SP^3 HYBRIDIZATION

Hybridization, in Chemistry, is defined as the concept of mixing two atomic orbitals to give rise to a new type of hybridized orbitals. This intermixing usually results in the formation of hybrid orbitals having entirely different energy, shapes, etc. The atomic orbitals of the same energy level mainly take part in hybridization. However, both fully-filled and half-filled orbitals can also take part in this process, provided they have equal energy.

During the process of hybridization, the atomic orbitals of comparable energies are mixed together and mostly involves the merging of two 's' orbitals or two 'p' orbitals or the mixing of an 's' orbital with a 'p' orbital, as well as 's' orbital with a 'd' orbital. The new orbitals, thus formed, are known as **hybrid orbitals.** More significantly, hybrid orbitals are quite useful in explaining atomic bonding properties and molecular geometry.

Sp^3 Hybridization

When one 's' orbital and 3 'p' orbitals belonging to the same shell of an atom mix together to form four new equivalent orbitals, the type of hybridization is called a **tetrahedral hybridization or sp^3**. The new orbitals formed are called **sp^3 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 109.28^0
- Each sp^3 hybrid orbital has 25% s character and 75% p character.
- Examples of sp^3 hybridization are ethane (C_2H_6) and methane
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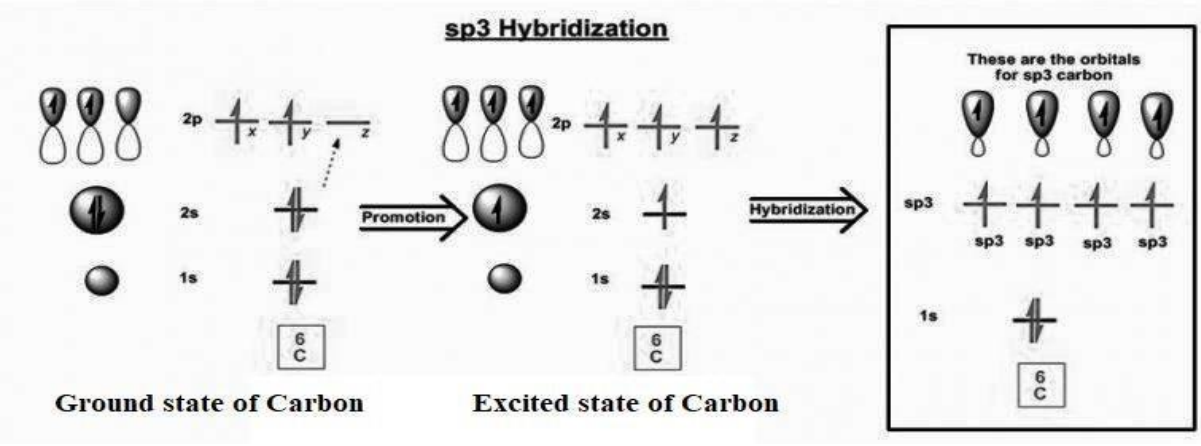
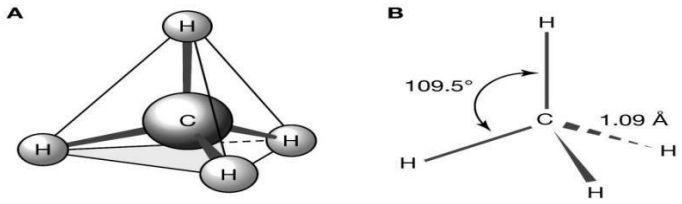
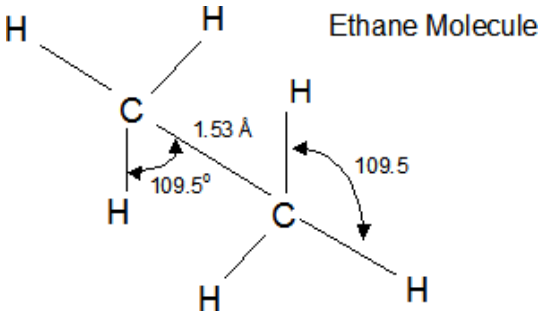


