Chemical Bonding and Molecular Structure.

→ [lecture-1]

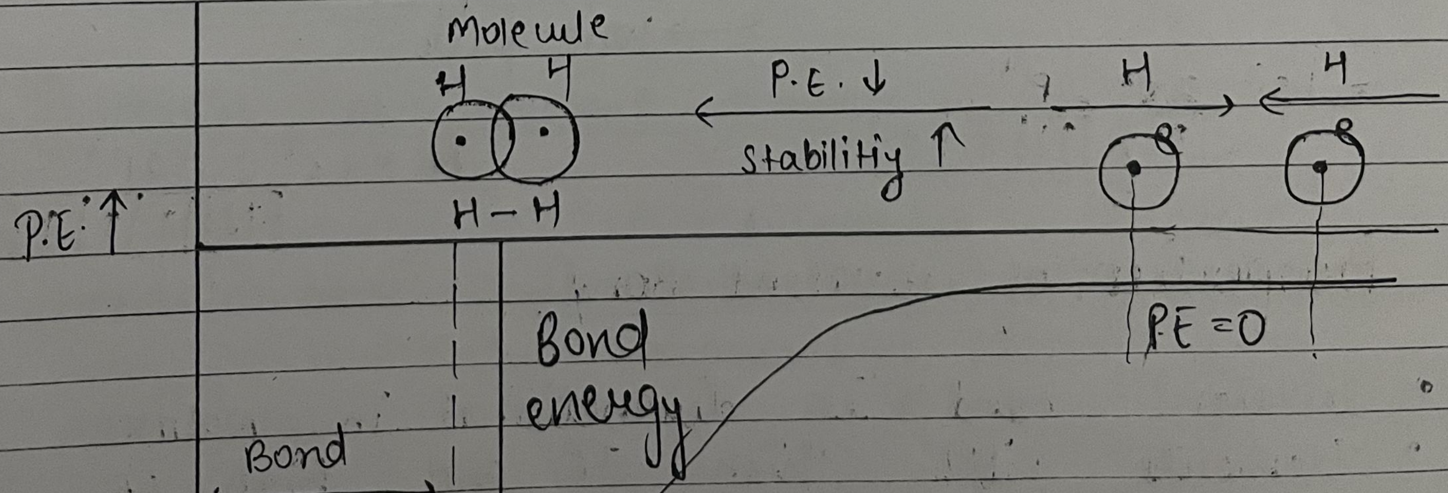
Que what is a Bond?

Ans Bond is a attraction froce by which two or more atoms ~~whole~~ + hold together in a Molecule.

Que why atoms do form bond?

Ans To attain stability or to reduce potential energy.

$$\boxed{P.E. \propto \frac{1}{\text{Stability}}}$$



Covalend Bond is directiona

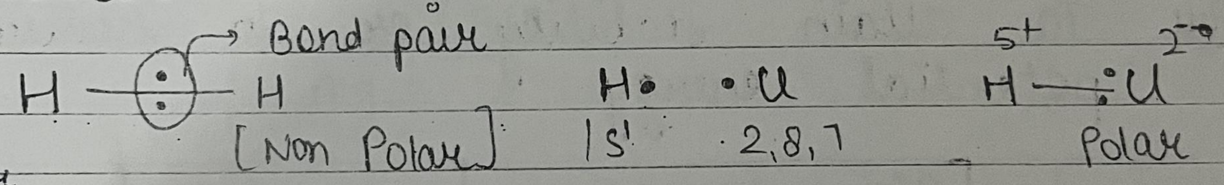
Bond

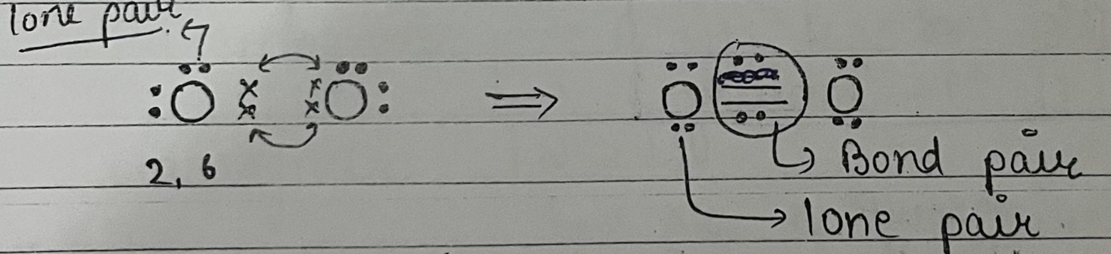
- Strong Bond (200-400 KJ/mole)
  - Covalent Bond
  - Co-ordinate Bond
  - Metallic Bond
  - Ionic Bond/ Electrovalent Bond
- Weak bond (12-40 KJ/mole)
  - Hydrogen Bond
  - Vander wall's forces

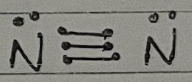
Inter Molecular
Intra Molecular

Covalent Bond

It is formed by sharing of unpaired electrons between two atoms.







$= 1s^2\ 2s^2\ 2p^4$

[↑↓] [↑↓|↑|↑]

$N = 1s^2\ 2s^2\ 2p^3$

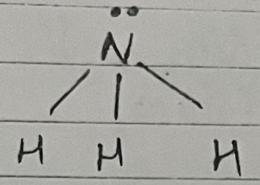
[↑↓|↑|↑|↑]

Properties of covalent Bond

- covalent bond is directional in Nature.
- Elements with high IP and high EA (generally Non-metals) form covalent bond.

- Covalency → It is Equals to Number of bonds formed by an atom.

Ex (1) $\ddot{N}H_3$



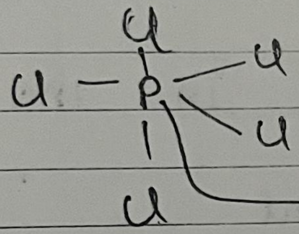
Covalency of N = 3
Covalency of H = 1

(2) CO_2 $O = C = O$

O ↓ covalency = 2

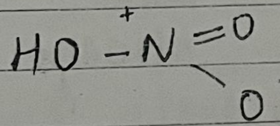
C ↪ Covalency = 4

(3)



→ Covalency of P = 5
Covalency of Cl = 1

$HNO_3 \Rightarrow HO-\overset{+}{N}(=O)-O^-$



Covalency of N = 4

→ [Lecture - 02]

Properties of Covalent Compounds.

- because covalent bonds have directional property that's why covalent compounds have a particular geometry & shape.

- Covalent compounds also show Isomersims.

H & F can Never be
central atom tries to remain in Maximum Covalency.
Nitrogen can Never be Pentavalent.

- Mostly covalent compounds have lower boiling points & Melting points except some covalently bonded Network Solid.

Ex Diamond, graphite, SiO_2 (silica), SiC, Quarts etc.

- Generally covalent compounds are bad conductor of Electricity Except graphite.

Rules of To write LDS

- Calculate Valance Electron in the given Molecule & ion.
- least / less electronegative element will be central atom (~~Hydrogen~~ H&F will always form single Bond).
- Guess most symmetric element & put a pair of electron in between central atom & ~~at~~ ~~a~~ other atom to make a bond.
- Now complete octet of outer atoms.
- After completing octet if valance e^- are remaining then put these valancy e^- in central atom.
- Now calculate formal charge for

also gives to corner atom &
Positive charge also gives to Central atom

each atom & the most Stable Structure will be the Structure which have minimum formal charges.

Lewis dot structure [LDS] :-

(1) Calculate valence e^-

Valence e^-	3	4	5	6	7	8
	B	C	N	O	F	Ne
	Al	Si	P	S	Cl	
						Xe

Covalency
O = 1, 2
S = 2, 4, 6
N = 3, 4
P = 3, 5
C = 4
Si = 4
Cl = 1, 3, 5, 7

(2) Guess the Skelton

Most Symmetric Skelton across central atom given better Result

⇒ Generally least / Less En atom will be central atom.

⇒ H & F Never be central atom.

Ex ① CO_2 COO ×
OCO ✓

(2) CO_3^{-2}

C O O O ✗

O · C O O ✗

O C · O ✓

O

(3) SO_4^{-2}

O

O S · O ✓

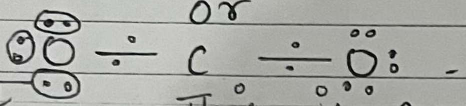
O

CO_2

① Valence e^- = 4 + 6 + 6 = 16 e^-

② O : C : O

or



This is a valid structure of CO_2 (unstable)

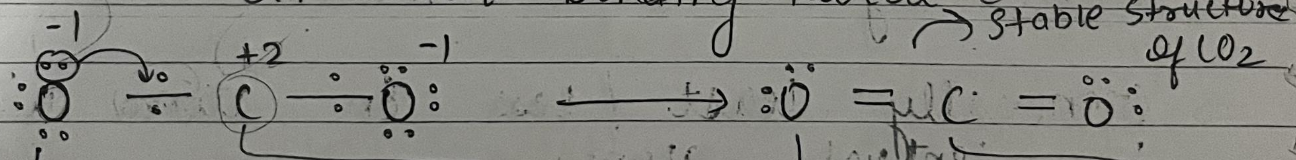
16
−4 (BP)
12 e
−12 e (octate)
0

16 − 12 − 2 ⇒ 2 Ans

Formal Charge [FC] :- 2

FC = no. of valance e^- − No. of bonds − 2 × No. of lP
= V − LP − $\frac{BP}{2}$
(No. of Non bonded e)

lP = Non bonding Paired e^-



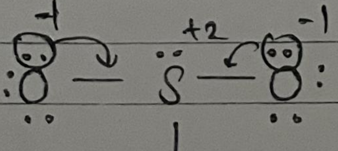
FC = 6 − 1 − 6
= −1

FC = 4 − 2 − 0
= +2

FC = 6 − 2 − 4
= 0

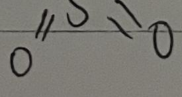
FC = 4 − 4 = 0
= 0

SO_2



FC = 6 − 2 − 2
= +2

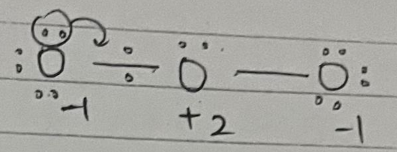
Total valence e^- = 18
−4 (BP)
14
−12 (octet)
2 e

