

H-B (3)
H-I (4)
H₂S is better
BDE of C-F > C-O

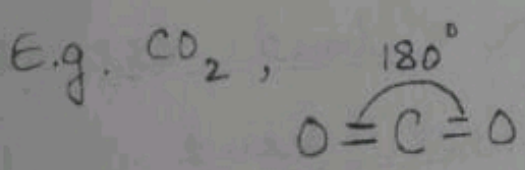
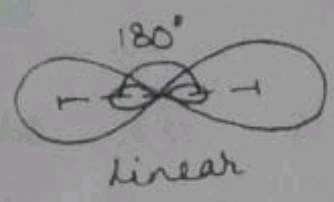
Hybridisation

When the atomic orbitals overlap then due to different energy of subshell the magnitude of overlap will be different due to which the molecules will be distorted having different bond length and bond angle.

However, it is observed that molecules are symmetrical having fixed bond length, bond angle and bond energy. Thus, atomic orbitals just do not overlap but before bond formation merging of atomic orbitals takes place resulting in equivalent energy of all atomic orbitals.

The process of merging of at. orbitals of same or nearly same energy level to give rise to an equal no. of degenerate (equal energy) set of orbital (hybrid orbitals), is called hybridisation.

one s + one p → two sp hybrid orbitals



one s + three p → three sp² hybrid orbitals

E.g. BCl₃,



trigonal or triangular planar

one s + three p → four sp³ hybrid orbitals

E.g. CCl₄

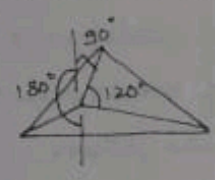


109.5° (109.5°)

Tetrahedral

one s + three p + one d (dz²) → five sp³d hybrid orbitals

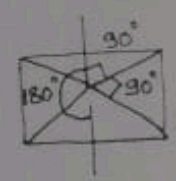
E.g. PCl₅



Trigonal bipyramidal

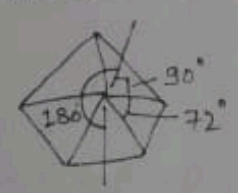
one s + three p + two d (dx²-y² & dz²) → six sp³d² hybrid orbitals

E.g. SF₆

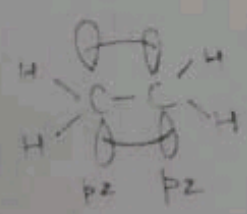
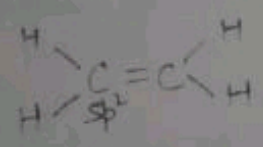


Octahedral

one s + three p + three d → seven sp³d³ hybrid orbitals

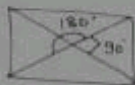


In molecules π-bond is formed due to lateral overlap of unhybridised orbitals. Hybrid Orbitals form σ-bond.



Other Types of Hybridisation Observed in Transition elements:-

dsp^2 $(n-1)dnsnp^1 \rightarrow$ square planar
(dx^2-y^2)



e.g. $[Ni(CN)_4]^{2-}$

dsp^3 $(n-1)d+nsnp^3$

d^2sp^3 $(n-1)d^2+nsnp^3$

Deviate Prediction for Hybridisation :-

* C.N. = $\frac{1}{2}(V+M-C+A)$ for inorganic molecules
(Coordination No.)

V = no. of valence e^- on central atom.

M = no. of monovalent atoms attached to central atom.

C = no. of +ve charge

A = no. of -ve charge

E.g. CO_2

$$C.N. = \frac{1}{2}(4+0-0+0) = 2 \rightarrow sp$$

CO_3^{2-}

$$C.N. = \frac{1}{2}(4+0-0+2) = 3 \rightarrow sp^2$$

SO_4^{2-}

$$C.N. = \frac{1}{2}(6+0-0+2) = 4 \rightarrow sp^3$$

NH_3

$$C.N. = \frac{1}{2}(5+3-0+0) = 4 \rightarrow sp^3$$

No. of Lone pair of e^- = C.N. - no. of attached atom to central atom.

H_2O

$$C.N. = \frac{1}{2}(6+2-0+0) = 4 \rightarrow sp^3$$



$$\text{C.N.} = \frac{1}{2}(5+5-0+0) = 5 \rightarrow \text{sp}^3\text{d}$$



$$\text{CN} = \frac{1}{2}(6+6-0+0) = 6 \rightarrow \text{sp}^3\text{d}^2$$



$$\text{CN} = \frac{1}{2}(7+7-0+0) = 7 \rightarrow \text{sp}^3\text{d}^3$$

Q

Give hybridisation state, no. of lone pair of E to C.N.



