

Hybridization

Definition: The phenomenon of mixing up of atomic orbitals of similar energies and formation of equivalent number of entirely new orbitals of identical shape and energy is known as "hybridization" and the new orbitals so formed is called as "hybrid orbitals".

Important points for understanding the hybridization:

- 1- The number of hybrid orbitals generated is equal to the number of pure atomic orbitals that participate in hybridization process.
- 2- Hybridization concept is not applicable to isolated atoms. It is used to explain the bonding scheme in a molecule.

3- Covalent bonds in polyatomic molecules are formed by the overlap of hybrid orbitals or of hybrid orbitals with unhybridized ones.

Types of Hybridization

sp Hybridisation	linear	180 °
sp ² Hybridisation	trigonal planar	120°
sp ³ Hybridisation	tetrahedral	109.5°
sp ³ d Hybridisation	trigonal bipyramidal	
dsp ² hybridisation	square planar	
sp ³ d ² Hybridisation	octahedral	

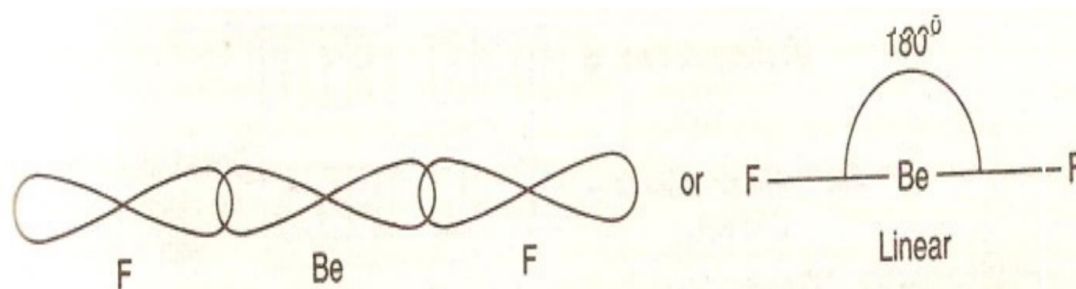
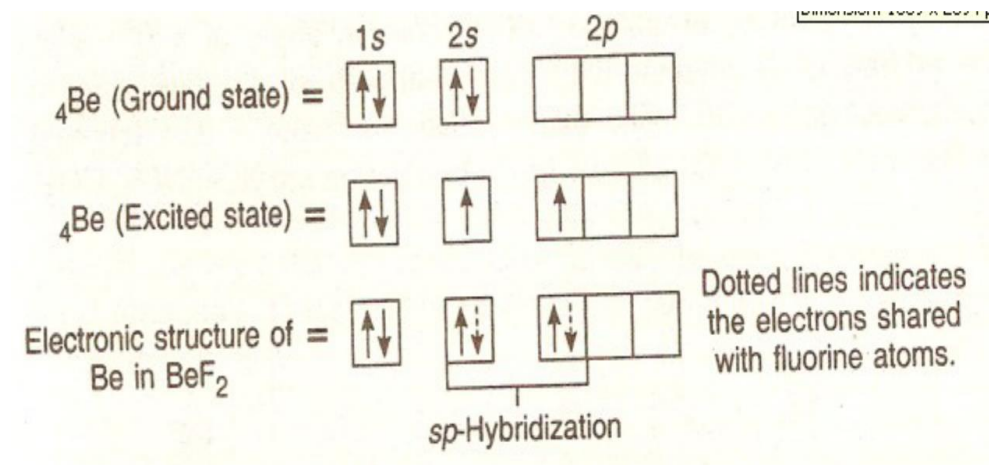
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Types of Hybridization

- (1) **sp-hybridization:** The combination of one s and one p-orbitals to form two hybrid orbitals of equal energy is known as sp-hybridization.

Example: In BeF_2 Molecule the sp -hybridized orbitals of Be overlap with the half-filled orbitals of two fluorine atoms to give a **linear shape**.

Structure of BeF_2 Molecule



Ethyne (C_2H_2) is a linear molecule with a triple bond between the two carbon atoms. Since each carbon atom is bonded to two other atoms and has no lone pairs, the hybridization of each carbon is sp .