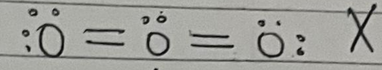


POPU

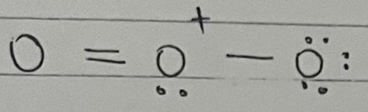
O_3 (Ozone)

$$\begin{aligned} ve &= 18 \\ &\underline{-4} \\ &14e \\ &\underline{-12e} \\ &\underline{2e} \end{aligned}$$

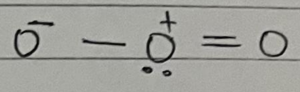




↳ valance e^- = 10



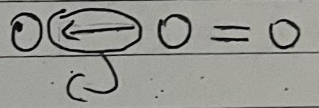
or



↳ 2nd Period element (B, C, N, O, F, etc.) Never expand their octate

or

They can have max^m 8e is outermost shell

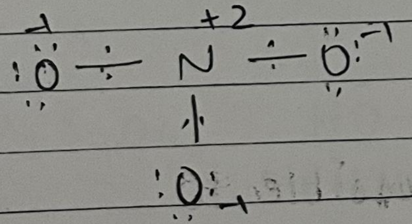


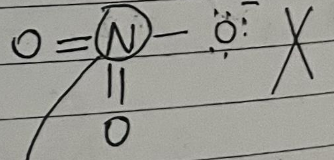
or

representation of Co-ordinate bond.

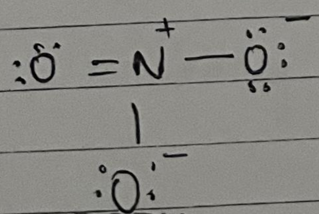
NO_3^-

$$\begin{aligned} ve = 5+18+1 &= 24 \\ &\underline{-6} \\ &18 \\ &\underline{-18} \\ &0 \end{aligned}$$

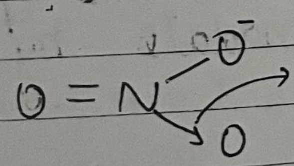




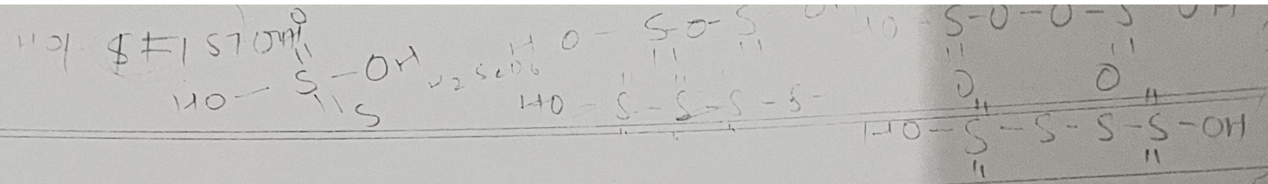
↳ outershell = 10e⁻



or



→ Co-ordinate bond head of Arrow will be toward -ive change



→ [Lecture - 03]

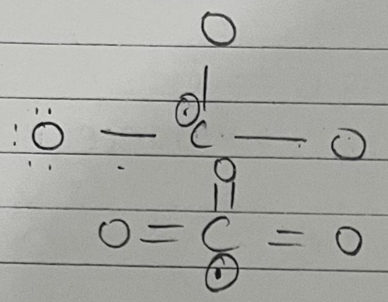
2, 8

2 c

ClO_3

= 7 + (6 × 3) = 7 + 18 = 25

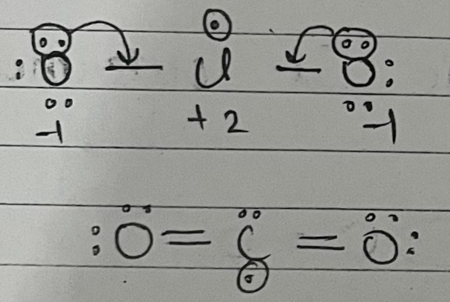
$$\begin{array}{r} 6 \\ \hline 19 \\ 18 \\ \hline 1 \end{array}$$



ClO_2

V.e. = 7 + 6 + 6 = 19e

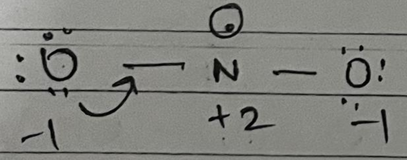
$$\begin{array}{r} 19e \\ -4\ (BP) \\ \hline 15 \\ -12 \\ \hline 3e \end{array}$$

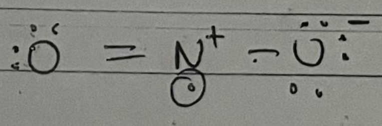


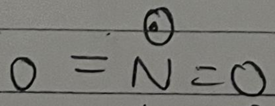
NO_2

V.e. = 5 + 6 + 6 = 17

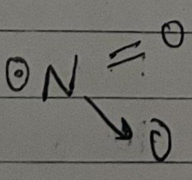
$$\begin{array}{r} 17 \\ -4 \\ \hline 13 \\ -12e \\ \hline 1e \end{array}$$





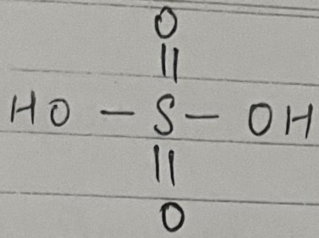


↳ 9e will not possible to accomadate by 'N'



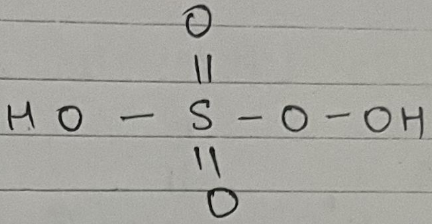
POPU

H_2SO_4



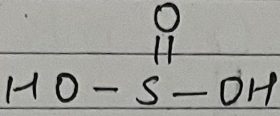
$HO-\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}-OH$

H_2SO_5
Corro's acid



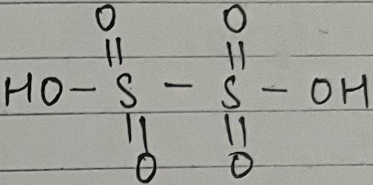
$HO-\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}-O-OH$

H_2SO_3



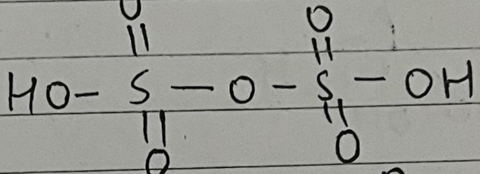
$HO-\overset{\overset{O}{\|}}{S}-OH$

** $H_2S_2O_6$



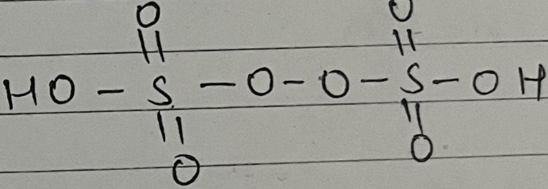
$HO-\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}-\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}-OH$

$H_2S_2O_7$
Oleum



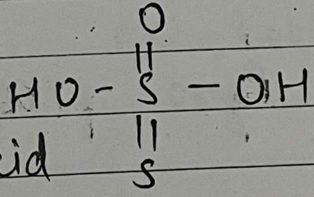
$HO-\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}-O-\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}-OH$

$H_2S_2O_8$
Marshell's acid



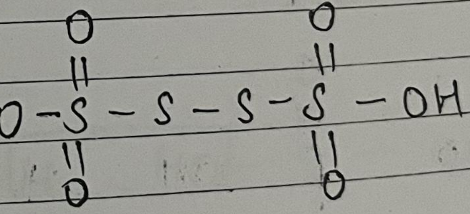
$HO-\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}-O-O-\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}-OH$

$H_2S_2O_3$
thio sulphuric acid



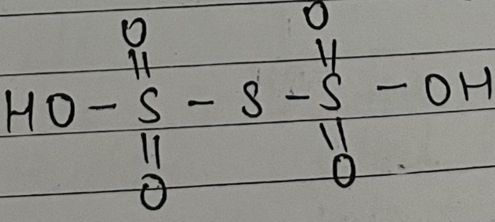
$HO-\overset{\overset{O}{\|}}{\underset{\underset{S}{\|}}{S}}-OH$

*** $H_2S_4O_6$



$HO-\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}-S-S-\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}-OH$

$H_2S_3O_6$

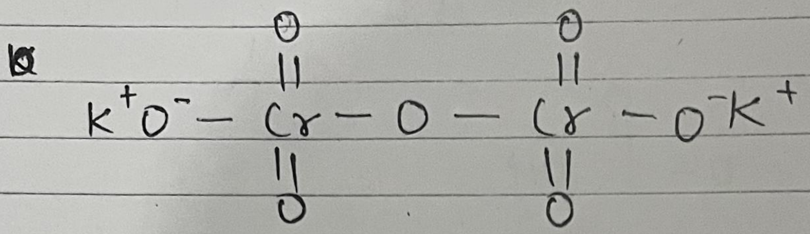


$HO-\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}-S-\overset{\overset{O}{\|}}{\underset{\underset{O}{\|}}{S}}-OH$

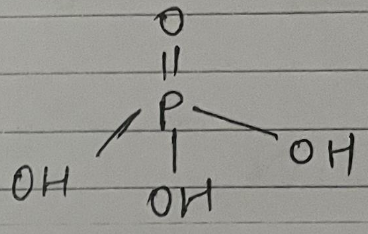
$H_2S_xO_y$ $x \geq 2,\ y \geq 7$ then there must be an oxygen b/w sulphur & sulphur

$y \leq 6$ No oxygen b/w Sulphur & sulphur.

