CHEMICAL BONDING - I

→ Force of attraction which hold the atoms to combine them as stable molecule is called as chemical bond.

→ As per old convention chemical bond is formed to achieve octet or duplet (in some cases) similar to Inert gases.

→ Compounds in which atom(s) have more than 8 e^- after bonding, they are called hypervalent. And if no. of e^-'s are less than 8 they are called Hypovalent.

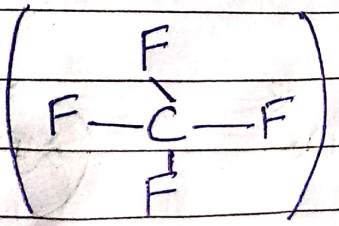
e.g.→ Hypervalent → SF_6, IF_7, PCl_5, $AsCl_5$
Hypovalent → BF_3, $BeCl_2$, $AlCl_3$

→ $H + H \longrightarrow H_2$ $(H—H)$ ← Bond

$O + O \longrightarrow O_2$ $(O=O)$ ← Bond

$2H + O \longrightarrow H_2O$ $\left(\begin{matrix} H \\ H \end{matrix}\!>\!O\right)$

$C + 4F \longrightarrow CF_4$



→ After Neil Bartlett experiment it is concluded that octet rule has no significance for chemical bonding.

→ Chemical bonding is further explained by energy calculations.

First Compound of Xenon

$$O_2 + [PtF_6] \longrightarrow O_2^+ [PtF_6]^-$$

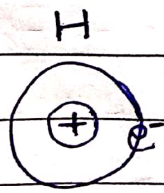
$$O_2 \longrightarrow O_2^+ + e^- \qquad \Delta H = +1175 \text{ kJ/mole}$$

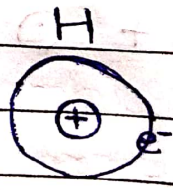
$$Xe + [PtF_6] \longrightarrow \underline{Xe^+ [PtF_6]^-} \quad \underline{1962}$$

First compound of Xenon

$$Xe \longrightarrow Xe^+ + e^- \qquad \Delta H = +1170 \text{ kJ/mole}$$

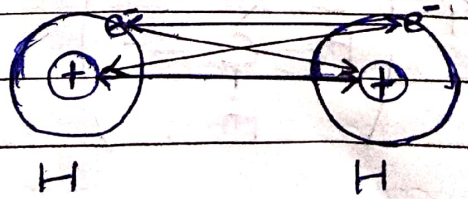
1.





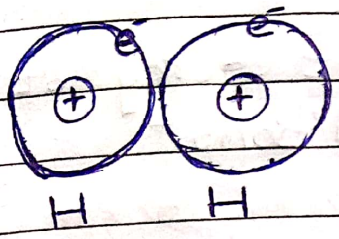
E = 0

2.

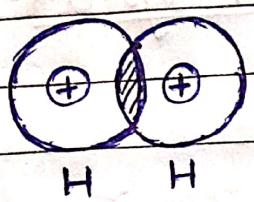


T.E = $+E_1 + E_2 - E_3 - E_4$

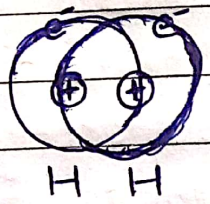
③

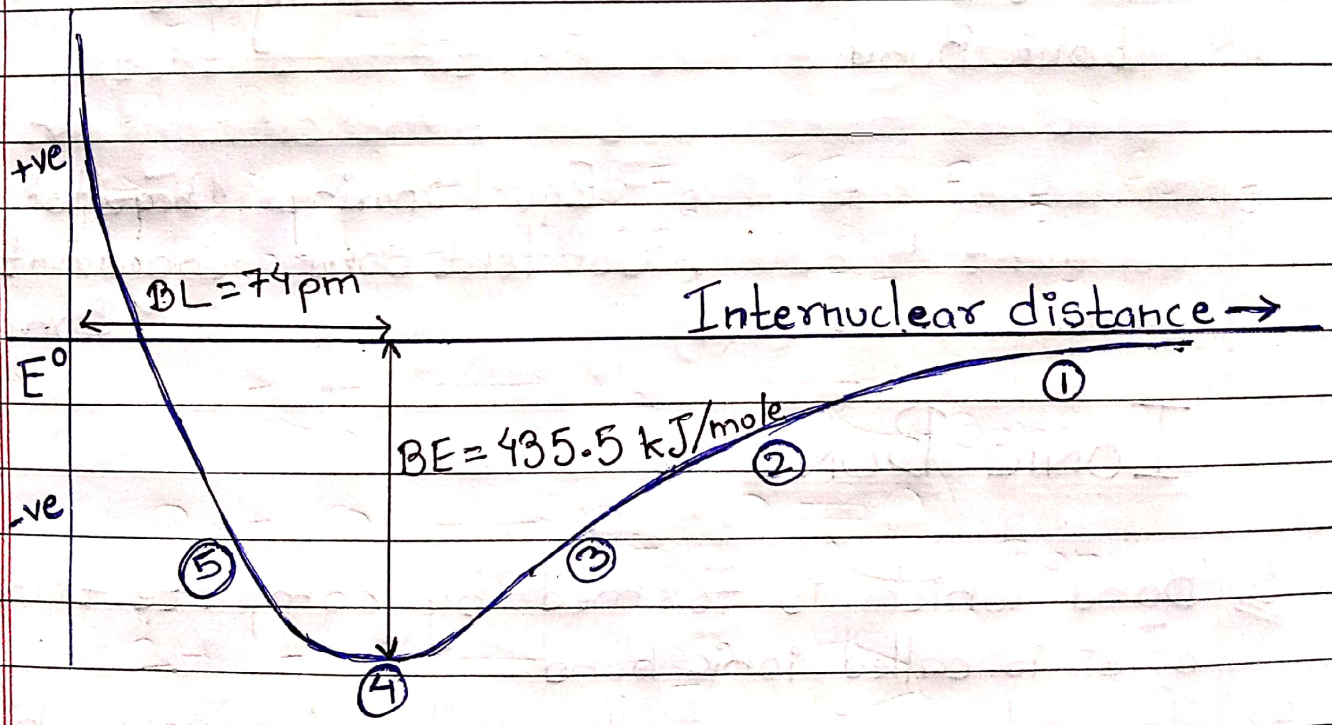


④



⑤

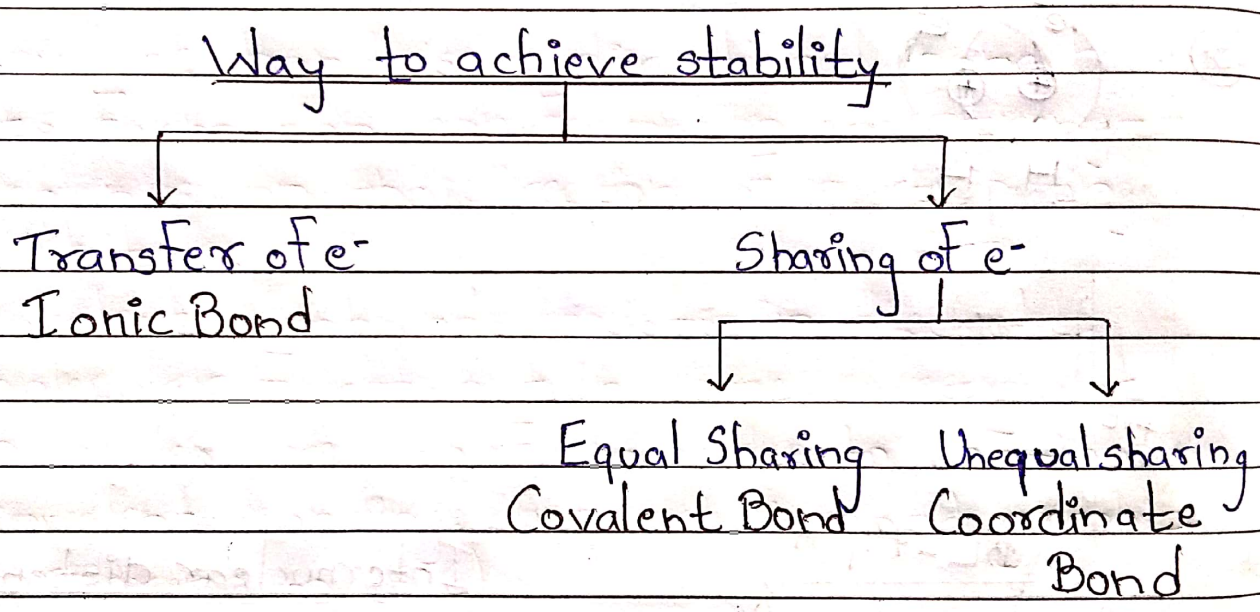




→ As per modern approach of chemical bonding when atoms are combine to each other they have attractive forces as well as repulsive forces b/w them but attractive forces are stronger as compared to repulsive forces so that atom are combined to

each other to attain lowest energy state in given set of ~~conti~~ conditions.

→ Chemical bond formation is always an exothermic process.



IONIC BOND

1. Bond which is formed by complete transfer of e⁻ is called ionic bond.
2. Ionic bond is actually coulombic force which exist between oppositely charged ions formed by complete transfer of electron.
3. The Ionic Bond is non-directional or omni-directional bond so that ionic compound does not exist in molecular form. They exist in the

Form of ionic lattice.

4. Ionic compound is generally formed between electropositive and electronegative element.

5. Favourable condition for ionic compound formation is energy consumed during the formation of ions must be smaller as compared to energy released by lattice formation.

e.g → $Na + Cl \longrightarrow Na^+ Cl^-$

→ Cs^+Au^-

$NO^+[BF_4]^-$

$O_2^+[PtF_6]^-$

$O_2^+[AsF_6]^-$

$NH_4^+Cl^-$

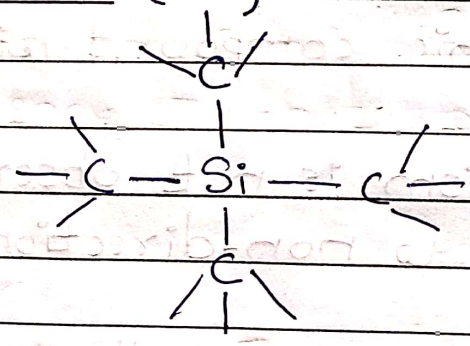
→ There is one ionic compound with one empherical formula.

→ Stereo isomerism is not observed in ionic compound due to non-directional nature of ionic bond.

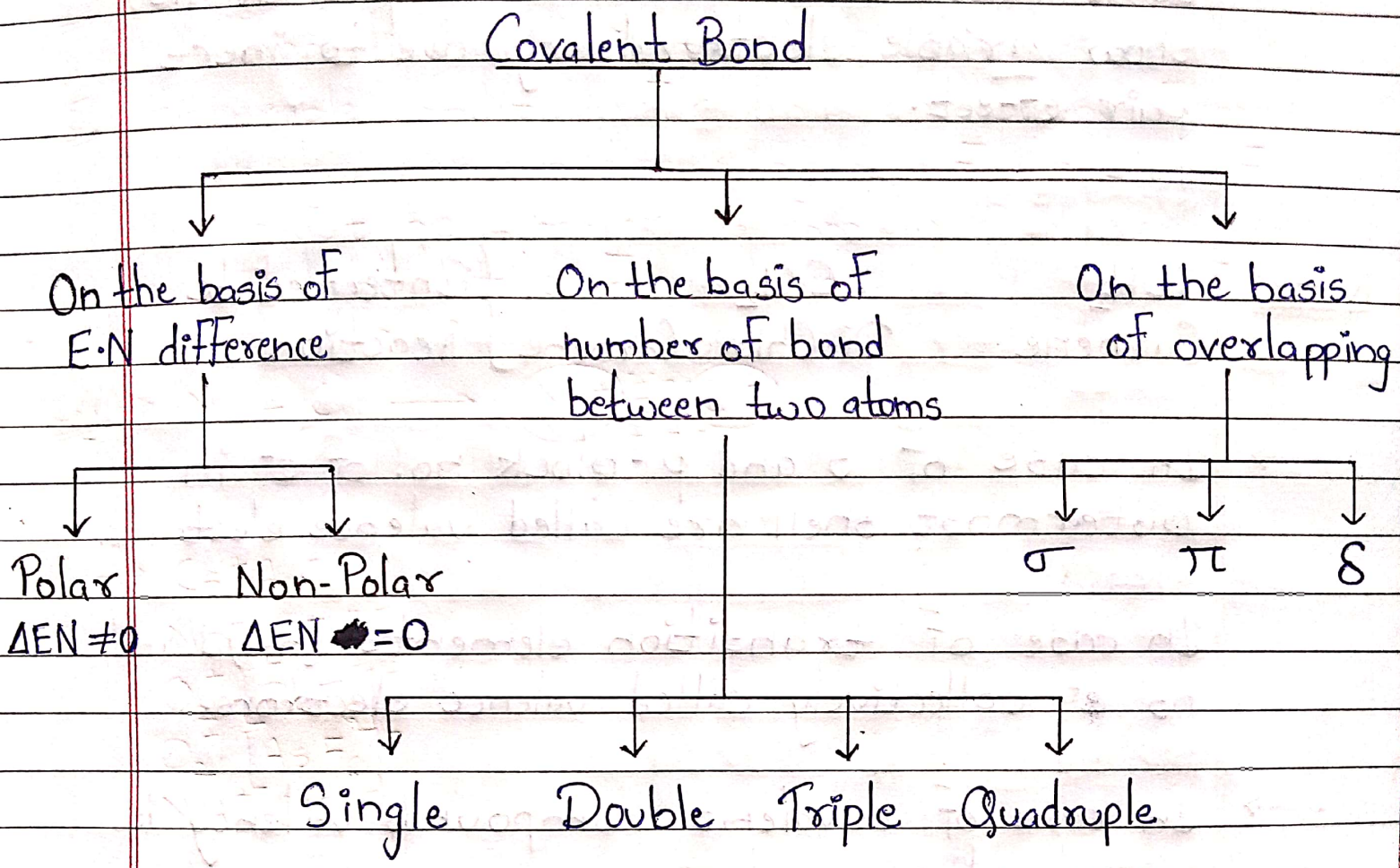
→ Ionic compounds are generally high melting solid and show conductivity in molten or aqueous form.

Covalent Bond

1. Bond which is formed by equal sharing of e^- between the atoms is called covalent bond.
2. During covalent bond formation each e^- of shared pair is contributed by each atom and counted in valence e^- For both.
3. Covalent bond is a directional bond because it's formation, non-formation and strength depends on the direction of participating orbitals.
4. Covalent compounds exists in discrete molecular form but in some cases giant molecules are also Formed due to continuous covalent bonding, such as diamond, graphite, carborandum (SiC)



Type of covalent bond :-



VALENCY

→ Combining capacity of element is called co-valency.
→ In case of ionic compound no. of electrons loss or gain by an atom to form ionic bond is called electrovalency.

I A elements have 1 or +1 electrovalency.
II A elements have 2 or +2 electrovalency.

→ d-block elements show variable electrovalency. Some heavy ~~elems~~ elements of p-block also show variable electrovalency due to inert pair effect.

Note: $:CH_2$ Carbene, $:CCl_2$ Di-Chloro Carbene } Intermediate Reaction

→ In case of s and p-block no. of e^- in outermost shell are called valence electrons.

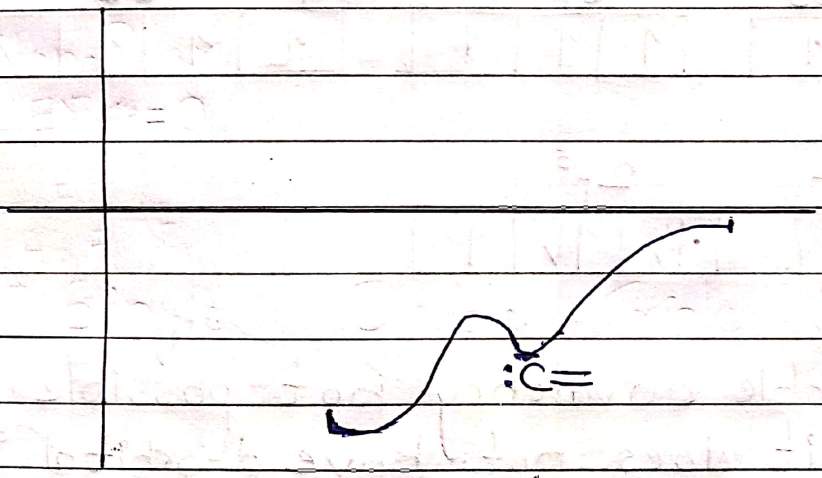
In case of transition elements (n-1)d and ns e^- collectively called valence electrons.

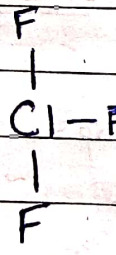
→ In case of covalent compounds valency is considered as covalency.
No. of unpaired e^- in ~~valency~~ valence shell are called as covalency of that atom.

Lone pair
No. of e^- pairs of outermost shell which not involved in sharing are called lone pair.

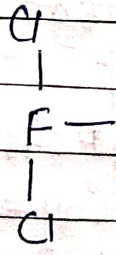
H	Li	Be	B	C	N	O	F
	$1s^2 2s^1$	$1s^2 2s^2$	$1s^2 2s^2 2p^1$	$1s^2 2s^2 2p^2$	$1s^2 2s^2 2p^3$	$1s^2 2s^2 2p^4$	$1s^2 2s^2 2p^5$
$1s^1$	~~$1s^2 2s^1$~~	~~$1s^2 2s^2$~~	~~$1s^2 2s^2 2p^1$~~	~~$1s^2 2s^2 2p^2$~~			
Cov = 1	Cov = 1	Cov = 2	Cov = 3	Cov = 4	Cov = 3	Cov = 2	Cov = 1
H–H		–Be–	–B<	–C–	–N–	–O–	:F–
			–B=		–N=	=O	:F–F:
				–C≡	N≡	:O=O:	
				=C=			
				>C=	N≡N		

C → | 1↓ | | 1 | 1 | |



Q→ 

is existing molecule

but 

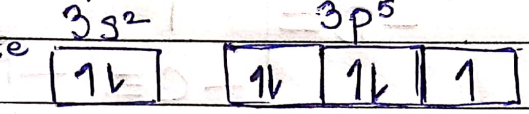
is not existing. Explain?

→ Some of elements which can increase their no. of unpaired e⁻ in their valence shell, they can show

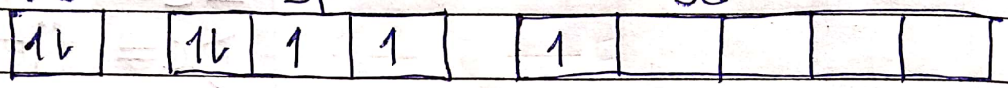
variable ~~valency~~ covalency.

→ It is observed in 3rd period and beyond 3rd period in periodic table.

