# Hybridization

Hybridization is the process of mixing two or more atomic orbitals to produce a new orbital called hybrid orbitals.

Atomic orbitals e.g s, p, d, g.

Hybridization:

1s + 1p ⟶ sp hybrid orbitals

1s + 2p ⟶ $sp^2$ hybrid orbitals

1s + 2p + d ⟶ $sp^2d$ hybrid orbitals.

1s + 3p ⟶ $sp^3$ hybrid orbitals.

Hybrid orbitals: sp, $sp^2$, $sp^3$, $sp^2d$, $sp^3d^2$

## Formation of sp3 hybrid orbitals:

The electronic configuration of carbon is $2s^2 2p^6$ or $2s^2 2p_x^1 2p_y^1$.

| Ground state | | Excited state | |
| --- | --- | --- | --- |
| | | $2p_z^1$ | |
| $2p_y^1$ | | $2p_y^1$ | sp3 |
| $2p_x^1$ | | $2p_x^1$ | sp3 |
| $2s^2$ | remove $1e^-$ from 2s to $2p_z$ ⟶ | $2s^1$ | sp3 |

Mixing of $2s^1$, $2p_x^1$, $2p_y^1$, $2p_z^1$ ⟶ gives rise to formation of $sp^3$ orbitals.

Shape or geometry of sp3 ⟶ tetrahedral,

methane.

Formation of $Sp^2$ ~~hybrid~~ orbitals.

Consider Boron → $2s^1\ 2p^1$ or $2s^1\ 2p_x^1$

Ground state — Excited state.

$2p_x^1$ — $2p_y^1$ } $sp^2$ hybrid orbitals

$2S^2$ —remove le⁻ from 2s to 2py.→ $2p_x^1$

$2s^2$.

Mixing → $2s^1\ 2p_x\ 2p_y^1$ → $sp^2$ hybrid orbitals

e.g $BF_3$

Shape: Planar or triangular.

Formation of sp hybrid orbitals.

Consider Beryllium (Be) — $2s^2$.

Ground state — Excited state.

$2s^2$ —remove 1e from 2s to $2p_x$→ $2px^1$ } sp hybrid orbitals

$2s^2$

Mixing of $2s^2\ 2p_x^1$ orbitals — sp hybrid orbitals

e.g $BeCl$.

Shape → linear.

→ Co-ordination Number And Geometry

Co-ordination number is the number of bonds attached to the central metallic atom. It helps us to predict the geometry of the molecules.

Consider the following general examples.

**$AB_2$ molecules**

B — A — B

Co-ordination number = 2

Shape — linear

Bond angle — $180^\circ$

E.g $BaCl_2$, $Ag(CN)_2^{+}$

**$AB_3$ molecules**

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B — A — B            B
    |                |
    B          B — A   B
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Co-ordination number = 3

Shape — Triangular or planar

Bond angle — $120^\circ$

E.g $BF_3$, $BCl_3$ etc.

**$AB_4$ molecules**

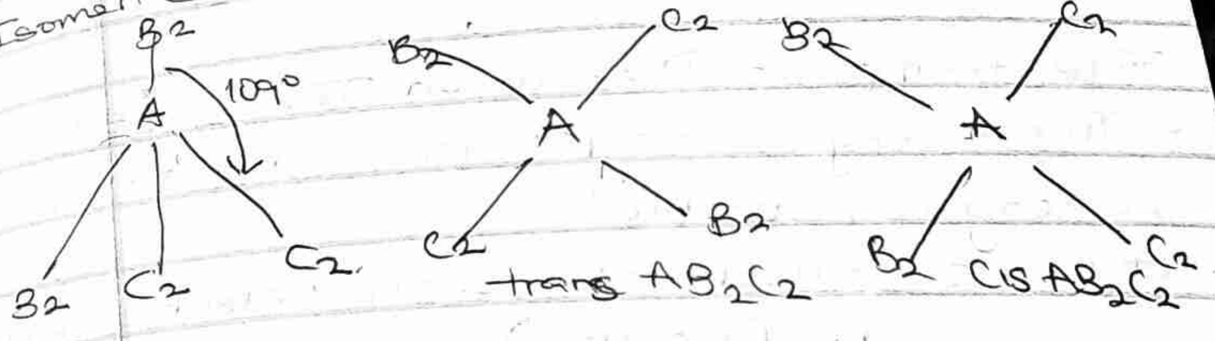
Co-ordination number = 4

Shape — Tetrahedral or square planar.

| Tetrahedral | Square planar |
| --- | --- |
| - $sp^3$ | $sp^2d$ |
| - No isomer | Isomers (cis or trans) |

109° | 90°

- Isomer (cis - trans) - eg $AB_2C_2$




tetrahedral

$AB_5$ or $\bar{A}B_4$ molecules

Co-ordination number = 5

Shape :- trigonal bipyramid or square pyramid.