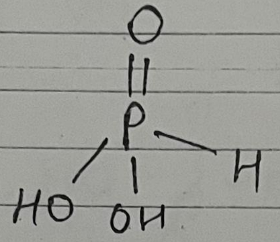
$K_2Cr_2O_7$ [Potessium dichromate]



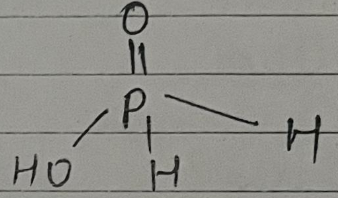
⇒ H_3PO_4



* H_3PO_3

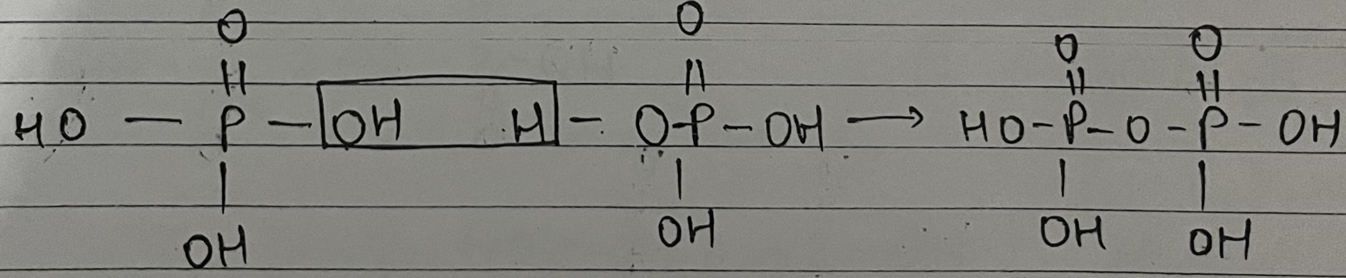


* H_3PO_2



$$2H_3PO_4 \xrightarrow{-H_2O} H_4P_2O_7$$

Phosphoric acid　　Pyro phosphoric acid



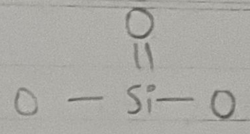
$$2H_2SO_4 \xrightarrow[-H_2O]{\Delta} H_2S_2O_7$$

Pyro Sulphuric acid or oleum

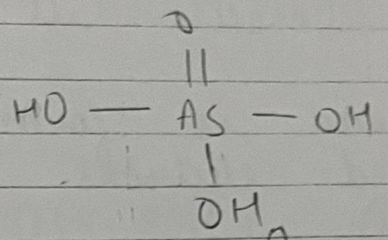
Sulphuric acid

Negative charge matlab single Bond &
Positive charge matlab Double Bond.

Ques (i) H_2SiO_3 ⟶ SiO_3^{-2}

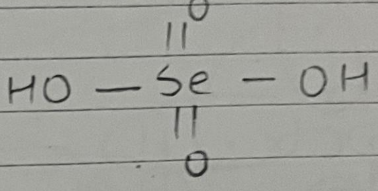


(ii) H_3AsO_4



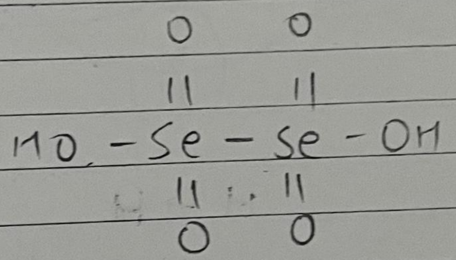
(iii) H_2SeO_4

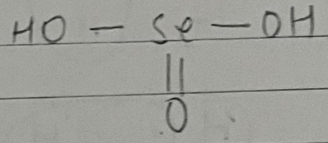
(iv) H_2SeO_3

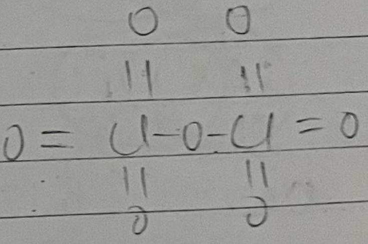


(v) $H_2Se_2O_6$

*
(vi) Cl_2O_7







⟶ [Lecture-04]

Theories of Bonding

(1) ocatate rule
(2) VBT (Valance Bond theory) & its Expansion
(3) MOT (Molecular orbital theory)

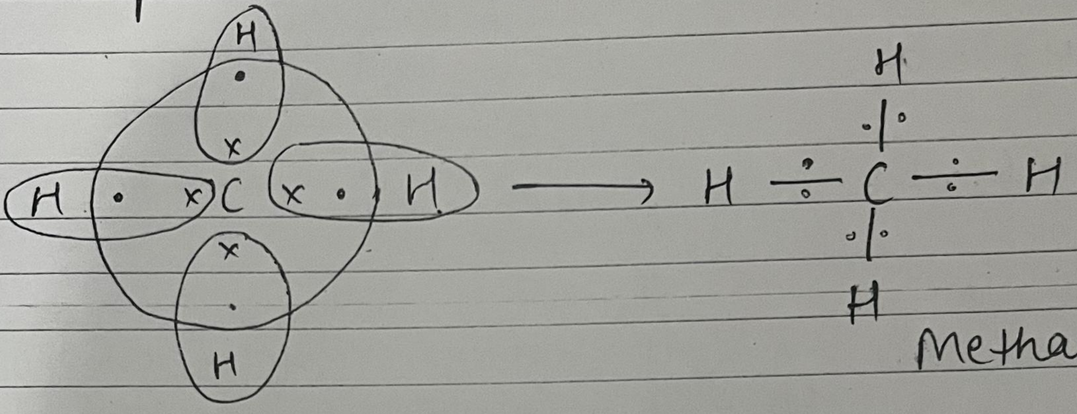
Octate Rule

- According to this rule every element

wants to complete its octate. (Hydrogen try to complete its duplete] ↳ (Two electoons)

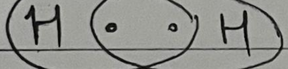
- Covalent Bond is formed by Sharing of unpaired electrons.

(1)



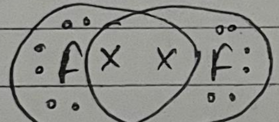
Methane

(2)



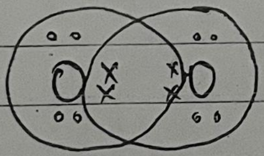
H – H

(3)



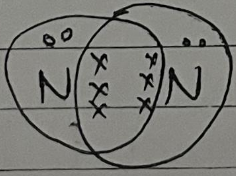
F – F

(4) O_2



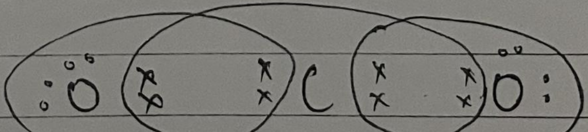
:Ö = Ö

(5) N_2



N≡N

(6) CO_2

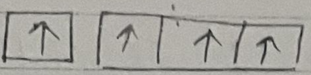


Ö=C=Ö

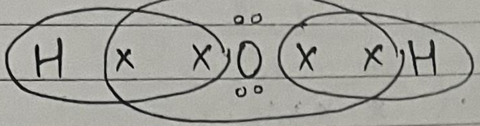
C = $1s^2 2s^2 2p^2$ [↑↓] [↑][↑][ ]

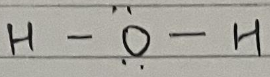
POPU (elemental)

$C = 1s^2 2s^1 2p^3$
(compound)

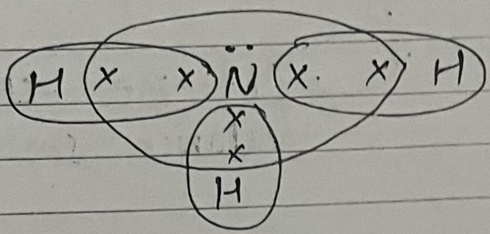


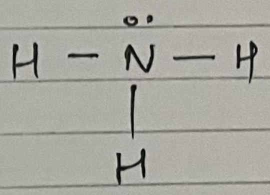
(7) H_2O





(8) NH_3

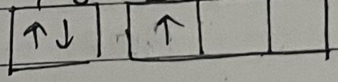




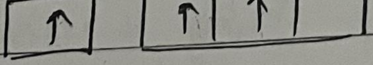
Exceptions

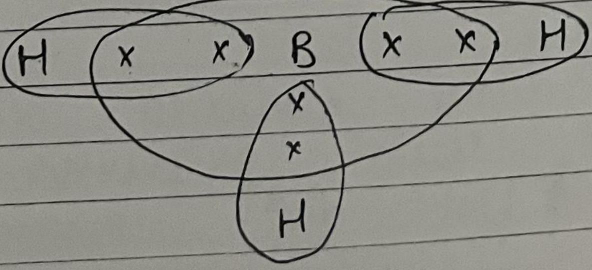
(1) Hypo valent :- Valence e^- of central atom is less than 8.