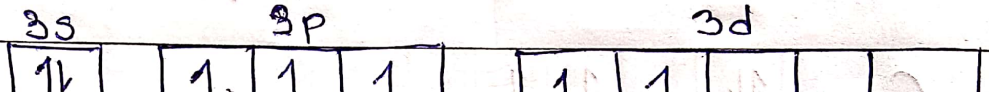
Ground state Cl = Cov = 1



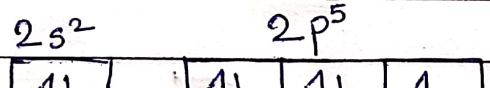
Cov = 3 Cl 1st ES



Cov = 5 Cl 2nd ES



Cov = 7 Cl 3rd ES

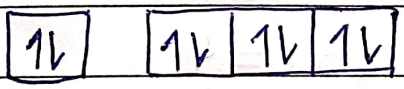
F = 

F ⇒ Variable covalency not possible by it because it does not have d-orbital in valence shell.

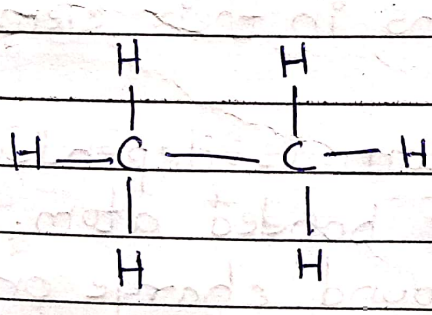
ns^1	ns^2np^0	ns^2np^1	ns^2np^2	ns^2np^3
Li	Be	B	C	N
Cov = 1	Cov = 2	Cov = 3	Cov = 4	Cov = 3
	Mg	Al, Ga, In, Tl	Si, Ge, Sn, Pb	P, As, Sb, Bi
	Cov = 2	Cov = 1, 3	Cov = 2, 4	Cov = 3, 5
		L·P = 1, 0	L·P = 1, 0	L·P = 1, 0

ns^2np^4	ns^2np^5
O	F
Cov = 2	Cov = 1
S, Se, Te, Po	Cl, Br, I
Cov = 2, 4, 6	Cov = 1, 3, 5, 7
L·P = 2, 1, 0	L·P = 3, 2, 1, 0

Q. Xe

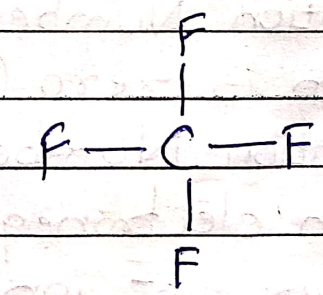
⇒ Xe = 

Possible covalency of Xe	Lone Pair in Xe
2	3
4	2
6	1
8	0

Q→ 

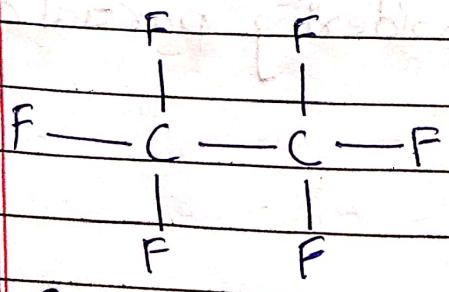
Cov = 4

O·N = -3



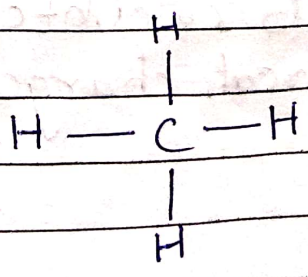
Cov = 4

O·N = +4



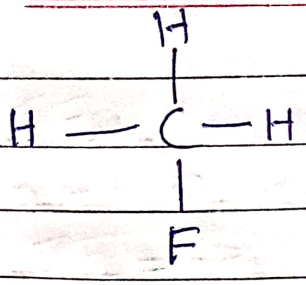
Cov = 4

O·N = +3

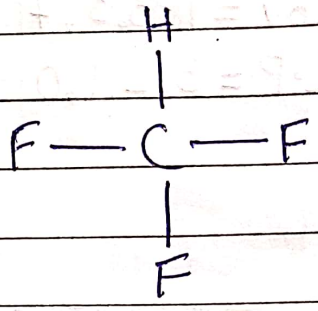


Cov = 4

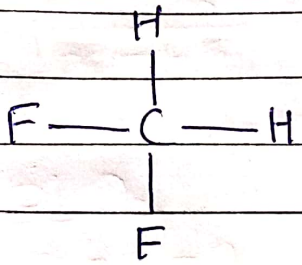
ON = -4



Cov = 4
ON = -2



Cov = 4
ON = +4



Cov = 4
ON = 0

Cov = 4
ON = +2

Oxidation Number

→ Oxidation Number represents state of oxidation of atom in given compound.
→ Oxidation Number of atoms in their elemental form is zero (0).
→ Oxidation Number of atom is dependent upon electronegativity of bonded atom.
→ In case of ionic compound charge on ion represent O.N.
→ In covalent compound or molecular ion O.N is calculated by considering partial charge as a real charge.

Or

ON of atom in covalent compound is calculated by shifting the both electron of shared pair on more electronegative atom.

O	F
-2	-1

In peroxide $= -1$

In Superoxide $= -\frac{1}{2}$

$O_3^- = -\frac{1}{3}$

in $OF_2 = +2$

in $O_2F_2 = +1$

IA	IIA	B, Al, Ga, In	C, Si, Ge, Sn	N, P, As, Sb, Bi	S, Se, Te
+1	+2	(-3 to +3)	(-4 to +4)	(-3 to +5)	(-2 to +6)

Range of ON = (n-8) to +n
n = no. of e^- in valence shell.

Cl, Br, I
(-1 to +7)

Q-① $[FeF_6]^{-3}$

$x - 6 = -3$

$\boxed{x = +3}$

② MnO_4^-

$x - 8 = -1$

$\boxed{x = +7}$

(3) $\underline{I}F_7$

$x - 7 = 0$

$\boxed{x = +7}$

(4) $H\underline{Cl}O_3$

$+1 + x - 6 = 0$

$\boxed{x = +5}$

(5) $\underline{Si}O_2$

$x - 4 = 0$

$\boxed{x = +4}$

(6) $\underline{B}F_4^-$

$x - 4 = -1$

$\boxed{x = +3}$

(7) $\underline{K}H$

$x - 1 = 0$

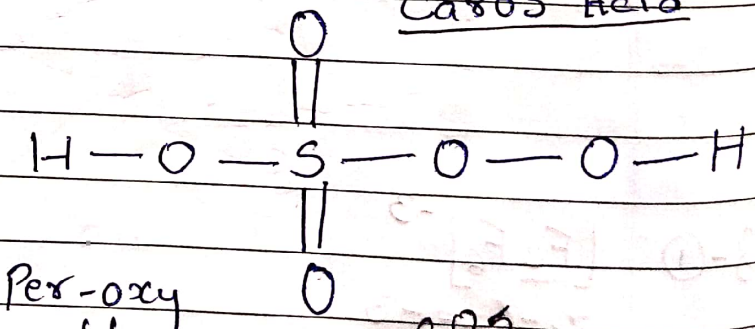
$\boxed{x = +1}$

(8) $H_2\underline{S}O_5$

$+2 + x - 6 - 2 = 0$

$\boxed{x = +6}$

Caro's Acid



Per-oxy sulphuric acid H_2SO_5

(9) $K_2\underline{Cr}_2O_7$

$+2 + 2x - 14 = 0$

$\boxed{x = +6}$

(10) $\underline{S_2O_6}^{2-}$

$2x - 12 = -2$

$\boxed{x = +5}$

(11) $\underline{ClO_4}^{-}$

$x - 8 = -1$

$\boxed{x = +7}$

(12) $\underline{NO_2}^{+}$

~~$x - 8 = +1$~~ $x - 4 = +1$

~~$\boxed{x = +7}$~~ $\boxed{x = +5}$

(13) $H\underline{N}O_2$

$1 + x - 4 = 0$

$\boxed{x = +3}$

(14) $\underline{Na}\,H$

$x - 1 = 0$

$\boxed{x = +1}$

(15) $\underline{Si_2}F_6$

$2x - 6 = 0$

$\boxed{x = +3}$

(16) $H\underline{S}O_5^{-}$

~~$+1 + x - 10 = +1$~~ $+1 + x - 2 - 6 = -1$

$\boxed{x = +6}$

(17) $N_2H_5^+$

$2x + 5 = +1$

$\boxed{x = -2}$

(18) XeO_3F_2

$x - 6 - 2 = 0$

$\boxed{x = +8}$

(19) C in C_{60}

$\boxed{0}$

(20) $P_3O_3^{-3}$

$3x - 6 = -3$

$\boxed{x = +1}$

(21) $K_2H_2P_2O_7$

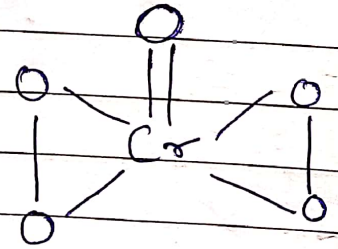
$+2 + 2 + 2x - 14 = 0$

$\boxed{x = +5}$

(22) CrO_5

$x - 8 - 2 = 0$

$\boxed{x = +6}$



(23) C_3O_2

$2x - 2 = 0$

$\boxed{x = +1}$

Co-ordinate Bond :-

→ Bond which is Formed by unequal sharing of e⁻ b/w the atoms is called co-ordinate bond.

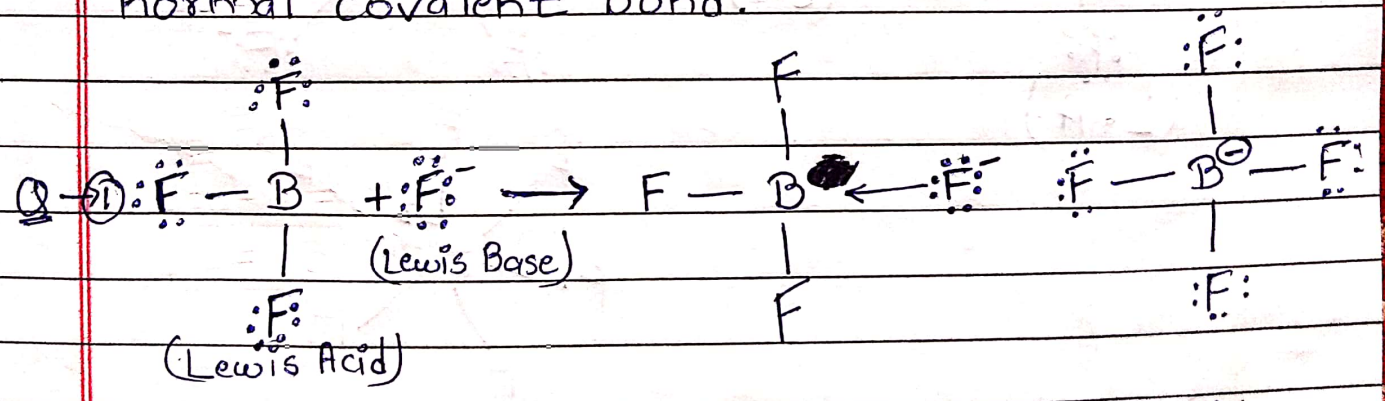
→ ~~Bond the~~ Both the e⁻ of the shared pair are given by 1 atom, but contribute in the stability of both.

→ During co-ordinate bond formation donar species is called lewis base and acceptor species is called lewis acid.

→ For co-ordinate bond Formation, donar species must have lone pair and acceptor species must have vacant orbital invalence shell.

→ Co-ordinate bond is differ From covalent bond only in the way of formation but once it is formed its is identical with covalent bond.

→ When co-ordinate bond is replaced by normal covalent bond.



$I_2 + KI \longrightarrow K^+ I_3^-$

Brown Colour (Betadine)

③ $CH_3-\ddot{O}: + H^+ \longrightarrow CH_3-\overset{\displaystyle CH_3}{\underset{|}{O}}:\rightarrow H^+ \quad CH_3-\overset{+}{O}-H$ (with CH_3 below the O^+)

(L·B) (L·A)

④ $F_3B: + H-N: \rightarrow F_3B\leftarrow N-H$

(L·A) (L·B)

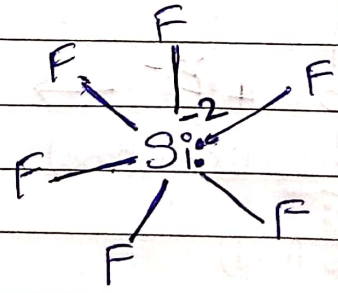
$F_3B^{\ominus}-N^{\oplus}-H$

⑤ $:\ddot{O}=\ddot{O}: + :\ddot{O}: \rightarrow :\ddot{O}=\ddot{O}:\rightarrow :\ddot{O}-\ddot{O}: \quad :\ddot{O}=\ddot{O}^+-:\ddot{O}:^-$

(L·B) (L·A)

⑥ $F-Si(F)(F)-F + 2F^- \rightarrow SiF_6^{2-}$

(L·A) (L·B)

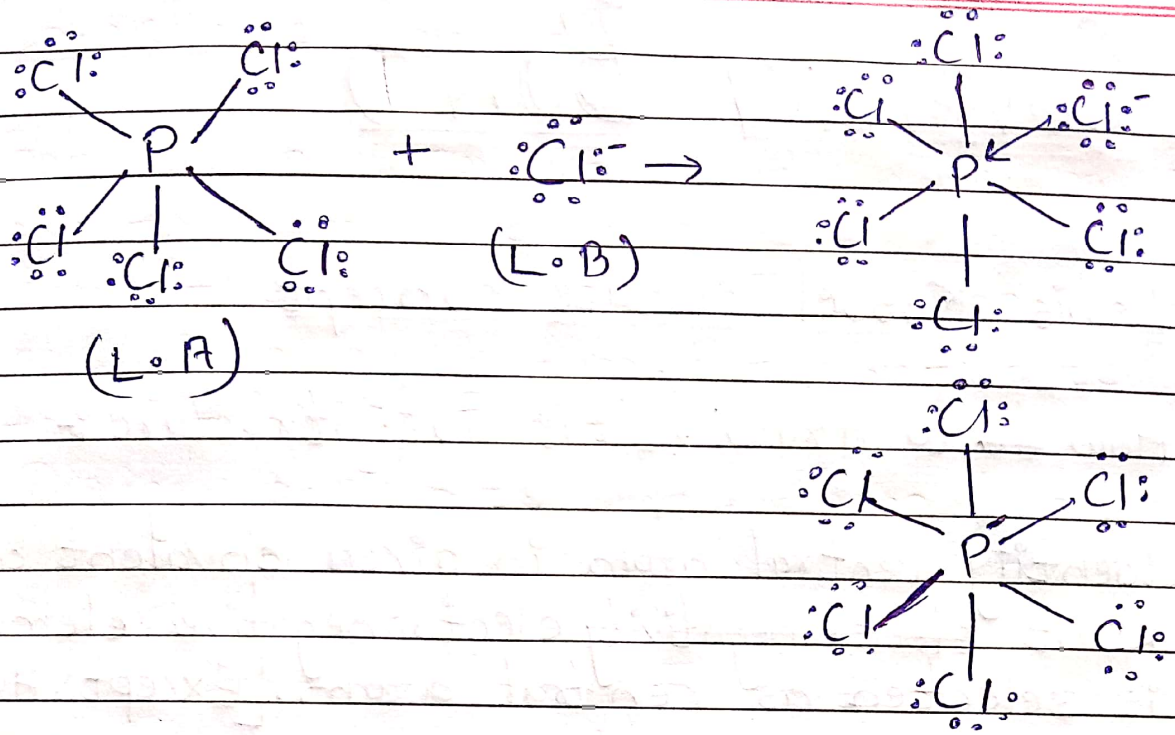


⑦ $I-I: + I^- \rightarrow I-I\leftarrow I^-$

(L·A) (L·B)

$I-I^-(:)-I$

(8)



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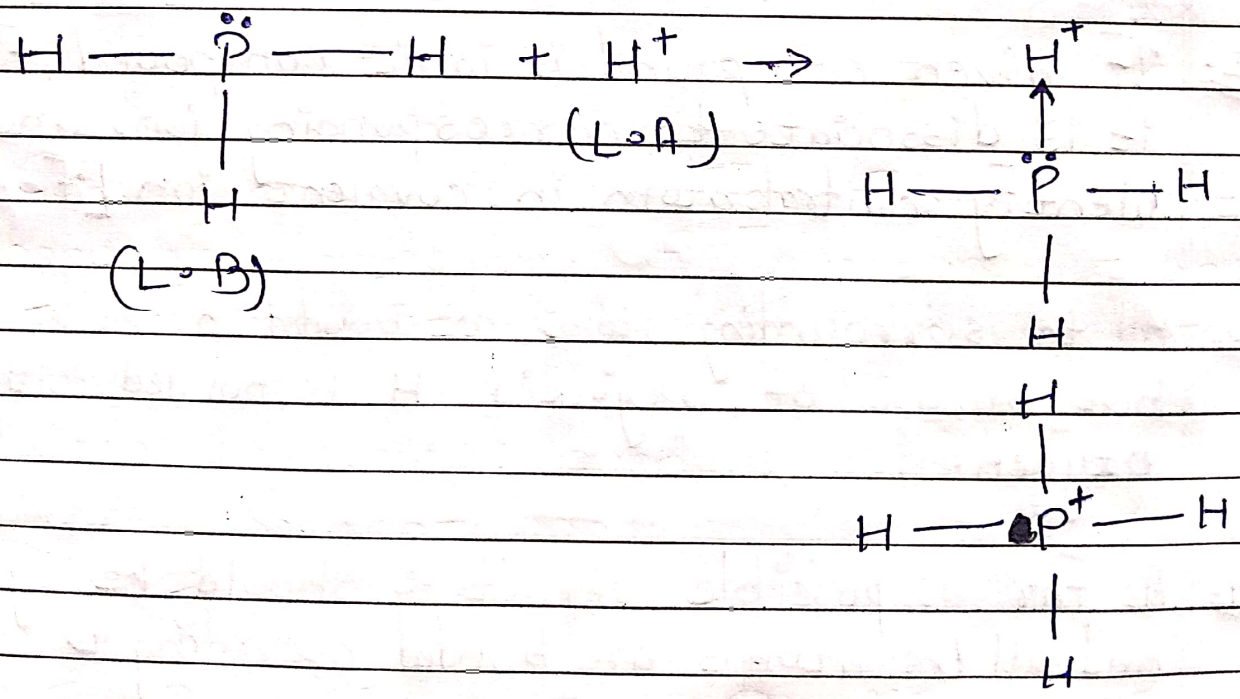


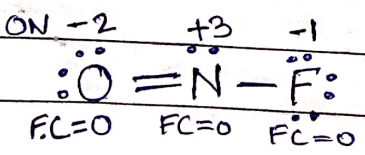
COVALENT BOND

Lewis Kossel Octate concept

How ~~do~~ to draw Lewis dot structure :-

1. Identify central atom in given covalent compound. Least ~~electronegativity~~ electronegative element is selected as central atom. [Except, Hydrogen]
2. If given compound is ionic compound, First it is dissociate to corresponding ions and identify central atom in covalent ion [if any]
3. All the surrounding atoms are bonded to central atom but in case of oxy-acid H is bonded with oxygen.
4. As far as possible structure should be symmetric and all the atoms are bonded according to their covalency.