$$\text{CN} = \frac{1}{2}(6+0-0+0) = 3 \rightarrow \text{sp}^2$$

$$\text{Lone pair} = 1$$



$$\text{CN} = \frac{1}{2}(6+0-0+0) = 3 \rightarrow \text{sp}^2$$

$$\text{Lone pair} = 0$$



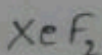
$$\text{CN} = \frac{1}{2}(6+0-0+2) = 4 \rightarrow \text{sp}^3$$

$$\text{Lone pair} = 1$$



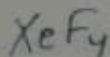
$$\text{CN} = \frac{1}{2}(5+0-0+1) = 3 \rightarrow \text{sp}^2$$

$$\text{Lone pair} = 0$$



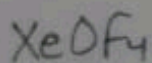
$$\text{CN} = \frac{1}{2}(8+2-0+0) = 5 \rightarrow \text{sp}^3\text{d}$$

$$\text{Lone pair} = 3$$



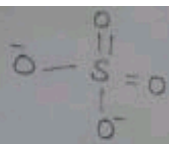
$$\text{CN} = \frac{1}{2}(8+4-0+0) = 6 \rightarrow \text{sp}^3\text{d}^2$$

$$\text{Lone pair} = 2$$

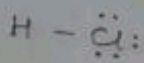


$$\text{CN} = \frac{1}{2}(8+4-0+0) = 6 \rightarrow \text{sp}^3\text{d}^2$$

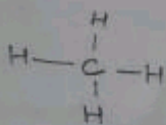
$$\text{Lone pair} = 1$$



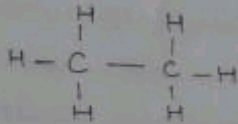
$$\text{CN} = 4 + 0 = 4 \rightarrow sp^3$$



$$\text{CN} = 1 + 3 = 4 \rightarrow sp^3$$



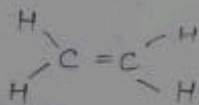
$$\text{CN} = 4 + 0 = 4 \rightarrow sp^3$$



$$\text{CN} = 4 + 0 = 4 \rightarrow sp^3$$

$$\text{CH}_3^-, \text{CN} = 3 + 1 = 4 \rightarrow sp^3$$

$$\text{CH}_3^+, \text{CN} = 3 + 0 = 3 \rightarrow sp^2$$



$$\text{CN} = 3 + 0 = 3 \rightarrow sp^2$$

Deviations from Hybridisation :-

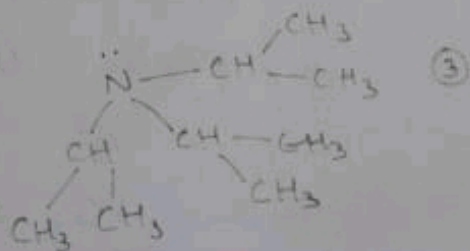
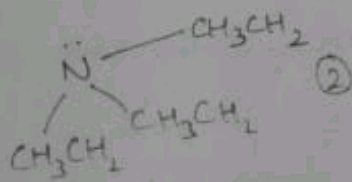
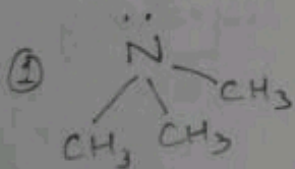
1. In case of fractional C.N.,

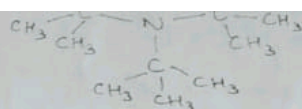
$$\text{CN} = \frac{1}{2} \times 5 = 2.5 \rightarrow \text{for } \text{NO}_2$$

NO_2 has intermediate characteristics between sp and sp^2 as its bond angle is in between 120° & 180° . The observed bond angle is closer to 120° . Hence, it can be predicted to be like sp^2 .

2. Steric hindrance \rightarrow When 2 group approach a position then depending upon their bulkiness, repulsion occurs which is known as steric repulsion. This repulsion increases bond angle.

steric rep \propto bulkiness of group

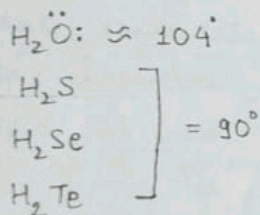
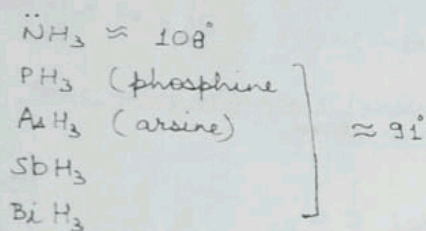




④ > ③ > ② > ① for bond angle.

With the increase in the bulkiness of the group due to steric repulsion the bond angle increases and in last case it comes closer to 120° due to which sp^2 characteristics develop in N.

3. Mixing of Atomic Orbitals Instead of Hybrid Orbitals



Thus in these species there is no hybridisation, rather the $1s$ orbital of Hydrogen overlaps with p orbital due to which the bond angle is around 90° .

S or P containing molecules show hybridisation state only when the E_n of the attached atom is greater than 2.6 and 2.5 respectively.