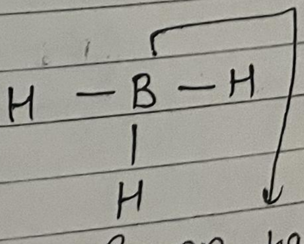
Ex BH_3 $B = 1s^2 2s^2 2p^1$



$B_{(E.S.)} = 2s^1 2p^2$



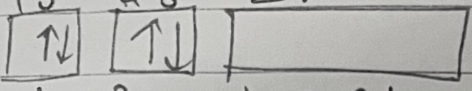




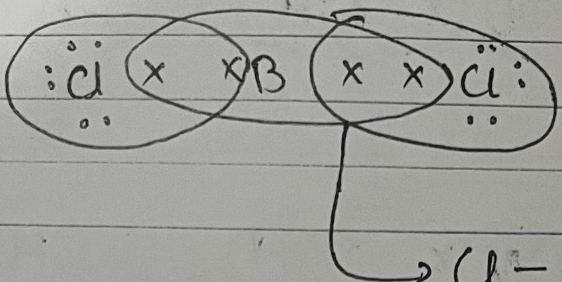
Boron have 6e

(2) $BeCl_2$

$B = 1s^2\ 2s^2\ 2p^0$



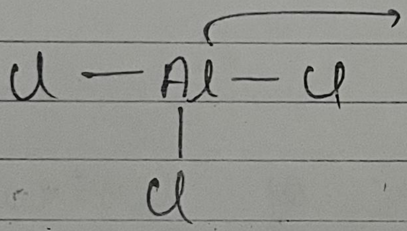
$Be = 1s^2\ 2s^1\ 2p^1$



→ Cl – Be – Cl

valance shell = 4e of Be

(3) $AlCl_3$



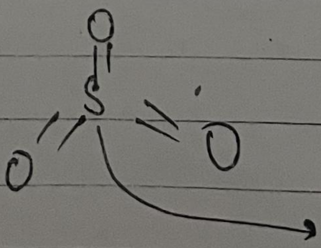
6e < octate

Hypervalent :-
central atom have more than 8e

Ex. PCl_5
→ valance shell = $10e^-$

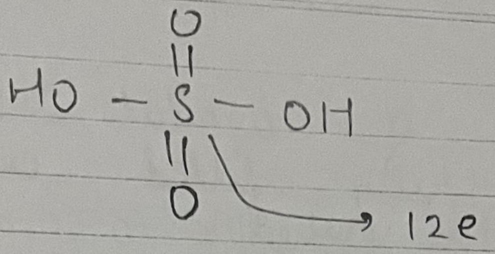
SF_6
→ $12e^-$

SO_3

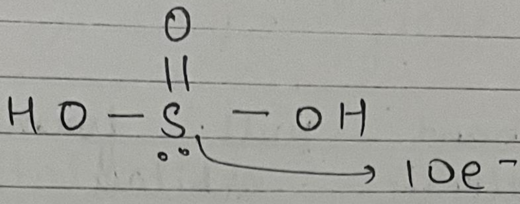


→ 12e

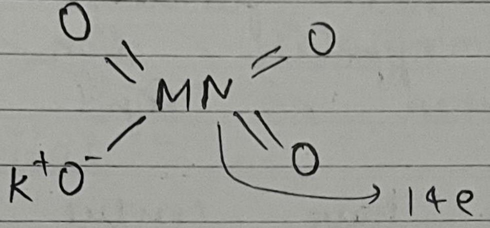
H_2SO_4



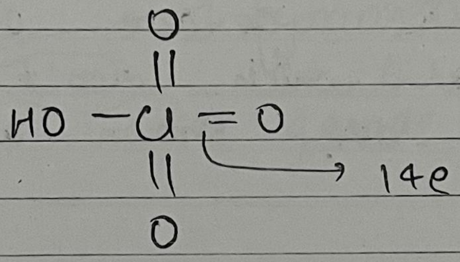
H_2SO_3



$KMnO_4$



$HClO_4$



VBT (valance Bond theory)

Postulate of VBT

- Lewis sharing of atomic orbitals takes place to form a covalent bond rather then sharing of electrons
- ~~Eo~~ Two orbitals which are taking part in overlaping must have unpaired e^- of opposite spin to form covalent Bond.

- If overlaping of orbitals taking place between fully filled orbitals and vacant orbital then co-ordinate bond will form.

- Covalent bond will formed by overlaping of two atomic orbitals of same sign of wave function. If two orbitals of opposite sign are overlaped then no bond will formed.

- ✱ Orbitals which have centre of symmetry are known as gerade orbitals and those orbitals which don't have centre of symmetry are known as Non gerade orbitals.

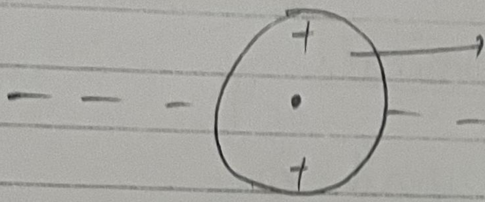
- Extent of overlaping is greater in the directional overlaping as compared to Non directional overlaping.

Gerade orbital:-

$l = 0, 2$ (grade)
s & d orbitals

$l = 1, 3$ (Non grade)
p & f

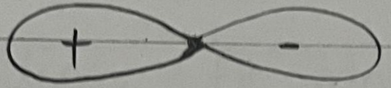
(1) S - orbital



Sign of wave funⁿ

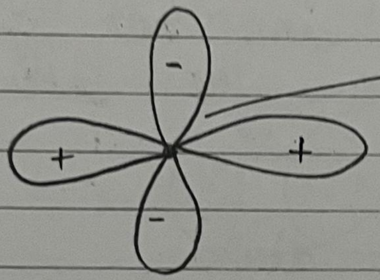
grade

(2) P - orbital :-



non gerade cos X
(Unsymmetrical w.r.t. center)

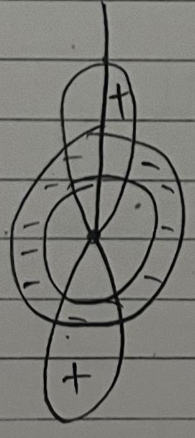
(3) d - orbital :-



Symmetric w.r.t. center
cos ✓
gerade

(4) f - orbital :- unsymmetric w.r.t. centre

Non grade



Ring Present in ⊥ Plane
cos ✓
gerade

→ [lecture - 05]

Overlaping of Atomic orbitals

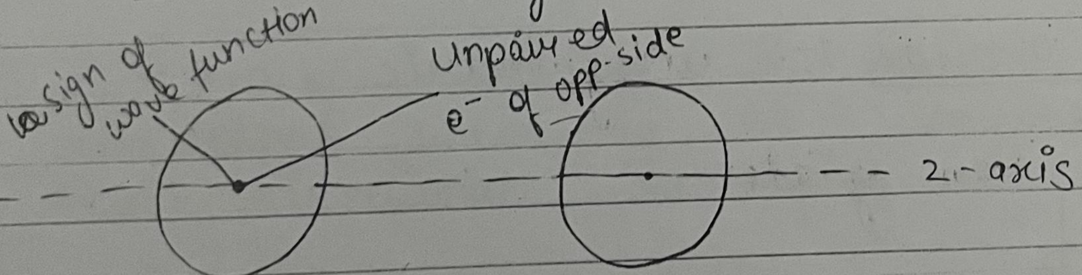
(1) Head to Head or Head - on
or
axial overlaping

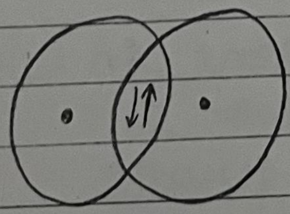
(2) Side overlaping or Co-lateral overlaping

Head on Overlaping :-

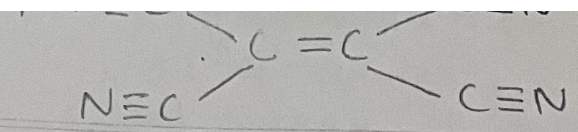
- If Internucleus ^occur axis in not given the z-axis will be the Internucleus axis.

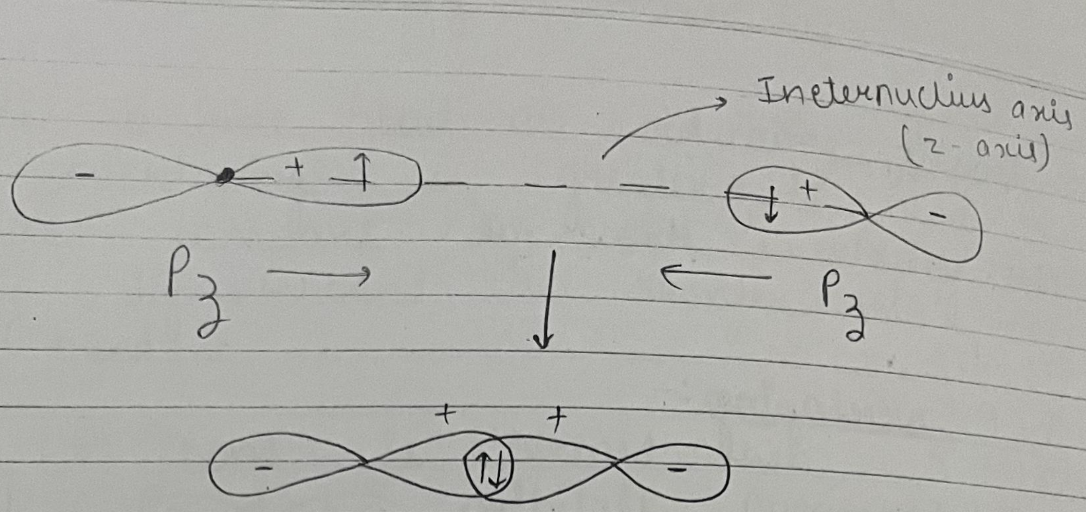
(1) S-S overlaping :- (non-dir^n)





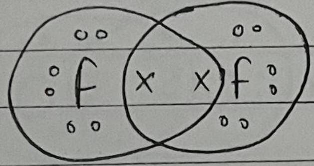
(2) P-P overlaping :- directional





formation f_2 Molecule :-

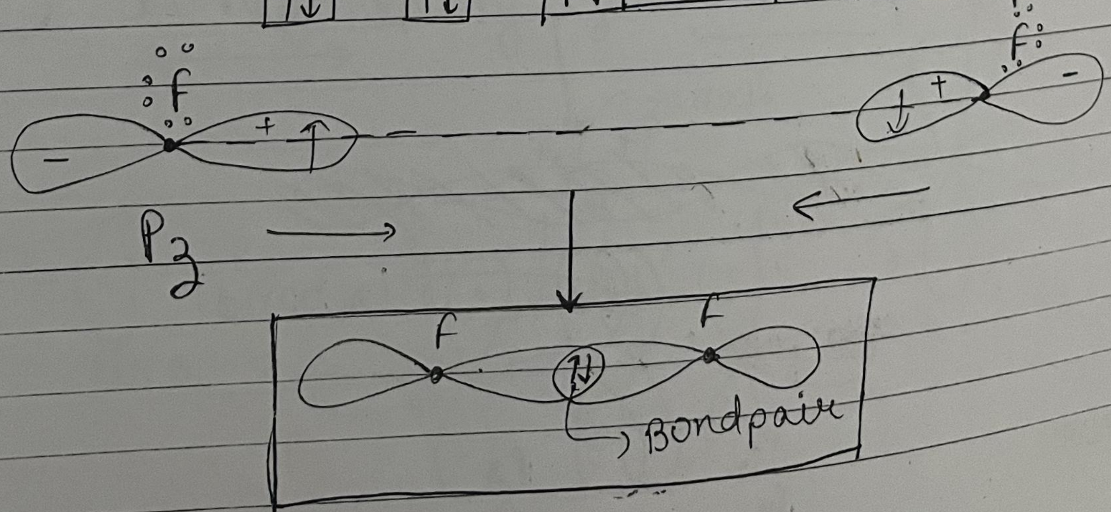
(1) According to octate rule :-



(2) According to VBT :-

f = $1s^2 2s^2 2p^5$

↑↓ ↑↓ ↑↓ | ↑↓ | ↑ → Non Bonding Paired e⁻ (lone pair)