e.g. → ① NOF

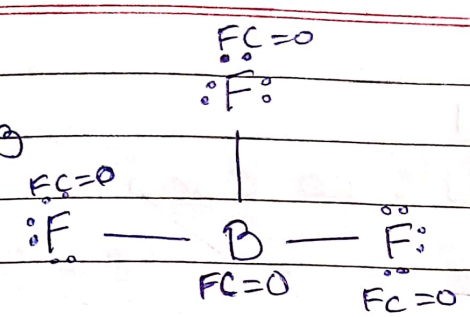


Covalency of O = 2, N = 3, F = 1
Bond → 3 Covalent Bond ; 2σ bond, 1π bond
Total L.P = 6

FC → Formal Charge

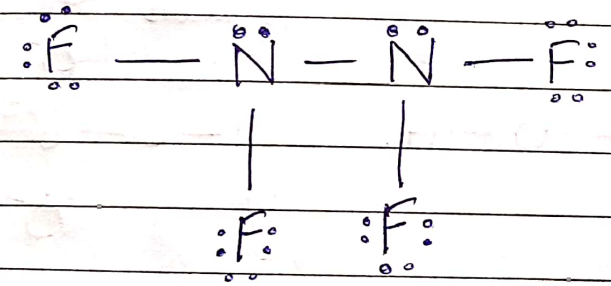
Date
Page

② BF_3



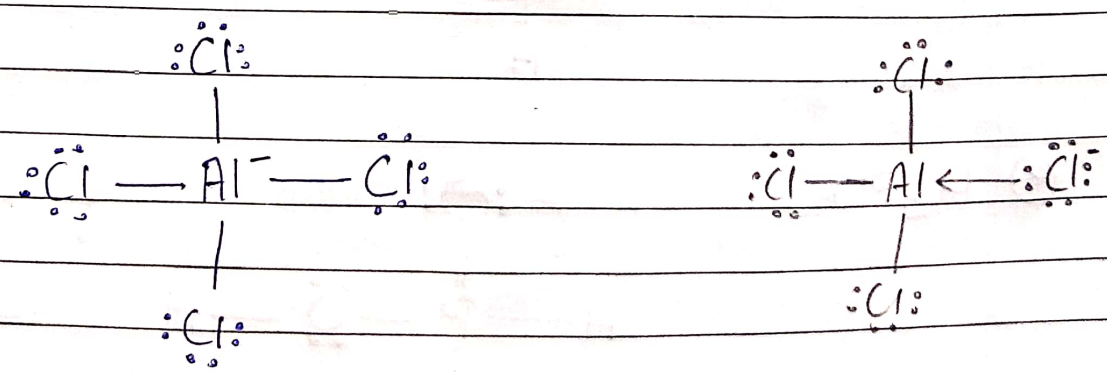
ON of B = +3 ; F = -1
Covalency of B = 3 ; F = 1
Total L.P = 9
Bond → 3 Covalent Bond ; 3σ Bond

③ N_2F_4



Covalency of N = 3 ; F = 1
FC on F = 0 ; N = 0
ON of N = +2 ; F = -1
Bond → 5 Covalent Bond ; 5σ bond
Total L.P = 14

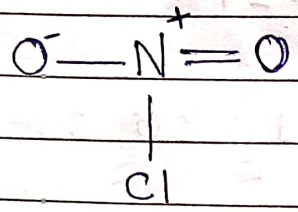
④ $AlCl_4^-$



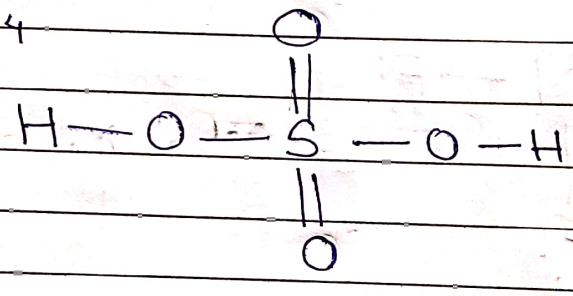
Covalency of Al^- = 4 ; Cl = 1
FC on Al = -1 ; Cl = 0

ON of Al = +3 ; Cl = -1
Bond → 4 covalent bond ; 4 σ Bond
Total L.P = 12

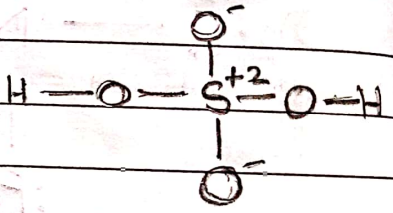
(5) NO_2Cl



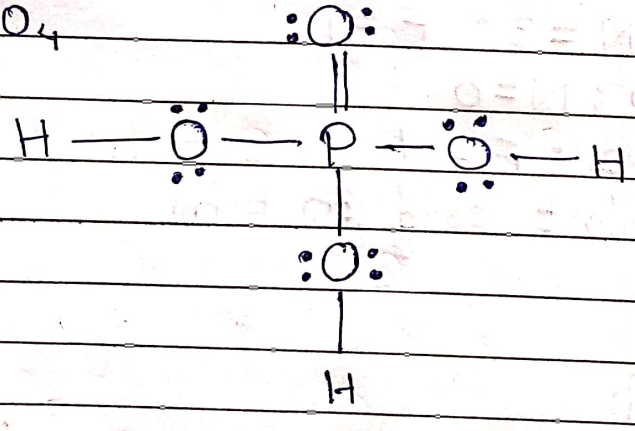
(6) H_2SO_4



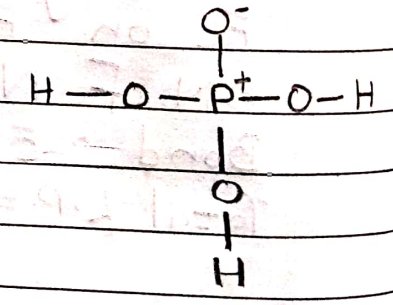
Lewis Structure



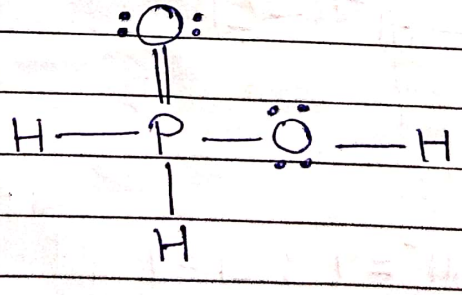
(7) H_3PO_4



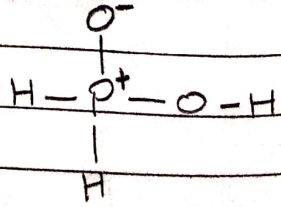
Lewis structure



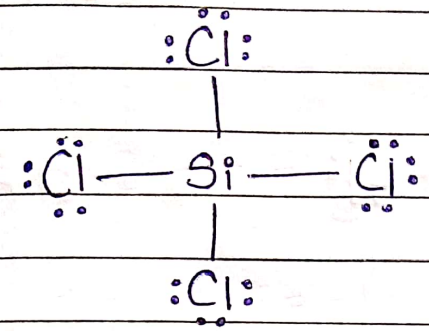
(8) H_3PO_2



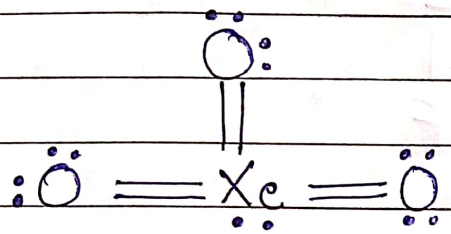
Lewis Structure



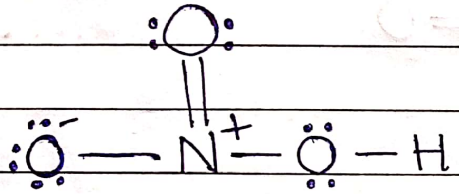
(9) $SiCl_4$



(10) XeO_3

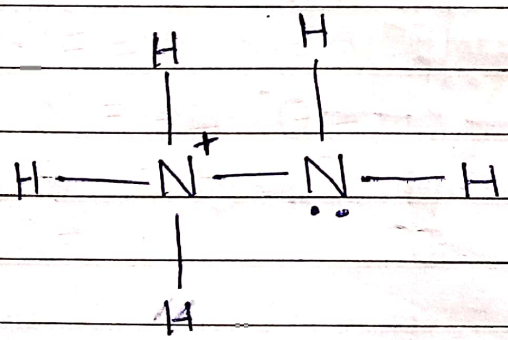


(11) HNO_3



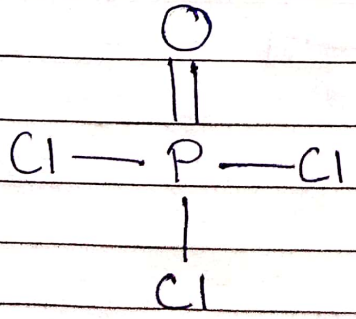
ON of N :→ +5

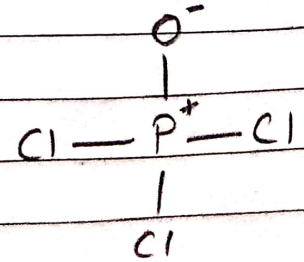
(12) $N_2H_5^+$



(13) $POCl_3$

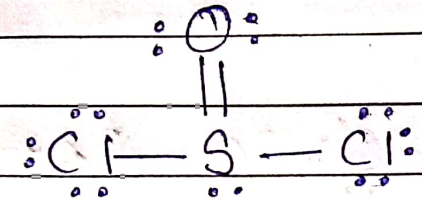
Lewis Structure

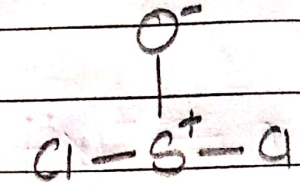




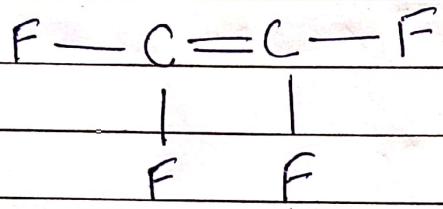
Lewis Structure

(14) $SOCl_2$

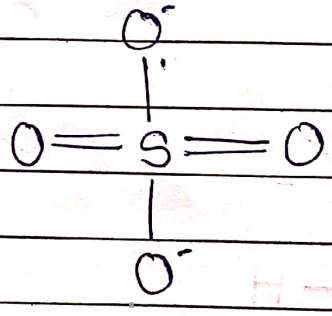




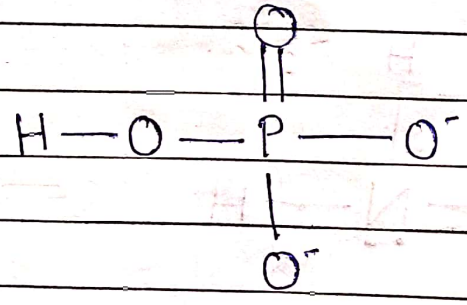
(15) C_2F_4



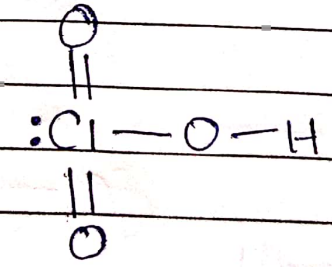
(16) SO_4^{2-}



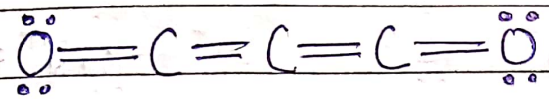
(17) HPO_4^{2-}



(18) $HClO_3$

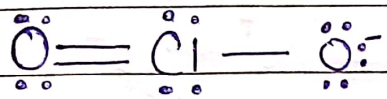


(19) C_3O_2

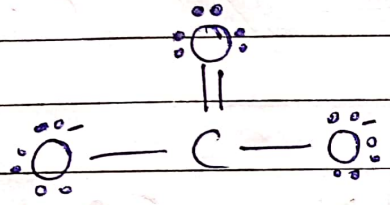


$\sigma = 4, \pi = 4, L.P = 4$

(20) ClO_2^-



(21) $CO_3^{2-} \rightarrow H_2CO_3$

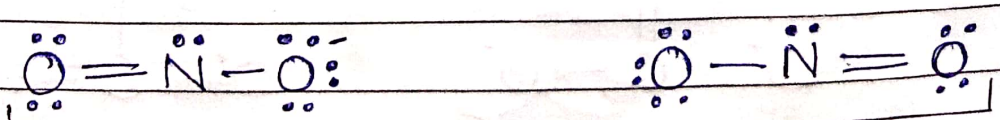


(22)

Resonance

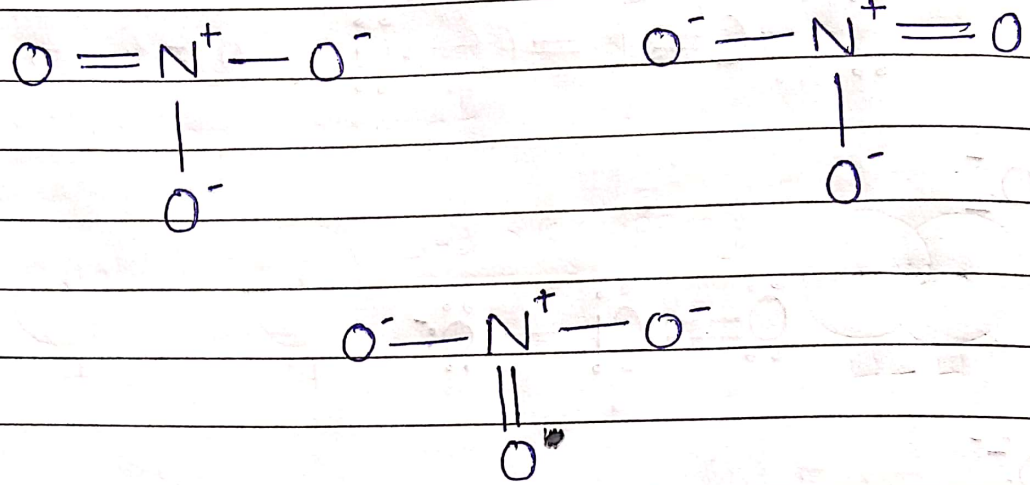
When more than one type of Lewis structure are possible for a molecule in which positions of atom is identical but different positions of multiple bond, ~~these are~~ they are considered as resonating structures and molecule/species is represented by resonance hybrid.

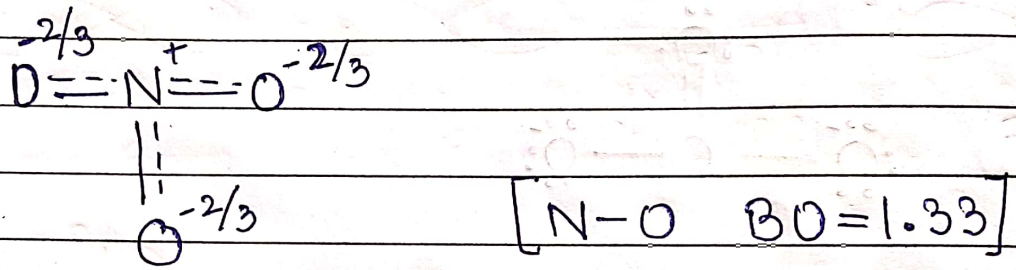
e.g → (1.) NO_2^-



$[O{=}N{-}O] \quad [N\text{-}O \ BO \rightarrow 1.5]$

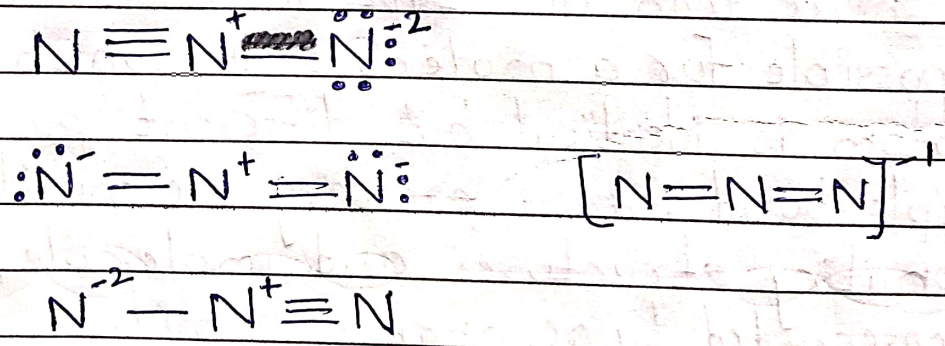
② NO_3^-



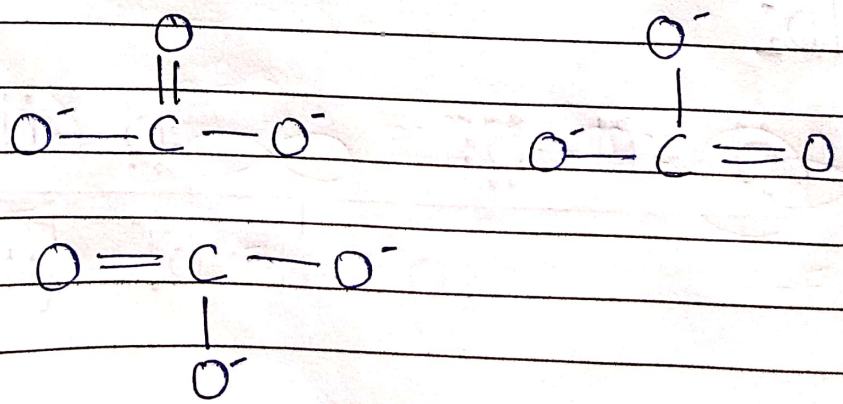


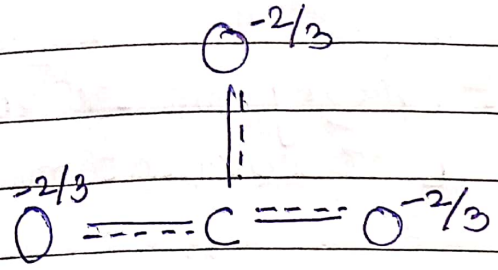
[N-O BO=1.33]