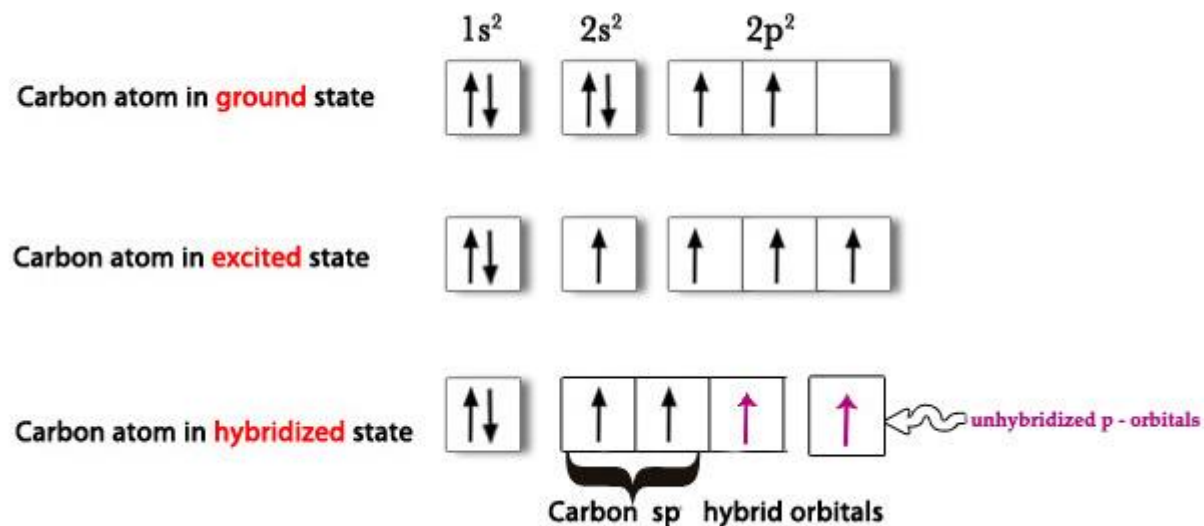
Again, the promotion of an electron in the carbon atom occurs in the same way. However, the hybridization now involves only the $2s$ orbital and the $2p_x$ orbital, leaving the $2p_y$ and the $2p_z$ orbitals unhybridized.

In acetylene molecule, the central carbon atom is sp hybridized.

Carbon (6) $1s^2 2s^2 2p^2 \rightarrow$ **Ground state.**

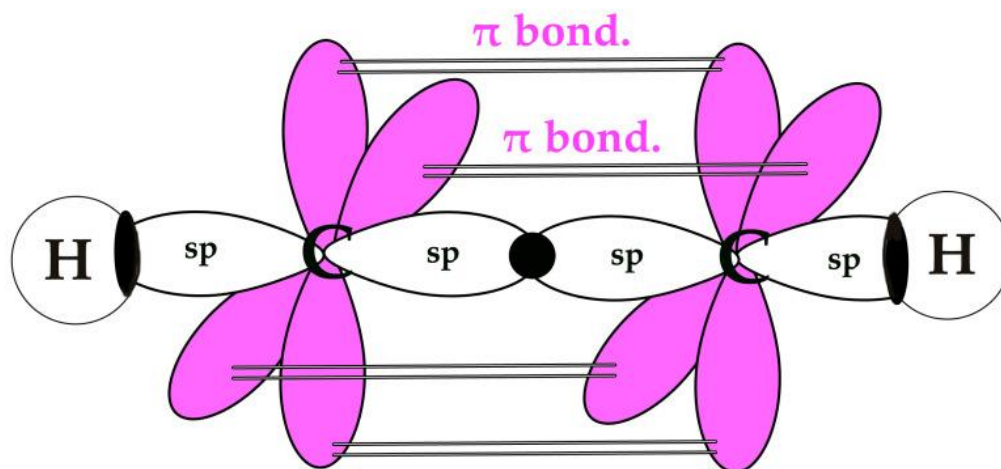
C(6) $1s^2 2s^1 2p^3 \rightarrow$ One 2s electron is promoted to 2p orbital.

Then, 2s and one 2p orbital hybridise to form two sp hybrid orbitals.



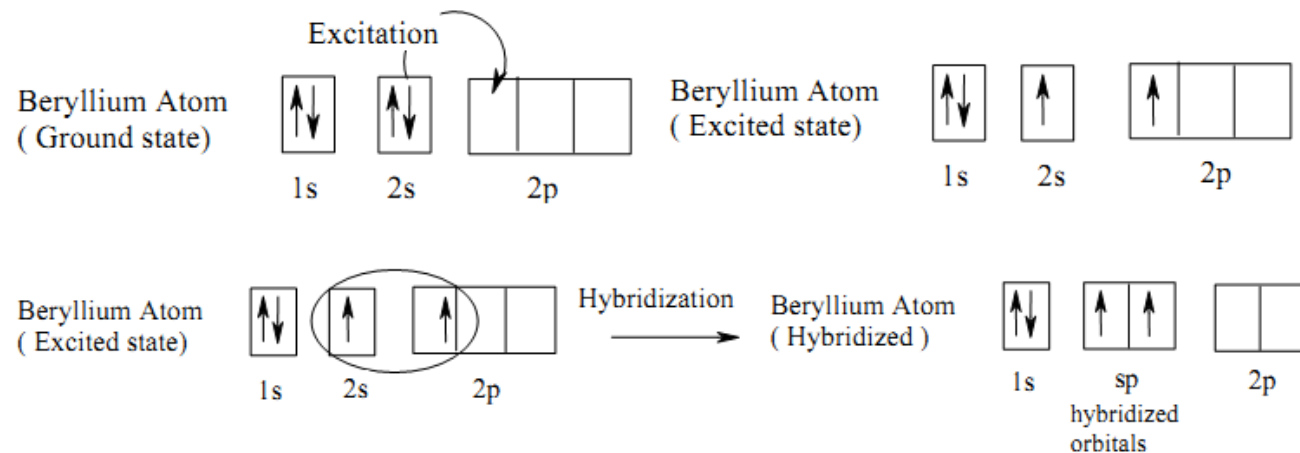
The sigma bond between the two carbon atoms is formed from **sp hybrid orbitals**, and the remaining hybrid orbitals form sigma bonds to the two hydrogen atoms. Both the p_y and the p_z orbitals on each carbon atom form pi bonds with each other. As with

