جامعة المستقبل
AL MUSTAQBAL UNIVERSITY

كلية العلـــــوم
قـســــــــــم الادلة الجنائية

المحاضرة السادسة

Hybridization

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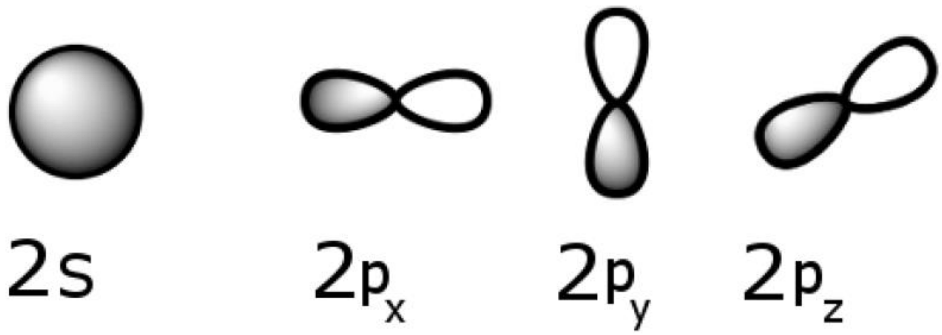
Definition of Hybridization

What is Hybridization?

- ✓ Hybridization happens when atomic orbitals mix to form a new atomic orbital.
- ✓ The new orbital can hold the same total number of electrons as the old ones. The properties and energy of the new, hybridized orbital are an 'average' of the original un hybridized orbitals.
- ✓ This process is called **hybridization**. The new orbitals thus formed are known as **hybrid orbitals.**
- ✓ The concept of hybridization was introduced because it was the best explanation for the fact that all the C - H bonds in molecules like methane are identical.

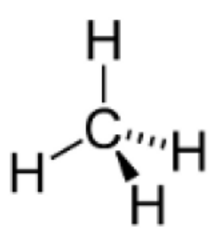
Example

In their ground state, carbon atoms naturally have electron configuration $1S^2 2S^2 2P^2$. The four outermost electrons, i.e. those in the 2S and 2P sublevels are available to form chemical bonds with other atoms. The 2S orbital is capable of holding up to two electrons, and there are three 2P orbitals, each capable of holding up to two electrons, which means the 2P orbitals can hold up to six electrons. Individually, these electron orbitals look something like this. (Each is centered on carbon's nucleus and the p orbitals make angles of 90° with one another.)

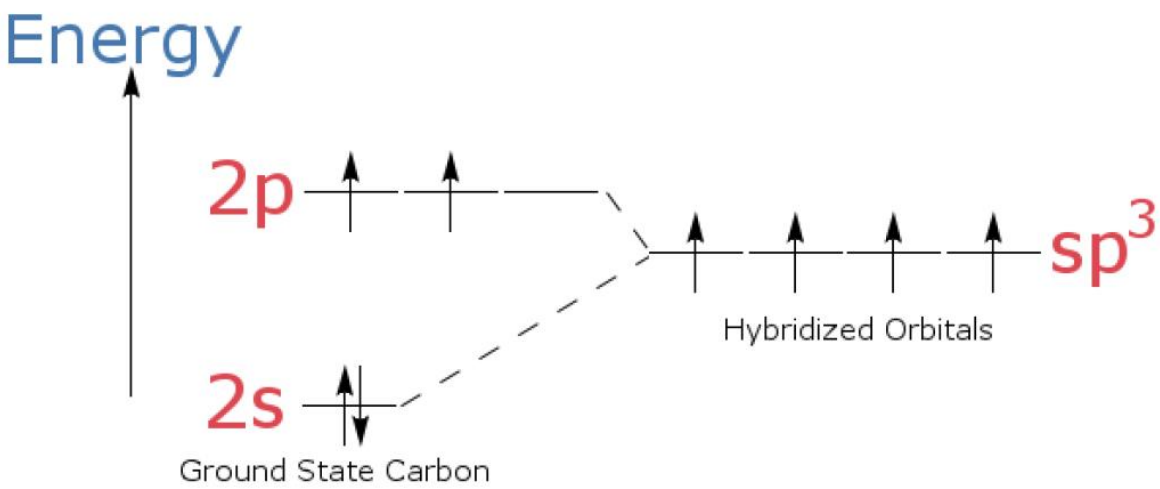


- ✓ The two lobes of a p orbital, one shaded, the other not, represent different phases of the wave function Ψ.
- ✓ When a p orbital meets another orbital, their phases can interfere constructively or destructively. This is shown in the schematic below: an s orbital and a p orbital come together and hybridize. Like sign phases interfere constructively. There is destructive interference if the signs of the phases are different.