③ N_3^-

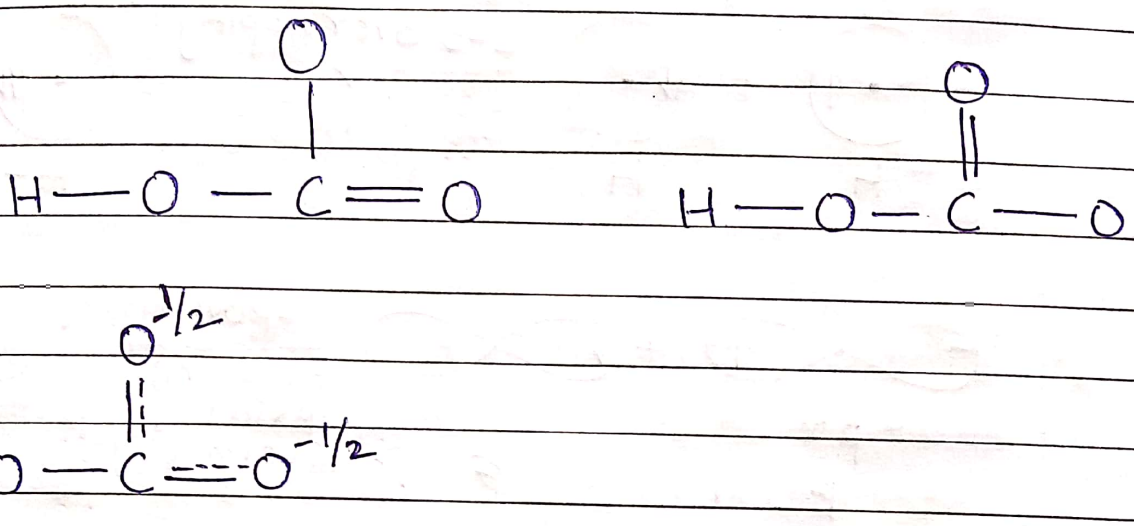


④ CO_3^{2-}





⑤ HCO_3^{2-}



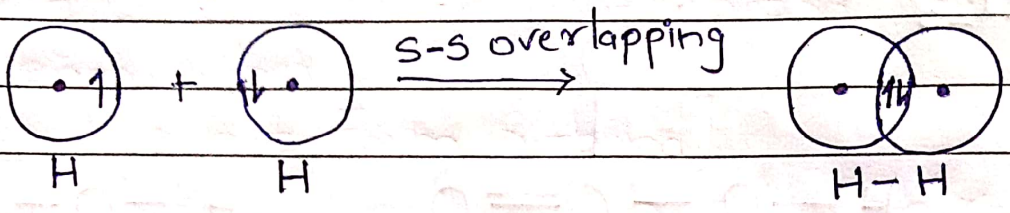
* IMPORTANT NOTE :-

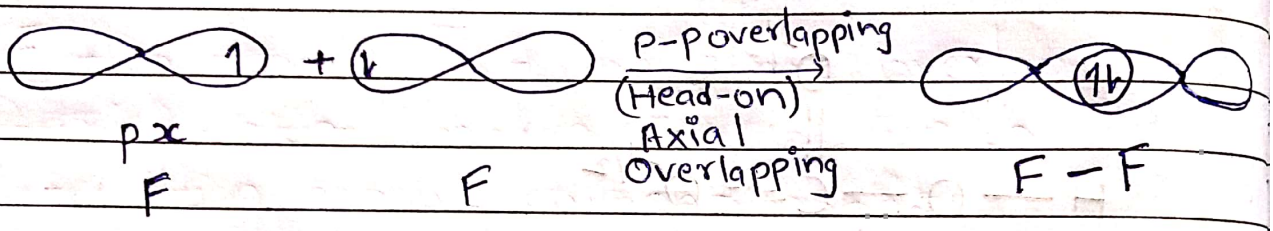
Some of compounds are covalent but dissociate into ions when dissolved in water.

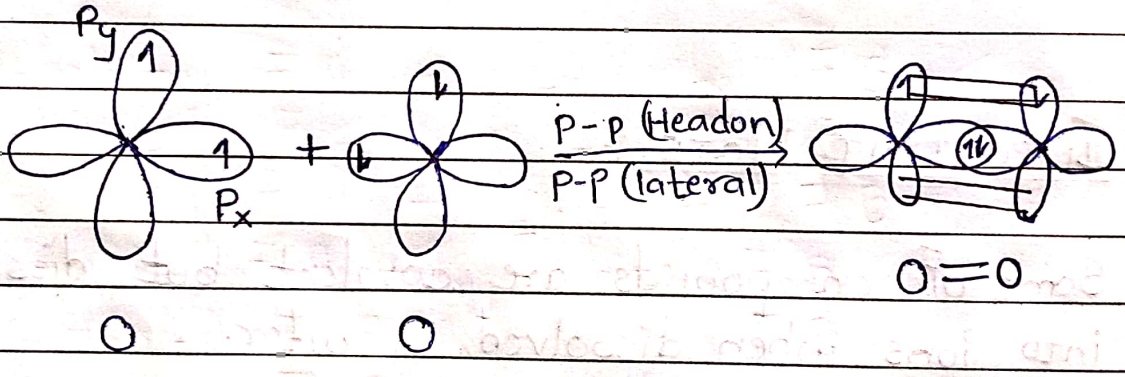
eg → HCl
AlX_3 [X = Cl, Br, I]
GaX_3 [X = Cl, Br, I]
$FeCl_3$, $FeBr_3$
$CuCl_2$, $CuBr_2$
$SnCl_2$, $SnCl_4$
$SnBr_2$, $SnBr_4$

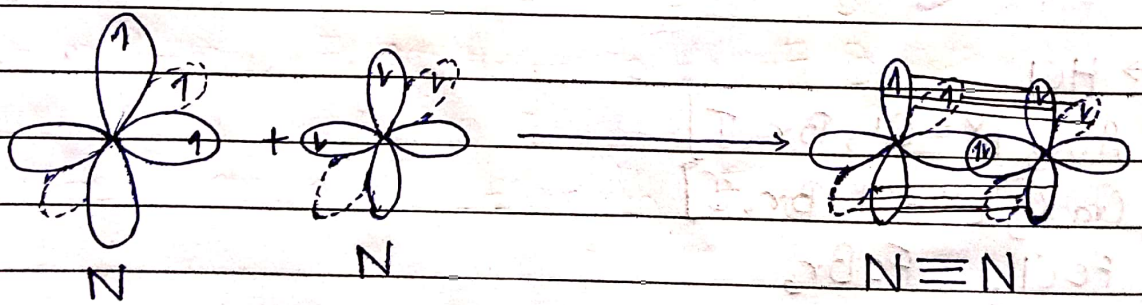
Valence Bond Theory :- [Theory for the formation of covalent molecule]

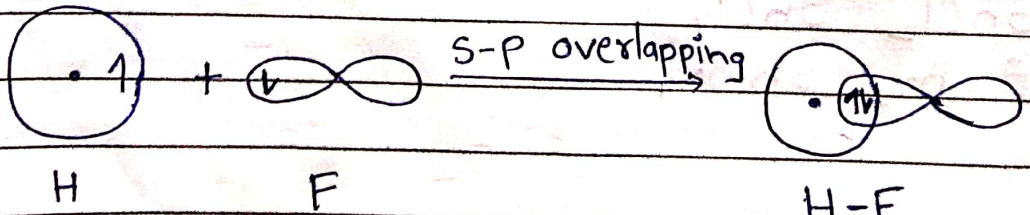
① Overlapping Concept











→ According to ~~ve~~ overlapping concept covalent bond is formed by equal sharing of e^- by the overlapping of valency shell orbitals of two different atoms.

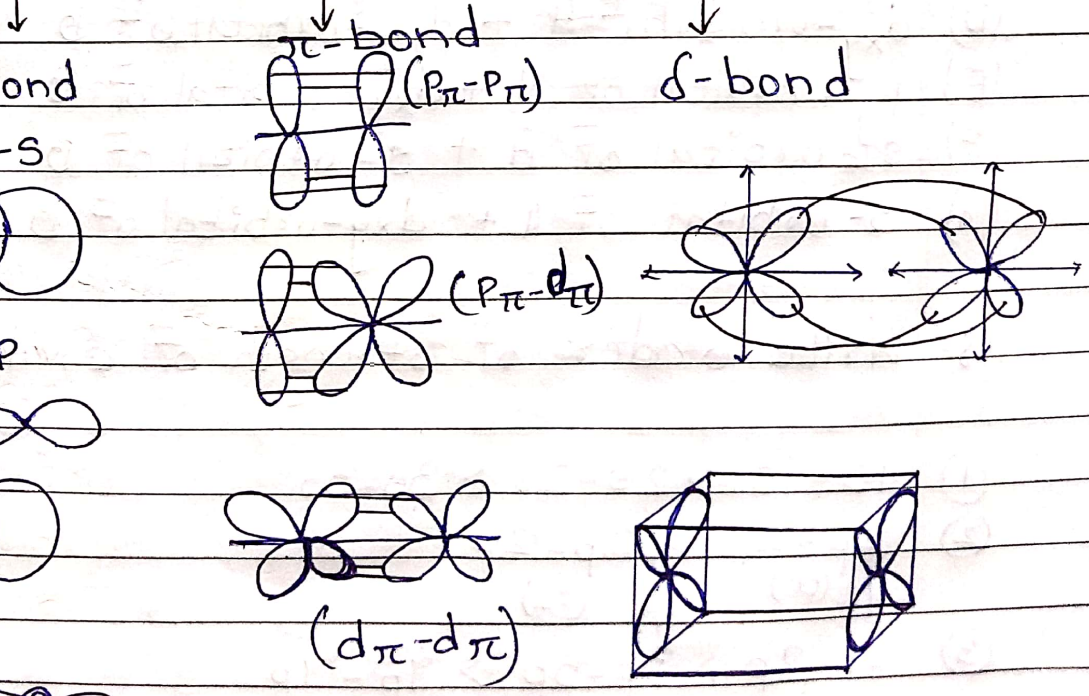
→ For overlapping, participating orbitals must have proper orientation and one unpaired e^- in each with opposite spin.

→ Strength of covalent bond is explained by extent of overlapping between the participating orbitals.

→ Different types of bonds are formed by overlapping $\sigma, \pi, \delta, \phi$, etc.

→ Extent of overlapping is depends on various factors.

Types of Bond



* Hybridised orbital always produce σ bond

δ-bond

Delta bond is formed by special type of sidewise overlapping of d-orbitals in which all the four lobes of d-orbitals are interact to each other.
[d_{z^2} does not form δ-bond]

Q- If two atoms of A and B are overlaps on ~~x-axis, which~~ common x-axis, which interaction produce covalent bond:-

(A) s-orbital of A + p_x-orbital of B ✓
(B) p_y-orbital of A + p_y-orbital of B ✓
(C) p_x-orbital of A + p_z-orbital of B X
(D) d_{xy}-orbital of A + d_{xy}-orbital of B ✓
(E) p_y-orbital of A + d_{xy}-orbital of B ✓
(F) s-orbital of A + s-orbital of B ✓
(G) s-orbital of A + dxy-orbital of B ✓

Q- Write order of strength of covalent bond (B.E)

① 1s-1s > 2s-2s > 3s-3s
② 2p-2p (σ) > 2p-2p (π)
③ 2p-2p (σ) > 3p-3p (σ) > 4p-4p (σ)

(4) $2p_{\pi}-2p_{\pi} > 3p_{\pi}-3p_{\pi}$

(5) $1s-2p > 1s-3p > 1s-4p$

(6) $\geq C-C \leq < \geq C=C \leq < -C\equiv C-$

(Carbon-carbon bond)

(7) $N_2 > N_2H_2 > N_2H_4$ (N–N B.E)

(8) $H-F > H-Cl > H-Br > H-I$

(9) $2s-2s < 2s-2p < 2p-2p$
(σ) (σ) (σ)

Q. Which has highest Thermal stability

(A) HF (B) HCl (C) HBr (D) HI

THERMAL Stability

$HF > HCl > HBr > HI$

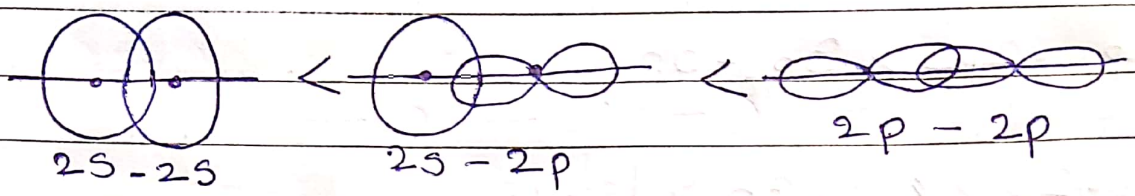
$H_2O > H_2S > H_2Se > H_2Te$

$NH_3 > PH_3 > AsH_3 > SbH_3$

$CH_4 > SiH_4 > GeH_4 > SnH_4$

$N_2 > O_2 > F_2$

★1(g)

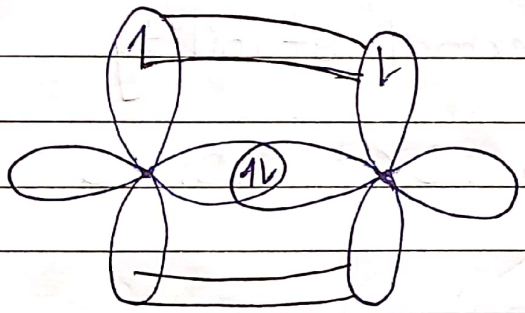


If n → same
strength (B.E) of directional bond is more.

Q. O=O is stable molecule but Sulphur does not form stable S=S. Explain

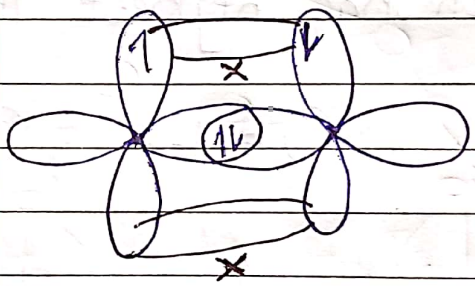
⟹

O = O



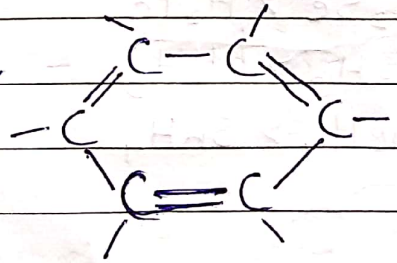
$2p_\pi - 2p_\pi$

less effective lateral overlapping of 3p-3p orbitals



Diamond — C —

Graphite



Diamond structure ✓ — Si —

Si

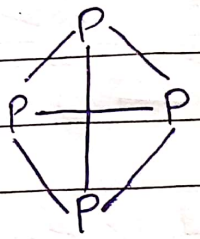
Graphite ✗

Pi-bond

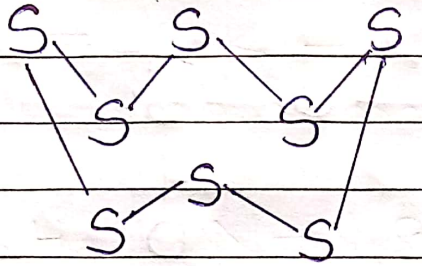
$N \equiv N$ $\quad O=O$ $\quad F-F$ ✓ $\quad Cl-Cl$ ✓

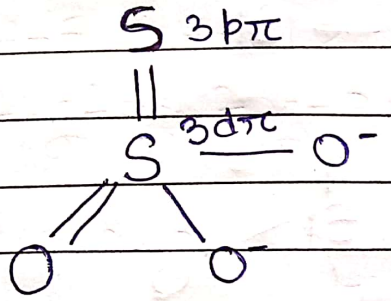
$P \equiv P$ ✗ $\quad S=S$ ✗ $\quad F \equiv F$ ✗ $\quad Cl \equiv Cl$ ✗

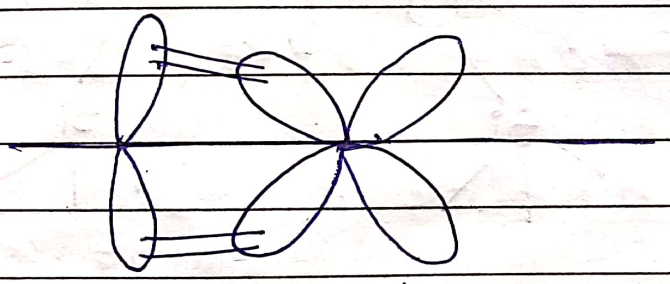
P_4



S_8



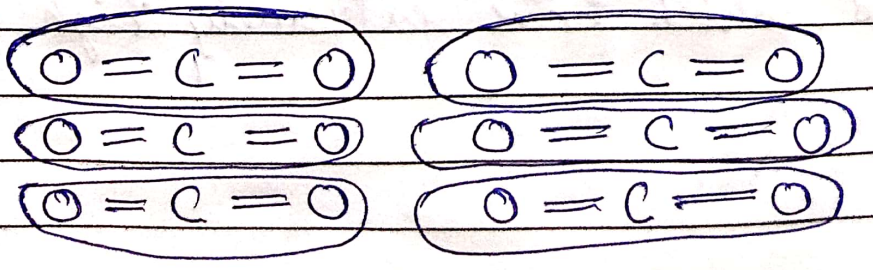
* 

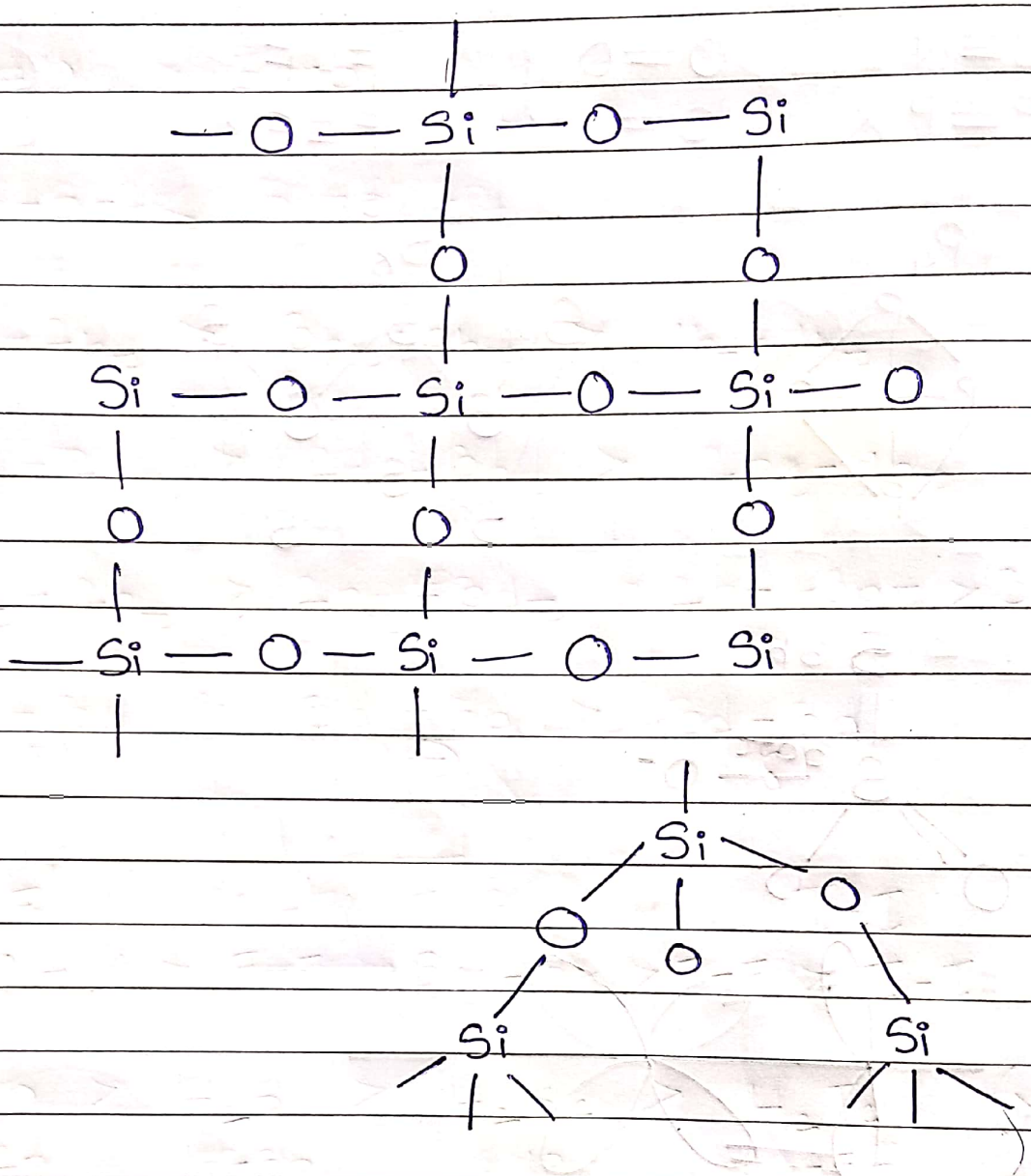


$3p_x$ $\quad 3d_{xy}$

Q→ CO_2 is gas at room temperature but SiO_2 is high melting solid. Explain?

