Hybridization

Hybridization : mixing of the pure atomic orbitals to obtain new orbitals (Hybrid orbitals) that are equivalent in shape and energy. The number of the hybrid orbitals is equal to the number of pure orbitals .

Types of Hybridization

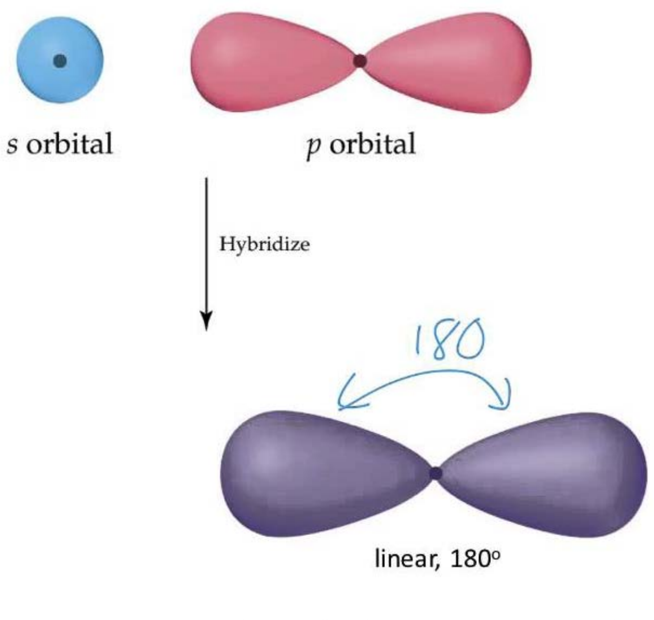
1- sp Hybridization

This type is compose participate of two orbitals one is a **s**, the other type is **p** to form important orbitals of sp located in a straight line at an angle of 180 degrees in order to get less repulsion between the two orbitals.

50% s and 50 % p

$$s + p \longrightarrow 2sp$$

pure orbital pure orbital Hyprid orbitals



sp hybrid orbitals shown together

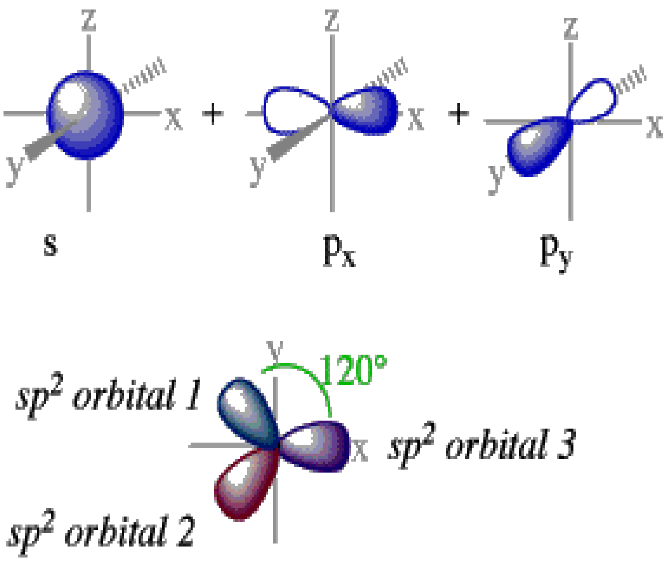
2- sp^2 Hybridization

This type consists of one atomic orbital type s, with two orbitals types is p to form important orbitals of sp^2 located in a same level with angle of 120 degrees in order to get less repulsion between the three orbitals

33

⟶ $3sp^2$

ital Hyprid orbitals



3- sp^3 Hybridization

This type of hybridization produce from one orbital atom type s with three orbital of p and formation four atom hybridization orbitals type sp^3 and take Tetrahedral regular figure with angle of 109.5 degree in order to get less repulsion between the orbitals.

25% s and 75 % p

$$s \quad + \quad 3p \longrightarrow 4sp^3$$

Applications of hybridization

1. Linear molecule

Orbital 1s is internally considered do not participate in hybridization.

