



CHEMICAL BONDING

Postulates of Valence Bond Theory

1. Overlapping is necessary for bond formation.
2. Only half filled atomic orbitals participate in bond formation.
3. Greater the overlapping, stronger will be the bond.
4. Electrons with opposite spin pair up to stabilize themselves during overlapping.
5. The bond formed by linear or head to head overlapping of partially filled orbitals is called sigma bond.
6. The bond formed by parallel or side by side overlapping of partially filled orbitals is called pi bond.

Q: Differentiate between sigma bond and pi bond.

Sigma Bond	Pi Bond
The bond formed by linear or head to head overlapping of partially filled orbitals	The bond formed by parallel or side by side overlapping of partially filled orbitals
In sigma bond, electron density is present between two nuclei.	In pi bond, electron density is above and below the bond axis.
It is comparatively inert bond	It is comparatively reactive.
It is a strong bond	It is a weak bond
Atoms are always bonded with sigma bond first.	Pi bond is formed when sigma bond is already present in atoms.
It is represented by σ	It is represented by π

Main Postulates of Molecular Orbital Theory:

1. The valence orbitals of two atoms overlap to form molecular orbitals.
2. The number of molecular orbitals formed is equal to number of atomic orbitals overlapped.
3. The half of the molecular orbitals has low energy than parent atomic orbitals called Bonding molecular Orbitals (BMO) while other half have high energy than parent atomic orbitals called anti bonding molecular orbitals (ABMO).
4. The bonding molecular orbitals formed by linear overlapping are called sigma (σ) orbitals while anti bonding molecular orbitals are called sigma star (σ^*) orbitals.
5. The bonding molecular orbitals formed by parallel overlapping are called pi (π) orbitals while anti bonding molecular orbitals are called pi star (π^*) orbitals.
6. The electrons are distributed in molecular orbitals according to following rules.
 - Auf bau principle
 - Pauli's Exclusion Principle

- Hund's rule
7. The no. of bonds between two atoms is given by bond order.

Bond Order: The half of the difference of no. of bonding and anti bonding electrons is called Bond order.

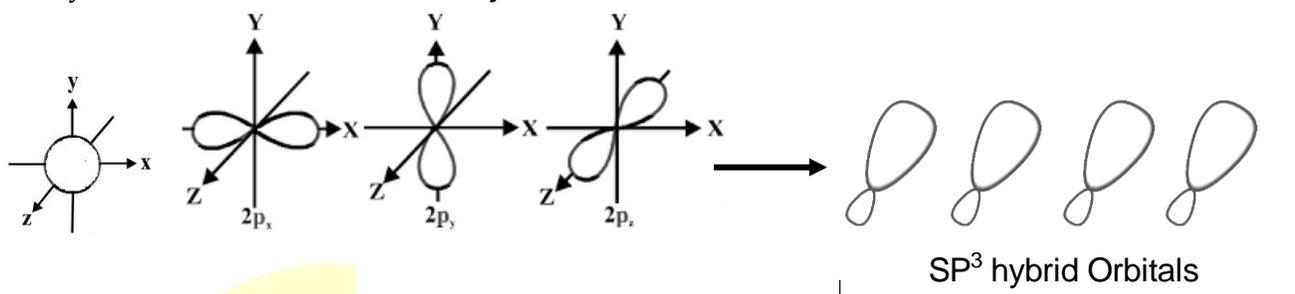
$$\text{Bond Order} = \frac{N_a - N_b}{2}$$

HYBRIDIZATION

Atomic Orbital hybridization.

The process of intermixing of atomic orbitals of different energy and shape to form new orbitals of same energy and shape is called hybridization.

Newly formed orbitals are called **Hybrid orbitals**.



TYPES

There are three types of hybridization.

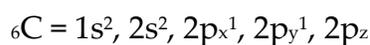
- sp³
- sp²
- sp

sp³ Hybridization:

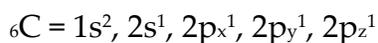
The process of inter mixing of one 's' orbital and three 'p' orbitals to form four hybrid orbitals is called sp³ hybridization.