$:\ddot{O} \overset{\pi}{\underset{\sigma}{=}} \ddot{O}:$ $\boxed{\text{Double bond} = \text{one } \sigma + \text{one } \pi}$

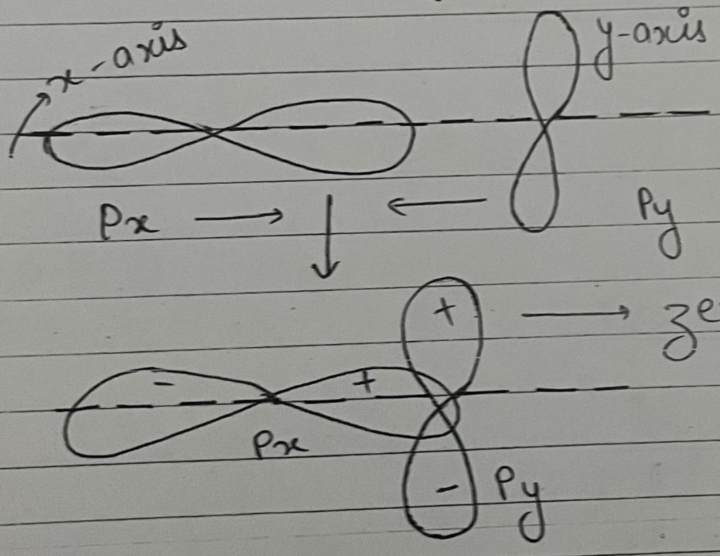
Ques. If Internucleus axis is x - axis

$P_y - P_y$ = π bond

$P_z - P_z$ = π bond

$P_x - P_x$ = σ bond

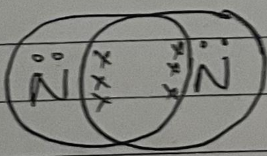
$P_x - P_y$ or $P_y - P_z$ = No bond will formed



→ zero overlaping no-bond will form

Formation of N_2 :-

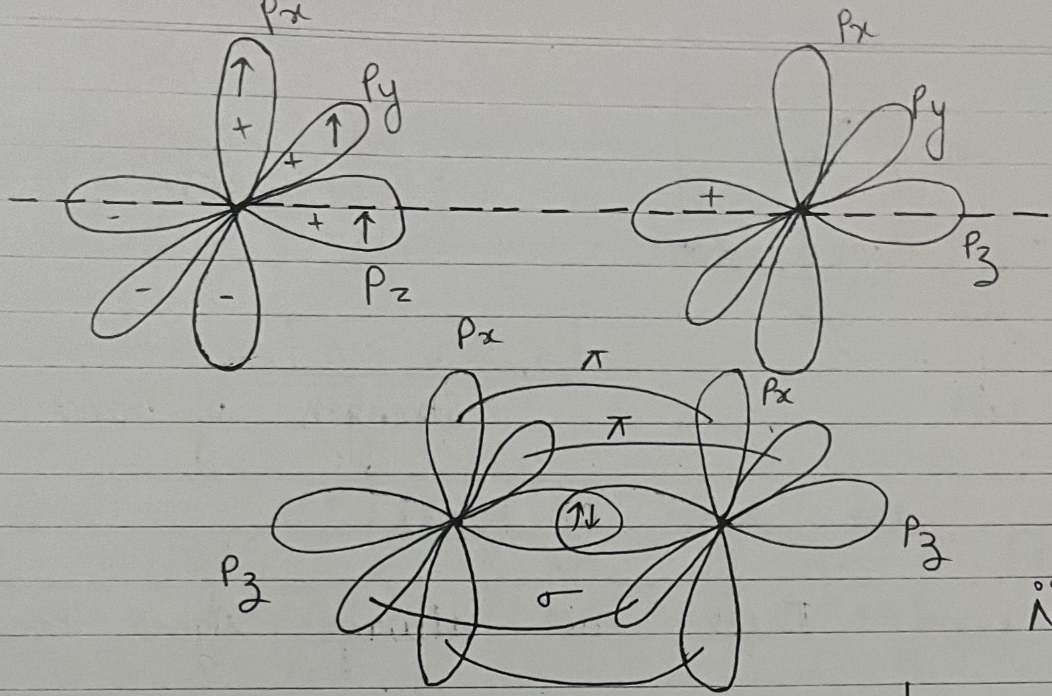
Octate rule



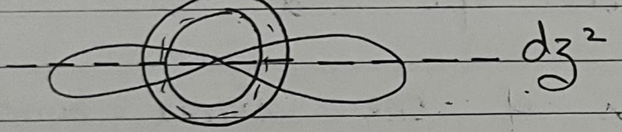
N≡N

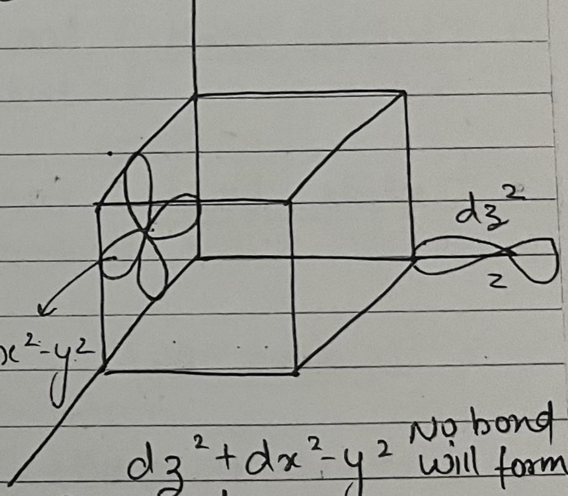
VBT $N = 1s^2\ 2s^2\ 2p^3$

$\boxed{\uparrow\downarrow}\ \boxed{\uparrow|\uparrow|\uparrow}$

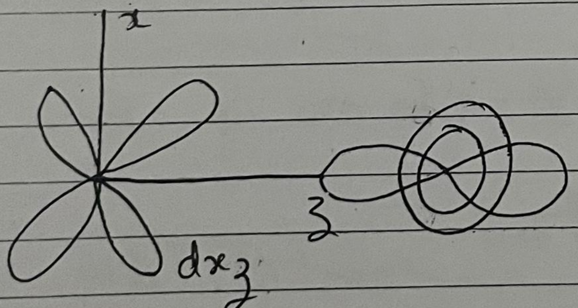


$\ddot{N}\equiv\ddot{N}$





$dz^2 + s|p_z|dz^2$



$dz^2 + dx^2-y^2$ No bond will form

$dz^2 + dxz|dyz$ No bond will form

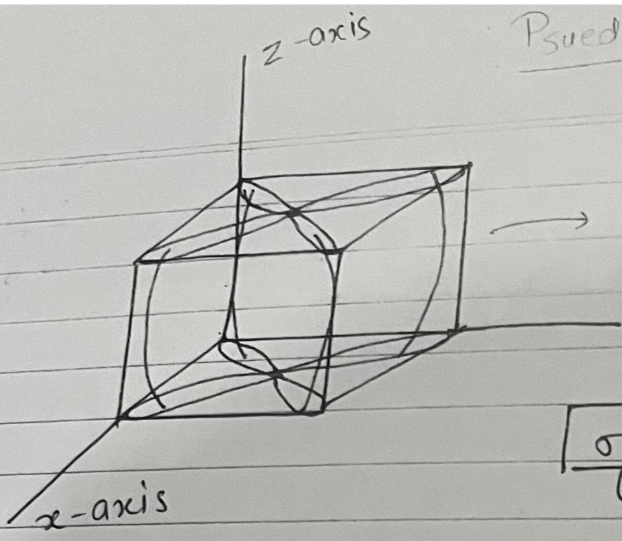
δ - bond :-

When '4' Lobes of each orbital get overlaped

$dxy + dxy \longrightarrow$ δ - bond

Inter nucleus axis is z-axis

Psuedo → fake /Nakli



→ S-bond (side overloding)

$\boxed{\sigma > S > \pi}$

↳ Strength of bond

Identify the types of bonds.

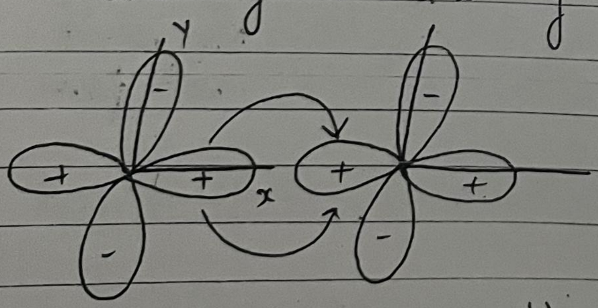
- **Single bonds**: These are always sigma bonds.
- **Double bonds**: Consists of one sigma bond and one pi bond.
- **Triple bonds**: Consists of one sigma bond and two pi bond.