In these orbitals can produce the molecular orbitals with orbital atoms of Cl to produce two covalent bonds between Be and Cl and formation $BeCl_2$ with angle of 180 degree.

$_4Be$ $1s^2$ $2s^2$ 2p

Be-atom ground state

Be-atom excited state

BCl_2 Linear molecules

Cl ——— Be ——— Cl =180 degree

2- Trigonal planar molecules

Example: BF_3

$_5B$ $1s^2$ $2s^2$ $2p^1$

B-atom ground stat

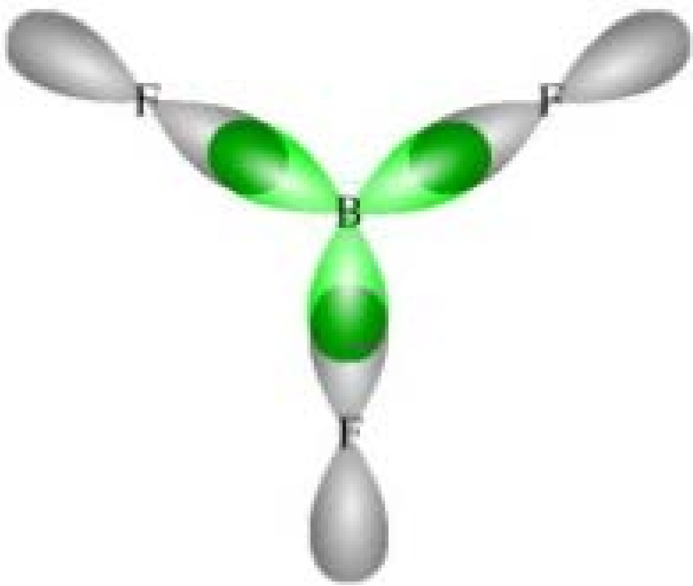
B-atom excited stat

Hyperdization (sp^2)

BF_3 molecules

Trigonal plane

For this of three orbitals can formation three hybrid orbitals molecule with three orbitals of three F atoms to formation BF_3 molecule with angle of 120 degree (Trigonal planar).



Angle of FBF = 120 degree

3- Tetrahedral molecules

Example: CH_4

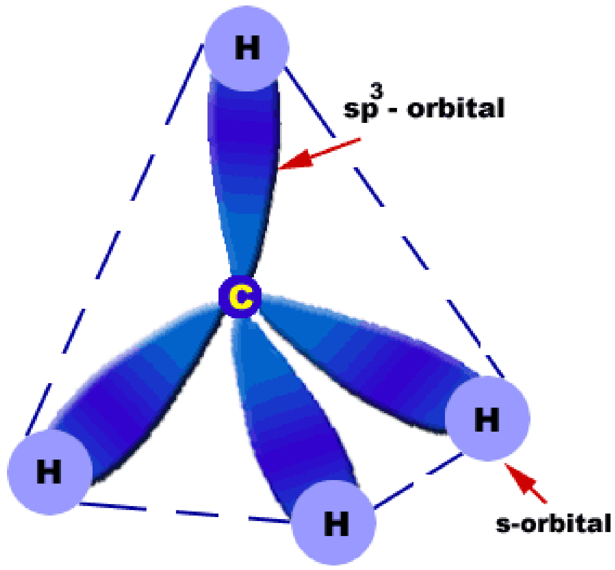
$_6C$ $1s^2$ $2s^2$ $2p^2$

C-atom ground stat

C-atom excited stat

Hyperdization (sp^3)

For this of four orbitals can formation four hybrid orbitals molecule with four orbitals of four H atoms to formation CH_4 molecule with angle of 109.5 degree (Tetrahedral).



