Hybridization

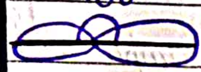
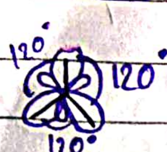
The process of mixing of pure orbital of an atom having nearly equal energy to produce a set of new equivalant orbitals (having the same shape and same energy containt) Is turnd as hybridization. The atom is said to be the hybridized state.

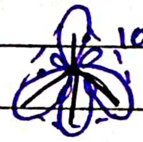
Types of hybridization

Hybridization is a three types in the carbon compound.

(i) SP hybridization structure Linear
(ii) sp^2 hybridization structure Trigonal
(iii) sp^3 hybridization structure Tetrahedral

Table - 1 - Summary of three types of hybridization of carbon

S. No.	No. of mixing orbital	No. of hybred orbital formed	Types of hybridization	Structure	Example
1.	One s or one p s = 50% p = 50%	Two sp hybrid orbital	sp	Linear 180° 	C≡C Acetylene
2.	One s or two p s = 33.3% p = 66.6%	Three sp^2 hybrid obital	sp^2	120°  Trigonal	Ethylene, Propylene (C=C) Ethen

3.	One s and three p $S = 25\%$ $P = 75\%$	Four sp^3 hybrid orbitals	sp^3	 109°28'	C—C CH_4, NH_4

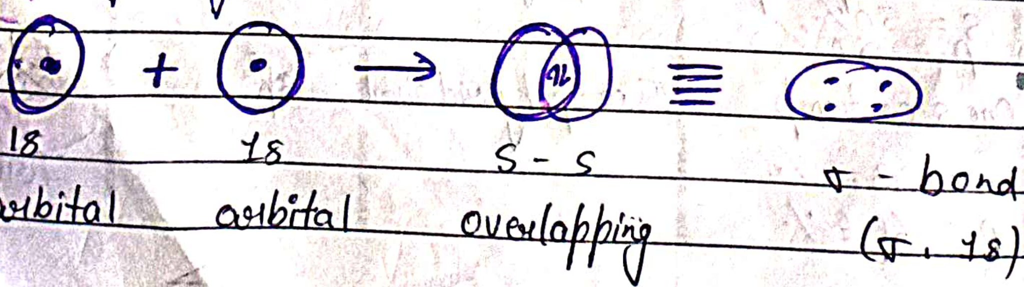
Decreasing order of s character in three type of hybrid orbital is $sp > sp^2 > sp^3$.
And the decreasing order of the size of three orbital could by $sp^3 > sp^2 > sp$.

Types of covalent bond

Covalent bonds can be divided into two types.
1. Sigma (σ) bond
2. Pi (π) bond

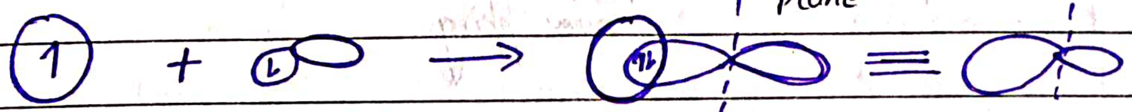
1. **Sigma (σ) bond** :- A sigma bond is formed by the linnear end to end or coaxial over lap of half filled orbitals of two atoms in an efficient way.
It has highest e- dinsity along the molecular axies.

By s-s overlapping
2 similar s atomic orbitals can overlap with each other to form of s-s molecular orbital.
Example:- Hydrogen molecule



By the s-p overlapping (Head on overlapping)
Sigma bonds by result and s or p orbitals
H - F

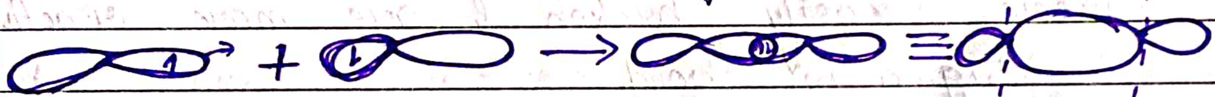
Nodal plone



s-orbital p_z-orbital s-p_z overlapping σ - bond

By the p_z-p_z overlapping (Head on overlapping)
Sigma bond result by a overlape a P_z orbital
For example :- (X - halogens)

