CHEM-102

HYBRIDIZATION OF ATOMIC ORBITALS

Hybridization was introduced to explain molecular structure when the valence bond theory failed to correctly predict them. Definition of Hybridization

Hybridization is actually a process in which atomic orbitals having different shape and energy intermix to form a set of same number of orbitals which have same shape and energy.

Hybridization is the combination of atomic orbitals like s, p, d or f to give the equivalent orbitals which are known as hybrid orbitals. This phenomenon is known as Hybridization. There is sp^3, sp^2, sp etc. hybridization and also dsp^2,dsp^3, sp^3d^2 etc. when considering d-orbital.

The new orbitals have the same total electron capacity as the old ones.

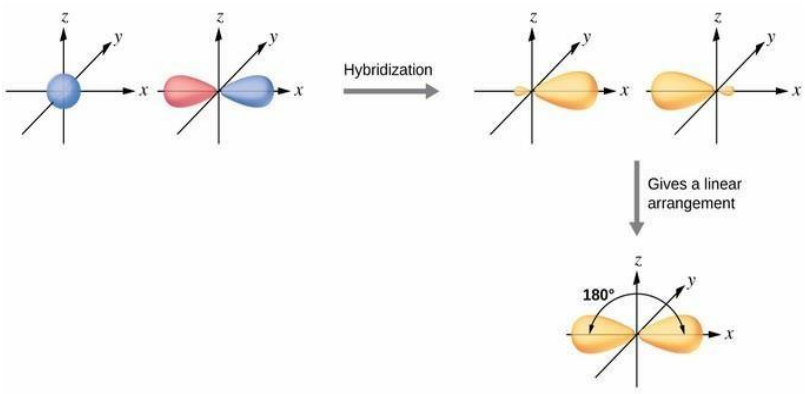
HYBRIDIATION RULES

- (1)Hybridize the CENTRAL ATOM ONLY (others as needed)
- Only use valence shell electrons.
- The number of hybrid orbitals formed = number of atomic orbitals used.
- Hybrid orbitals get 1 electron for a σ-bond, 2 electrons for a lone pair.
- Remaining electrons go into un-hybridized orbitals = π bonds.

SP Hybridization Definition

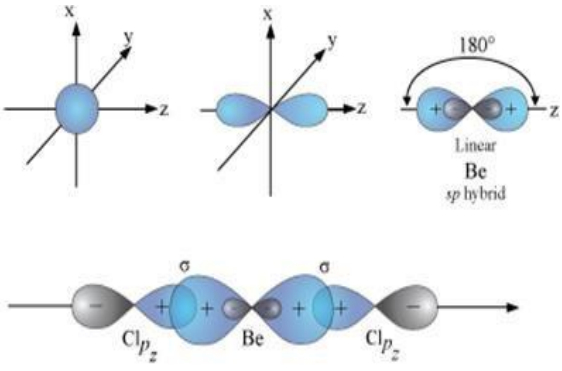
The process of hybridization in which one s orbital and one p-orbital of the same atom overlap to produce two hybrid orbital is known as sp-hybridization.

- In *sp* hybridization *sp* orbitals are linearly oriented.
- two *sp* orbitals will be at 180 degrees to each other.
- Remaining P_y and P_z un hybrid orbitals lie perpendicular to the plane of sp-orbital. s and p Orbitals
- Combining to Form Two sp Orbitals



