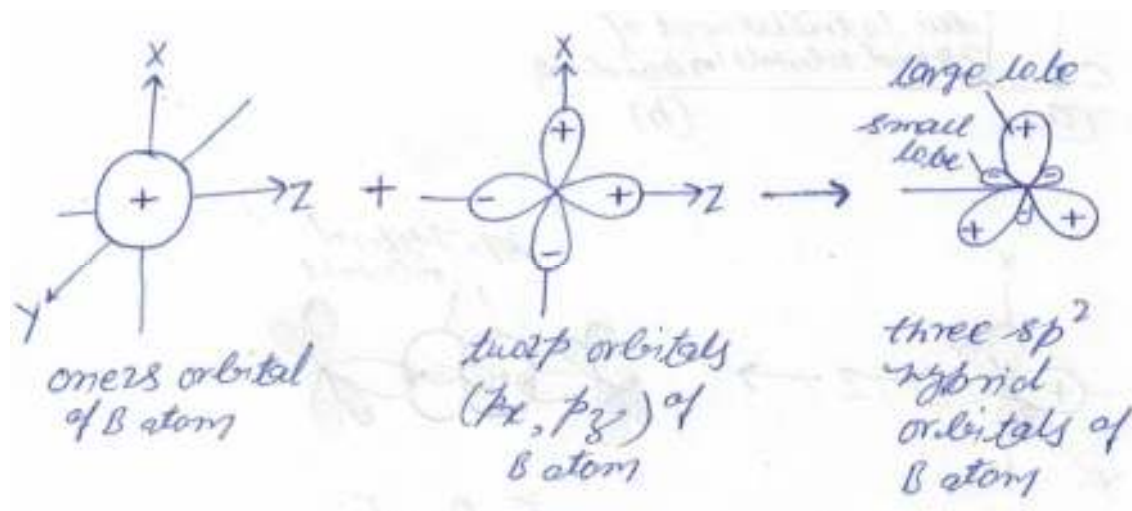
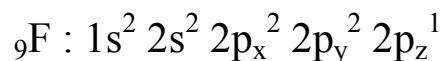


Fig. Formation of three sp^2 hybrid orbitals.

The electronic configuration of F atom is,



In the formation of boron trifluoride molecule, the half-filled p_z orbital of each fluorine atom overlaps with each of the three half-filled sp^2 hybrid orbitals of the boron atom, as shown in Fig.

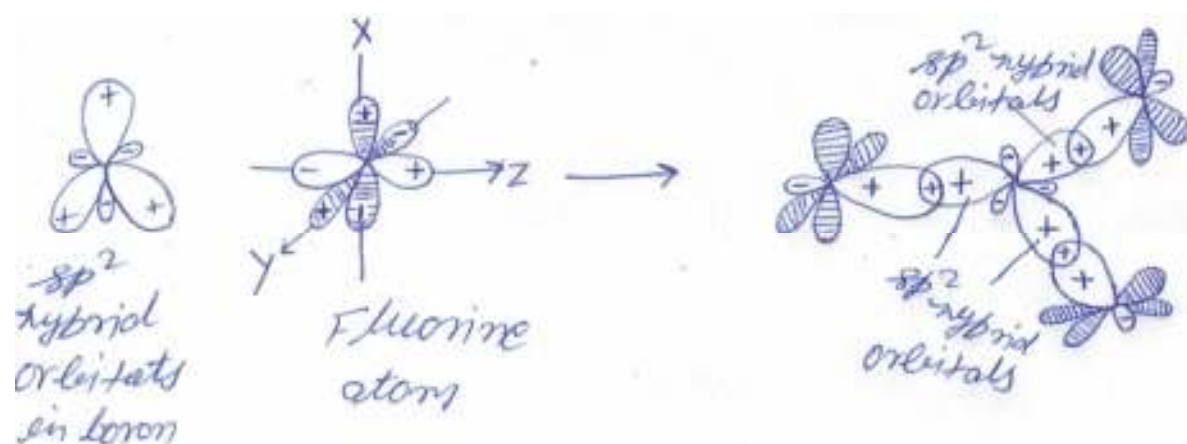


Fig. Formation of boron trifluoride molecule by the overlapping of the half-filled p_z orbitals of three fluorine atoms with the three sp^2 hybrid orbitals of boron atom. The shaded orbitals of fluorine are fully occupied.