ethene, these side-to-side overlaps are not directly on the line between the two bonded atoms. Additionally, these two pi bonds are perpendicular to one another (**Figure below**); one pi bond is above and below the line of the molecule, while the other is in front of and behind the page.



The bond angle is 180° and the molecule has linear geometry. Other molecules with sp hybridized central atom are BeCl₂, XeF₂.

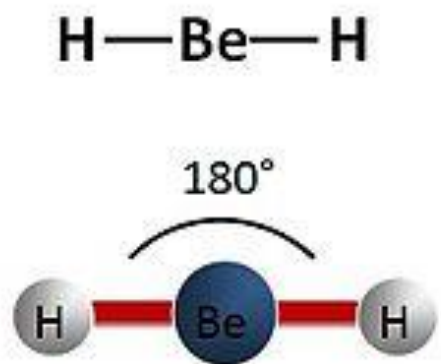
A beryllium hydride (BeH₂) molecule is predicted to be linear by VSEPR. The beryllium atom contains all paired electrons and so must also undergo hybridization. One of the 2s electrons is first promoted to the empty 2p_x orbital (see figure below.



Now the hybridization takes place only with occupied orbitals and the result is a pair of sp hybrid orbitals.

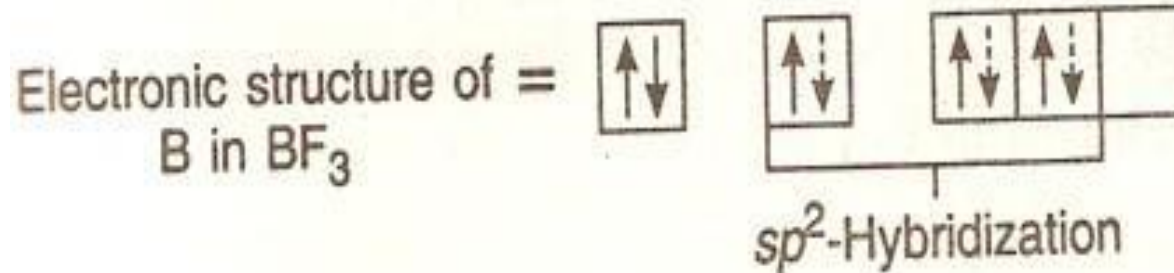
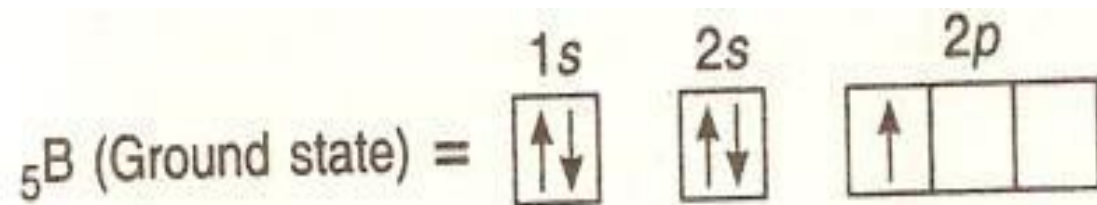
The two remaining p orbitals (p_y and p_z) do not hybridize and remain unoccupied (see figure below)

The geometry of the sp hybrid orbitals is linear, with the lobes of the orbitals pointing in opposite directions along one axis. Each can bond with a $1s$ orbital from a hydrogen atom to form the linear BeH_2 molecule.