sp Hybridization in $BeCl_2$

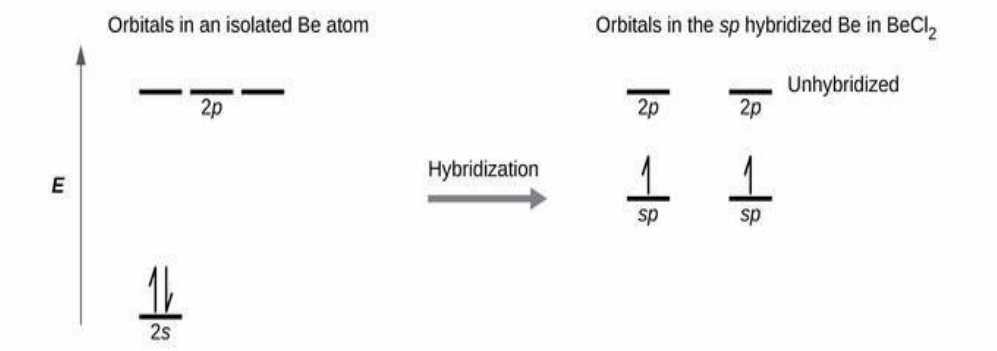
- Two of the Be atom's four valence orbitals will mix to yield two hybrid orbitals.
- When atomic orbitals hybridize, the valence electrons occupy the newly created orbitals.
- The Be atom had two valence electrons, so each of the *sp* orbitals gets one of these electrons.
- Each of these electrons pairs up with the unpaired electron on a chlorine atom.



- The two electrons that were originally in the *s* orbital are now distributed to the two *sp* orbitals, which are half filled.
- These half-filled hybrid orbitals will overlap with orbitals from the chlorine atoms to form two identical σ bonds.

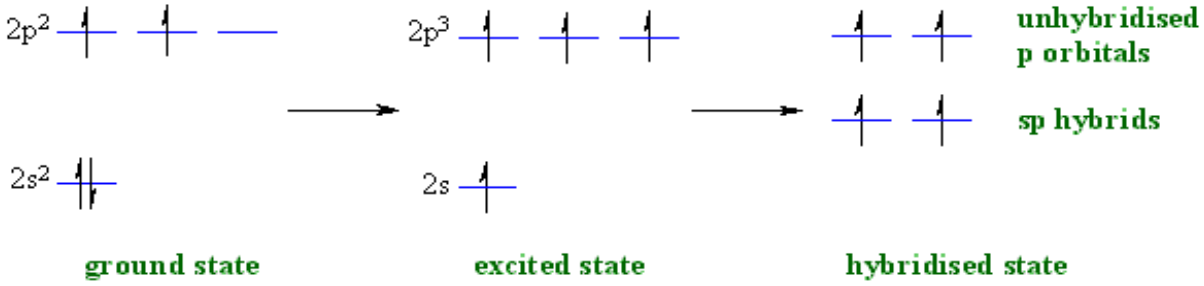
Energy Level Diagrams for sp Orbitals

Orbital Energy-Level Diagrams For Isolated and Bonded Be.

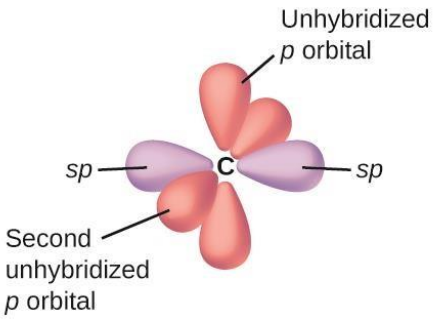


sp Hybridization in Ethyne

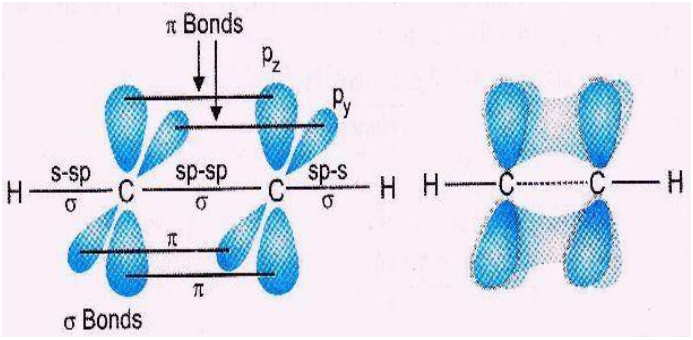
Molecular formula of ethyne is C_2H_2. In ethyne, each carbon atom is sp-hybridized. In this way, four sp-orbital are generated.