Bond angle and bond length of methane

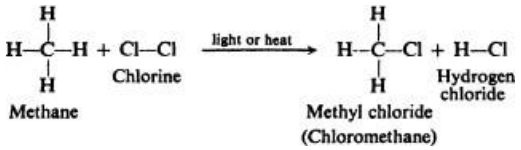


Bond angle and bond length of ethane



Halogenation of alkanes:

- When the substitution of alkane hydrogen by a halogen atom under the influence of UV light or250-400^{0}C.
- Chlorination is a typical example of a broad class of organic reactions known as substitution.
- A chlorine atom has been substituted for a hydrogen atom of methane, and the hydrogen atom thusreplaced is found combined with a second atom of chlorine.

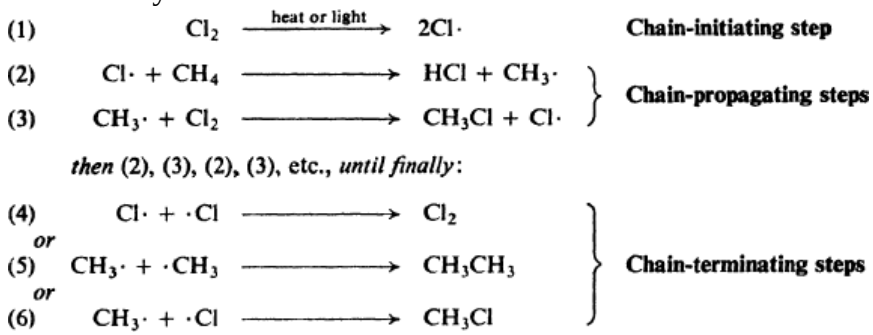


- Bromination takes place somewhat less readily than chlorination.
- Methane does not react with iodine at all.
- With fluorine it reacts so vigorously that, even in the dark and at room temperature, the reaction mustbe carefully, controlled: the reactants, diluted with an inert gas, are mixed at low pressure.
- We can, therefore, arrange the halogens in order of reactivity.

Reactivity of halogens $F_2 > Cl_2 > Br_2 (> I_2)$

Reaction mechanisms (Free radical):

- The detailed, step-by-step description of a chemical reaction, is called a mechanism.
- An atom or group of atoms possessing an odd (unpaired) electron is called a free radical.
- The chlorination of methane is an example of a chain reaction, a reaction that involves a series of steps,each of which generates a reactive substance that brings about the next step.
- **Chain-initiating step:** In this energy is absorbed and a reactive particle generated; in the present reaction it is the cleavage of chlorine into atoms (step 1).
- **Chain-propagating steps:** In this step consumes a reactive particle and generates another; here they are the reaction of chlorine atoms with methane (step 2), and of methyl radicals with chlorine (step 3).
- **Chain-terminating steps**: in which reactive particles are consumed but not generated; in the chlorination of methane these would involve the union of two of the reactive particles, or the capture of one of them by the walls of the reaction vessel.



- considered synthetic paraffin waxes with non-oxidized saturatedalkanes.