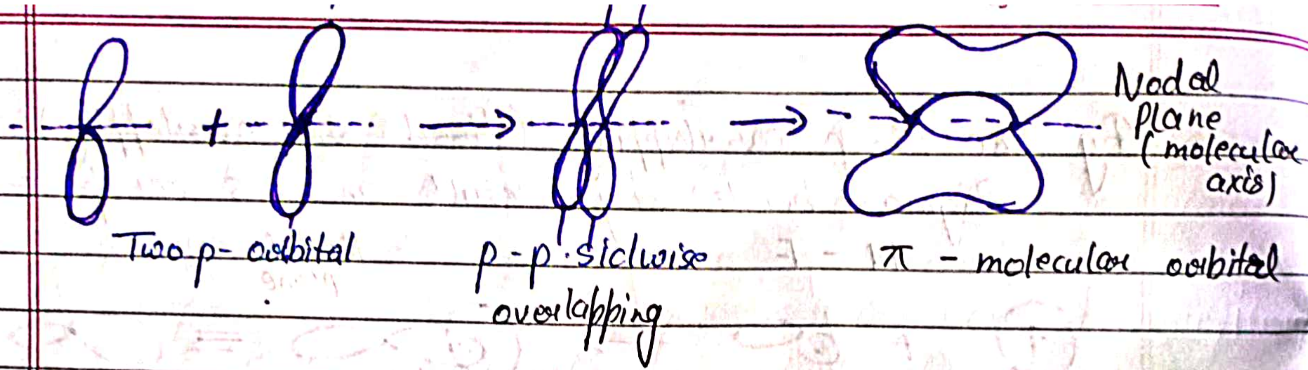
nodal plons



P_z- orbital P_z - orbital P_z-P_z overlapping σ bond

Sigma bond is symmetorical about the line joining two nuclei. They are represented by a single line b/w two atoms.
The electorons of sigma bond are called Sigma electoron.

2. **Pi (π) bond :-** It is formed by the sidewise (lateral) overlapping & ~~two~~ 2p atomic orbitals. (Which have their lops perpendicular to the molecular axis).
Pi(π) bond consist of halves.
One halfes of the (π) bond lies above the plane contaning two nuclei and the other half lies below the plane.



These bonds have following characterstics

- π - electrons are lossely heald then a pair of electrons in a sigma bond.
  Due to parsial overlape the π bond are more easily broken & are more reactive than sigma bond.

- The π bond locks the molecule is one fixed position So rotation is not possible around the π bond. This restriection in rotation around the π bond is ressponsible of the occurenc by a Cis and Trans isomerism in alkene.
- This do not have independent existence and exit along with a sigma bond in a molecule.

Bond length

- The distance b/w two atomic nuclei in a covalent molecule is called the bond distance are or bond length.

- Bond lengths are very small this are usually expressed in Angstroan unit (Å) (1 Å = 10^{-8} c.m or 10^{-10} m)

- This distance insure maximum stability of covalent bond b/c the repulsition b/w atomic nuclei is balanced by the stablising affect of overlapping atomic orbital.

- The bond length are characteristic properties of an molecule & give information about it's structure and properties.

- Bond length are measured by a X-ray Crystallography and Microwave Spectroscopy.

- The distance b/w atoms of a bond is not constant due to vibrating molecule.