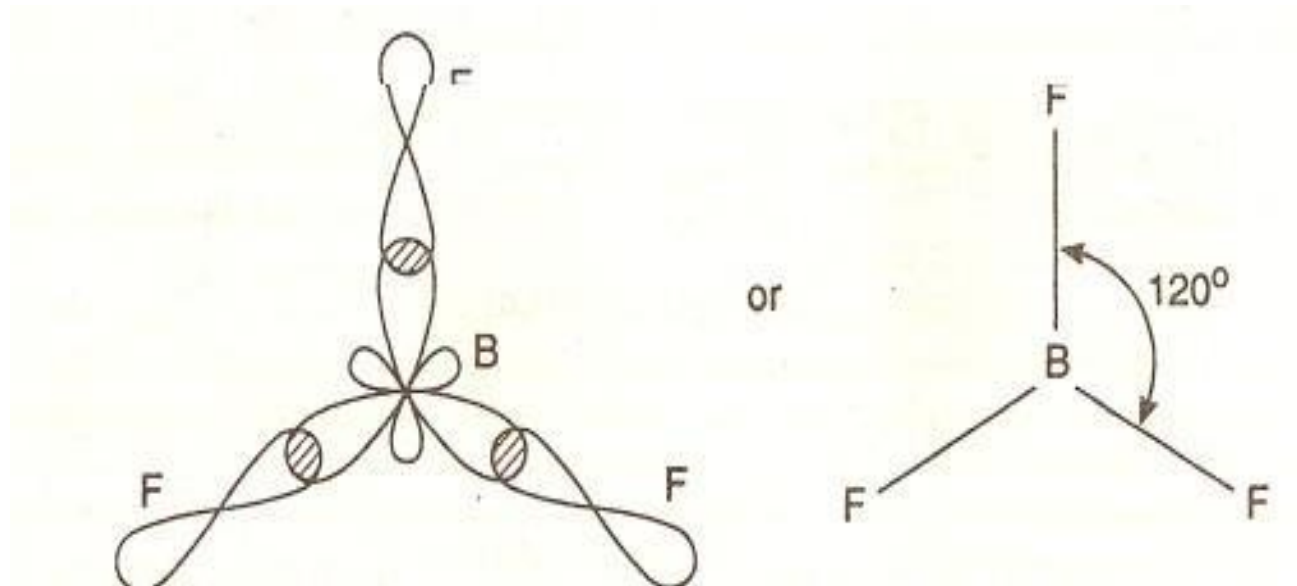
2- sp^2 -hybridization: The combination of one s and two p-orbitals to form three hybrid orbitals of equal energy is known as sp^2 -hybridization.

Example : BF₃ Molecule.

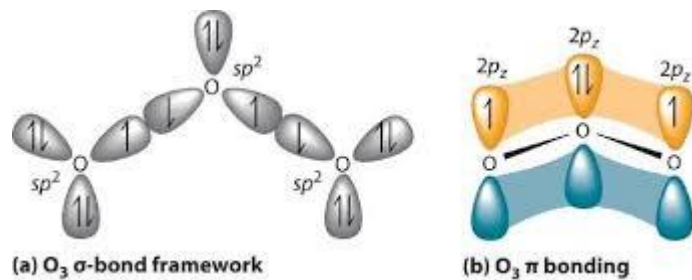


Dotted lines indicates the electrons shared with F atoms

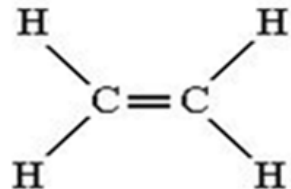
These sp^2 hybridized orbitals are oriented at an angle of 120° . When three sp^2 hybridized orbitals of B overlaps with three p-orbitals of fluorine, three σ -bonds are formed with bond angle 120° . The shape of BF_3 molecule is thus trigonal planar



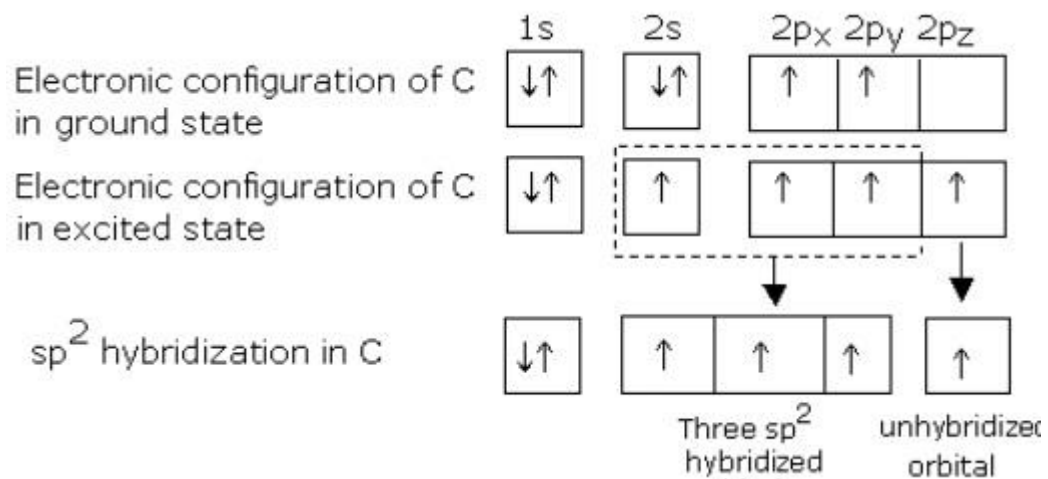
Other molecules with a trigonal planar electron domain geometry form sp^2 hybrid orbitals. Ozone (O_3) is an example of a molecule whose electron domain geometry is trigonal planar, though the presence of a lone pair on the central oxygen makes the molecular geometry bent. The hybridization of the central O atom of ozone is sp^2 .