Bond angle :- 90°, 120°.

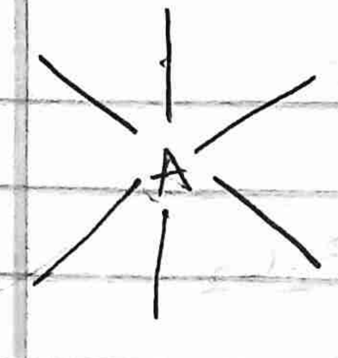
E.g $Fe(CO)_5$ Ferrocarp, $SbCl_5$, $\bar{T}eCl_4$

$AB_6$ Molecules

Coordination number = 6

Shape :- Octahedral

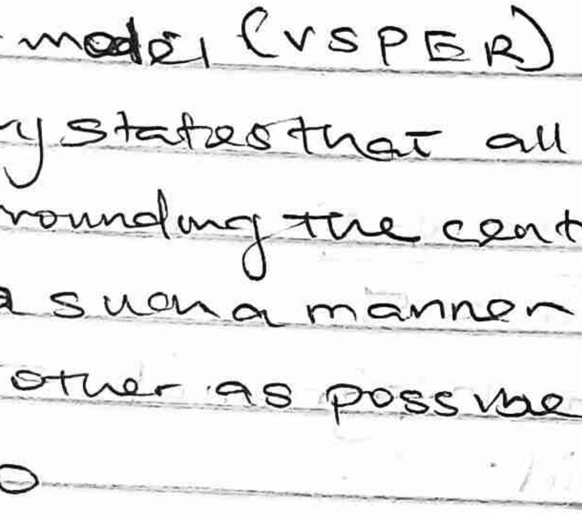
Bond angle :- 90°



eg $Co(NH_3)_4Cl_2$; $SF_6$

Electron pair Repulsion Theory (EPRT)
- This theory is used to predict the shape or geometry of molecules.
- It is also called valence shell electron pair repulsion model (VSPER)
- The theory states that all valence shell electron pairs surrounding the central atom locate themselves in such a manner as to be as far away from each other as possible.

E.g $H_2O$



ab - covalent bonds (bonding electron pairs)
cd - non bonding electron pair

# Hybridization And Multiple Bonds:

Lets consider the hybridization of compounds containing multiple bonds e.g ethylene,

ethylene — $C_2H_4$

its hybridization — $sp^2$

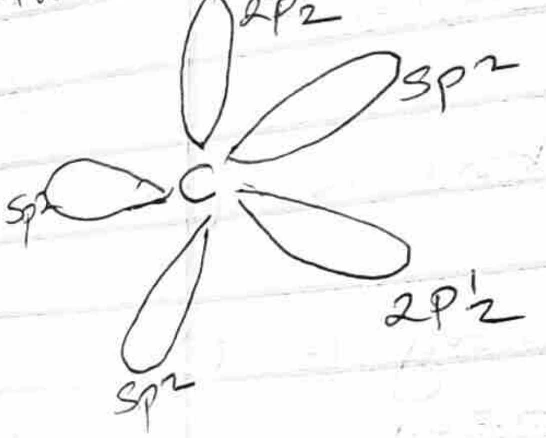
Ground state = $2s^2\ 2p_x^1\ 2p_y^1$

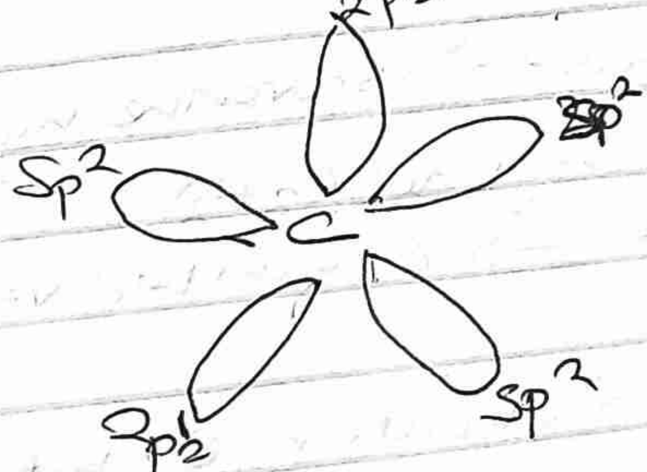
Ground state ——> Excited state,

| Ground state | Excited state |
| --- | --- |
| | $2p_z^1$ |
| $2p_y^1$ | $2p_y^1$ |
| $2p_x^1$ | $2p_x^1$ |
| $2s^2$ | $2s^2$ |