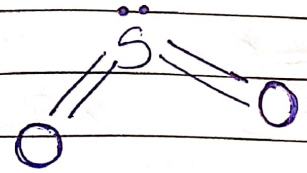
⇒ $O \overset{2p_\pi - 2p_\pi}{=} C \overset{2p_\pi - 2p_\pi}{=} O$ $\quad$ ✗ $O \overset{3p_\pi - 2p_\pi}{=} Si = O$





CO_2 is gas at room temperature because it has discrete molecules which are interact by vanderwaal forces only C and O can form stable $2P_\pi - 2P_\pi$ bond so that CO_2 ~~is~~ gas.

Silicon is unable to form $3P_\pi - 2P_\pi$ bond with oxygen so it form covalent network like solid, which have extremely high melting point.



S = [↿⇂] [1] [1] [1] [1] [ ] [ ] [ ] [ ]

S can form $3p_\pi - 2p_\pi$ bond

★ (Al) (Si) (P) (S) (Cl)

Size decreases, π-bond formation ability increases

★ $2p_\pi - 3p_\pi$

It depends on size of 3p

Q→ Write order of B.E in :-

(1.) 1s-1s , 2s-2s , 2p-2p (σ)

→ 1s-1s > 2p-2p > 2s-2s

(2.) 1s-2p , 2s-2p , 2p-2p (σ)

→ 1s-2p > 2p-2p > 2s-2p

✓ (3.)

H_2	HF	F_2
1s-1s	1s-2p	2p-2p

→ HF > H_2 > F_2

(4.) -O-O- < -S-S-

(5.) $O=O > S=S$

(6.) $-S-S- < S=S$

(7.) $2p_\pi - 2p_\pi > 3p_\pi - 3p_\pi > 4p_\pi - 4p_\pi$

(8.) $2p_\pi - 2p_\pi > 2p_\pi - 3p_\pi > 2p_\pi - 4p_\pi$

(9.) $2p_\pi - 2p_\pi > 2p_\pi - 3d_\pi > 2p\pi - 3p\pi > 3p\pi - 3p\pi$

(10.) $3d - 3d > 3d - 3d > 3d - 3d$
(σ) (π) (δ)

(11.) F-F , Cl-Cl , Br-Br , I-I
→ Cl-Cl > ~~F-F~~ → Br-Br > F-F > I-I

(12.) $H_2O > H_2S > H_2Se > H_2Te$ (M-H BE)
1s-2p 1s-3p 1s-4p 1s-5p

(13.) $-\overset{|}{\underset{|}{C}}-\overset{|}{\underset{|}{C}}- > -\overset{|}{N}-\overset{|}{N}- > -O-O-$

(14.) $H_2 > Li_2$
1s-1s 2s-2s

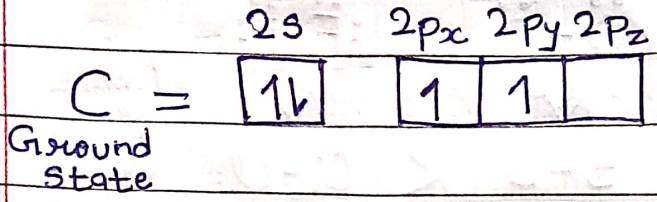
B.E.

C–C	> N–N	> O–O	> F–F
∨	∧	∧	∧
Si–Si	< P–P	< S–S	< Cl–Cl

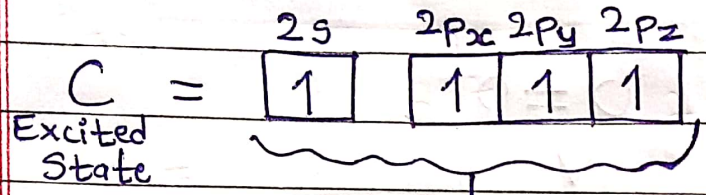
C=C	N≡N	O=O
∨	∨	∨
Si=Si	P≡P	S=S

Only overlapping concept unable to explain shape, geometry, bond angles of molecules which contain more than two molecules. [Polyatomic molecules] like BF, PCl_5, SF_6, CH_4, etc.

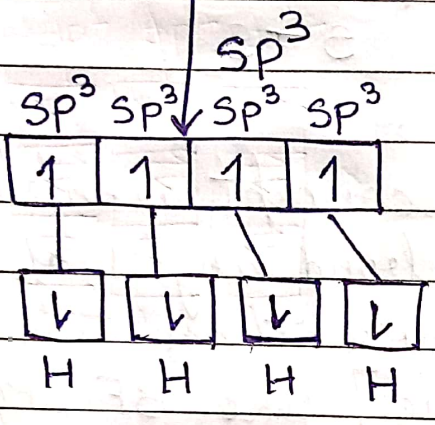
(2.) Hybridization Theory :-

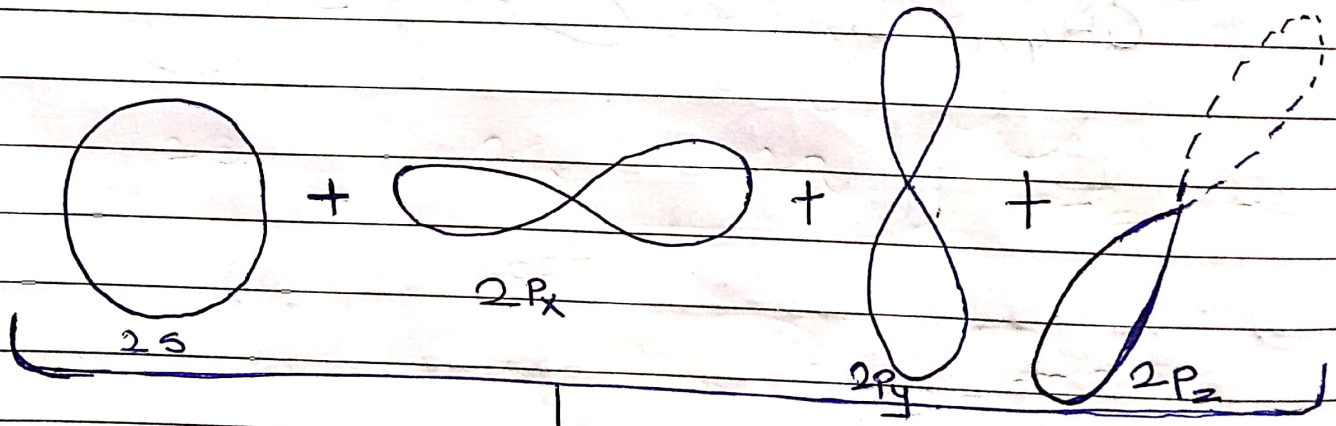


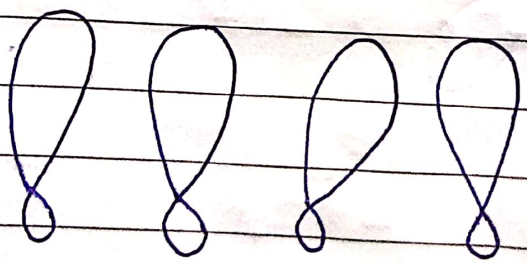
Ground State



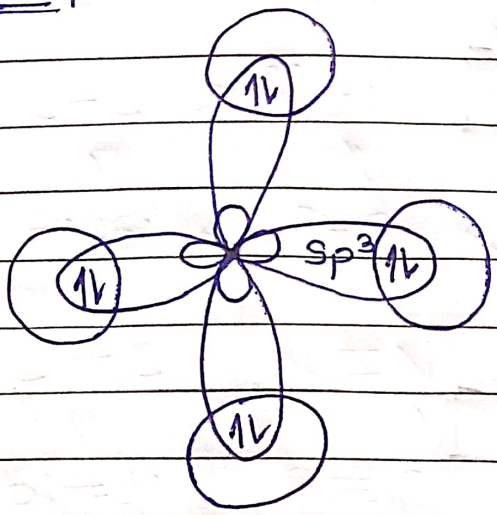
Excited State

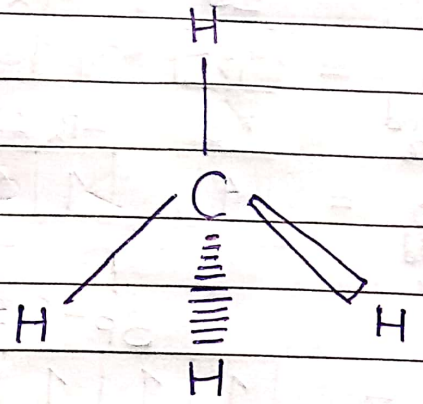






* CH_4

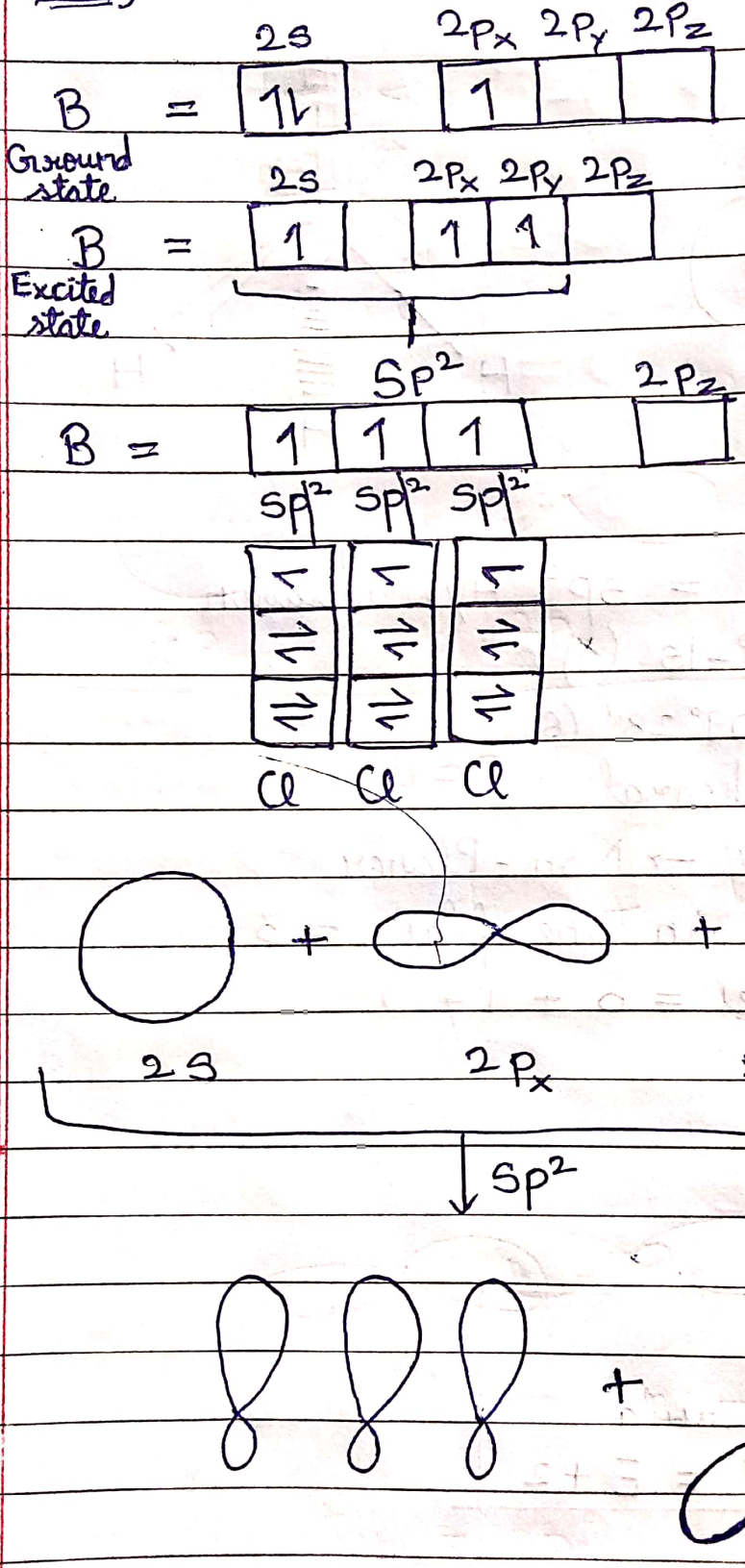


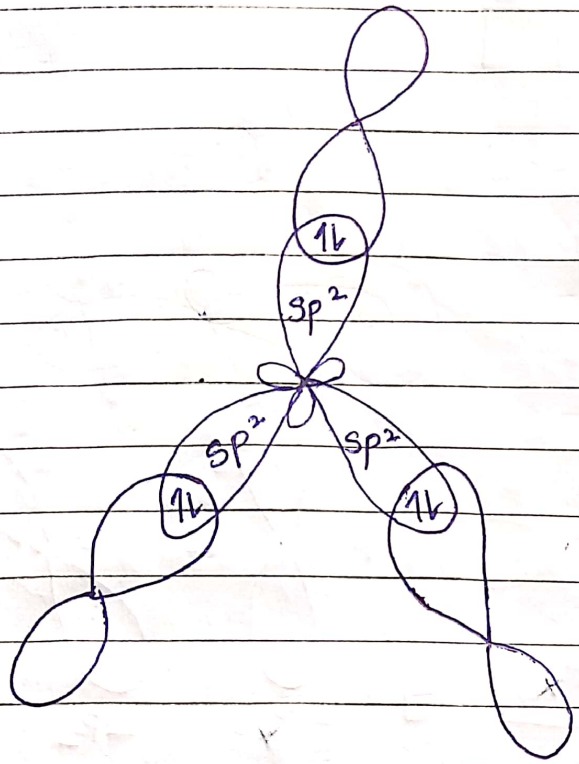


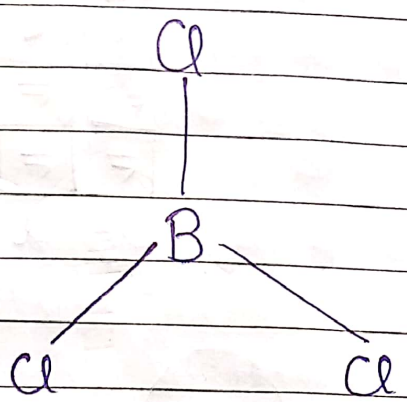
Hybridisation of C = sp^3 Hybridisation
Overlapping = sp^3-1s (4)
Bond Angle = 109°28' (6)
Geometry = Tetrahedral
Planer / Non Planer → Non-Planer
Maximum atom in one plane = 3
No. of such planes = 6 + 4 = 10
V = 4
E = 6
F = 4

Note:
Euler's Formula
V + F = E + 2

BCl_3


2s
2Px 2Py 2Pz
B =
Ground state
B =
Excited state
Sp²
2Pz
B =
sp² sp² sp²
Cl Cl Cl
2s
2Px
2Py
2Pz
Sp²





Hybridisation = sp^2

Overlapping = $sp^2 - 3p$

Bond Angle = 120° (3)

Geometry = Trigonal planer

→ Planer

Maximum atom in one plane = 4

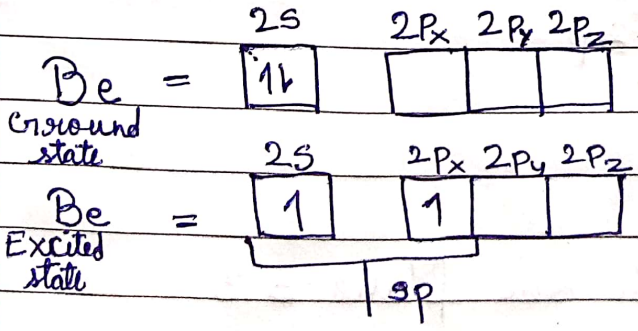
No. of such plane = 1

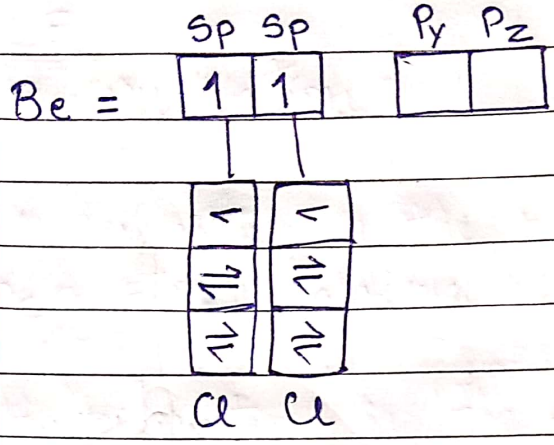
~~V~~

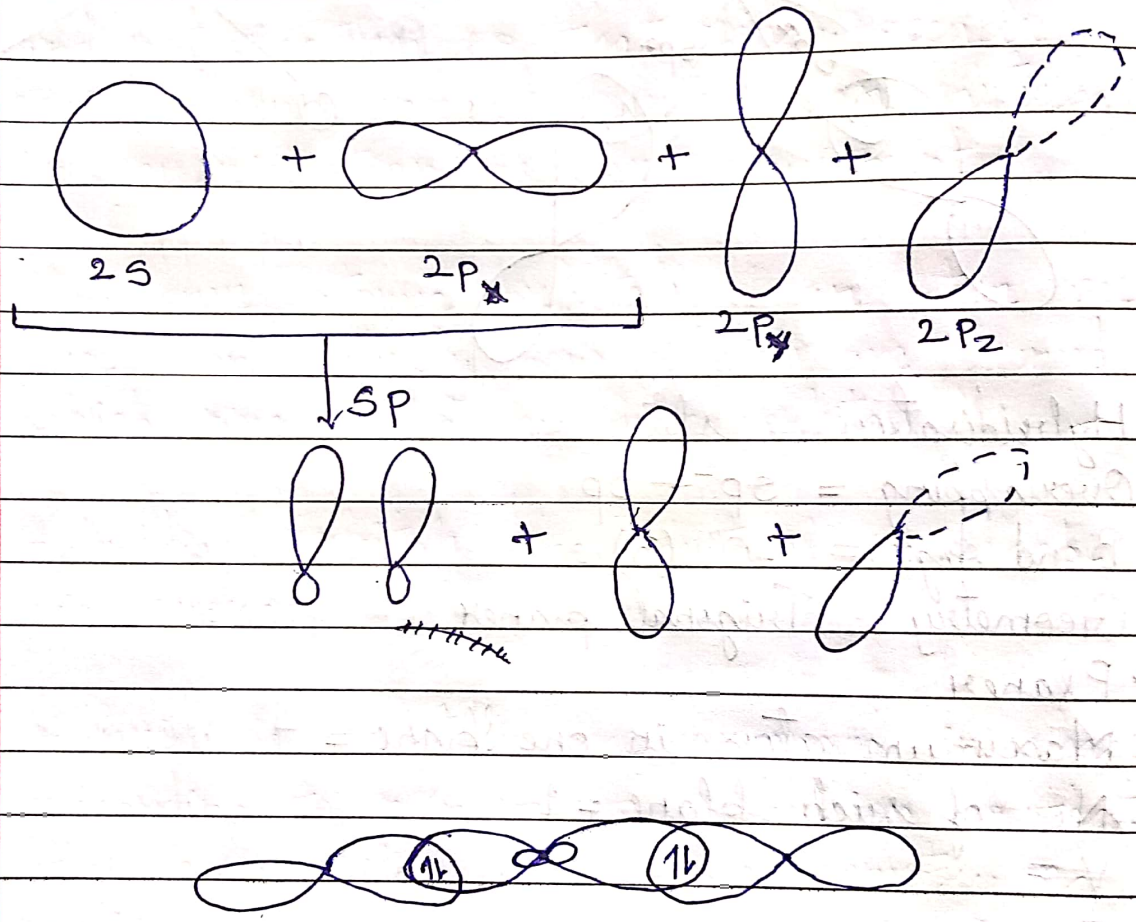
~~E~~

~~F~~

$BeCl_2$







Cl — Be — Cl

Hybridisation = sp
Overlapping = sp - 3p
Bond Angle = 180°
Geometry = Linear
→ Planer
Maximum atom in one plane = 3
No. of such plane = 1