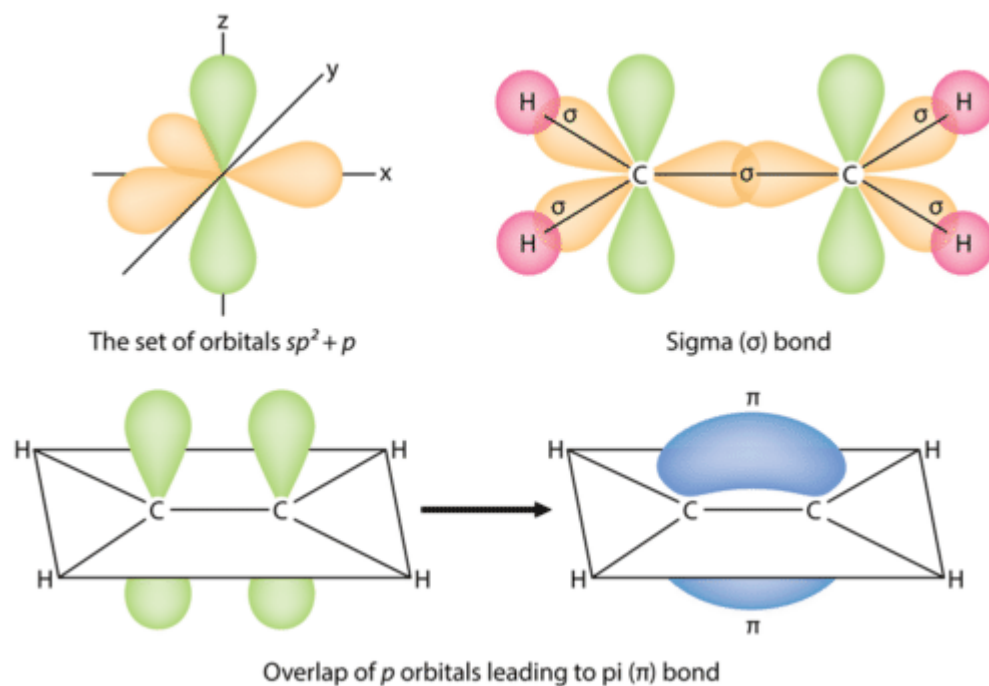
Ethylene molecule



As can be seen above (**Figure above**), the electron domain geometry around each carbon atom is trigonal planar, which corresponds to sp^2 hybridization. Previously, we saw carbon undergo sp^3 hybridization in a CH_4 molecule, so how does it work in this case? As seen below, the electron promotion is the same, but the hybridization occurs only between the single s orbital and two of the three p orbitals. Thus generates a set of three sp^2 hybrids along with an unhybridized $2p_z$ orbital. Each orbital contains one electron and is capable of forming a covalent bond.



The three sp^2 hybrid orbitals lie in one plane, while the unhybridized $2p_z$ orbital is oriented perpendicular to that plane. The bonding in C_2H_4 is explained as follows. One of the three sp^2 hybrids forms a bond by overlapping with the identical hybrid orbital on the other carbon atom. The remaining two hybrid orbitals form bonds by overlapping with the $1s$ orbital of a hydrogen atom. Finally, the $2p_z$ orbitals on each carbon atom form another bond by overlapping with one another sideways.