- SP^3 hybrid orbitals have a tetrahedral shape - each orbital makes an angle of 109.5° with the others.
- This angle maximizes the distance between the orbital limbs, which is natural given that the electrons in each of the limbs repel one another.
- The shape of molecules like methane, CH_4, with bond angles of 109.5°, is consistent with sp3hybridization of carbon atoms.



Here is an energy level diagram showing how electron energies change in hybridization.



Hybridization is defined as the concept of mixing two atomic orbitals with the same energy levels to give a degenerated new type of orbitals.

Types of Hybridization

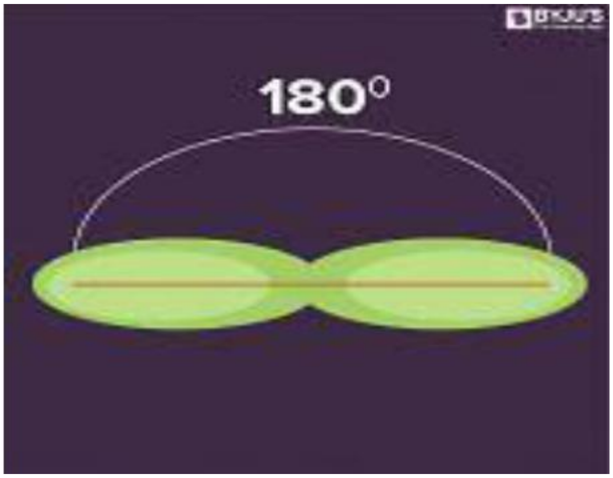
- Based on the types of orbitals involved in mixing, the hybridization can be classified as SP^3, SP^2, SP, sp^3d, sp^3d^2, sp^3d^3.
- Let us now discuss the various types of hybridization along with their examples. Almost always, some sort of intermixing i.e.,
- hybridization of pure atomic orbitals is observed before the bond formation to confer maximum stability to the molecule.
- You can find selected illustrations of different types of hybridizations in the following sections.
- sp (Beryllium chloride, $BeCl_2$; Acetylene, C_2H_2)
- sp^2 (Boron tri chloride, BCl^3; Ethylene, C^2H_4)
- sp^3 (Methane, CH^4; Ethane, C_2H_6)
- sp^3d (phosphorus pentachloride, PCl_5)
- sp^3d^2 (sulfur hexafluoride, SF_6)

- sp^3d^3 (Iodine heptafluoride, IF_7)

1. sp Hybridization

sp hybridization is observed when one s and one p orbital in the same main shell of an atom mix to form two new equivalent orbitals. The new orbitals formed are called **sp hybridized orbitals.** It forms linear molecules with an angle of 180°

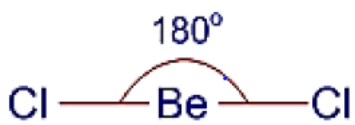
- This type of hybridization involves the mixing of one 's' orbital and one 'p' orbital of equal energy to give a new hybrid orbital known as an sp hybridized orbital.
- sp hybridization is also called diagonal hybridization.
- Each sp hybridized orbital has an equal amount of s and p character, i.e., 50% s and p character.

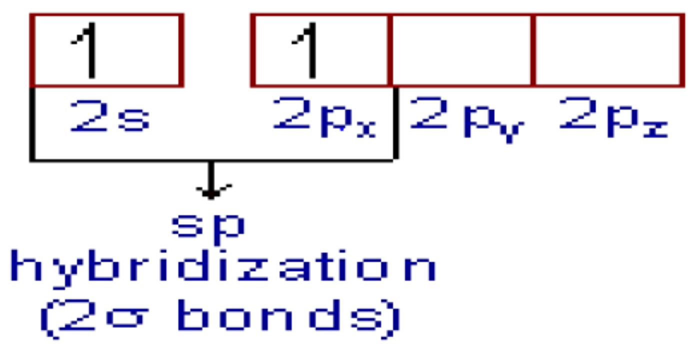


Examples of sp Hybridization: All compounds of beryllium like BeF_2, BeH_2, $BeCl_2$

- The ground state electronic configuration of beryllium (Be) is **$1s^2$ $2s^2$**, so it has no unpaired electrons.

- To form bonds, Be undergoes **excitation**, where one electron from the 2S orbital is promoted to the 2p orbital. The excited state configuration becomes **$1S^2$ $2S^1$ $2P^1$**, producing two unpaired electrons.
- If Be used pure s and p orbitals for bonding, the molecule might have an angular shape.
- However, the observed shape of **$BeCl_2$** is **linear**.
- To explain this, **sp hybridization** occurs: one 2S orbital mixes with one 2P orbital to form two equivalent **sp hybrid orbitals**.
- These two sp orbitals are arranged at **180°**, giving $BeCl_2$ its **linear geometry**.