A large amount of energy is released during the formation of sp^2 - p sigma bonds in BF_3 molecule. This is illustrated in Fig.

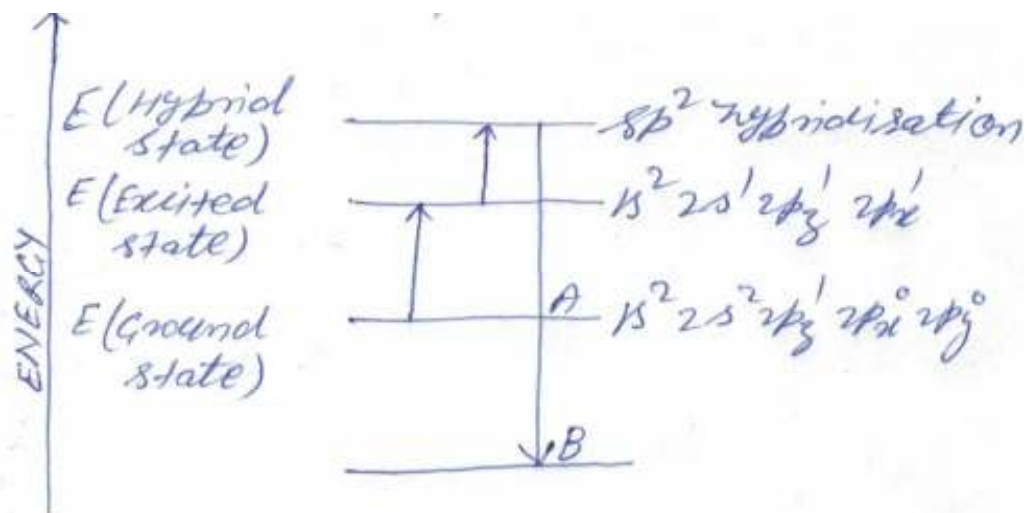


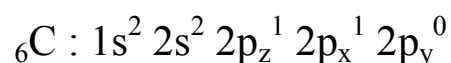
Fig. Energy required (i) for the promotion of a 2s electron to a 2p orbital (ii) for the hybridisation of s and p orbitals to give sp^2 hybrid orbitals in case of boron atom and (iii) energy released (represented by AB) in the formation of covalent bonds involving sp^2 hybrid orbitals.

The amount of energy thus released is much more than the energy which might have been released if pure s and p orbitals of boron had overlapped with the half-filled p orbitals of fluorine atoms. This accounts for the greater stability of sp^2 -p sigma bonds as compared to the stability of s-p and p-p sigma bonds.

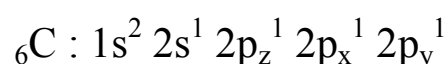
Example.

Formation of CH₄ molecule (sp³ hybridisation of orbitals of carbon atom).

The electronic configuration of carbon in ground state is,



Promotion of one of the 2s electrons into one of the vacant 2p orbitals due to the energy released in the formation of CH₄ molecule gives rise to excited state configuration,



There are now four half-filled orbitals which account for tetra-covalency of carbon. The four orbitals, one s and three p hybridise to give four sp³ hybrid orbitals of equivalent energy. The formation of sp³ hybrid orbitals is shown in Fig.