For example: Methane (CH₄)

In methane, the central atom is carbon. The electronic configuration of central atom (carbon) at ground level is

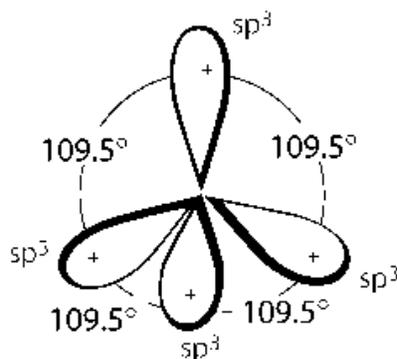
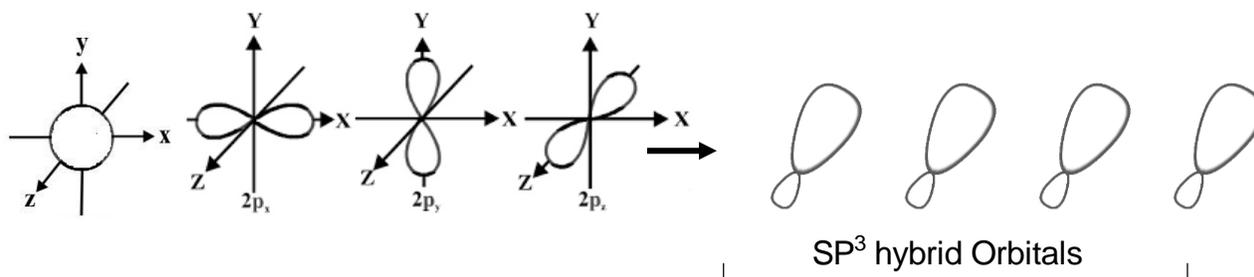


In excited state, One electron from 2s orbital jumps to empty 2pz orbital. The electronic configuration of carbon at excited state is



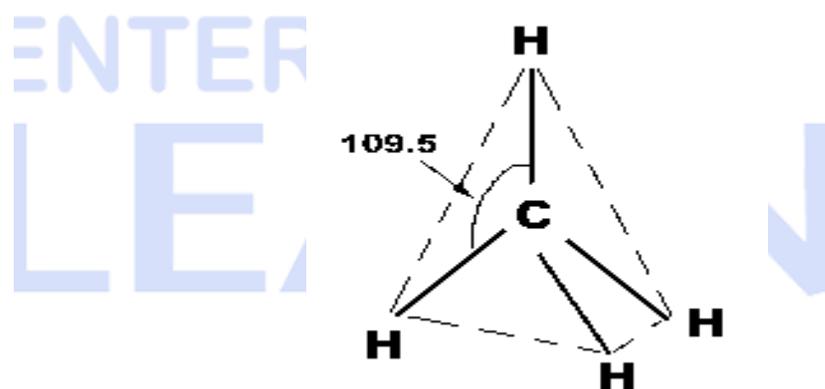
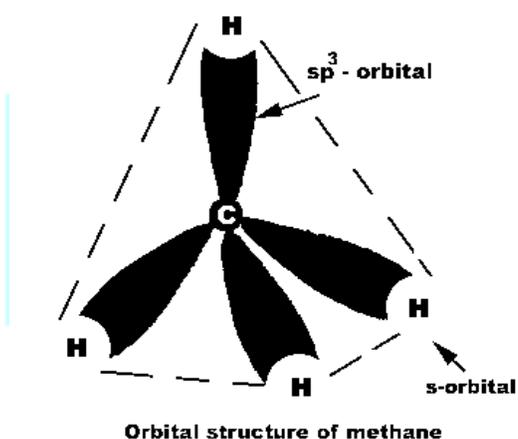
Now mixing of orbitals take place. Four orbitals 2s, 2p_x, 2p_y, 2p_z mix together to form four sp³ hybrid orbitals





- Shape = Tetrahedral
- Bond Angle = 109.5°

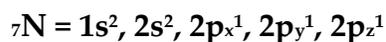
s-orbital of hydrogen atom overlap with sp³ orbitals to give s-sp³ overlapping which results in bond formation.