→ [Lecture-06]

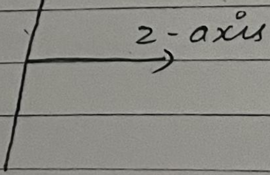
$d_{x^2-y^2} + d_{x^2-y^2}$

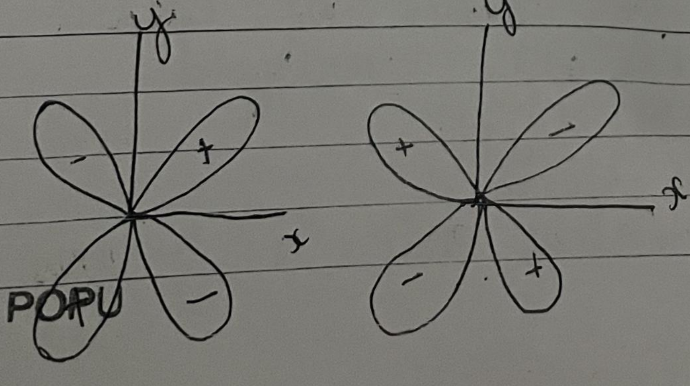
$\xrightarrow[z\text{-axis}]{\text{INA}} \delta$

$\xrightarrow[x \text{ or } y\text{-axis}]{\text{INA}} \sigma$



$d_{xy} + d_{xy}$

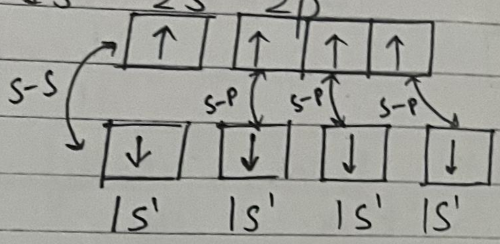


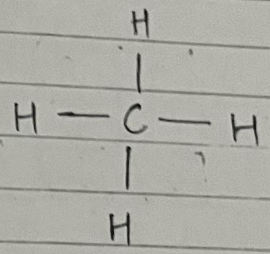


- Overlaping of one-one orbital can formed only one type of bond which is either sigma, Delta or pi.

Formation of CH_4 :-

$C = 1s^2 \; 2s^1 \; 2p^3$
(E.S.)





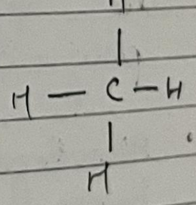
Extent of overlaping

S–S < S–P < P–P
overlaping overlaping overlaping

→ they should have same value of 'n'

Example :- 2s – 2s < 2s – 2p < 2p – 2p

Extent of overlaping ∝ Bond strength
or
Bond energy

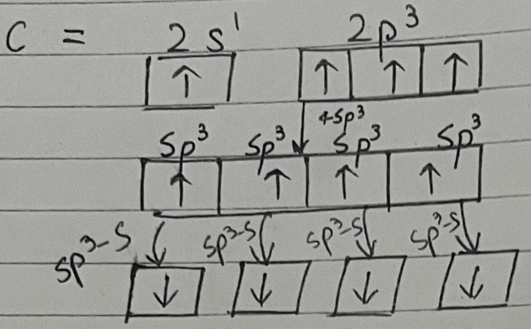


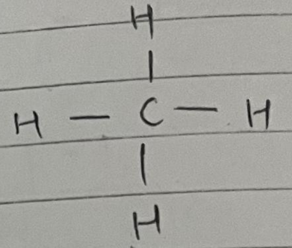
According to VBT in CH_4 one C–H bond is formed by S–S overlaping, and remaining 3 are formed by S–P overlaping

So, according to VBT all 4 C–H bonds should be not equal in energy.

- Hybridisation → Intermixing of Atomic orbitals of Same or nearly Same energy to gives new orbitals of Exactly Same energy.

But pratically it was found that all C-H bonds have equal energy this is the failure of VBT.





All C-H bond are formed by sp^3-s overlaping so, they all have equal energy.

Hybridisation

- To Support VBT hybridisation came into the frame to explain bonding of poly-atomic compounds.

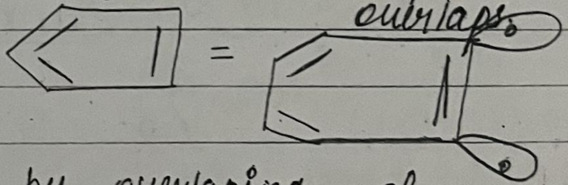
- According to Hybridisation Concept first before bonding atomic orbitals of same energy and near equals energy get mixed with each other and formed new orbitals of same energy and same shape are known as hybrid orbitals.

- After hydrisation atomic orbitals lost

Identity.

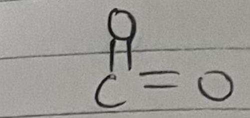
- Hybridisation is a therotical concept.
- Number of atomic orbital participating in the hybridisation process will be equals to Number of Hybrid orbital formed.
- Fully filled orbital, half filled or vaccant can participate in the hybridisation.
- Hybrid Orbital can form σ bond only they never form π and δ

∴ Exception → Benzyne $\longrightarrow sp^2-sp^2$ overlaps



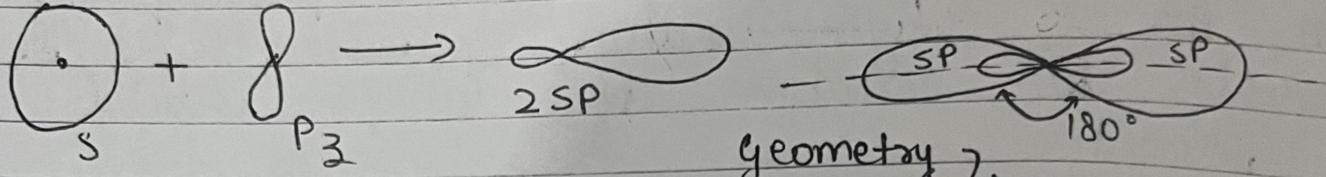
- π bond is formed by overlaping of unhybrid orbitals.
- Hybrid orbitals are more directional as compare to any of atomic orbitals.
- Hybrid and Unhybrid orbitals of same Element always present in perpendicular plane.
- The No. of hybrid orbitals = No. of Intermixing orbitals.

Types of Hybridisation



$O=C=O$

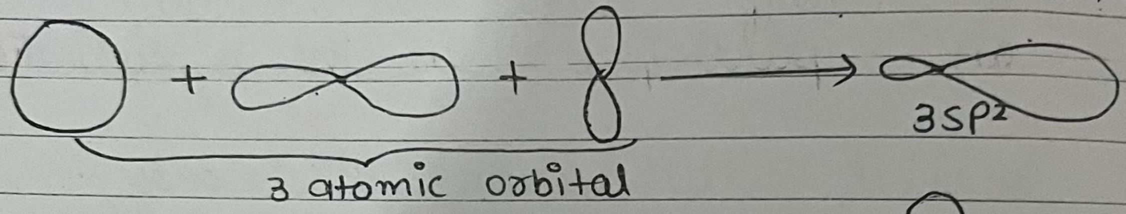
① S-P Hybridisation



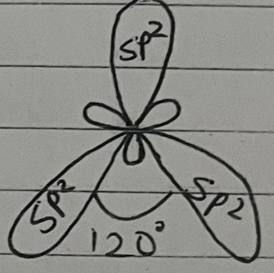
geometry ↳ Linear

Ex – $BeCl_2$, CO_2, etc.

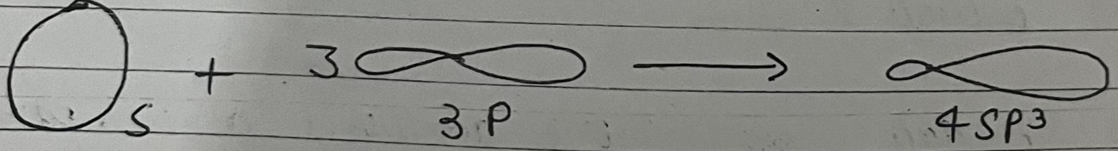
SP^2 :-

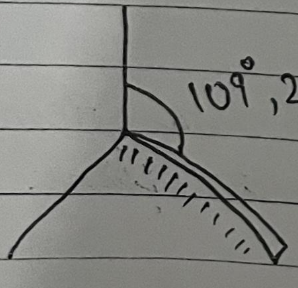


Triangular Planner

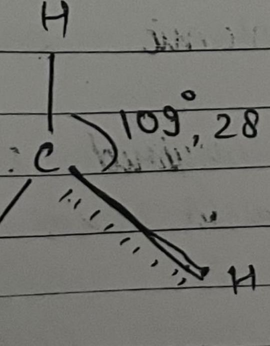


SP^3 :-





Ex –



POPU

→ [Lecture - 7]

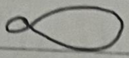
Valence Shell Electron pair replusion theory [VSEPR]

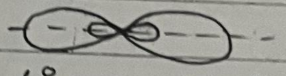
- According to it hybrid arranged itself in such a way that they feel or experience minimum replusion.

lP - lP rep^n > lP - BP rep^n > BP - BP rep^n

Hybridisation Hybrid orbital Geometry.

SP 2

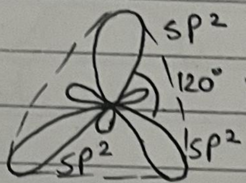




Linear Bond angle 180°

Ex - $BeCl_2$, CO_2

SP^2 3

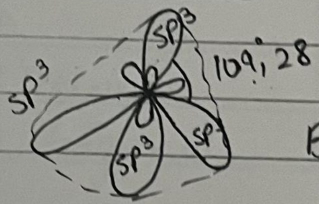


Trigonal planner

Bond angle 120°

Ex - BF_3

SP^3 4



Tetrahedral

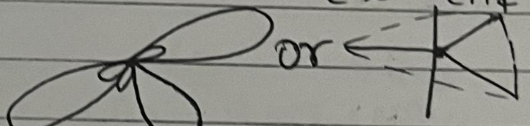
Bond angle = 109°,28'

Ex - CH_4

SP^3d 5

└ Ex - PCl_5

  ↳ d_{z^2}



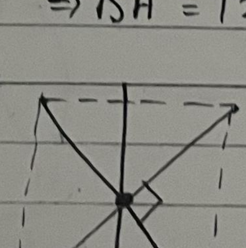
TBP (Trigonal planner Bi pyramidal)

⇒ BA = 120° & 90° No. of 90° angle = 6.