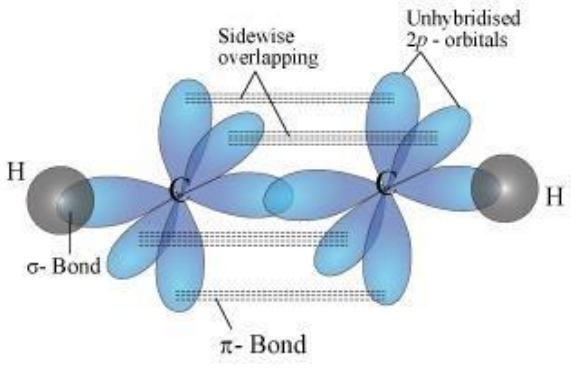


Energy level diagram of C atom in s-p hybridization



S-p hybridization of central C atom in ethyne





The linear shape, or 180° angle, is formed because electron repulsion is minimized the greatest, in this position.

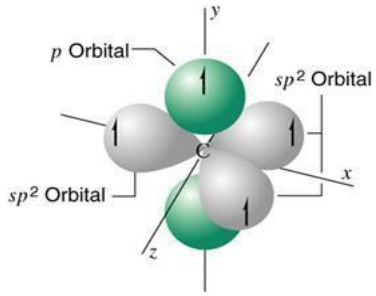
Summary

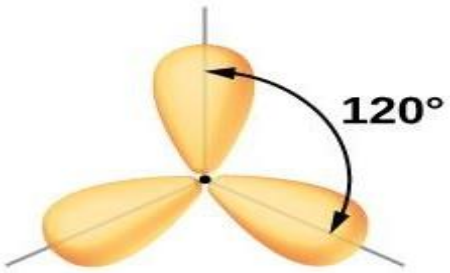
- **sp** occurs when a C has 2 attached groups
- **sp** has 50% s and 50% p character
- The 2 **sp** hybrids point in opposite directions at 180° to each other
- Each **sp** hybrid is involved in a σ bond
- The remaining **p** orbitals forms the 2π bonds
- View a triple bond as a σ + 2π bonds

Sp^2 Hybridization Definition

The process of hybridization in which one s orbital and two p-orbital overlap to produce three hybrid orbitals is known as sp^2 HYBRIDIZATION or TRIGONAL HYBRIDIZATION.

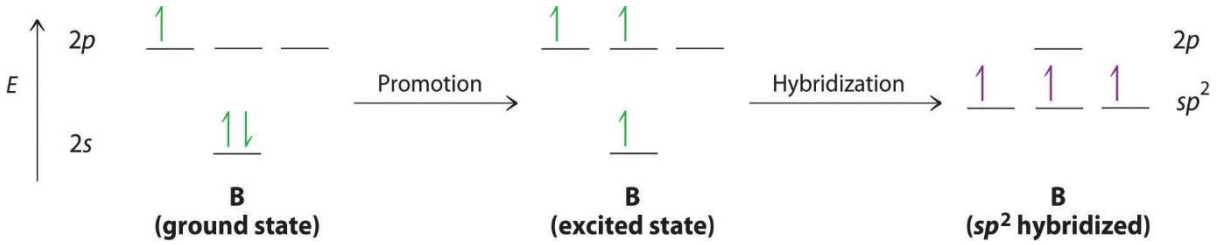
These orbital are coplanar and directed towards the corners of an equilateral triangle at an angle of 120° from each other. The fourth un hybrid Pz-orbital lies at right angle to the plane of Sp^2-orbitals.