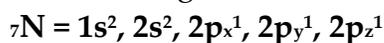
Example 2:

Ammonia (NH₃):

In ammonia, the central atom is nitrogen. The electronic configuration of central atom (nitrogen) at ground level is

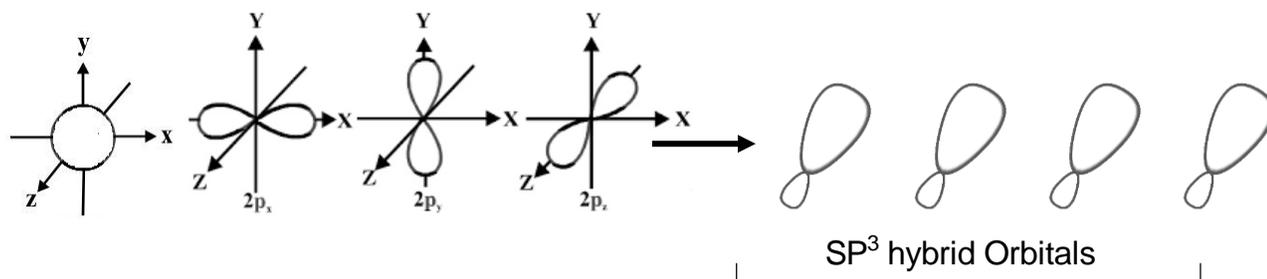


In excited state, there is no free orbital, so its ground state also considered as excited state.



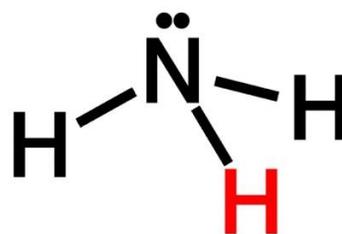
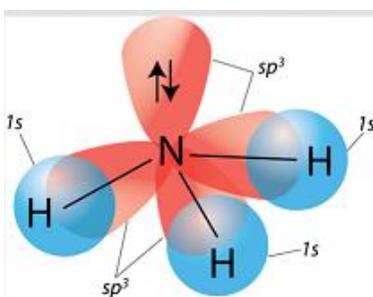
Now mixing of orbitals take place. Four orbitals 2s, 2p_x, 2p_y, 2p_z mix together to form four sp³ hybrid orbitals





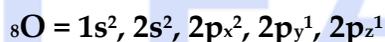
- **Shape = Triangular Planar**
- **Bond Angle = 107.5°**

As one sp^3 orbital is completely filled so it does not participate in overlapping. s-orbital of hydrogen atom overlap with three sp^3 hybrid orbitals to give s- sp^3 overlapping which results in bond formation.

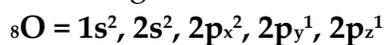


Example 3: Water (H₂O):

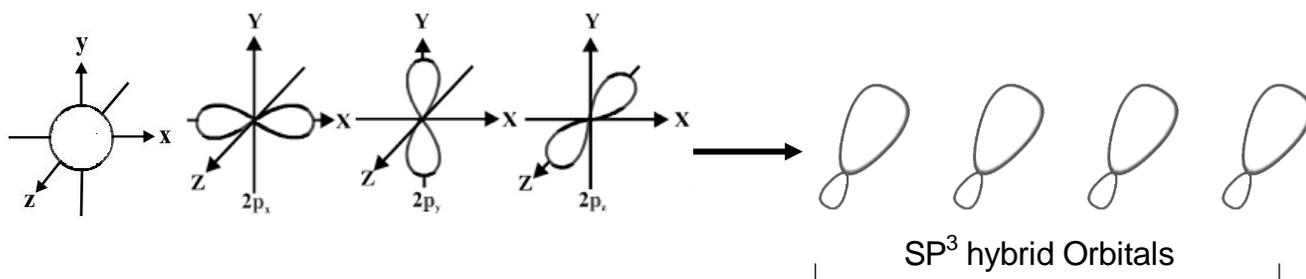
In water, the central atom is oxygen. The electronic configuration of central atom (oxygen) at ground level is



In excited state, there is no free orbital, so its ground state also considered as excited state.