2. sp^2 Hybridization

- **sp^2 hybridization** occurs when **one s orbital and two p orbitals** from the same shell mix together.
- This mixing forms **three equivalent sp^2 hybrid orbitals**.
- It is also called **trigonal hybridization**.

Main Characteristics

❖ Involves mixing of **1 s orbital + 2 p orbitals** of equal energy.

- The three sp^2 orbitals are arranged in a **trigonal planar geometry**.
- All three orbitals lie in **one plane**.
- The angle between them is **120°**.
- Each sp^2 orbital has:
    - **33.33% s character**
    - **66.66% p character**

Shape

- When the central atom is bonded to **three atoms** and is sp^2 hybridized, the molecule has a **trigonal planar shape**.

Examples

- Boron compounds such as:
    - **BF_3**
    - **BH_3**
    - **BCl_3**
- Carbon compounds containing a **C=C double bond**, such as **Ethylene (C_2H_4)**.

Boron Chloride (BCl_3)

- The ground state electronic configuration of boron (B) is:
  $1s^2\ 2s^2\ 2p^1$
  So, it has only **one unpaired electron**.
- To form **three bonds** with three chlorine atoms, boron needs **three unpaired electrons**.

❖ Therefore, one electron from the **2s orbital is promoted to the 2p orbital** by absorbing energy.

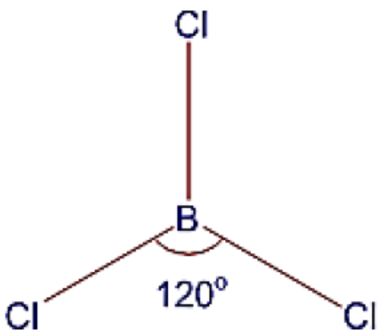
The excited state configuration becomes:

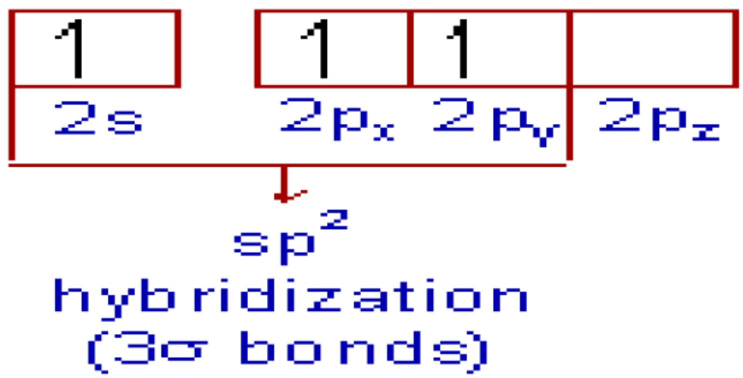
$1s^2\ 2s^1\ 2p_x^1\ 2p_y^1$

❖ Before bond formation, boron undergoes **sp^2 hybridization**:

- ❖ One 2s orbital mixes with two 2p orbitals.
- ❖ This forms **three equivalent sp^2 hybrid orbitals**.

❖ These three sp^2 orbitals lie in the same plane at **120° angles**, giving **BCl_3 a trigonal planar shape**.





3. sp^3Hybridization

When one 's' orbital and 3 'p' orbitals belonging to the same shell of an atom mix together to form four new equivalent orbital, the type of hybridization is called a **tetrahedral hybridization or sp3**. The new orbitals formed are called **sp3 hybrid orbitals.**

❖ These are directed towards the four corners of a regular tetrahedron and make an angle of 109°28' with one another.

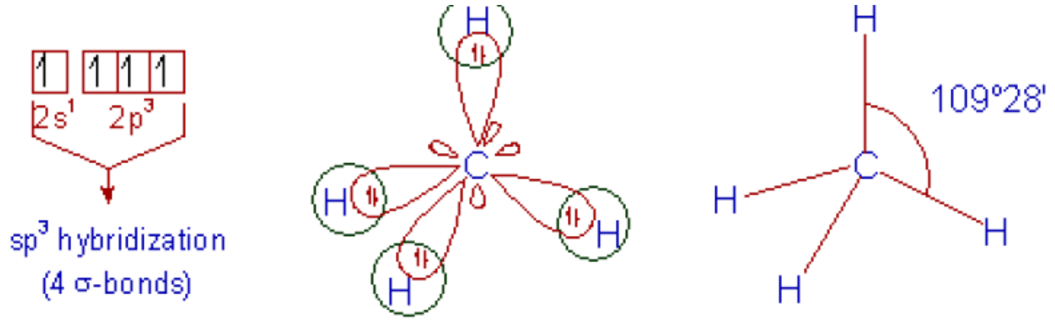
❖ The angle between the sp3 hybrid orbitals is 109.