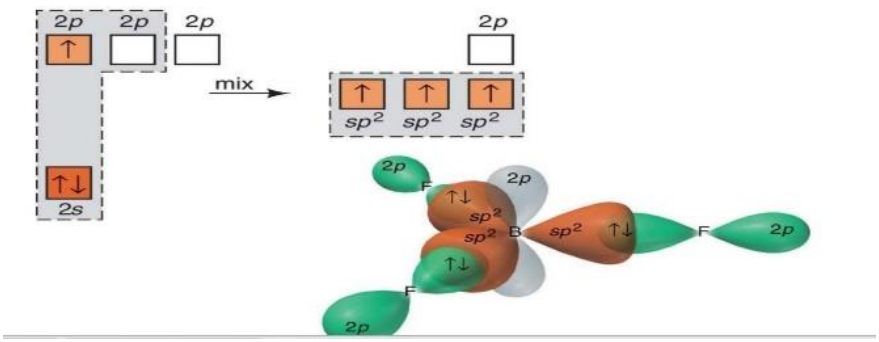


Sp^2 hybridization in BF_3

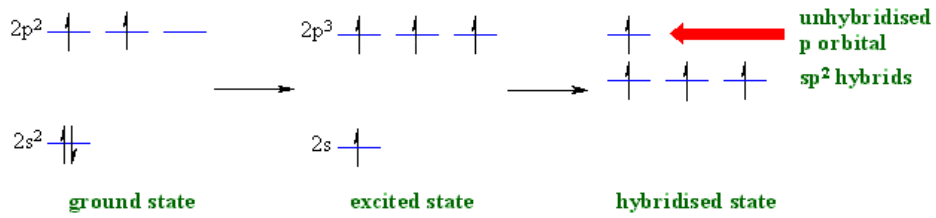
In boron tri fluoride Boron atom has three outer-shell electrons in its ground state. The 2s orbital and two of the 2p orbitals hybridize; one empty p-orbital remains.



Energy level diagram

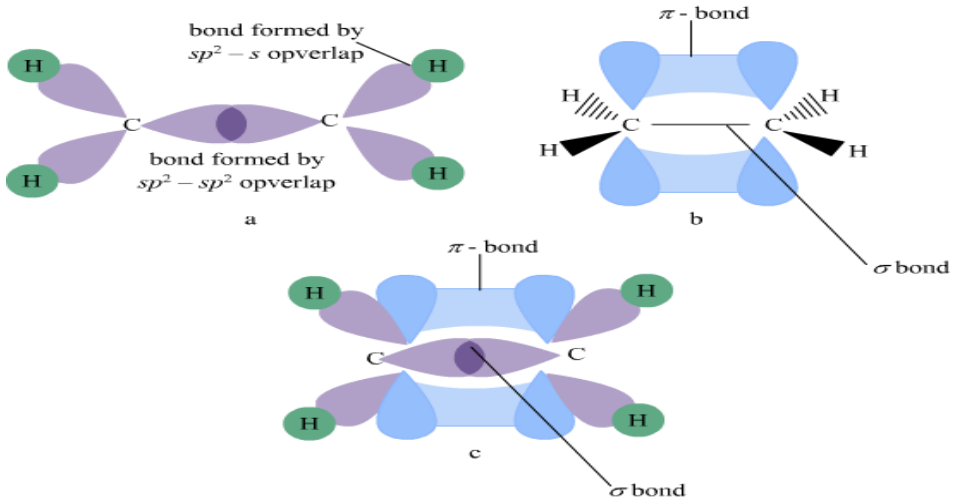


Sp2 Hybridization in Ethene



Energy level diagram of C in sp^2 hybridization

These hybridized orbitals align themselves in the tri-gonal planar structure.



Summary

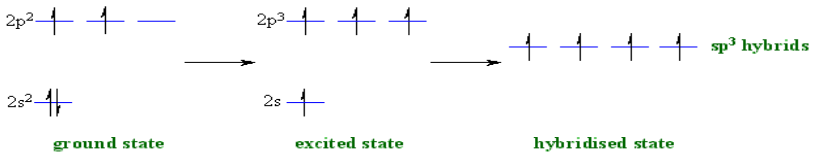
- **sp^2** occurs when a C has 3 attached groups.
- **sp^2** has 33% s and 67% p character.
- the 3 **sp^2** hybrids point towards the corners of a triangle at 120^o to each other.
- each **sp^2** hybrid is involved in a σ bond.
- the remaining **p** orbital forms the π bond.
- view a double bond as a σ + π bond.
-

Sp^3 hybridization Definition

- The process of hybridization in which one s orbital and three p-orbitals overlap to produce
  four hybrid-orbital is known as Sp^3 hybridization.
- These hybrid-orbital are identical in shape and energy.
- sp^3 hybrid orbitals are oriented at bond angle of 109.5^o from each other.