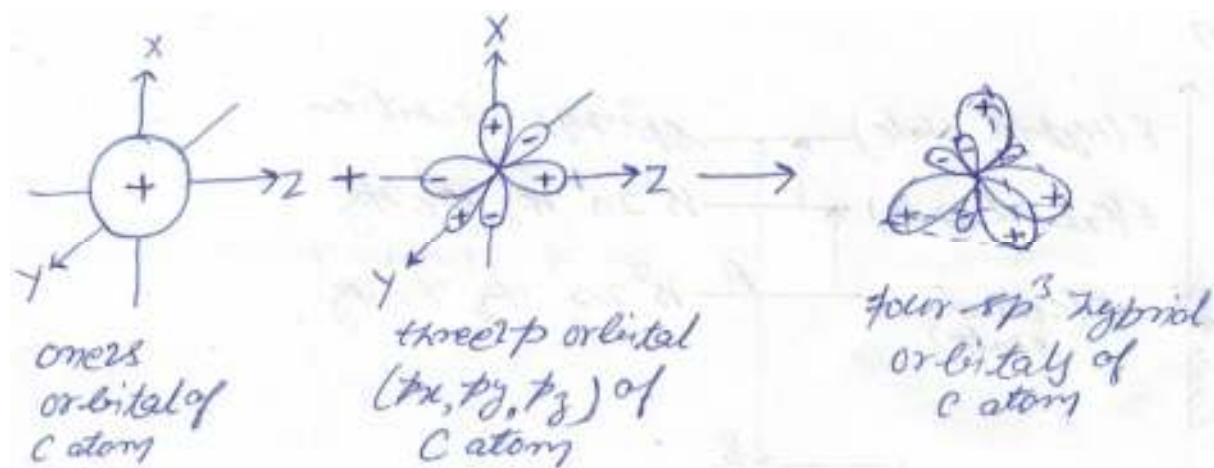
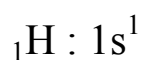


Fig. Formation of four sp^3 hybrid orbitals by overlapping of one s and three p orbitals.

The electronic configuration of H atom is,



In the formation of methane molecule, the half-filled $1s$ orbital of each hydrogen atom overlaps with each of the four half-filled sp^3 hybrid orbitals of carbon atom, as shown in Fig.

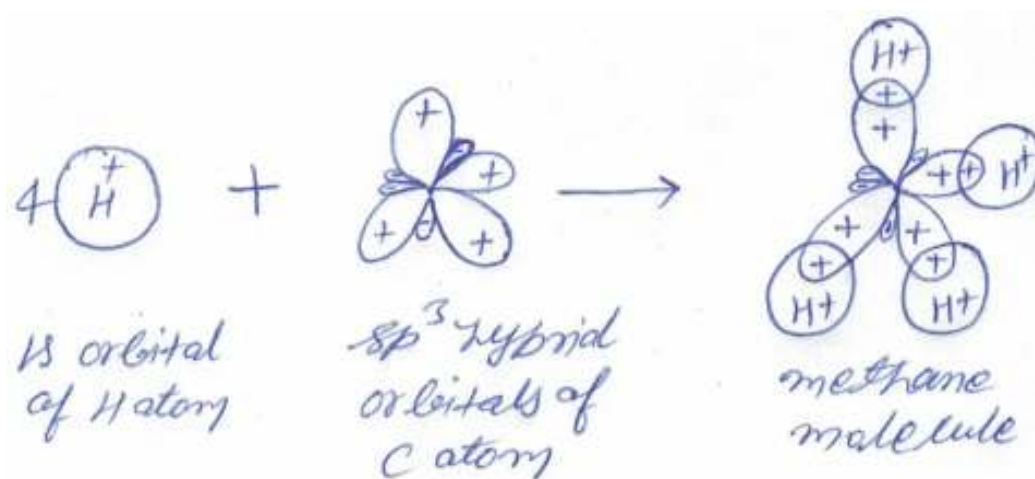


Fig. Formation of methane molecule by the overlapping of half-filled 1s orbitals of four hydrogen atoms with the four sp^3 hybrid orbitals of carbon atom.

As before, a large amount of energy is released during the formation of sp^3 -p sigma bonds.