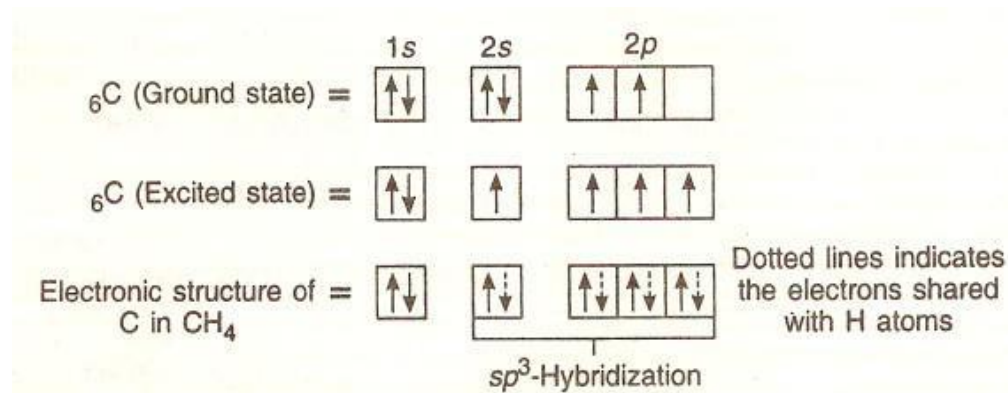


In a conventional Lewis electron-dot structure, a double bond is shown as two lines between the atoms, as in $\text{C}=\text{C}$. It is important to realize, however, that the two bonds are different; one is a sigma bond, while the other is a pi bond.

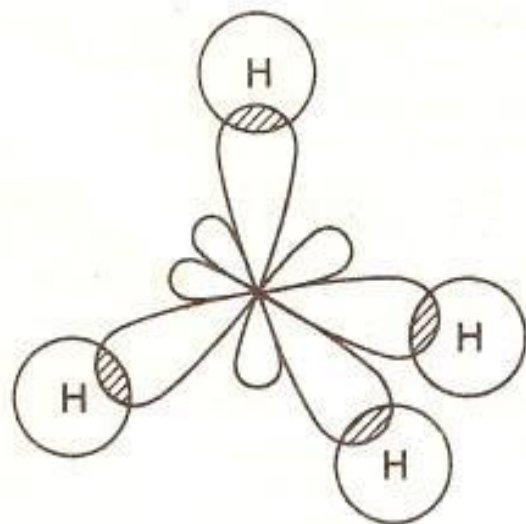
In the ethene molecule, C_2H_4 , there are five σ bonds. One $\text{C}-\text{C}$ σ bond results from overlap of sp^2 hybrid orbitals on the carbon atom with one sp^2 hybrid orbital on the other carbon atom. Four $\text{C}-\text{H}$ bonds result from the overlap between the sp^2 orbitals with s orbitals on the hydrogen atoms. The π bond is formed by the side-by-side overlap of the two unhybridized p orbitals in the two carbon atoms, the two lobes of the π bond are above and below the plane of the σ system. In an ethene molecule, the four hydrogen atoms and the two carbon atoms are all in the same plane

3- sp^3 -hybridization: The combination of one s and three p-orbitals to form four hybrid orbitals of equal energy is known as sp^3 -hybridization.

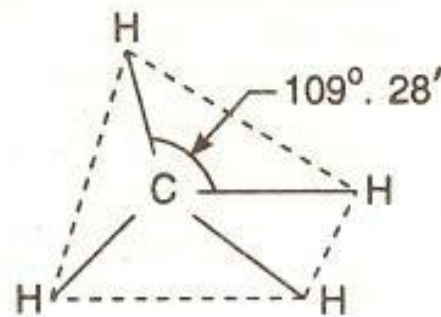
Example: Methane (CH_4) molecule.



These sp^3 -hybridized orbitals are oriented at an angle of $109^\circ 28'$. When these four sp^3 hybrid orbitals overlaps with four $1s$ orbitals of hydrogen, a symmetrical tetrahedral shaped CH_4 molecule form.