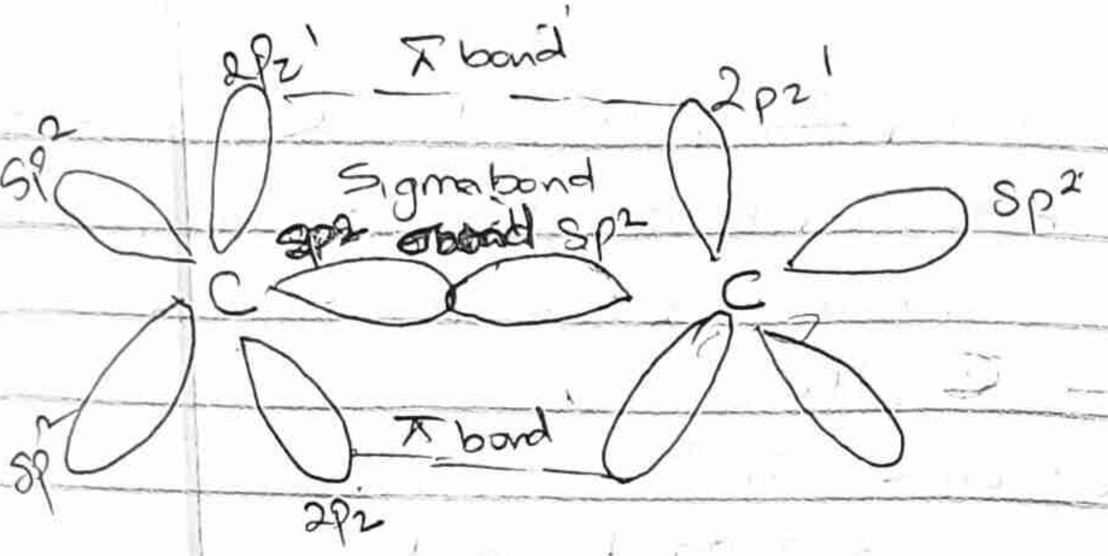
$sp^2 \rightarrow 2s^1\ 2p_x^1\ 2p_y^1$

The $2p_z^1$ would be in unhybridized state. Therefore, for each of carbon in $C_2H_4$ we have this diagram




Combining the two carbon atoms or bringing the two carbons together we have




Sp² – horizontal overlap of 2sp² → gives σ bond (sigma)

vertical overlap of Sp² → gives π bond (pi)

NB: (i) Simple covalent bonds contain σ bonds (sigma bonds)

(ii) Double covalent bonds contain 1σ bond and 2π (pie) bonds

Exercise:- Discover the hybridization and bonding in acetylene ($C_2H_2$)

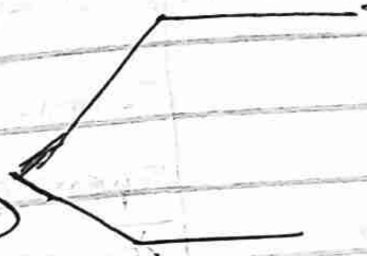
EPRT → Also called valence bond theory (VBT).

## Molecular Orbital Theory (MOT).

- It consist of two atomic orbitals combining form 2 molecular orbitals.

- Two molecular orbitals formed have differ energies

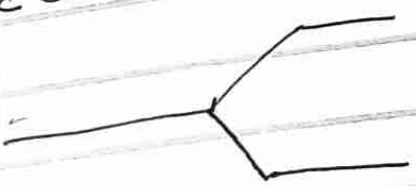
n+n ->2m
(atomic orbital) (MO)




Hybridization -> atomic orbital -> hybrid orbital
(VBT / EPRT -

MOT -> Atomic orbitals -> molecular orbitals :
2 atomic orbitals - 2 molecular orbitals :

2 MO



Molecular orbital -> lower energy -> favourable for bond formation and it is called bonding molecular orbital (BMO)

MO -> lower energy -> favourable for bond formation -> Bonding molecular orbitals (BMO)

MO -> higher energy -> unfavourable for bond formation -> called Antibonding molecular orbital (AMO)

Summary On Hybridization,

| Hybridization | No of electron pairs (co-ord no) | Orientation/ Shape | Bond Angle | Example |
| --- | --- | --- | --- | --- |
| $Sp^3$ | 4 | Tetrahedral | 109° | $CH_4$, $NH_4$ |
| $Sp^2d$ | 4 | Square planar | 90° | $Pt(NO_3)_2Cl$ |
| $Sp^2$ | 3 | Triangular | 120° | $BF_3$ |
| Sp | 2 | linear | 180° | $BeCl_2$, $BeF$ |