SIGMA BOND (σ)	Pi Bond (π)
(i) This bond is formed by overlap of orbitals along their internuclear axis.	(i) This is formed by sideways overlapping of orbitals / lateral overlapping.
(ii) It is formed by overlapping of s-s, s-p, p-p orbitals.	(ii) This is formed by overlapping of p-p orbitals only.
(iii) Extent of overlapping is large.	(iii) Extent of overlapping is small.
(iv) Sigma bond is strong bond.	(iv) Pi Bond is weak
(v) It consists of only one electron cloud, which is symmetrical about the internuclear axis.	(v) It consists of two e^- clouds, one above the plane of atomic nuclei and the other below it.
(vi) Free rotation about a σ-bond is possible.	(vi) Free rotation about a π-bond is not possible because on rotation, overlapping vanishes.

Hybridisation

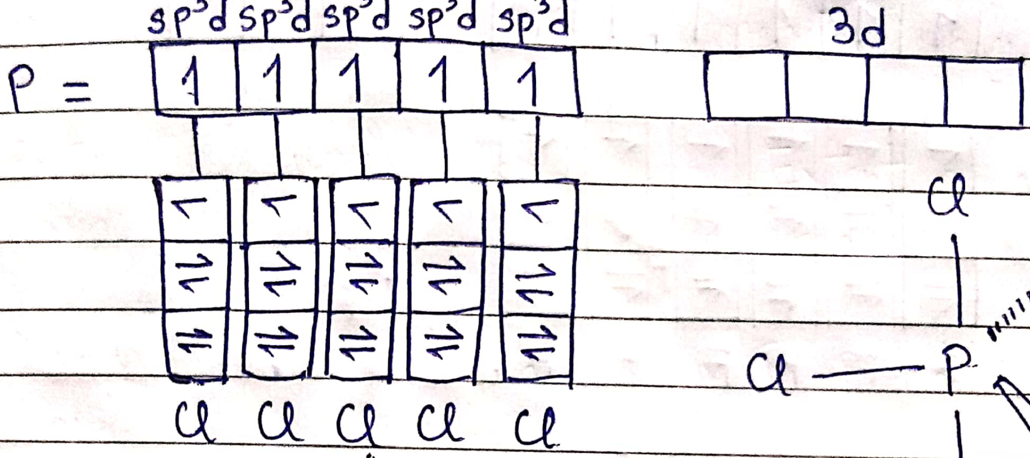
- Hybridisation is the mixing of atomic orbitals of a atom having nearly same energy.
- Hybridisation is the ~~mixing~~ property of orbital and not electron so that singly occupied, doubly occupied and vacant orbitals can participate in hybridisation as per requirement.
- When pure atomic orbitals of an atom are mix then entirely new orbitals are formed which are called hybridised orbitals.
- Hybridised orbitals are identical in shape and energy.
- Hybridised orbitals are arranged in space according to minimum repulsion so that they can decide shape and geometry of molecule.
- Hybridisation theory is required to explain shape and geometry of molecule observed by different spectroscopy methods.
- Hybridised orbitals always from σ bond, because shape and geometry of molecule is depends on σ bond.

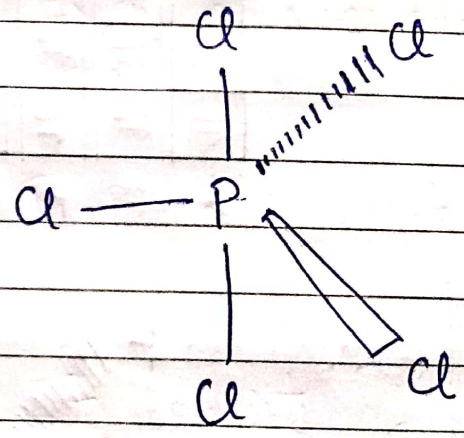
PCl_5

	3s	3px	3py	3pz
P =	↑↓	↑	↑	↑

	3s	3px	3py	3pz	3d				
P =	↑	↑	↑	↑	↑				

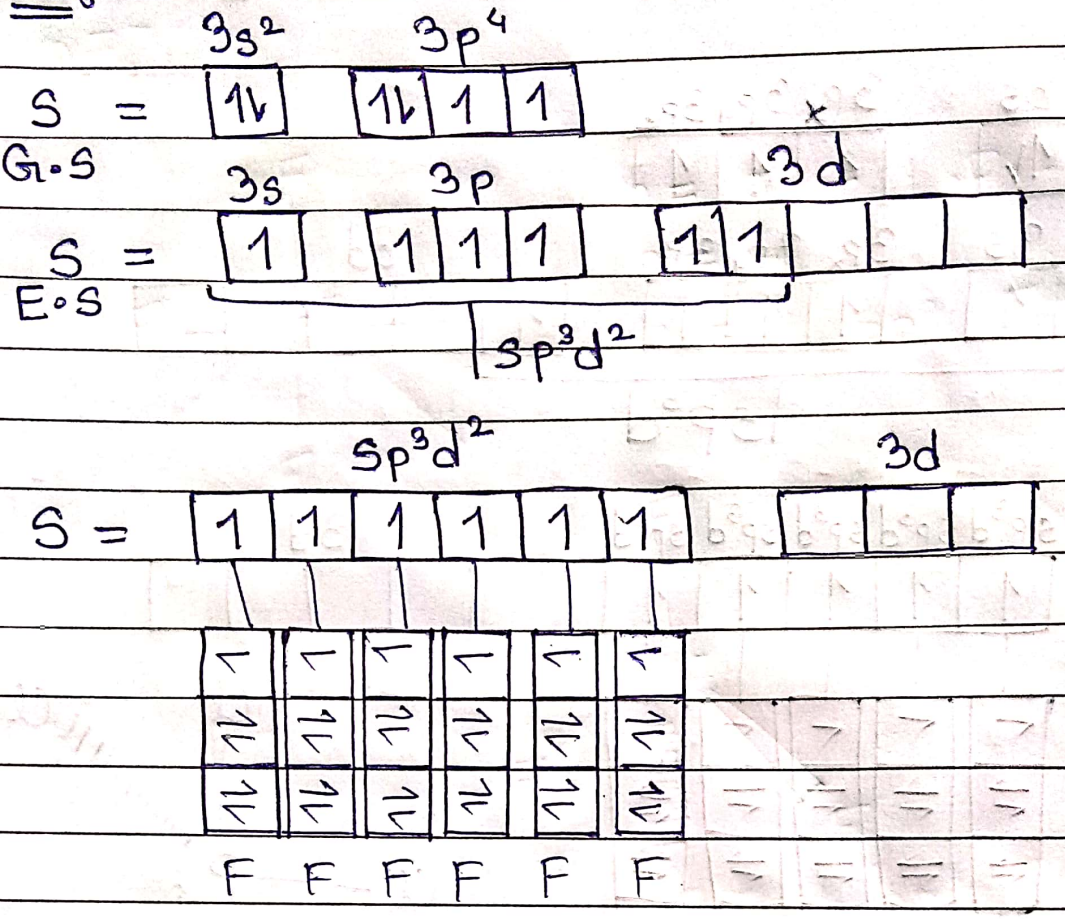
sp^3d

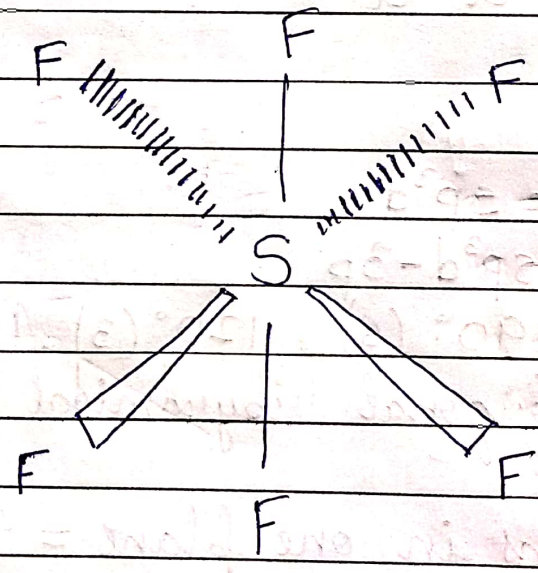




Hybridisation = sp^3d
Overlapping = $sp^3d - 3p$
Bond Angle = 90° (6), 120° (3), 180°
Geometry = Trigonal bipyramidal
→ Non-Planer
Maximum atoms in one plane = 4
No. of such planes = 4
V = 5
E = 9
F = 6

SF_6





Hybridisation = sp^3d^2

Overlapping = $sp^3d^2 - 2p$

Bond angle = 90° (12), 180° (3 bond pairs)

Geometry = Octahedral or Square bipyramidal

→ Non-Planer

Maximum no. of atom in one plane = 5
No. of such planes = 3

V = 6
E = 12
F = 8

* Steps to find hybridisation :-

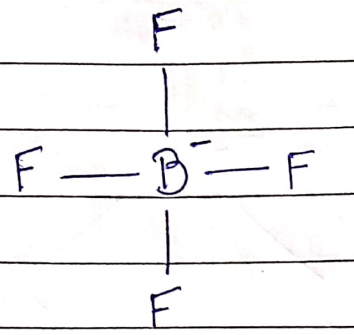
(1.) Draw structure of given species

(2.) Find n on central atom

n = No. of σ bond on that atom + L.P on that atom

(3.)
n = 2 sp
n = 3 sp^2
n = 4 sp^3
n = 5 ~~3p~~ sp^3d
n = 6 sp^3d^2
n = 7 sp^3d^3

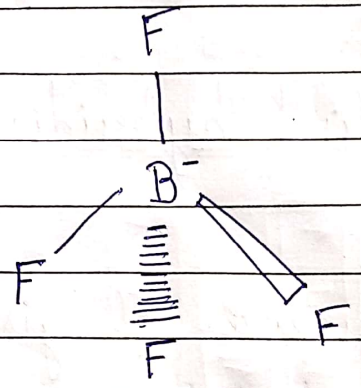
eg:- ① BF_4^-



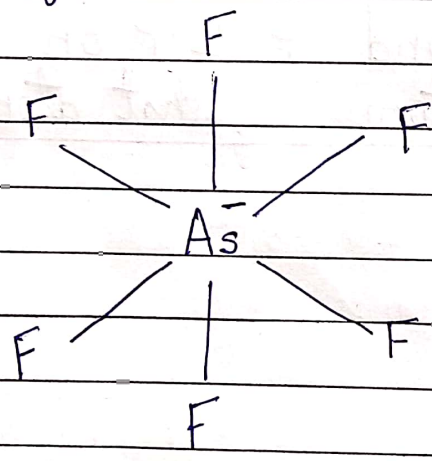
$n = \sigma + L.P$

$n = 4$

$n = 4$, sp^3, Tetrahedral



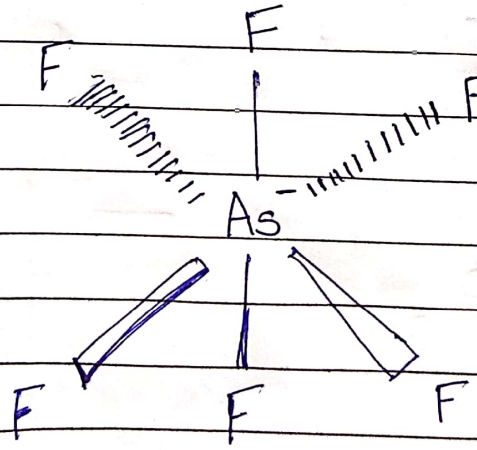
② AsF_6^-



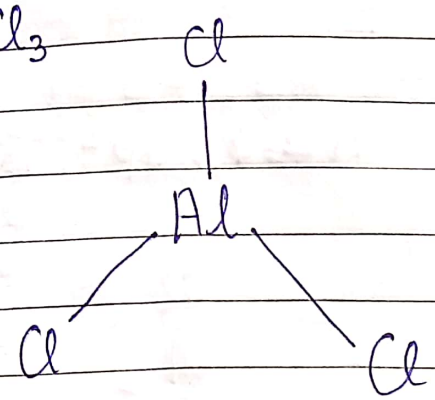
$n = \sigma + L.P$

$n = 6$

$n = 6$, sp^3d^2, Octahedral or Square bipyramidal



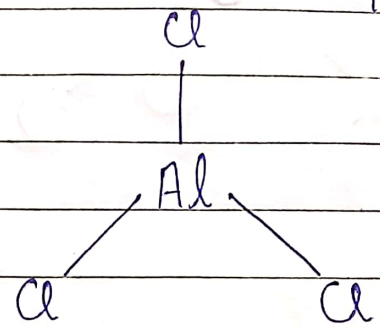
③ $AlCl_3$



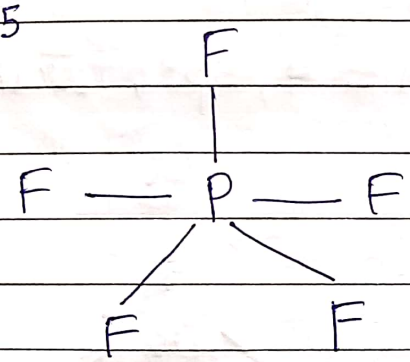
$n = \sigma + L.P$

$n = 3$

$n = 3$, sp^2, Trigonal Planer

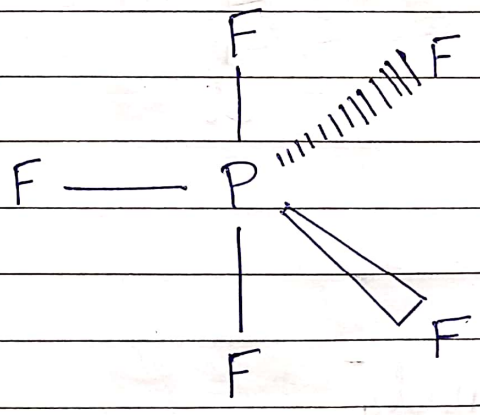


④ PF_5



$n = 5$

$n = 5$, sp^3d, Trigonal bipyramidal



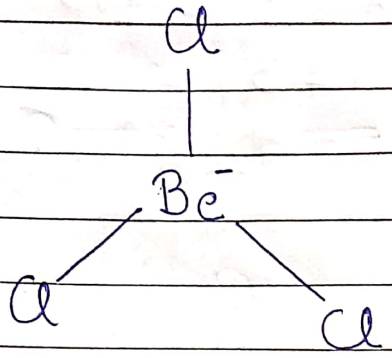
⑤ CO_2

$O = C = O$

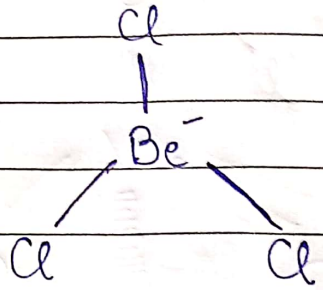
$n = 2$, sp, Linear

$O = C = O$

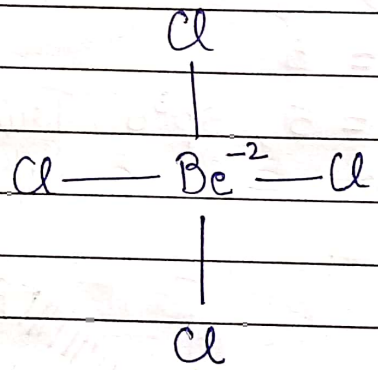
⑥ $BeCl_3^-$



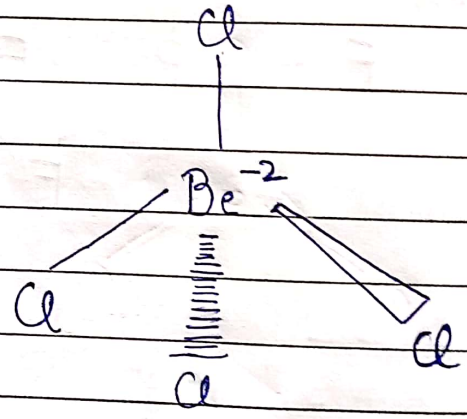
$n = 3$, sp^2, Trigonal Planar



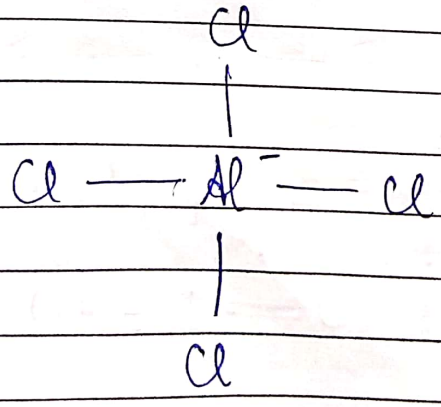
⑦ $BeCl_4^{-2}$



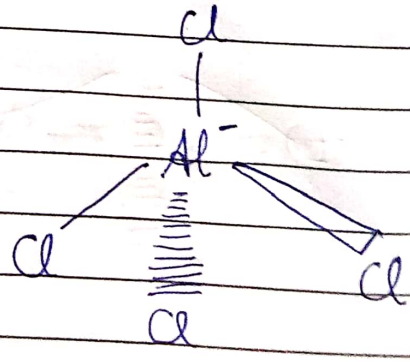
$n = 4$, sp^3, Tetrahedral



⑧ $AlCl_4^-$

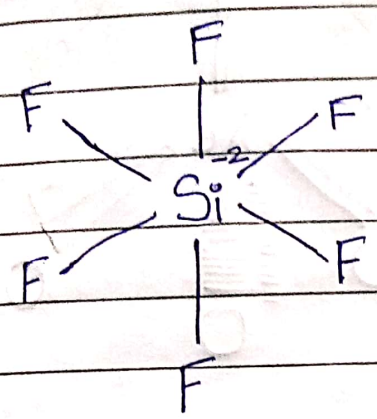


$n = 4$, sp^3, Tetrahedral

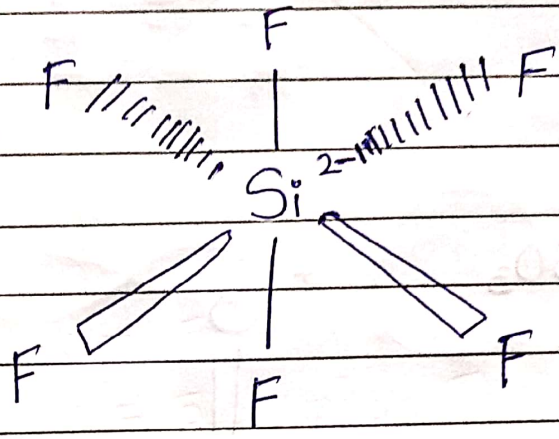


(8) Maximum no. of atom in one plane = 3
No. of such planes = 6 + 4 = 10

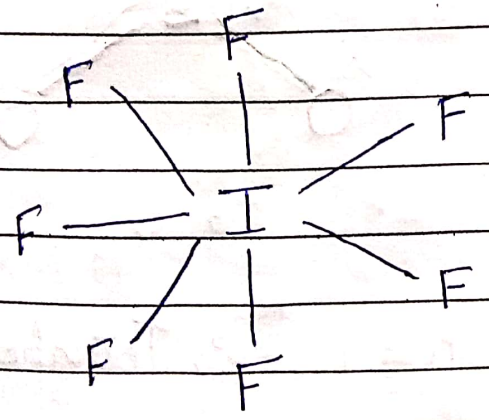
(9) SiF_6^{2-}



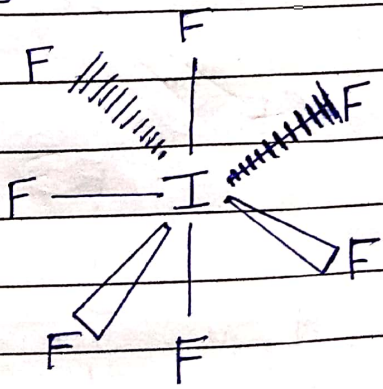
n = 6, Octahedral or Square bipyramidal, sp^3d^2