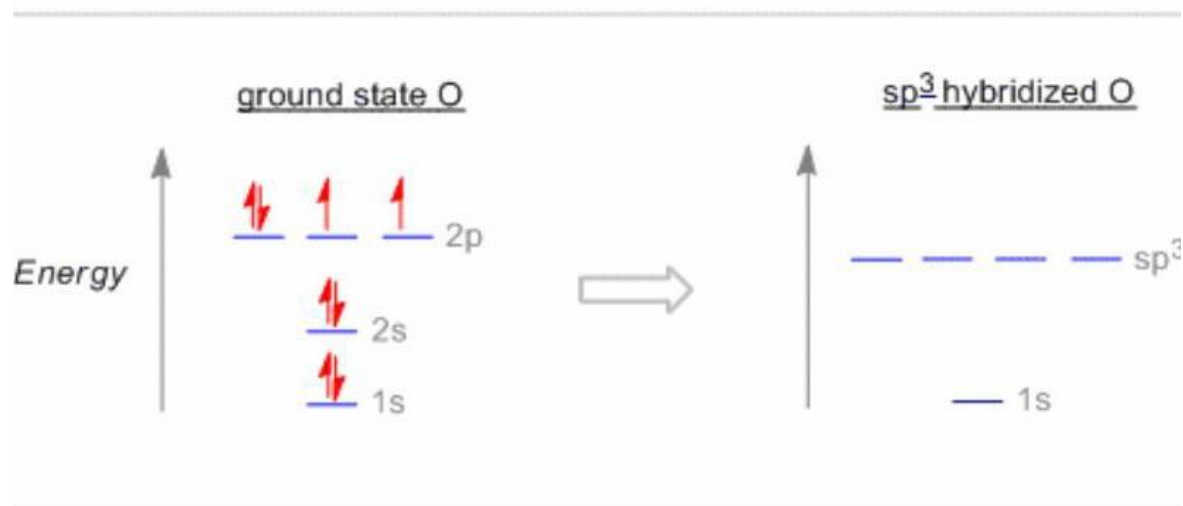


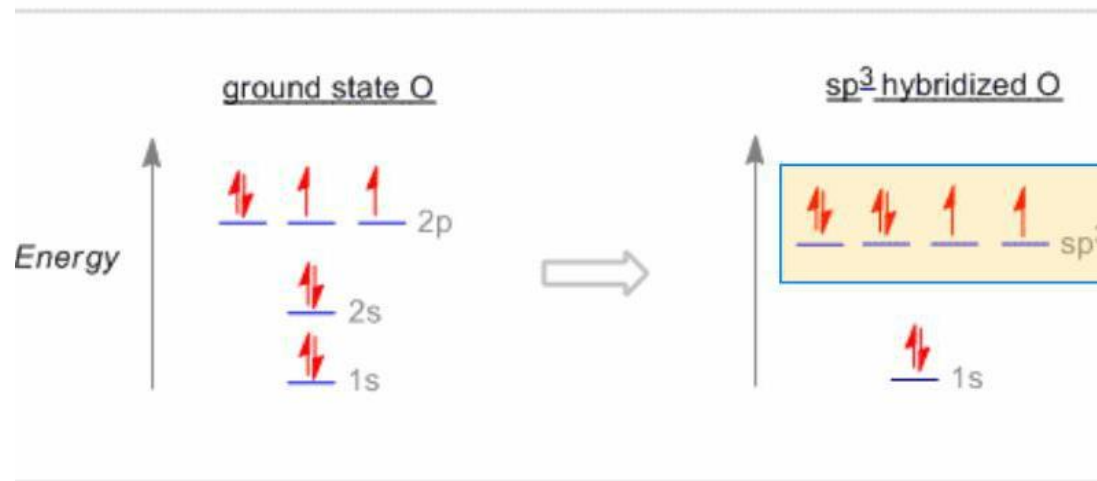
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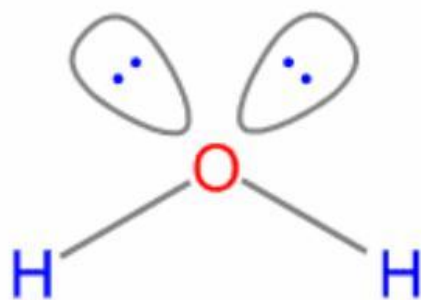
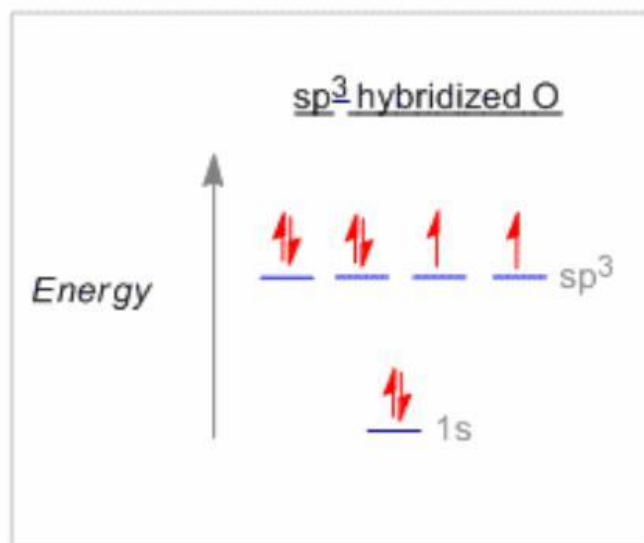
For example the molecule of water H_2O

The electron configuration is $\text{O} = 1s^2 2s^2 2p^4$



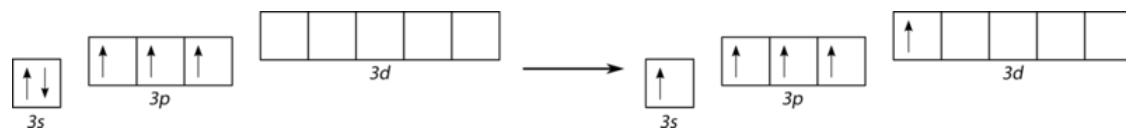


The **atomic orbitals** on O and that they must overlap with 1s orbitals from H to give H₂O

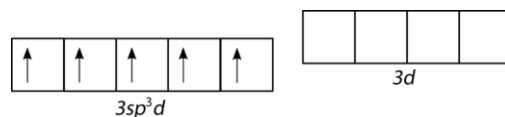


4-sp³d-hybridization: The combination of one *s*, three *p* and one *d*-orbitals to form five hybrid orbitals of equal energy is known as sp³d-hybridization.