Table :- Bonds length of some important Covalent bond

Bond	Bond lengths (Å)	Bond	Bond length (Å)
H−H	0.74 Hydrogen	C=O	1.20 Formaldehyde
C−C	1.54 Ethane		1.16 Carbon dioxide
	1.48 Butadiene	C−N	1.47 Methyl amine
C=C	1.34 Ethylene	C−Cl	1.78 Methyl chloride
C≡C	1.20 Acetylene	C−Br	1.94 Methyl bromide
C−H	1.11 Methane	C−I	2.14 Methyl iodine
	1.09 Benzene	O−H	0.96 Methanol
	1.06 Acetylene	N−H	1.01 Methyl amine
C−O	1.41 Ethanol	C−F	1.42 Methyl flouride
	1.34 Formic Acid		

- The length of a covalant bond is equal to ~~sum seme~~ of the covalant readii of the two concerned.

Example :- The bond length a C — C is 1.54 Å (supp) and theis covalant readius of C atom.

$$\frac{1.54}{2} = 0.77\ \text{Å}$$

Note :- Bond length given in Å can be converted into Picometer (pm) by multipling by 100.
(1 Å = 100 pm)

Factors affecting Bond length

1. Hybridization
2. Electeronegativity
3. Delocalization.

1. Hybridization :- Theire is a carelation b/w bond length & hybridization. As the amount of s character relative to the amount of p character in a hybrid orbital increases (↑) the bond length decreases (↓).

Table :- Carelation of bond length with hybridization

Types of hybridization	% of s character	C — H bond length (Å)	C — C bond length (Å)
sp^3	25%	1.11	1.54 Å
sp^2	33.3%	1.083	1.34 Å
sp^3	50%	1.057	1.20 Å

s character (↑) — bond length (↓) — bond length (↓)

2. **Electoronegativity** :- When a covalant bond is made up of two atoms having different electoronegativityes becomes some what more ionic in chardcter and possesses a slightly different length.

For Example :- As the electoronegativity of an atom attached to C atom in $C-X$ increases (↑), the valance e- of $C-X$ bond are attracted more towards the electoronegtive (X) atom which dicreases the affactive atomic radius & thus their is dicrease in $C-X$ bond length. This also explains while the $C-X$ bond in F_3C-X molecule is always shorter then in the corresponding H_3C-X molecule.

Table :- Effect of electoronegativity of C on the bond length of $C-X$

Bond length (Å) of C–H bond		Bond length (Å) of C–Cl		Bond length (Å) of C–F	
CH_3CH_2-H	1.11	H_3C-Cl	1.780	H_3C-F	1.391
H_3C-H	1.11	ClH_2C-Cl	1.772	F_3C-F	1.323
Cl_3C-H	1.06	Cl_2HC-Cl	1.763		
		Cl_3C-Cl	1.755		
		F_3C-Cl	1.720		

Dilocalization :- Dilocalization happen when electric charge spred over more then one atom. Example:- Bonding electrons may be distributed among severall atom that are bonded together.

The bond length are also affected by dilocalization of π ~~bo~~ electrons.
For example:- In Benzeen their three ~~C=C~~ C–C and three C=C 6, thus the bond length should be 1.54 Å and 1.34 Å respectivily. But actualy it lies in b/w single & double bond length and it is e 1.39 Å due to dilocalization of π electrons

Bond Angles (θ)

- The bond angle is difined as the angle b/w the direction of two neighbouring covalent bonds.
- sp^3, sp^2 and sp orbitals in hybridised carbon atoms have an angle of 109°28', 120° and 180° respectivily.
- The bond angles can be determind by X-ray diffraction, electron diffraction and spectroscopic method.

Factors affecting the bond angles

1. Hybridization
2. Lone pair repultension
3. Effect of substituents
4. Electronegativity of central atom

1. **Hybridization** :- Hybridization of bonding orbitals also play an important role in determining the value of bond angles.
It has been observed that as the s-character in a hybrid orbital increases (↑), the bond angle also increases (↑).

Hybrid orbitals		Bond angles	
increases(↑) s-character ↓	sp^3	$109°28'$	increase in bond angle (↑) ↓
	sp^2	$120°$	
	sp	$180°$	

This place has higher value of bond angle of esytelene is due to greather s-character that in ethylene, ethane and water having lower s-character.