(10) IF_7



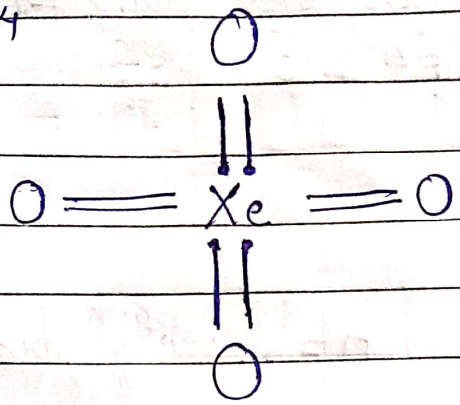
n = 7, Pentagonal bipyramidal
sp^3d^3



V = 7
E = 15
F = 10

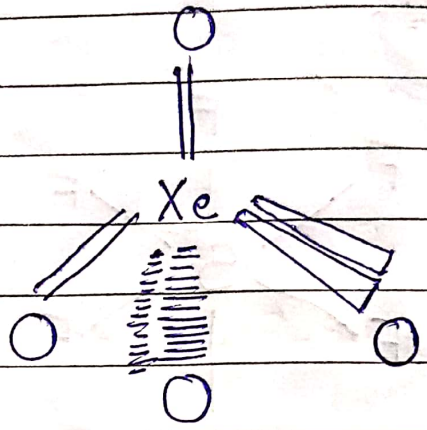
B.A = 90° (10), 72° (5), 180° (1)
Maximum atom in one plane = 5
No. of such planes = 1

(11) XeO_4

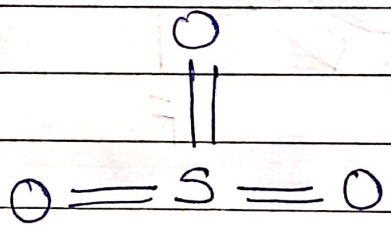


$n = 2 + 2 = 4$

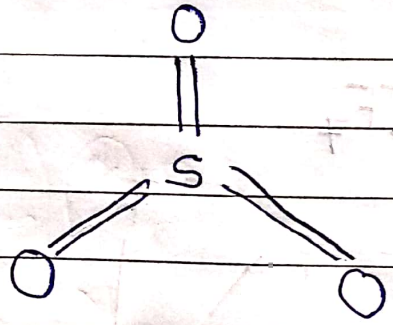
$n = 4$, sp^3, Tetrahedral



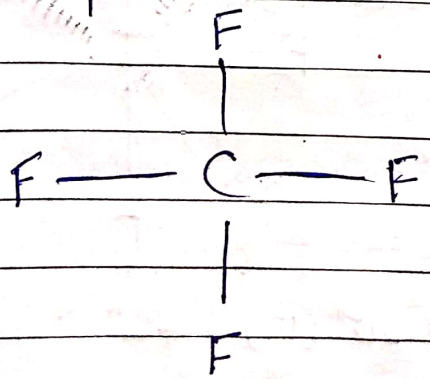
(12) SO_3



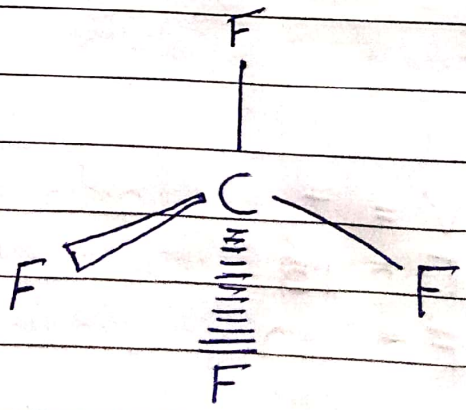
$n = 3$, sp^2, Trigonal Planar



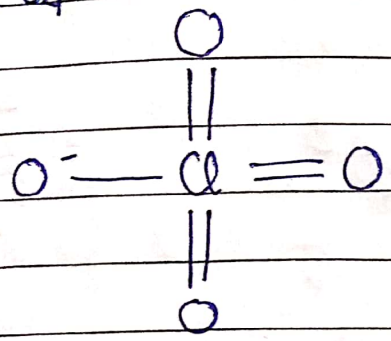
(13) CF_4



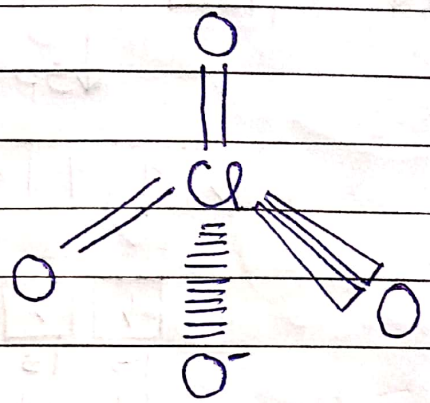
$n = 4$, sp^3, Tetrahedral



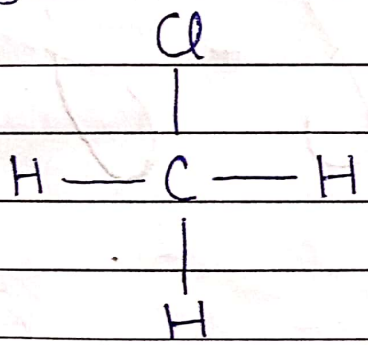
(14) ClO_4^-



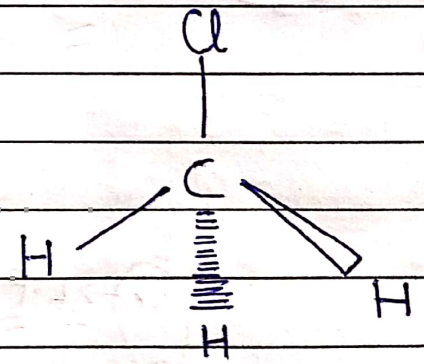
$n = 4, sp^3$, Tetrahedral



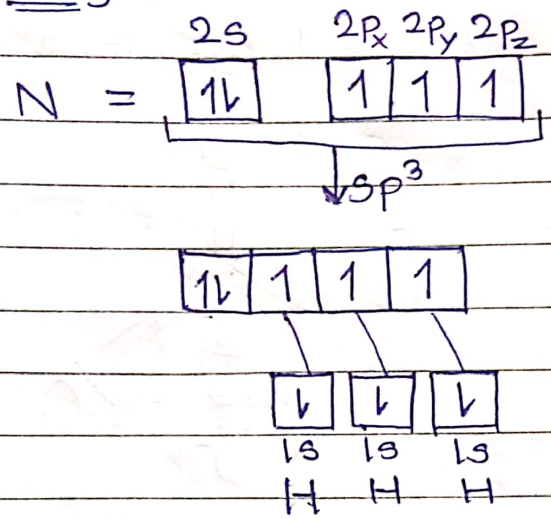
(15) CH_3Cl

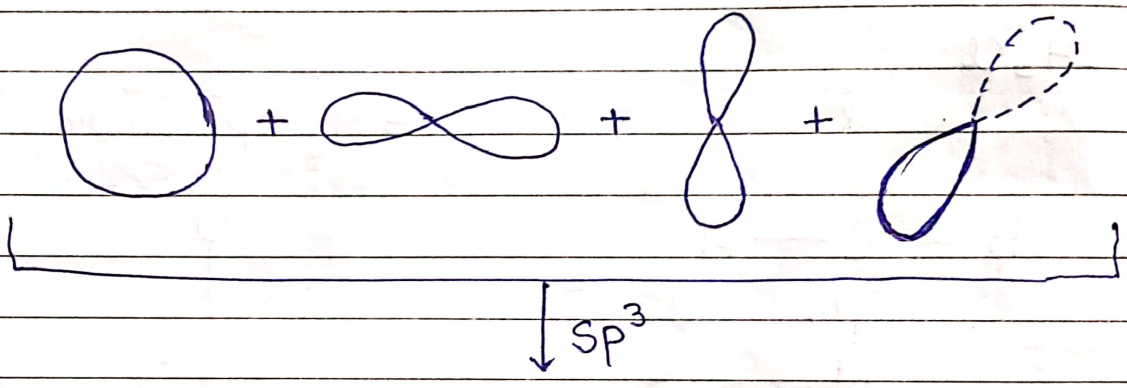


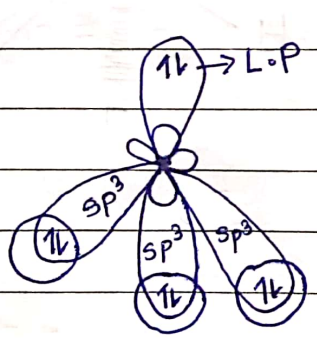
$n = 4, sp^3$, Tetrahedral

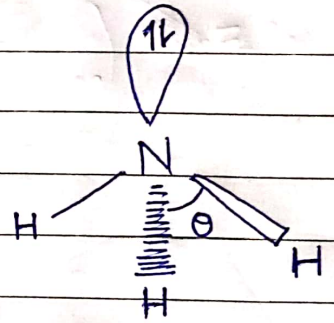


★ NH_3









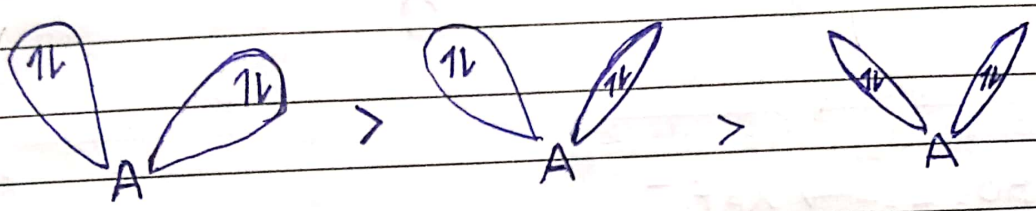
∴ θ = 107°

Hybridisation = sp^3
Overlapping = $sp^3 - 1s$ (3)
Electronic Geometry = Tetrahedral
Molecular Geometry = Triangle base pyramidal or Triangular pyramidal
Bond Angle = 107°

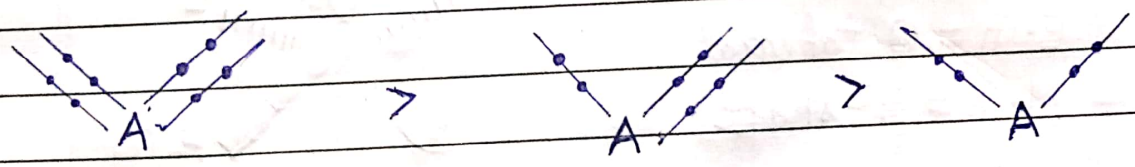
★ VALENCE SHELL ELECTRON PAIR REPULSION THEORY (VSEPR)

According to VSEPR theory, valence shell pair (Bond pair Or Lone pair) of central atom are arranged in space in such direction which cause minimum repulsion between them.

1. Repulsion



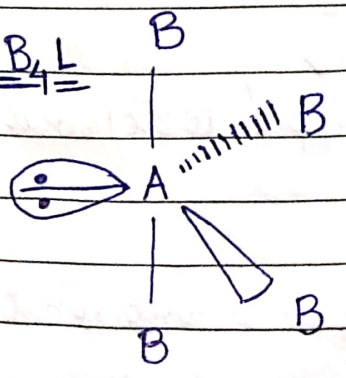
2.



Repulsion

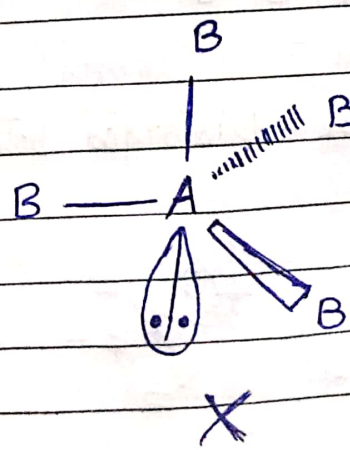
3. Stronger type of repulsion are must be minimum at 90° or below 90°

Q → AB_4L



✓

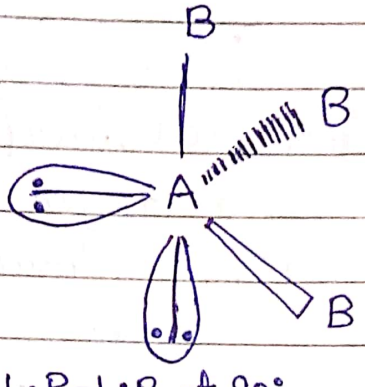
L·P – B·P of 90° = 2



✗

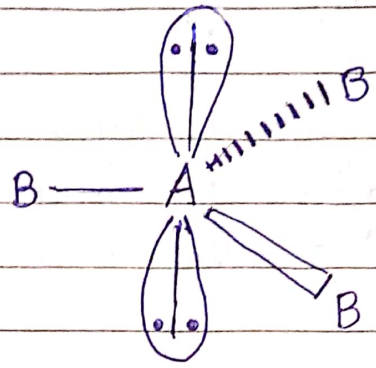
L·P – B·P at 90° = 3

Q → AB_3L_2



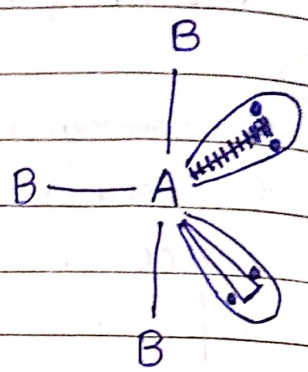
L·P-L·P at 90°

✗



L·P-B·P at 90° = 6

✗



L·P-B·P at 90° = 4

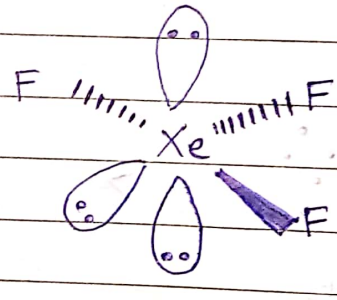
✓

★★ Q → AB_3L_3 → XeF_3^-

n = 6, sp^3d^2

E·G = Octahedral

M·G = T-shape

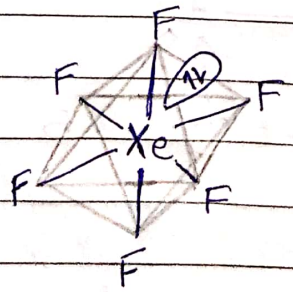


Q → AB_6L → XeF_6

n = 7, sp^3d^3

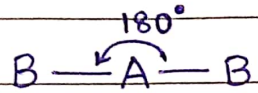
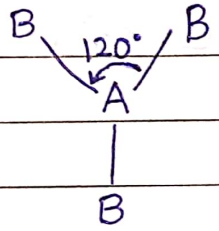
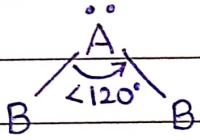
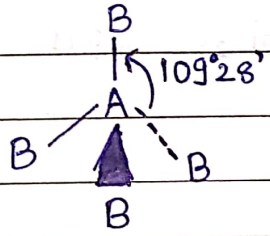
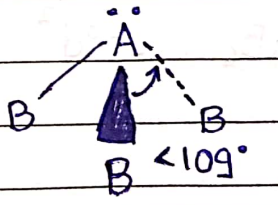
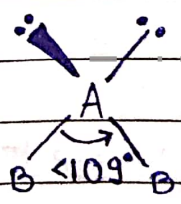
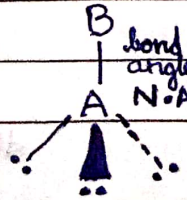
E·G = Pentagonal Bipyramidal

M·G = Distorted Octahedral or Capped Octahedral

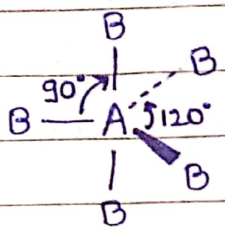
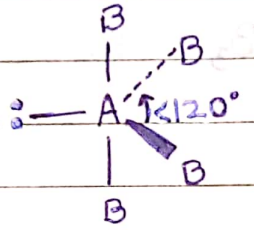
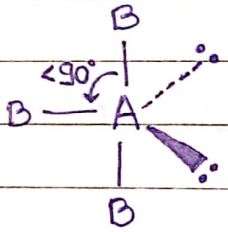
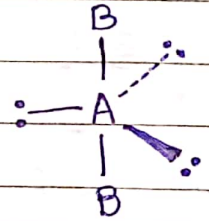
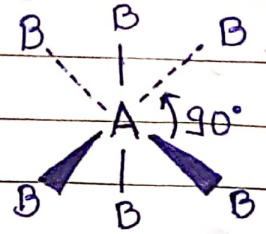
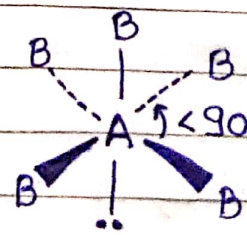


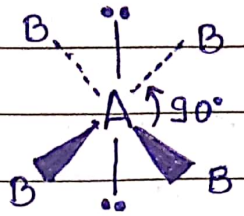
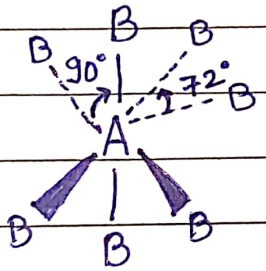
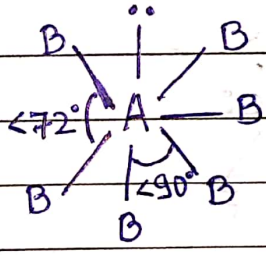
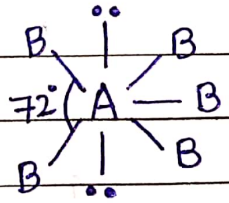
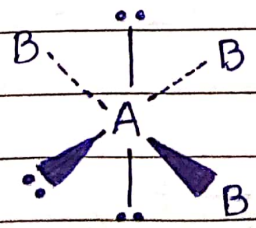
* Lone pair placement is not fixed.