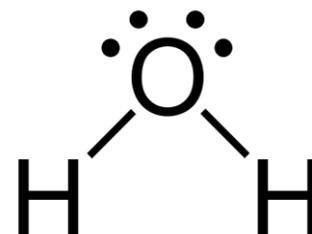
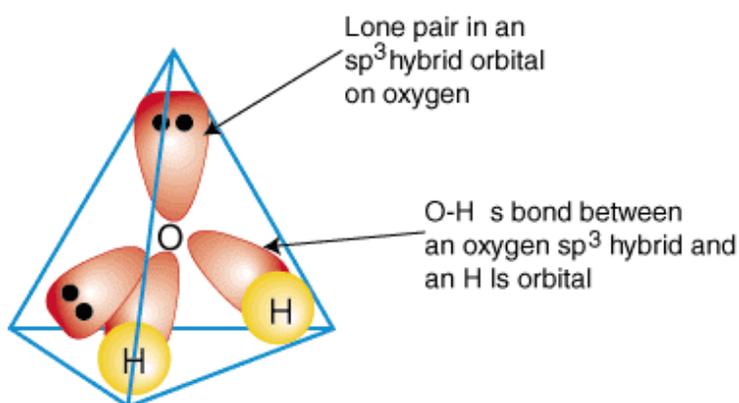


Now mixing of orbitals take place. Four orbitals $2s, 2p_x, 2p_y, 2p_z$ mix together to form four sp^3 hybrid orbitals.



- **Shape = Bent/ Angular**
- **Bond Angle = 104.5°**

As two sp^3 orbitals are completely filled so it does not participate in overlapping. s-orbital of hydrogen atom overlap with two sp^3 hybrid orbitals to give s- sp^3 overlapping which results in bond formation.

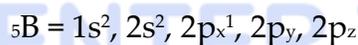


SP² HYBRIDIZATION

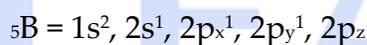
The process of inter mixing of one 's' orbital and two 'p' orbitals to form three hybrid orbitals is called sp^2 hybridization.

For Example: Boron Trifluoride (BF₃)

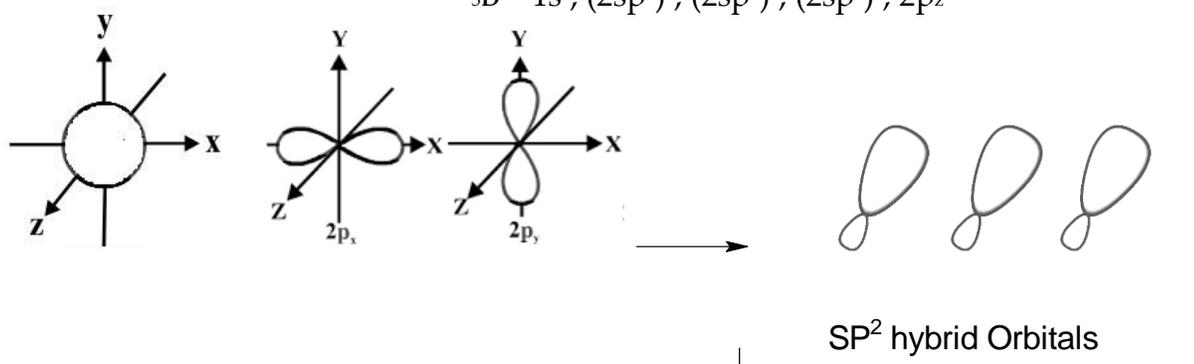
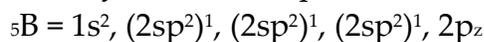
In **Boron Trifluoride**, the central atom is Boron (B). The electronic configuration of central atom (B) at ground level is



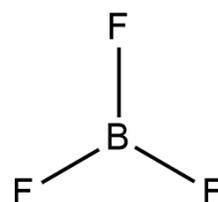
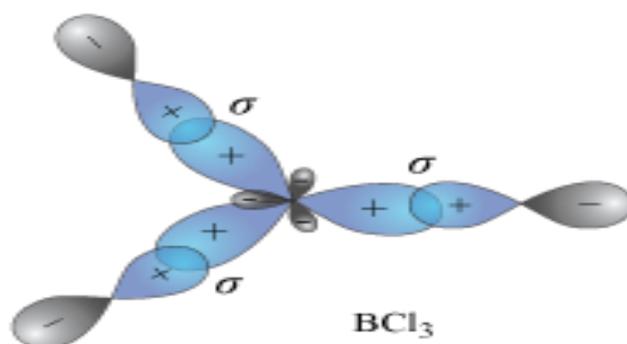
In excited state, One electron from 2s orbital jumps to empty $2p_y$ orbital. The electronic configuration of Boron (B) at excited state is



Now mixing of orbitals take place. Three orbitals $2s, 2p_x, 2p_y$ mix together to form three sp^2 hybrid orbitals whereas $2p_z$ orbital remain unhybrid to form pi bond.