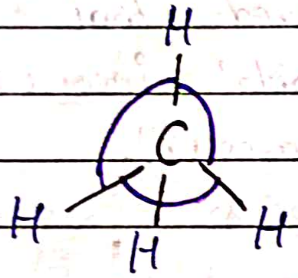
2. **Lone pair repulsion** :- The bond angle decreases (↓) with an increase (↑) in no. of lone pair.
Since the magnitude of repulsion b/w the e- pairs

around central atom decreases (↓) in the following order -

lone pair - lone pair > lone pair - bond pair > bond pair - bond pair

lp - lp > lp - bp > bp - bp

For example :- Methan (CH_4) molecule has 4 bond pairs with equal repulsive force. Which completely balanced each other.



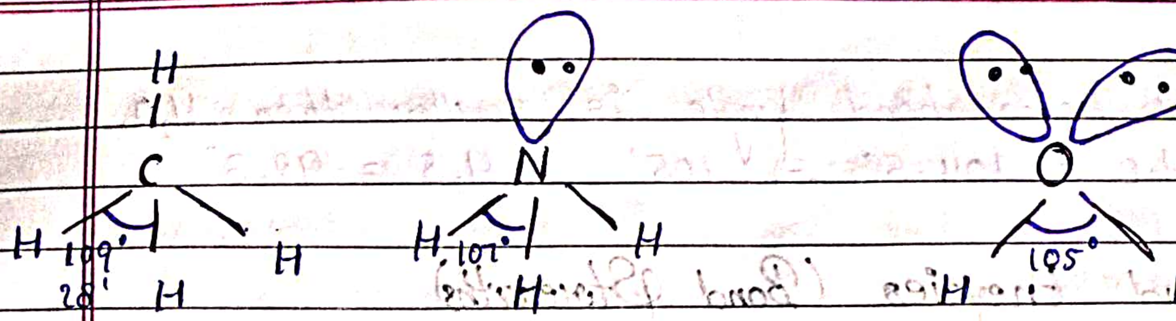
Tetrahedral
bond angle = 109° 28'
between H C H

Amonia (NH_3)

There are three bond pairs & one lone pair. Since has a greater repulsive force, the bond pairs are forced closer together resulting in the H - N - H bond angles of 107°

Water (H_2O)

In water molecule there are two bond pair and two lone pairs. Which cause greater repulsion than that in amonia molecule and thus forcing the bond pair stil closer together resulting in the H - O - H bond angle of 109.5° = 105°.



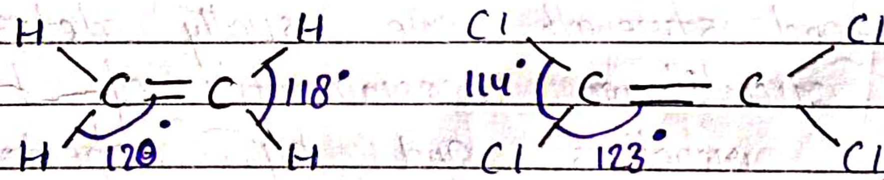
Methane (4 bond pair) tetrahedral shape

Amonia (3 bond pair & one lone pair) Pyramidal shape

Water (2 bond pair and 2 lone pair) bent -V- shape

3. **Effect of substituents :-** In sp^2 hybrid orbito the three lops of sp^2 hybrid orbital are directed towards the carner of and equlaterial triangle.

The angle b/w two sp^2 hybrid orbitals each 120° in ethylene molecule. However, this angle also deviates slightly when different substituents are attached to it.



4. **Electronegativity of central atom :-**

The increase in electronegativity of central atom increases the bond angle. ~~Th~~

For example :- H_2O and H_2S, Sulphur is less electronegative than Oxygen.

The bond pairs of H_2S are more away from the ~~cel~~ central atom, the repulsive forces b/w bond pair are small then in H_2O.

And hence bond angle is smaller then H_2O.
$H_2O = 104.5°$, = 105° , H_2S = 92.3°