Orbital structure of methane

Angle of HCH = 109.5 degree

Tetrahedral

4- Tetrahedral molecule (Pyramidel)

Example: NH_3

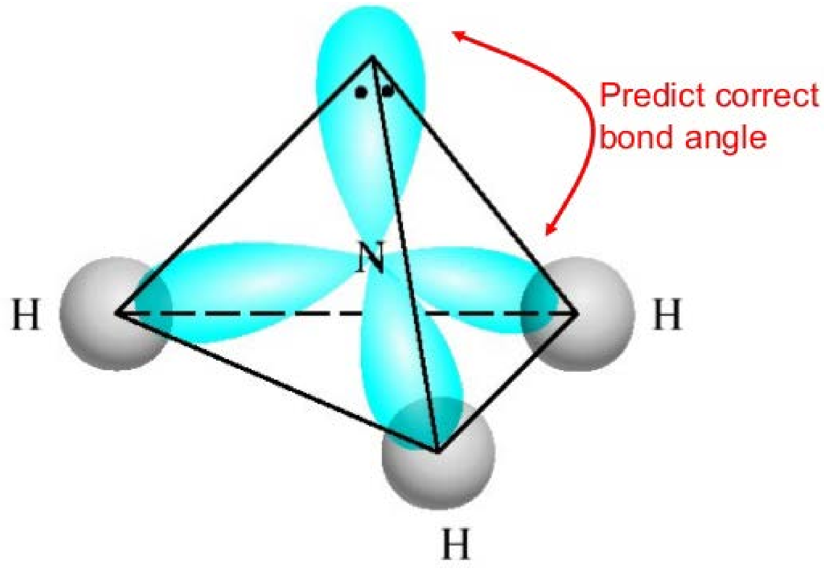
$_7N$ $1s^2$ $2s^2$ $2p^3$

N-atom ground stat

N-atom excited stat

Hyperdization (sp^3)

Four hybrid orbitals type sp^3 interfere with three orbitals atoms of three H atoms to formation three covalent bonds type σ and cannot this hybrid orbitals participated for interfere that contain one pair electron, So NH_3 molecule is formed Tetrahedral with angle of 107 degree.



Angle of HNH = 107 degree

5- Tetrahedral molecule (V-Shape)

Example: H_2O

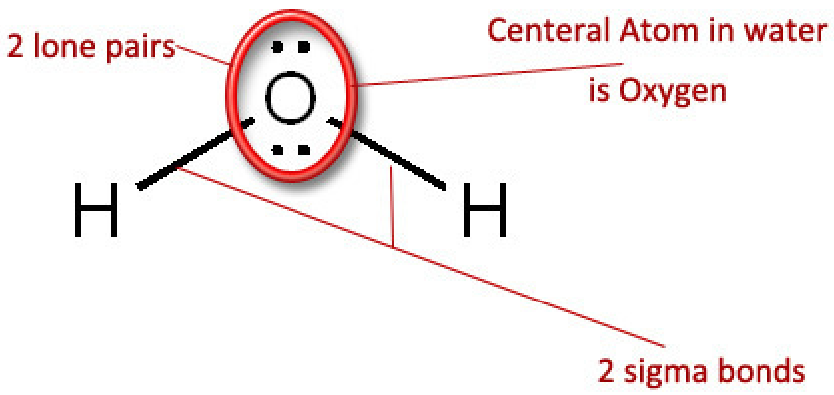
$_8O$ $1s^2$ $2s^2$ $2p^4$

O-atom ground stat

Hyperdization (sp^3)

Four hybrid orbitals type sp^3 interfere with two orbitals atoms of H atoms to formation two covalent bonds type σ and cannot this hybrid orbitals participated for interfere that contain two pair electrons, So H_2O molecule is formed irregular tetrahedral with angle of 105 degree.