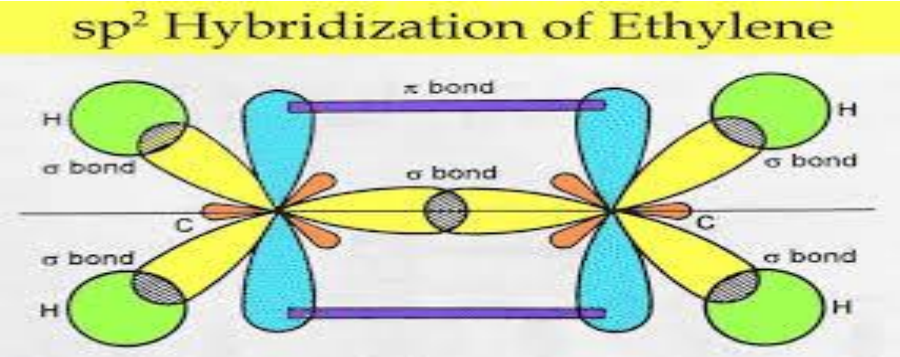
Uses of Paraffin

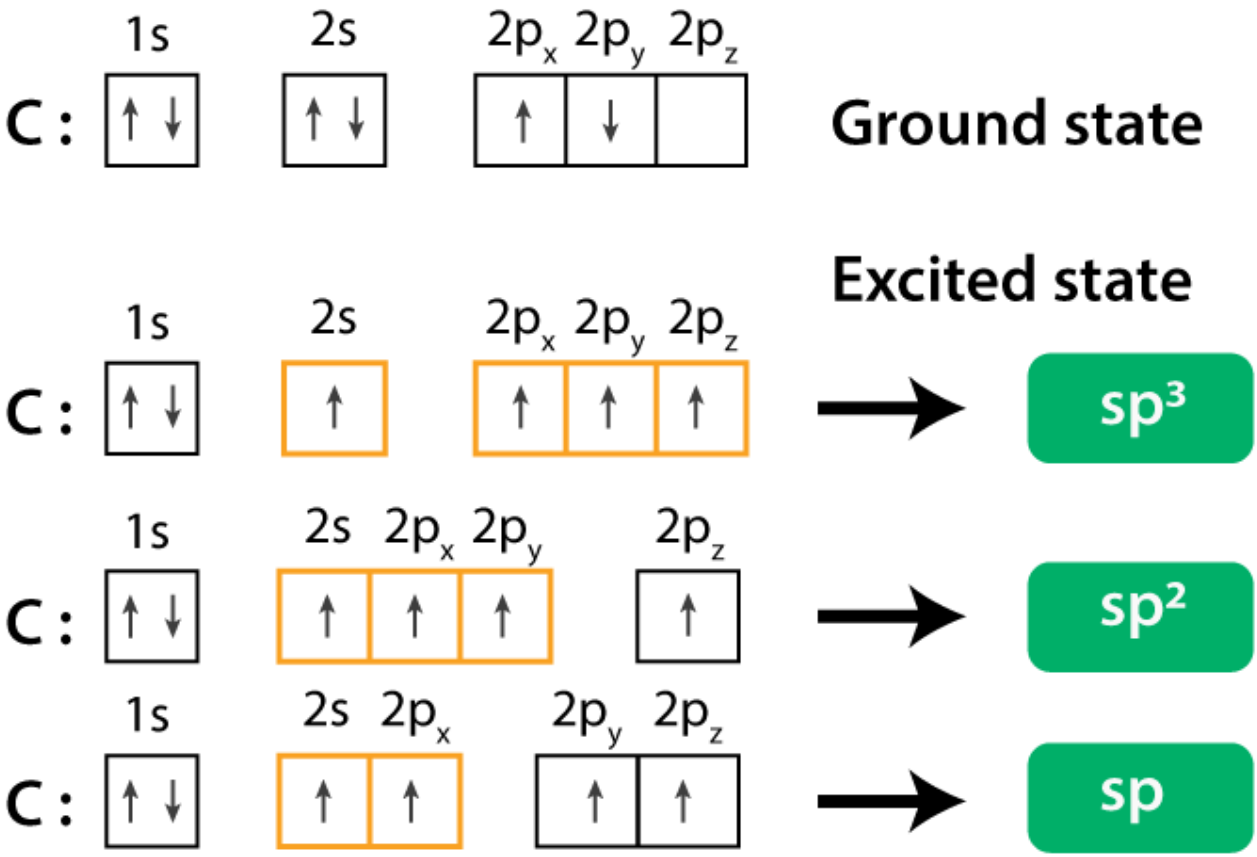
- Medicinal liquid paraffin, also known as ***paraffinum liquidum***, is a very highly refined mineral oil used in cosmetics and for medical purposes.
- Liquid paraffin has many uses in the medical field. Because liquid paraffin passes through the body's intestinal tract without being absorbed, it can be used as a laxative to limit the amount of water removed from the stool and ease constipation.
- Liquid paraffin is considered to have a limited usefulness as an occasional laxative.
- Paraffin wax were developed, the most popular of which was giving hot wax baths to patients suffering from a variety of ailments, in particular rheumatism and joint pain. The wax would be used to soften the skin andthe intense heat would soothe the muscles and ready them for massage treatment.