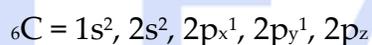
- **Shape: Triangular planner**
- **Bond Angle: 120°**



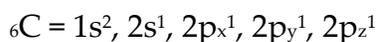
boron trifluoride

For example: Ethene (C₂H₄) or Ethylene

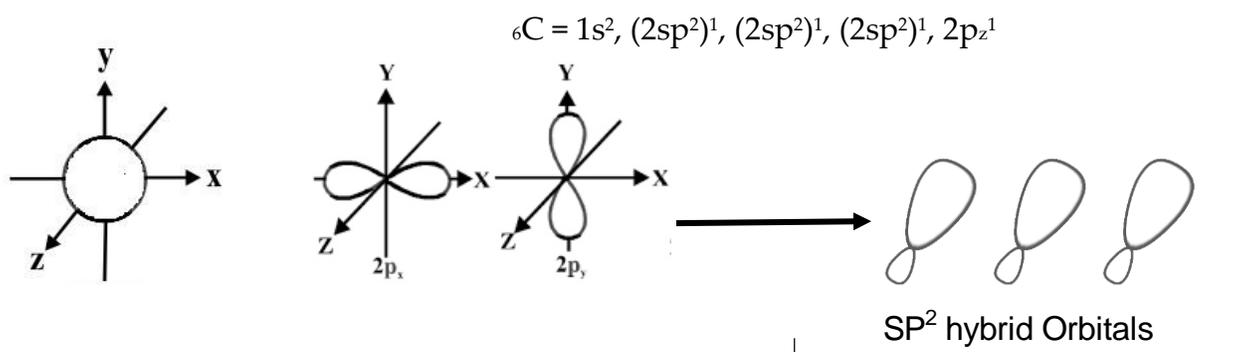
In ethene, the central atom is carbon. The electronic configuration of central atom (carbon) at ground level is

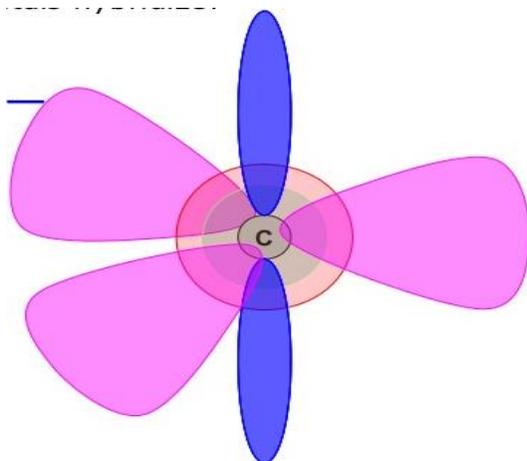


In excited state, One electron from 2s orbital jumps to empty 2p_z orbital. The electronic configuration of carbon at excited state is

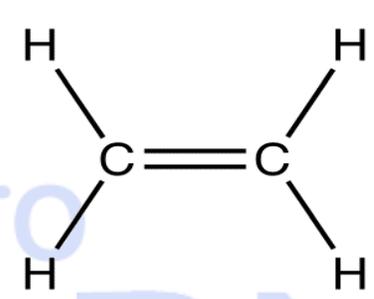
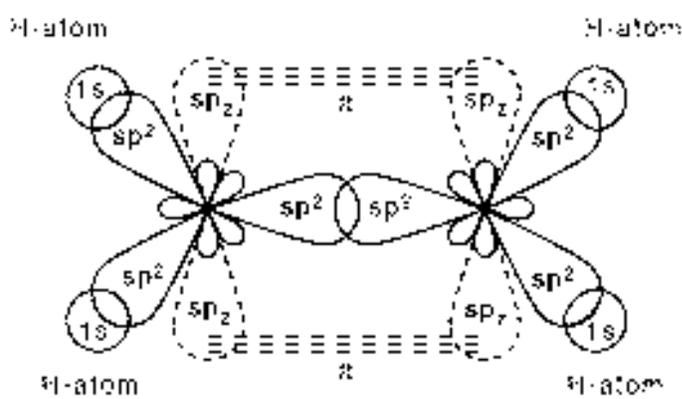