SP^3d^2 6

↳ dx^2-y^2 & dz^2

Ex - SF_6



Square planner Bi pyramidal or Octahedal

all Bond angle = 90°

No. of 90° Bond angle = 12

POPU

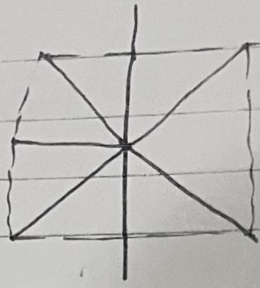
* we

we consider it in geometry.

sp^3d^3 7

↳ $d_{xy}, d_{x^2-y^2}, d_{z^2}$

Ex – IF_7



Pentagonal Bi pyramidal

BA = 72° (5)

BA = 90° (10)

Determination of Hybridisation :- (Basic)

Steric No. (SN) = (no. of 'σ' bond + no. of lP/ −ive charge)

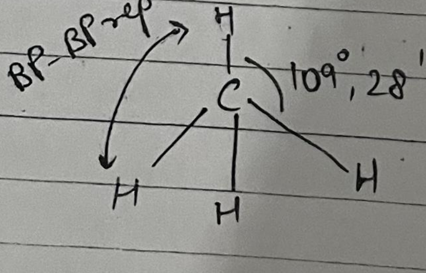
we never consider π bonds and +ive charge in hybridisation.

S.N.	2	SP
S.N.	3	SP^2
S.N.	4	SP^3
S.N.	5	SP^3d
S.N.	6	SP^3d^2
S.N.	7	SP^3d^3

Ex CH_4

SN = 4 + 0 = 4

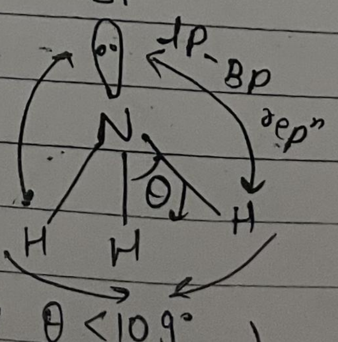
SP^3



$\ddot{N}H_3$

3 + 1 = 4

SP^3

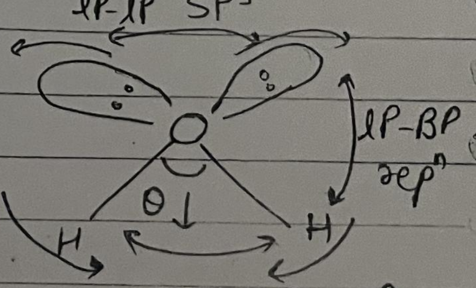


(θ < 109°
θ = 107°)

$H_2\ddot{O}:$

2 + 2 = 4

lP-lP SP^3



BP-BP repⁿ

(θ = 104.5°)

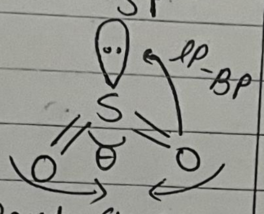
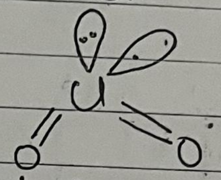
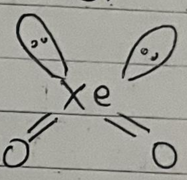
POPU

Shape = Geometry
= Tetrahedral
BA = 109°, 28'

Shape :- Pyramidal
Geo :- Tetrahedral
Molecular :- Pyramidal Geometry

Geo. :- Tetrahedal
Shape :- V-Shape
or
Bent shape

Ex Determine shape, hybridisation of following:

	CO_2	SO_2	ClO_2	XeO_2
Rough Structure	$:\ddot{O} \overset{\pi}{\underset{\sigma}{=}} C = \ddot{O}:$	$O = \ddot{S} = O$	$O = \ddot{Cl} = O$	$O = \ddot{Xe} = O$
Hybridisation	SP	SP^2	SP^2	SP^3
Shape	O = C = O Linear 180°	 Bent shape $\theta < 120°$ $\theta \approx 118°$	 Bent Shape	 Bent shape
Geometry	Linear	planner trigonal	Planner trigonal	Tetrahedral

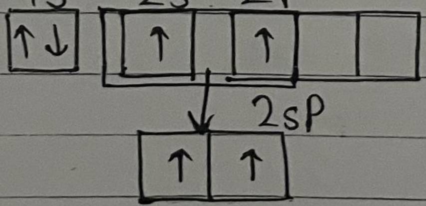
SN = 2, Hyb : SP

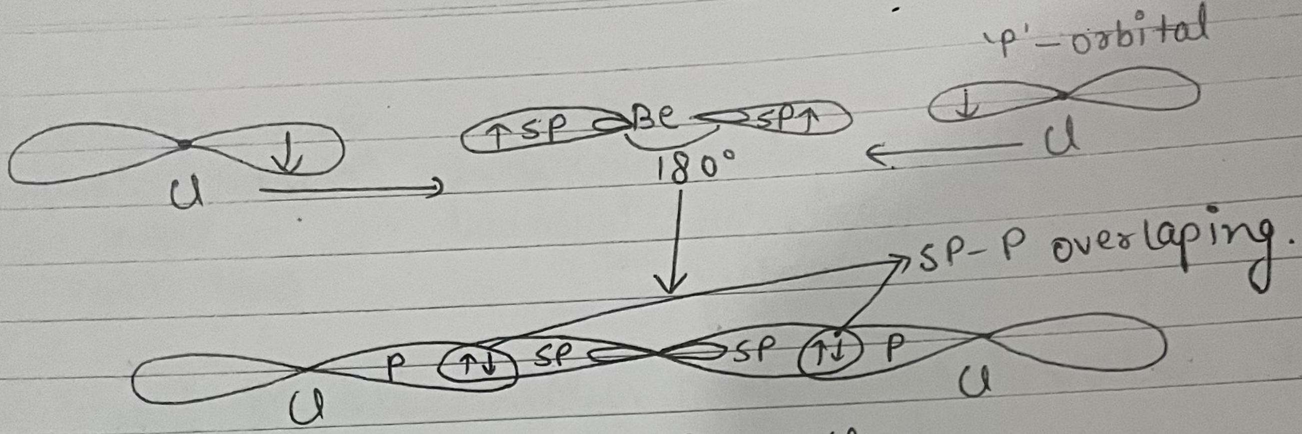
Ex AB_2
CO_2, $BeCl_2$, BeH_2,
$H-C \equiv C-H$

Formation of $BeCl_2$:-

Be = $1s^2$ $2s^2$ $2P^0$
(g.s.) [↑↓] [↑↓]

Be = $1s^2$ $2s^1$ $2P^1$
(g.s.)





Cl — Be — Cl

→ [lecture-08]

Formation of CO_2 :-

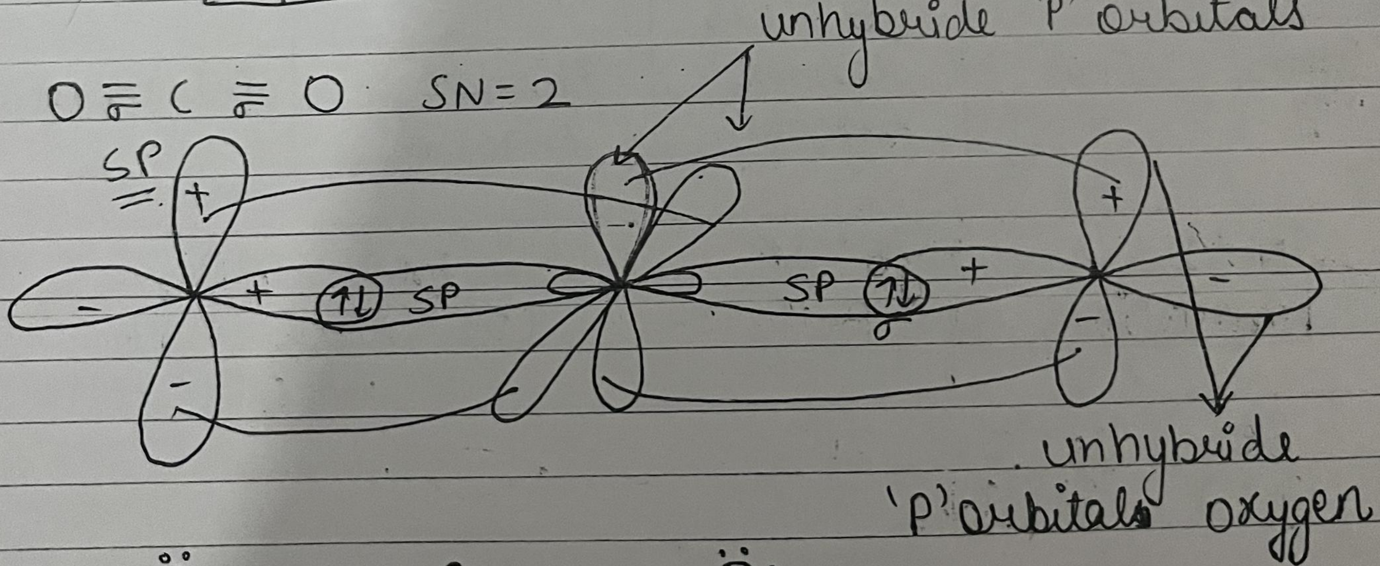
$C = 1s^2\ 2s^1\ 2p^3$

(E.S.) [↑] [↑] [↑] [ ]

2SP [↑][↑] [↑][↑] ↱ unhybride

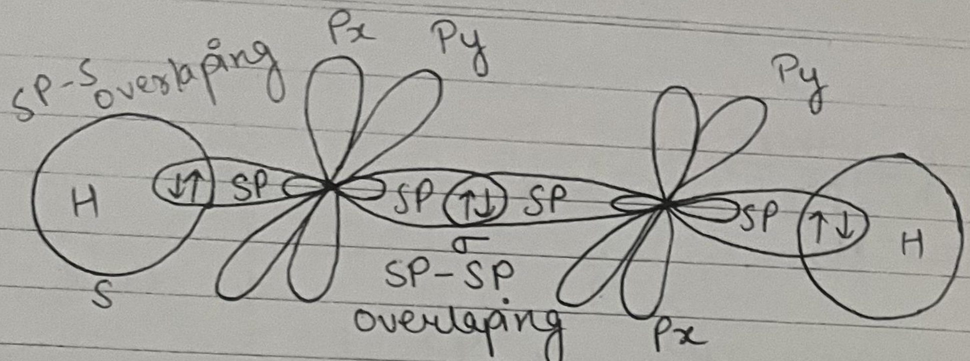
$O = 1s^2 2s^2 2p^4$ [↑↓] [↑↓][↑][↑]