sp^2 Hybridization

sp^2 hybridization is observed when one s and two p orbitals of the same shell of an atom mix to form 3 equivalent orbitals. The new orbitals formed are called **sp^2 hybrid orbitals.**

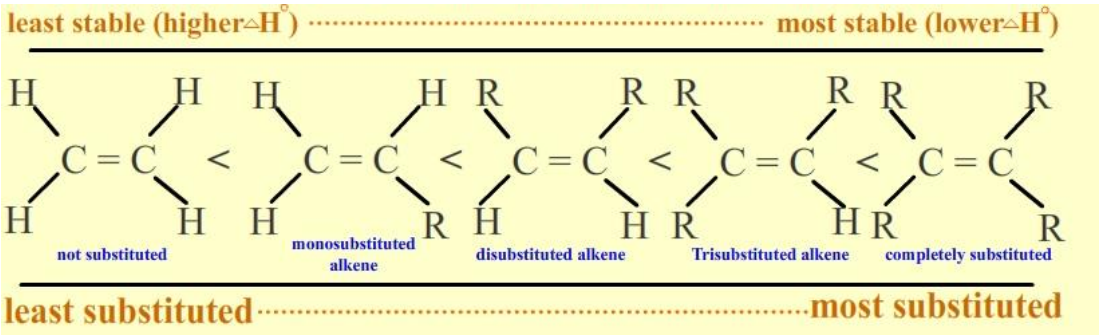
- sp^2 hybridization is also called trigonal hybridization.
- It involves the mixing of one 's' orbital and two 'p' orbitals of equal energy to give a new hybrid orbital known as sp^2.
- A mixture of s and p orbital formed in trigonal symmetry and is maintained at 120^0.
- All three hybrid orbitals remain in one plane and make an angle of 120° with one another. Each of the hybrid orbitals formed has a 33.33% 's' character and 66.66% 'p' character.
- The molecules in which the central atom is linked to 3 atoms and is sp2 hybridized have a triangular planar shape.



