

Hybridization in Organic Compounds.

(1) The process of mixing atomic orbitals to form a set of new equivalent orbitals is termed as **hybridization**. There are three types of hybridization encountered in carbon atom. These are,

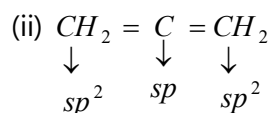
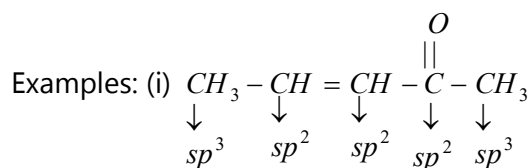
- (i) sp^3 **Hybridization** (involved in saturated organic compounds containing only single covalent bonds),
- (ii) sp^2 **Hybridization** (involved in organic compounds having carbon linked by double bonds) and
- (iii) sp **Hybridization** (involved in organic compounds having carbon linked by a triple bonds).

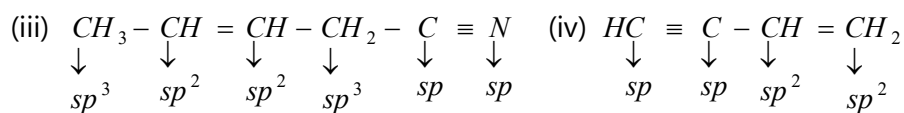
Type of Hybridization	Number of orbitals used	Number of unused p-orbitals	Bond	Bond angle	Geometry	% s-character
sp^3	1s and 3p	Nil	Four σ	109.5°	Tetrahedral	25 or 1/4
sp^2	1s and 2p	One	Three σ One π	120°	Trigonal	33.33 or 1/3
sp	1s and 1p	Two	Two σ Two π	180°	Linear	50 or 1/2

(2) **Determination of hybridization at different carbon atoms:** It can be done by two methods,

- (i) **First method:** In this method hybridization can be known by the number of π – bonds present on that particular atom.

Number of π – bond/s	0	1	2
Type of hybridization	sp^3	sp^2	sp





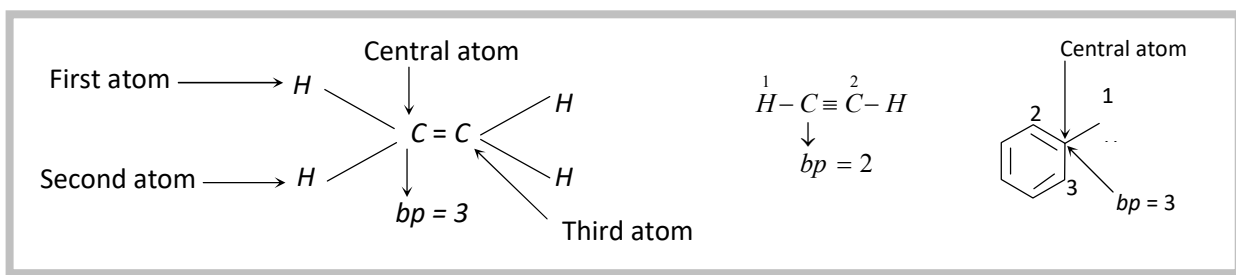
Note: In diamond carbon is sp^3 hybridized and in graphite carbon is sp^2 hybridized.

This method cannot be used for those atoms of the molecule which have positive charge, negative charge or odd electron.

(ii) **Second method:**(Electron pair method)

ep = bp + lp; where ep = electron pair present in hybrid orbitals, bp = bond pair present in hybrid orbitals

Number of bp = Number of atoms attached to the central atom of the species



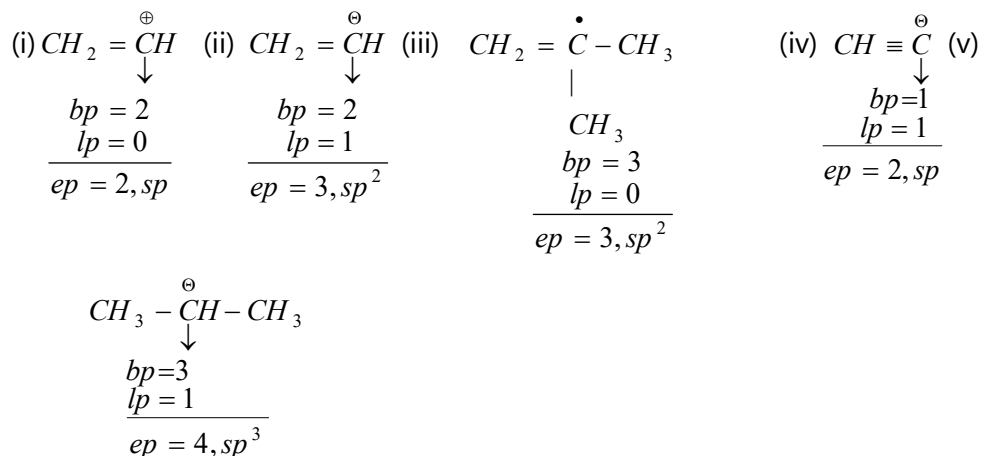
Number of lp's can be determined as follows,

- (a) If carbon has π - bond/s or positive charge or odd electron, then lp on carbon will be zero.
- (b) If carbon has negative charge, then lp will be equal to one.