❖ Each sp3 hybrid orbital has 25% s character and 75% p character.

❖ Example of sp3 hybridization: ethane ($C2H_6$), methane.

Methane (CH_4)

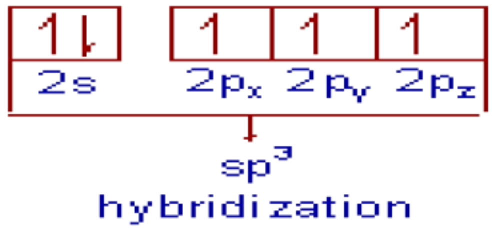
- During the formation of methane molecule, the carbon atom undergoes sp3 hybridization in the excited state by mixing one '2s' and three 2p orbitals to furnish four half filled sp3 hybrid orbitals, which are oriented in tetrahedral symmetry in space around the carbon atom.
- Each of these sp3 hybrid orbitals forms a σsp3-s bond with one hydrogen atom. Thus carbon forms four σsp3-s bonds with four hydrogen atoms.
- Methane molecule is tetrahedral in shape with $109^{o\prime}$ bond angle.

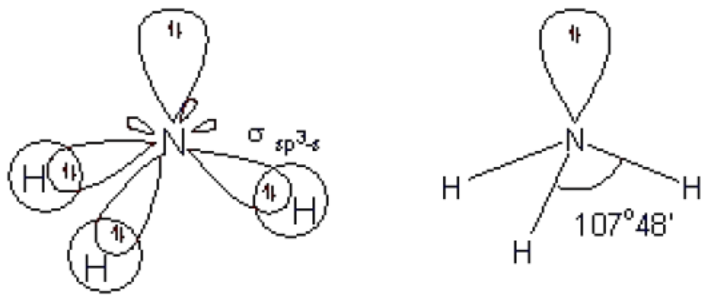


Tetrahedral structure of methane

Ammonia (NH_3)

- The ground state electronic configuration of nitrogen (N) is: $\mathbf{1s^2\ 2s^2\ 2p_x^1\ 2p_y^1\ 2p\_z^1}$
- Nitrogen has **three unpaired electrons** in the 2p orbitals, so it can form **three bonds** with three hydrogen atoms.
- If only pure p orbitals were used, the bond angle would be **90°**.
- However, the observed bond angle in NH_3 is **107°′**.

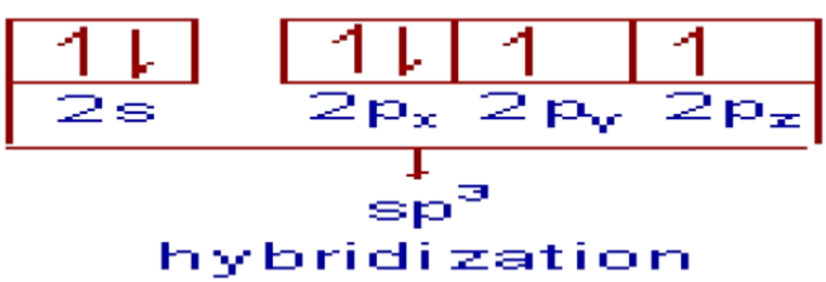




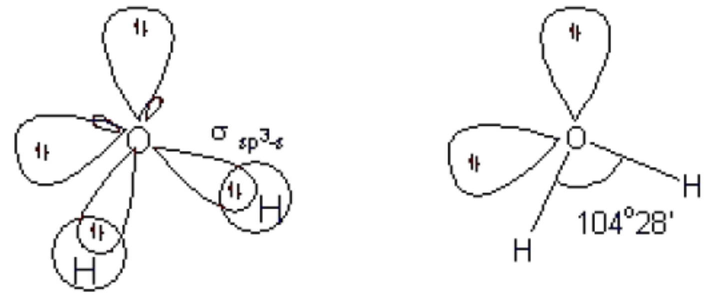
Trigonal pyramidal structure of ammonia molecule

Water Molecule (H_2O)

- The ground state electronic configuration of oxygen (O) is:
  $1s^2\ 2s^2\ 2p_x^2\ 2p_y^1\ 2p\_z^1$
- Oxygen has **two unpaired electrons**, so it can form **two bonds** with two hydrogen atoms.
- If only pure p orbitals were involved, the expected bond angle would be **90°**.
- However, the experimental bond angle in water is **104°′**.



The reported bond angle is 104o28' instead of regular tetrahedral angle: $109^{o'}$. It is again due to repulsions caused by two lone pairs on the bond pairs. Thus water molecule gets angular shape (V shape).



Angular shape of water molecule