Angle of HOH = 105 degree



6- Trigonal bipyramid molecule

Example: PCl_5

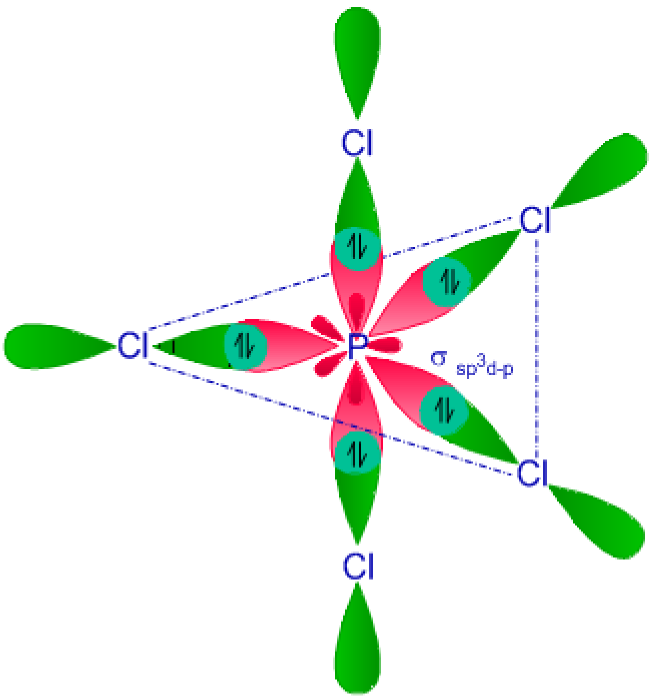
$_{15}P$ $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3P^3$ 3d

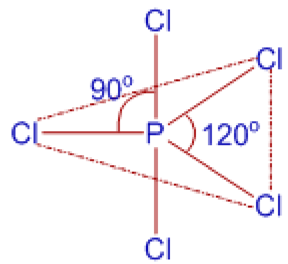
P-atom ground stat

P-atom excited stat

Hyperdization (sp^3d)

Five hybrid orbitals each is half filled overlap with p- orbital of each Cl atom, So PCl_5 molecule is formed Trigonal bipyramid .





Trigonal bipyramidal structure of PCl_5

Angle = 90 and 120 degree

7- Octahydral molecule

Example: SF_6

$_{16}S$ $1s^2$ $2s^2$ $2p^6$ $3s^2$ $3P^4$ $3d$

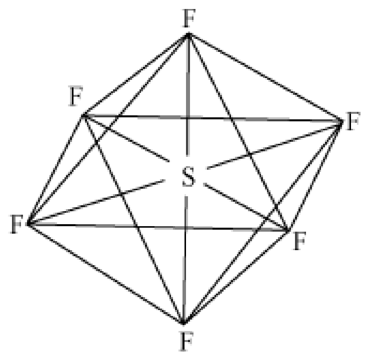
S-atom ground stat

S-atom excited stat

Hyperdization (sp^3d^2)

Octahydral molecule for SF_6

Six hybrid orbitals each is half filled overlap with p- orbital of each F- atom, So SF_6 molecule is formed Octahydral with angle 90 degree.



Conclusion:

1.Number of hybrid orbitals =

Number of σ + Number of lone pairs (n)

2.Geometrical shape of the molecule depend on the type of hyperdization.

Hyperdization	**Number of electron pairs**	**Geometrical shape (Example)**	**Angle around central atom**
sp	2	Linear ($BeCl_2$)	180
sp^2	3	Trigonal planar (BF_3)	120
sp^3	4	Tetrahedral (CH_4)	109.5
sp^3d	5	Trigonal bipyramide (PCl_5)	120, 90
sp^3d^2	6	Octahedral (SF_6)	90

3. If all hyperdization Orbital forming bonding pairs , regular structure is obtained.

4. If one or more hyperdization Orb. Occupied by lone pair – non-bonding- (n), distortion from the regular structure obtained as in:

CH_4 **NH_3** **H_2O**

Teh. Pyramidel V-Shape

HCH	HNH	HOH
109°	104°	105°

This is because non-bonding pair (n) occupied larger space so it repulse the bonding pairs, so the angle is reduced as in NH_3 . In H_2O two non-bonding orbitals the repulsion increases , so the angle is reduced more.