Now mixing of orbitals take place. Three orbitals 2s, 2p_x, 2p_y mix together to form three sp² hybrid orbitals whereas 2p_z orbital remain unhybrid to form pi bond.





Three sp² hybrid orbitals and one 2p_z unhybrid orbital



- Shape: Triangular planner
- Bond Angle: 120°

SP HYBRIDIZATION

The process of inter mixing of one 's' orbital and one 'p' orbitals to form two hybrid orbitals is called sp hybridization.

For Example: Beryllium Chloride: (BeCl₂)

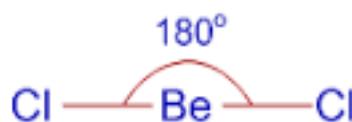
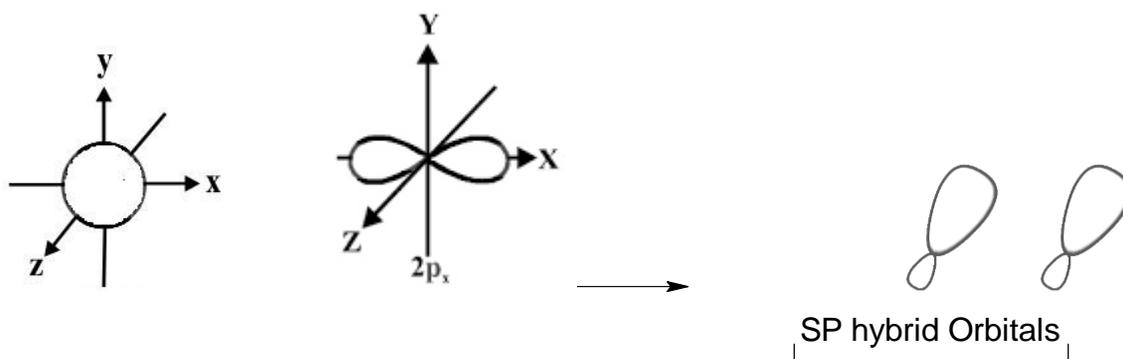
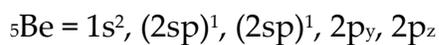
In Beryllium Chloride, the central atom is Beryllium (Be). The electronic configuration of central atom (Beryllium) at ground level is

$$4\text{Be} = 1s^2, 2s^2, 2p_x, 2p_y, 2p_z$$

In excited state, One electron from 2s orbital jumps to empty 2p_x orbital. The electronic configuration of Beryllium at excited state is

$$4\text{Be} = 1s^2, 2s^1, 2p_x^1, 2p_y, 2p_z$$

Now mixing of orbitals take place. Two orbitals $2s$, and $2p_x$ mix together to form two sp hybrid orbitals.

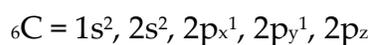


Shape: Linear
Bond Angle: 180°

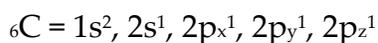


For Example: Ethyne (C_2H_2)

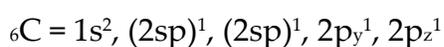
In ethyne, the central atom is carbon. The electronic configuration of central atom (carbon) at ground level is