For phosphorus pentachloride (PCl₅), the electron domain and molecular geometries are trigonal bipyramidal. The electron promotion is from the 3*s* orbital to an empty 3*d* orbital.



The hybridization then occurs with a single *s* orbital, three *p* orbitals, and a single *d* orbital. The set of five hybrid orbitals are called *sp*³*d* hybrids.

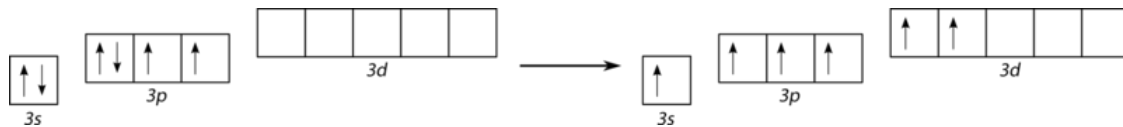


The overlap of the five hybrid sp^3d orbitals with the $3p$ orbital of each chlorine atom results in the five covalent bonds of PCl_5 . Other molecular geometries derived from trigonal bipyramidal electron domain geometry (seesaw, T-shaped, linear) also display the same hybridization.

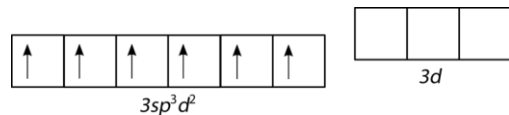
(5) sp^3d_2 -hybridization: The combination of one s , three p and two d -orbitals to form six hybrid orbitals of equal energy is known as sp^3d_2 -hybridization.

Examples: SF_6 Molecule.

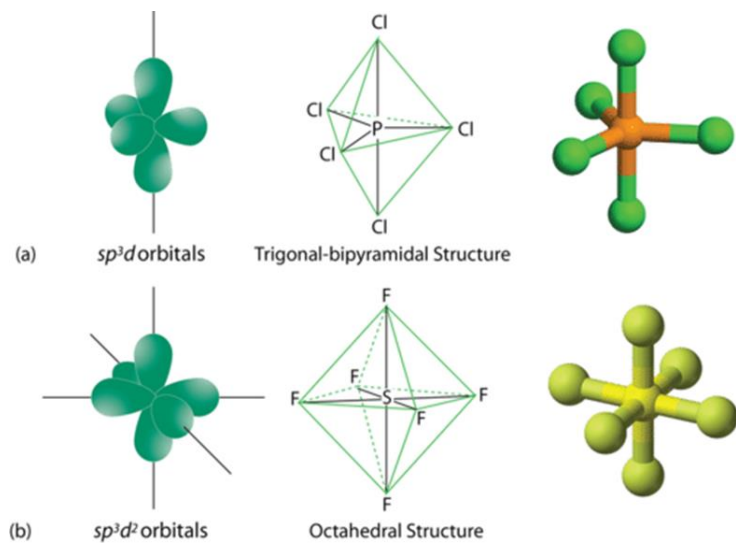
Sulfur hexafluoride (SF_6) has an octahedral electron domain and molecular geometry. In this case, a $3s$ and a $3p$ electron are each promoted to two empty $3d$ orbitals.



The hybridization now occurs with one s orbital, three p orbitals, and two d orbitals. The resulting set of six equivalent orbitals is called sp^3d^2 hybrids.



The overlap of the six hybrid sp^3d^2 orbitals with the $2p$ orbital of each fluorine atom results in the six covalent bonds of SF_6 . Other molecular geometries derived from octahedral electron domain geometry (square pyramidal, square planar) also exhibit this type of hybridization. The figure below (**Figure below**) shows the shape and orientation of the sp^3d and sp^3d^2 hybrid orbital sets



Summary of Hybrid Orbitals

Electron Domain Geometry	Hybridization of the Central Atom	Number of Hybrid Orbitals	Possible Molecular Geometries	Examples
Linear	sp	2	linear	BeH_2 , CO_2
Trigonal Planar	sp^2	3	trigonal planar, bent	BF_3 , CO_3^{2-} , O_3
Tetrahedral	sp^3	4	tetrahedral, trigonal pyramidal, bent	CH_4 , NH_3 , H_2O
Trigonal Bipyramidal	sp^3d	5	trigonal bipyramidal, seesaw, T-shaped, linear	PCl_5 , SF_4 , ClF_3 , I_3^-
Octahedral	sp^3d^2	6	octahedral, square pyramidal, square planar	SF_6 , BrF_5 , XeF_4