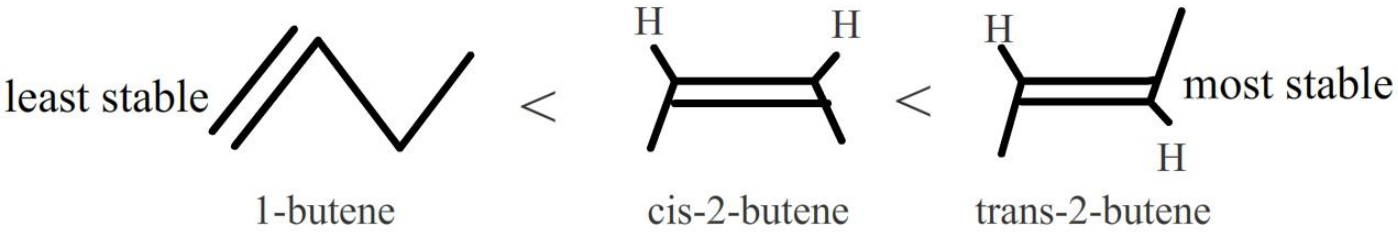


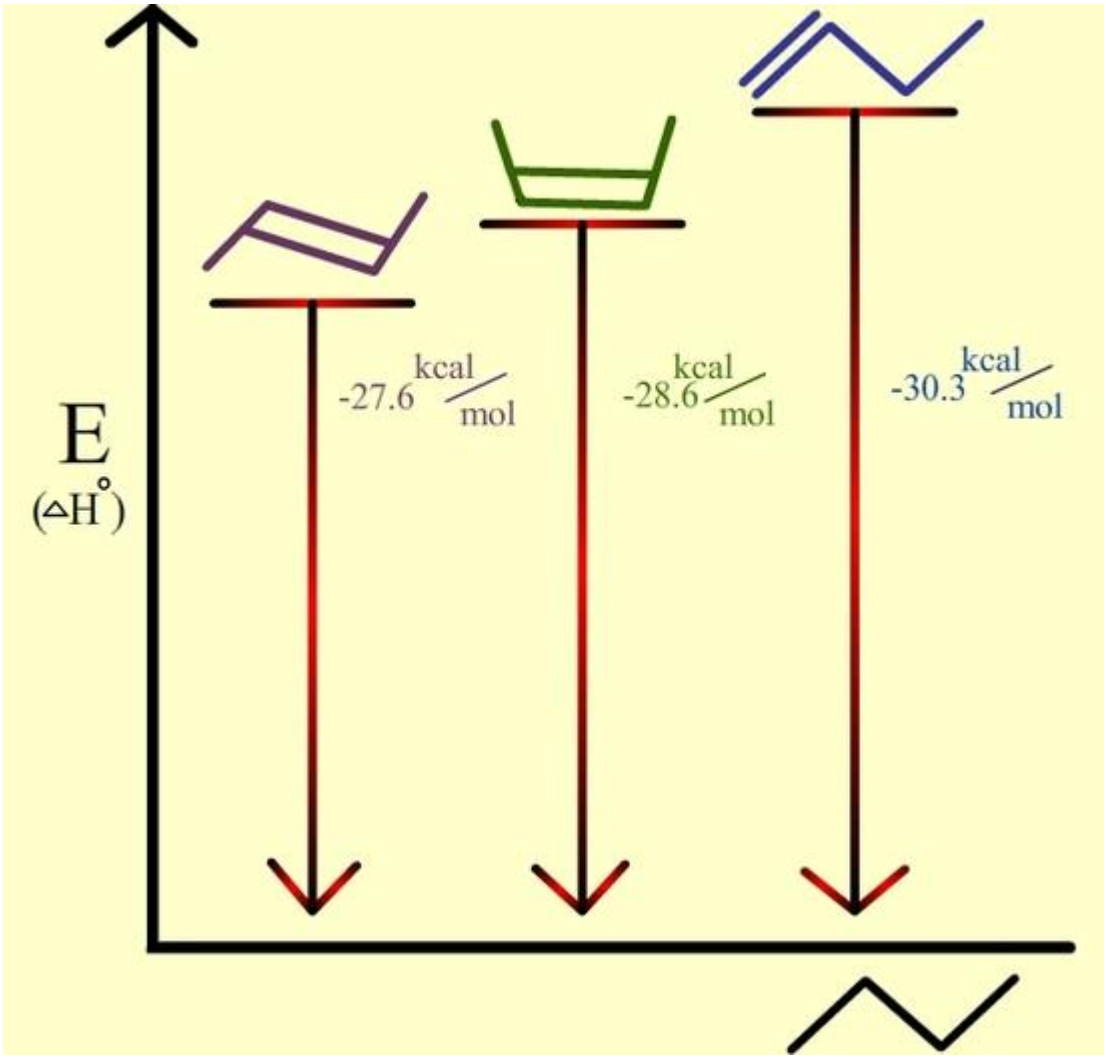
Stability of alkanes

The stability of alkene can be determined by measuring the amount of energy associated with the hydrogenation of the molecule. Since the double bond is breaking in this reaction, the energy released in hydrogenation is proportional to the energy in the double bond of the molecule. This is a useful tool because heats of hydrogenation can be measured very accurately. The is usually around -30 kcal/mol for alkenes. Stability is simply a measure of energy. Lower energy molecules are more stable than higher energy molecules. More substituted alkenes are more stable than less substituted ones due to **hyperconjugation**. They have a lower heat of hydrogenation. The following illustrates stability of alkenes with various substituents:



In disubstituted alkenes, trans isomers are more stable than cis isomers due to steric hindrance. Also, internal alkenes are more stable than terminal ones. See the following isomers of butene:




E
(ΔH°)
-27.6 kcal/mol
-28.6 kcal/mol
-30.3 kcal/mol