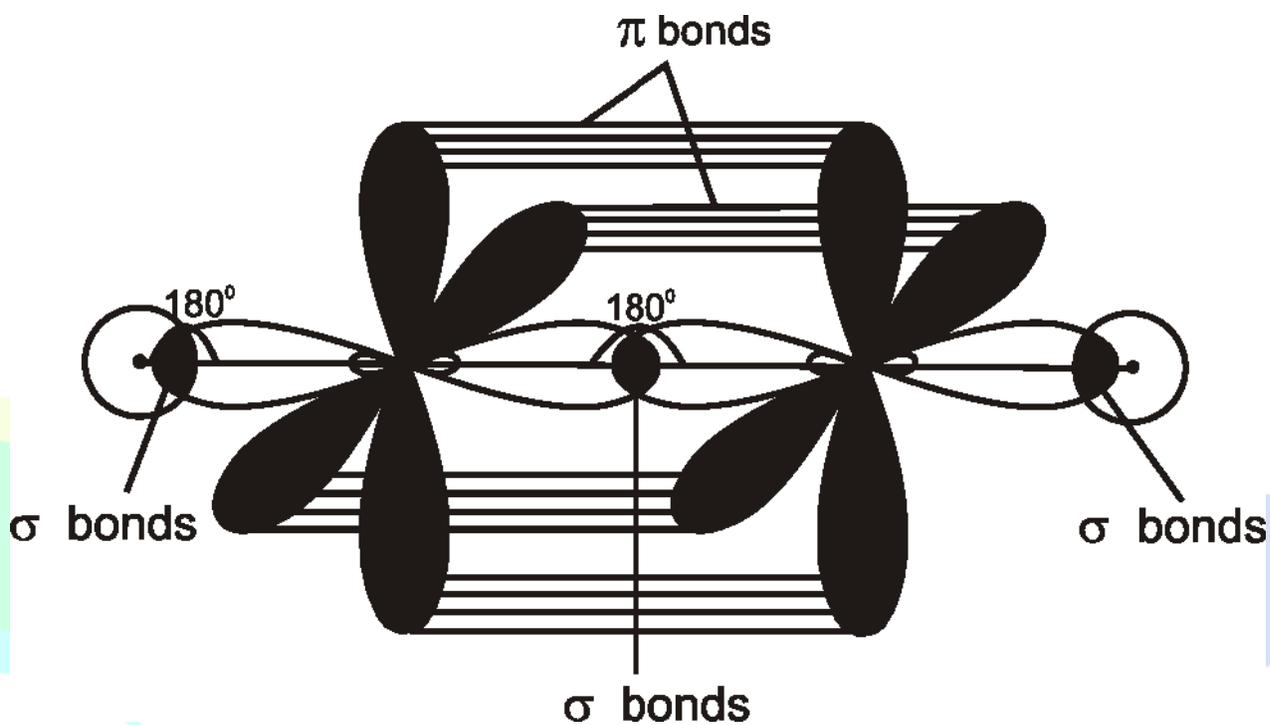
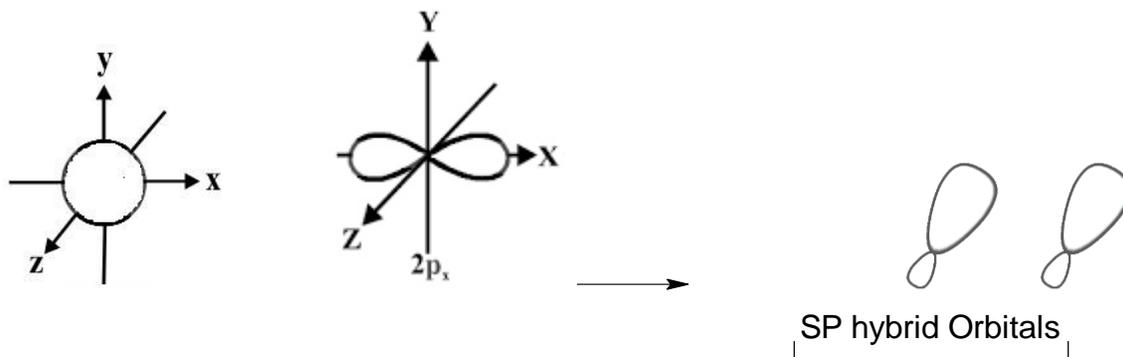


In excited state, One electron from $2s$ orbital jumps to empty $2p_z$ orbital. The electronic configuration of carbon at excited state is



Now mixing of orbitals take place. Two orbitals $2s$, and $2p_x$ mix together to form two sp hybrid orbitals whereas $2p_y$, $2p_z$ orbital remain unhybrid to form two pi-bond.





- Shape: Linear
- Bond Angle: 180°