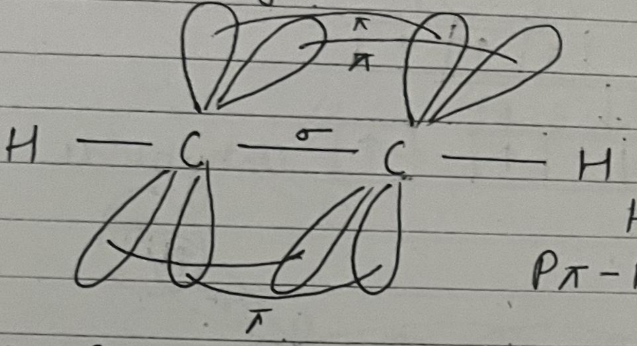
$O \underset{\sigma}{\equiv} C \underset{\sigma}{\equiv} O$ SN = 2



:Ö ═══ C ═══ Ö:

Formation of $H - \underset{SP}{C} \equiv \underset{SP}{C} - H$





$H-C\equiv C-H$

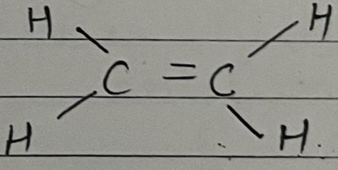
$P\pi - P\pi$

<u>SP^2 Hybridisation</u> :- <u>Geometry planner trigonal</u>

S.N. = 3 = No. of σ bond + No. of lP

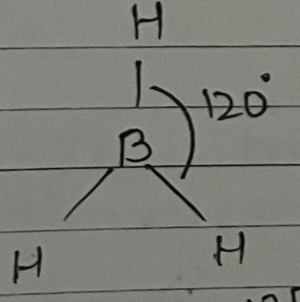
$AB_3 \Rightarrow BH_3$, BF_3, BCl_3, BBr_3

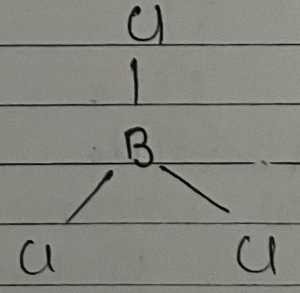
$\overset{\oplus}{C}H_3$

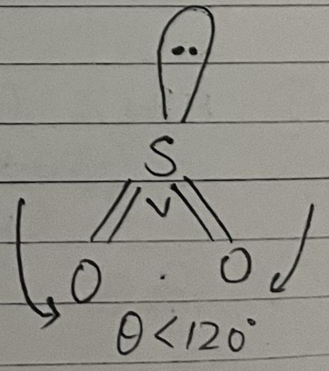


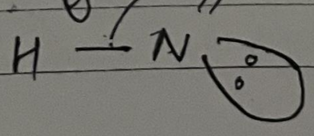
etc.

$\ddot{A}B_2$, $\ddot{S}O_2$, $H\ddot{N}O_2$ etc.









Formation of ethene :-

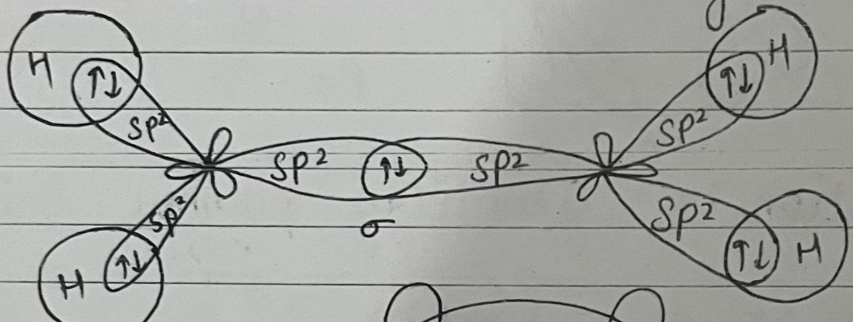
$\overset{sp^2}{H_2C} = \overset{sp^2}{CH_2}$

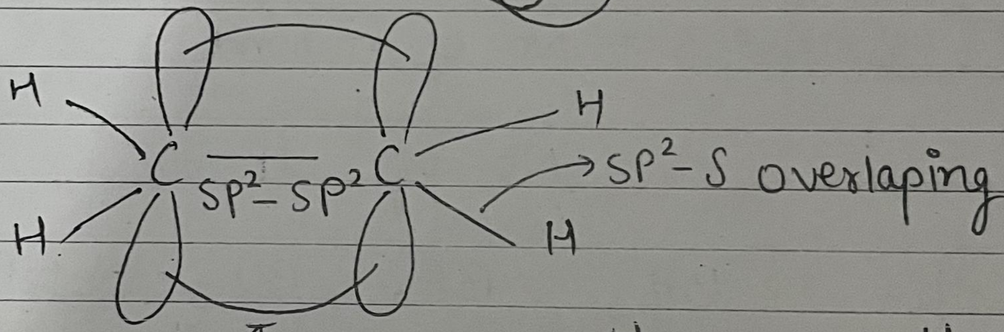
C = $1s^2$ $2s^1$ $2p^3$

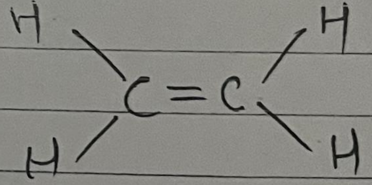
[↑] [↑ | ↑] [↑]

↓ $3sp^2$

[↑ | ↑ | ↑] [↑] unhybride



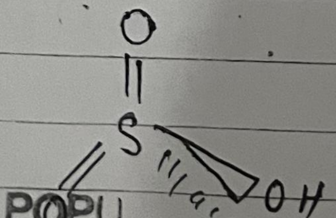


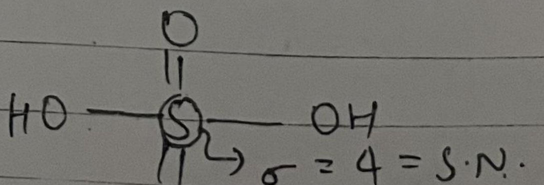


sp^3 Hybridisation:→ Geometry tetrahedral

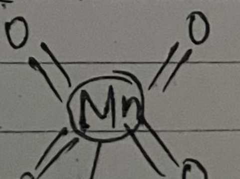
↳ S.N. = 4

① AB_4 : CH_4, CCl_4, $CHCl_3$,
SiH_4, $SiCl_4$, Diamond
H_2SO_4, $KMnO_4$, $K_2Cr_2O_7$ etc.

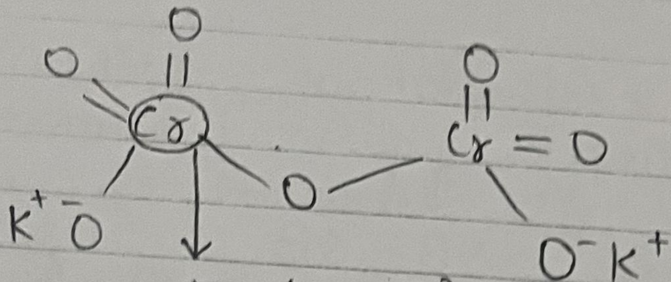




↳ σ = 4 = S.N.
lP = 0
sp^3

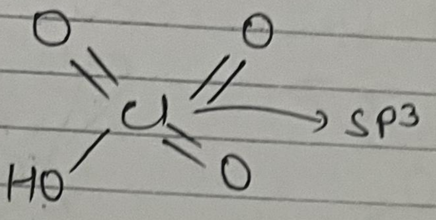


↳ sp^3



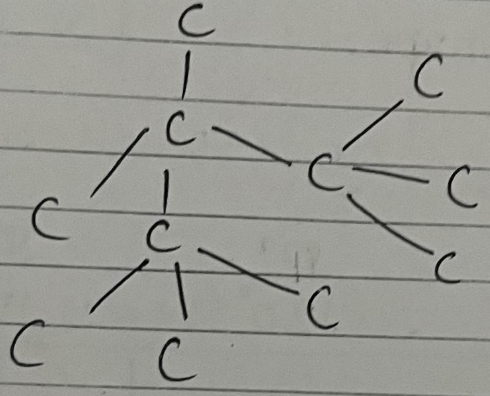
σ = 4 SP³

$HClO_4$



lP = 0
σ = 4

Diamond

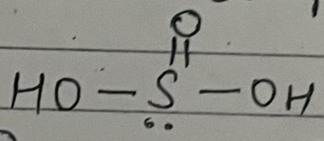


SP³

② $\ddot{A}B_3$ $\ddot{N}H_3$, $\ddot{P}Cl_3$, $\ddot{P}Br_3$, $\ddot{A}sCl_3$, $H_2\ddot{S}O_3$, $\overset{\ominus}{C}H_3$, etc. (Shape :- Pyramidal)

σ = 3
lP = 1

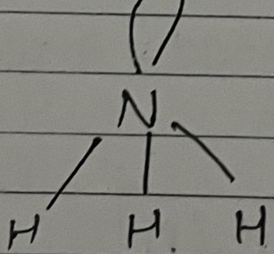
∴ H_2SO_3



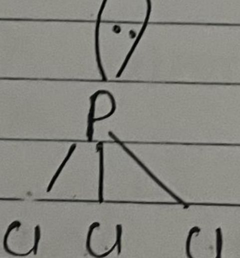
$HO-\underset{\cdot\cdot}{\overset{\overset{O}{\|}}{S}}-OH$

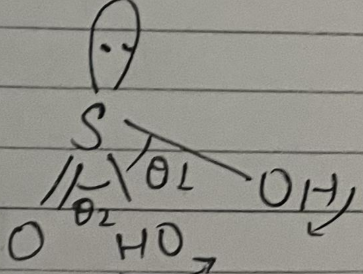
$\overset{\ominus}{C}H_3$

SN = 3+1
= 4

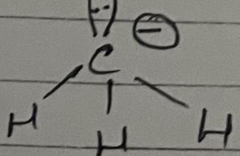


Pyramidal





θ2 > θ1



POPU