Number of electron pairs (ep) tells us the type of hybridization as follows,

ep	2	3	4	5	6
Type of hybridization	sp	sp^2	sp^3	$sp^3 d$	$sp^3 d^2$

Example:



(3) Applications of hybridization

(i) **Size of the hybrid orbitals:** Since s - orbitals are closer to nucleus than p - orbitals, it is reasonable to expect that greater the s character of an orbital the smaller it is. Thus the decreasing order of the size of the three hybrid orbitals is opposite to that of the decreasing order of s orbital character in the three hybrid orbitals.

$$sp^3 > sp^2 > sp$$

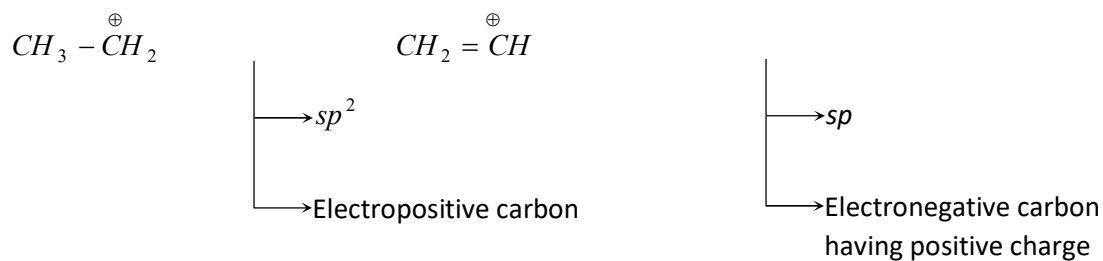
(ii) Electronegativity of different orbitals

(a) Electronegativity of s -orbital is maximum.

(b) Electronegativity of hybrid orbital \propto % s -character in hybrid orbitals

Orbital	sp	sp^2	sp^3
% s - character	50	33.33	25
s-character in decreasing order and electronegativity in decreasing order			

Thus sp -hybrid carbon is always electronegative in character and sp^3 - hybrid carbon is electropositive in character. sp^2 -hybrid carbon can behave as electropositive (in carbocation) as well as electronegative (in carbanion) in character.



(c) Electronegativity of different hybrid and unhybrid orbitals in decreasing order is as follows

$$\xrightarrow{s > sp > sp^2 > sp^3 > p}$$

% s - character in decreasing order and electronegativity in decreasing order.

(iii) **Bond length variation in hydrocarbons**

$$\% \text{ s orbital character} \propto \frac{1}{C - C \text{ bond length}} \propto \frac{1}{C - H \text{ bond length}}$$

Bond type (C – H)	Bond length	Bond type (C – C)	Bond length
$sp^3 - s$ (alkanes)	1.112Å	$sp^3 - sp^3$ (alkanes)	1.54 Å
$sp^2 - s$ (alkenes)	1.103Å	$sp^2 - sp^2$ (alkenes)	1.34Å
$sp - s$ (alkynes)	1.08Å	$sp - sp$ (alkynes)	1.20Å

Note: C–C bond length in benzene lies between single and double bond due to resonance. (1.40Å).

(iv) **Bond strength in hydrocarbons:** The shorter the bond, the greater the compression between atomic nuclei and hence greater the strength of that bond is. Thus the bond formed by sp hybridized carbon is strongest (i.e., it has maximum bond energy) while that formed by sp^3 hybridized carbon is the weakest (i.e., it has minimum bond energy). This is evident by the bond energies of the various types of C – H and C – C bonds.

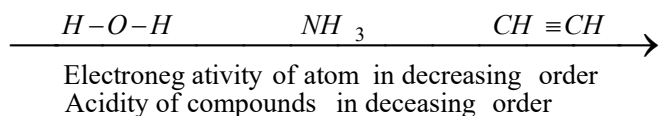
Bond type (C – H)	Bond energy (kcal/mole)	Bond type (C – C)	Bond energy (kcal/mole)
$sp^3 - s$ (in alkanes)	104	$sp^3 - sp^3$ (in alkanes)	80 – 90
$sp^2 - s$ (in alkenes)	106	$sp^2 - sp^2$ (in alkenes)	122 – 164
$sp - s$ (in alkynes)	121	$sp - sp$ (in alkynes)	123 – 199

(v) **Acidity of hydrocarbons**

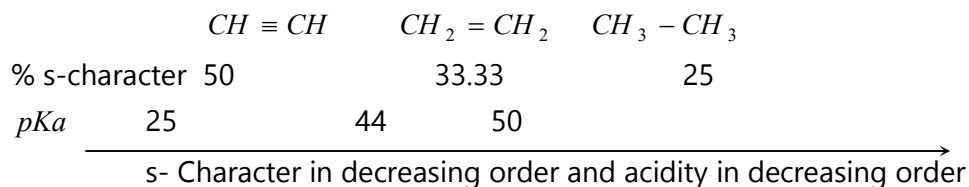
(a) Hydrogen present on electronegative carbon is acidic in character.

(b) Acidity of hydrogen is directly proportional to the electronegativity of atom on which hydrogen is present.

Thus



(c) Acidity of hydrocarbon \propto % s-character



Note: Acidity $\propto K_a$ and Acidity $\propto \frac{1}{pK_a}$ ($pK_a = -\log K_a$)

Order of acidic nature of alkynes is, $HC \equiv CH > HC \equiv C - CH_3$

The relative acidic character follows the order;



Obviously, the basic character of their conjugate bases follows the reverse order, i.e.