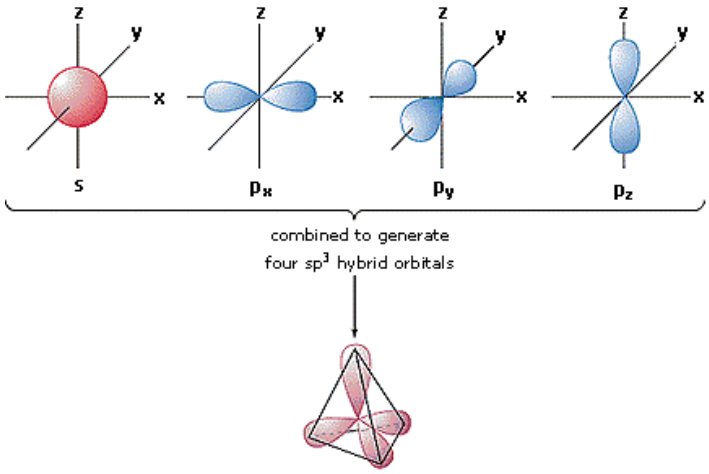
- sp^3-orbital are arranged in tetrahedral fashion.

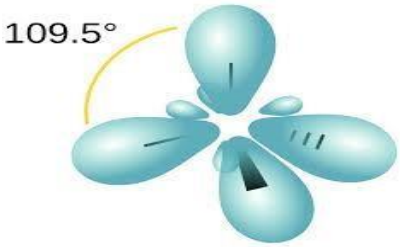
Sp^3 hybridization in CH_4



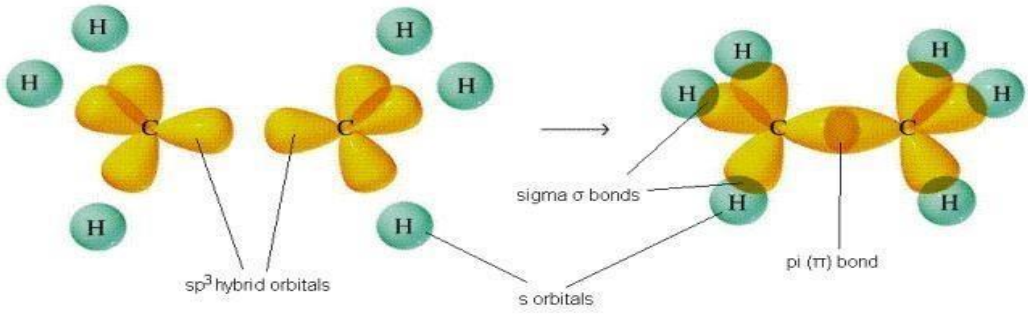
Energy level diagram of C in CH4

- One s-orbital (2s) and three p-orbital (2px, 2py, 2pz) overlap to produce four Sp^3-hybrid orbitals.
- These Sp^3- hybrid orbital are at a angle of 109.5^o from each other.
- These Sp^3-orbitals are attached at the corner of a tetrahedron.

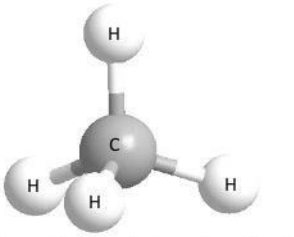




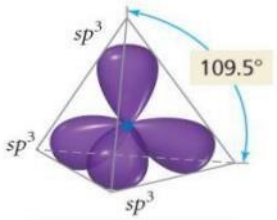
Sp^3 Hybridization in Ethane



After this hybridization, carbon now has four equivalent orbitals that are used to bond to the hydrogens in methane



Carbon with 4 bonds in methane (CH_4)



Arrangement of the hybrid orbitals in carbon

sp^3 hybridization in ethane

Summary

- **sp^3**occurs when a C has 4 attached groups
- **sp^3** has 25% s and 75% p character
- the 4 **sp^3** hybrids point towards the corners of a tetrahedron at 109.5^o to each other
- each **sp^3**hybrid is involved in a σ bond