SHAPES OF MOLECULES BASED ON VSEPR THEORY

Total no. of hybrid orbitals	No. of b.p. (bond pairs)	No. of unshared pair i.e lp	General Formula	Type of hybridisation	Stereo chemical formula/ structure	Shape	Example
2	2	0	AB_2	sp		linear	$BeCl_2$
3	3	0	AB_3	sp^2		Trigonal planar	BCl_3, NO_3^-, GaF_3, CO_3^{2-}
3	2	1	AB_2L	sp^2		V or Bent or angular	$SnCl_2$, O_3, SO_2
4	4	0	AB_4	sp^3		Tetrahedron	CH_4, SiF_4, NH_4^+
4	3	1	AB_3L	sp^3		Trigonal pyramidal	NH_3, CH_3^-
4	2	2	AB_2L_2	sp^3		V or Bent or angular	H_2O, SF_2
4	1	3	ABL_3	sp^3		linear	ClO^-

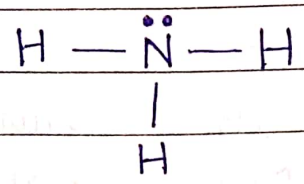
★★

Total no. of hybrid orbitals	No. of b.p. (bond pairs)	No. of unshared pair i.e. l_p	General formula	Type of hybrid-isation	Stereo chemical formula/ structure	Shape	Example
5	5	0	AB_5	sp^3d		Trigonal bipyramidal	PF_5, SF_5^+, $SbBr_5$, XeO_3F_2
5	4	1	AB_4L	sp^3d		Seesaw/ Teetar-Tauter/ Distorted Tetrahedral/ Folded square.	SF_4
5	3	2	AB_3L_2	sp^3d		T-shaped/ Bent T-shaped.	ClF_3, BrF_3
5	2	3	AB_2L_3	sp^3d		Linear	ICl_2^-, XeF_2, I_3^-
6	6	0	AB_6	sp^3d^2	 All bond $\angle = 90°$	Octahedral or Square bipyramidal	SF_6, IF_6^+
6	5	1	AB_5L	sp^3d^2	 All less than 90°	Square pyramidal	IF_5, $XeOF_4$, BrF_5

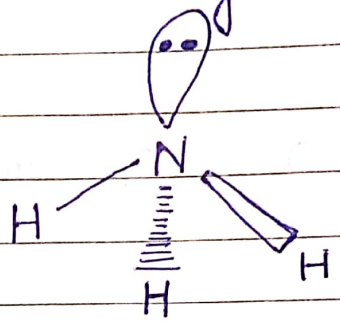
Total no. of hybrid orbitals (bond pairs)	No. of b.p.	No. of unshared pair i.e. lp	General formula	Type of hybridisation	Stereo chemical formula / structure	Shape	Example
6	4	2	AB_4L_2	sp^3d^2		Square planar	IF_4^-, XeF_4, ICl_4^-
7	7	0	AB_7	sp^3d^3		Pentagonal bipyramidal.	IF_7
7	6	1	AB_6L	sp^3d^3		Distorted octahedral	XeF_6, IF_6^-
7	5	2	AB_5L_2	sp^3d^3		Pentagonal planar	XeF_5^-
6	3	3	AB_3L_3	sp^3d^2		T-shape	XeF_3^-

**

e.g. 1. NH_3

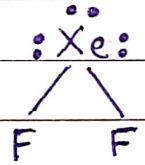


n = 4, sp^3
E.G = Tetrahedral
M.G = Trigonal Pyramidal

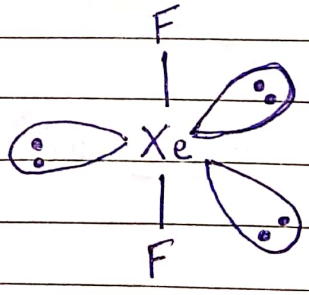


• Non-Planar

2. XeF_2

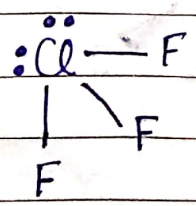


n = 5, sp^3d
E.G = Trigonal bipyramidal
M.G = Linear

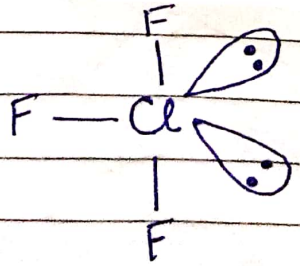


• Planar

3. ClF_3

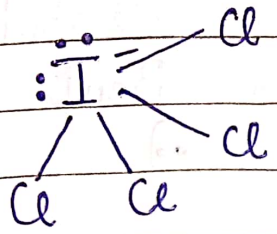


n = 5, sp^3d
E.G = Trigonal bipyramidal
M.G = T-shaped



• Planar

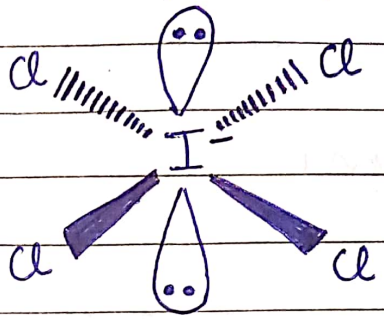
4. ICl_4^-



$n = 6$, sp^3d^2

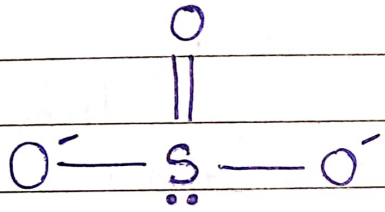
E·G = Octahedral

M·G = Square planar



• Planar

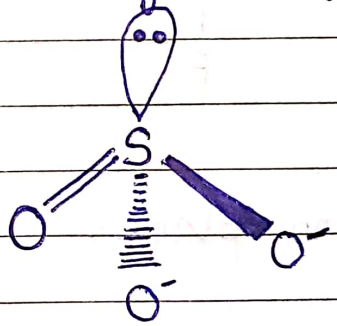
5. SO_3^{2-}



$n = 4$, Tet sp^3

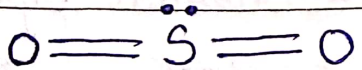
E·G = Tetrahedral

M·G = Trigonal Pyramidal



• Non-Planar

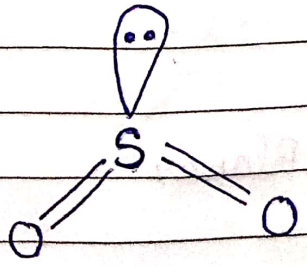
6. SO_2



$n = 3$, sp^2

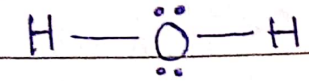
E·G = Trigonal Planar

M·G = Bent



• Planar

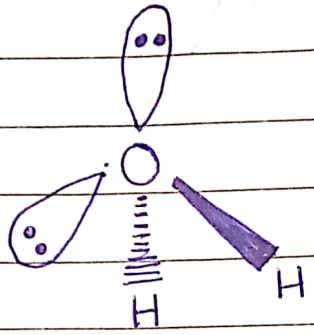
7. H_2O



$n = 4, sp^3$

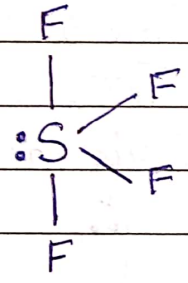
E·G = Tetrahedral

M·G = Bent



- Planar

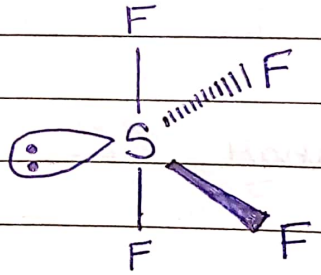
8. SF_4



$n = 5, sp^3d$

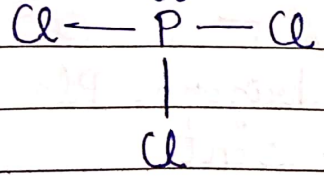
E·G = Trigonal bipyramidal

M·G = See-saw



- Non-planar

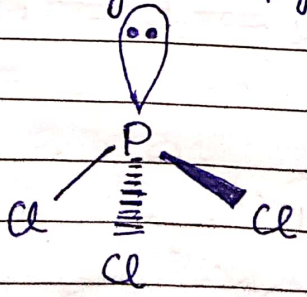
9. PCl_3



$n = 4, sp^3$

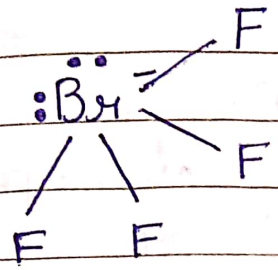
E·G = Tetrahedral

M·G = Trigonal pyramidal



- Non- Planar

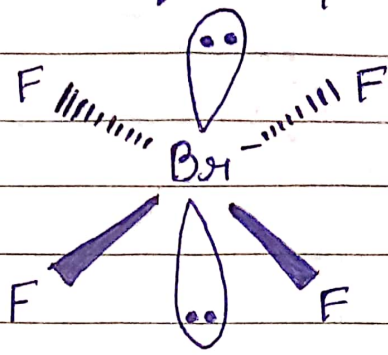
10. BrF_4^-



n = 6, sp^3d^2

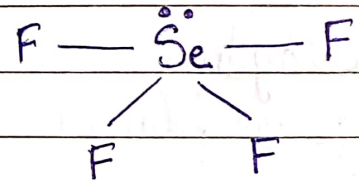
E·G = Octahedral

M·G = Square planar



• Planar

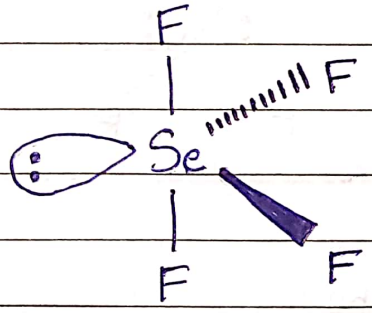
11. SeF_4



n = 5, sp^3d

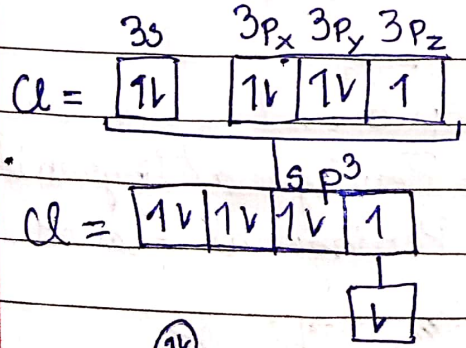
E·G = Trigonal bipyramidal

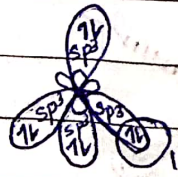
M·G = See-saw



• Non-Planar

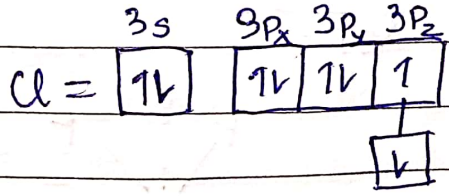
★ HCl

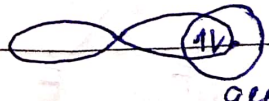




Linear geometry explain by hybridisation

HCl



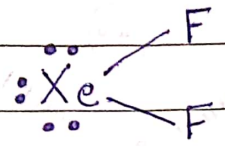


Linear geometry by p-s overlapping

Race #14

Q1]

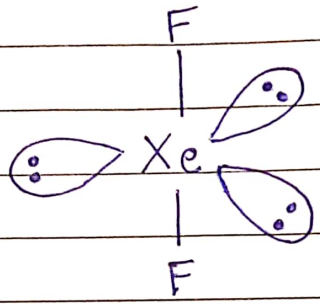
(1) XeF_2



n = 5, sp^3d

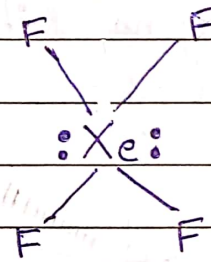
E·G = Trigonal bipyramidal

M·G = Linear



• Planar

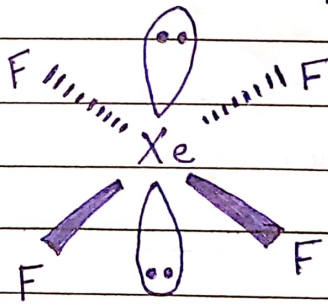
(2) XeF_4



n = 6, sp^3d^2

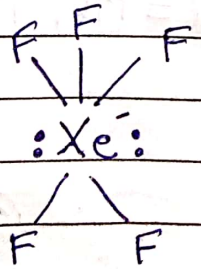
E·G = Octahedral

M·G = Square planar



• Planar

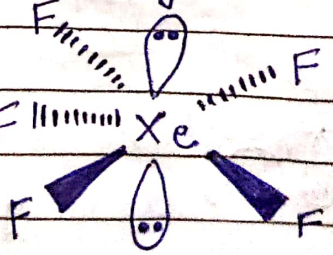
(3) XeF_5^-



n = 7, sp^3d^3

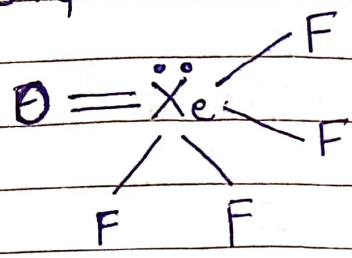
E·G = Pentagonal bipyramidal

M·G = Pentagonal planar



• Planar

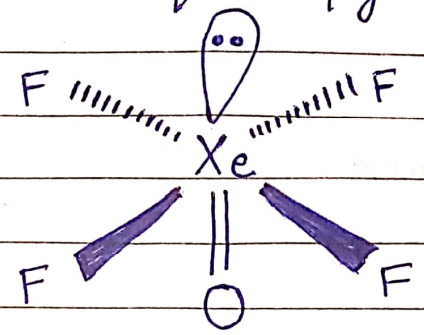
(4) $XeOF_4$



$n = 6, sp^3d^2$

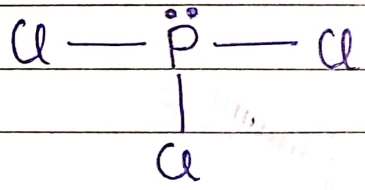
E·G = Octahedral

M·G = Square pyramidal



- 1 $(2p_\pi - 5d_\pi)$
- Non-Planar

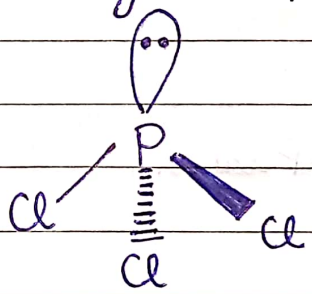
(5) PCl_3



$n = 4, sp^3$

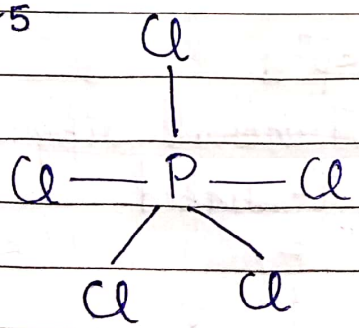
E·G = Tetrahedral

M·G = Trigonal pyramidal



- Non-Planar

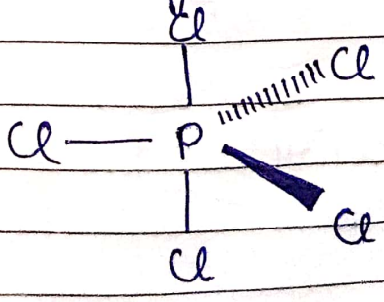
(6) PCl_5



$n = 5, sp^3d$

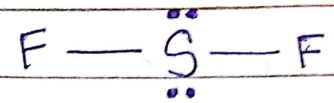
E·G = Trigonal bipyramidal

M·G = Trigonal bipyramidal



- Non-Planar

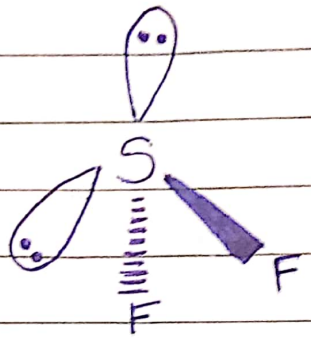
(7) SF_2



n = 4, sp^3

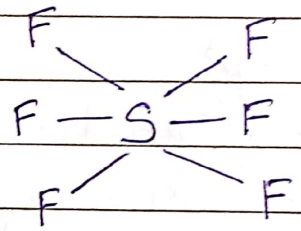
E·G = Tetrahedral

M·G = Bent



• Planar

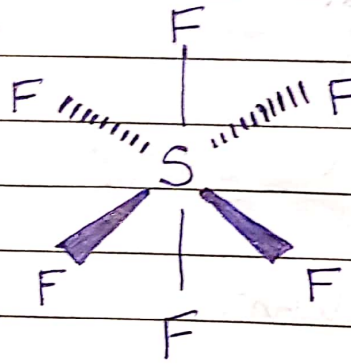
(8) SF_6



n = 6, sp^3d^2

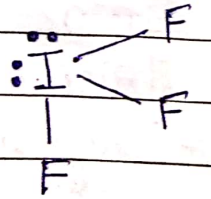
E·G = Octahedral

M·G = Octahedral



• Non-Planar

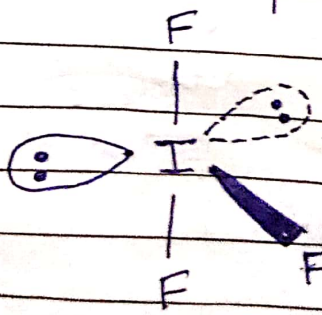
(9) IF_3



n = 5, sp^3d

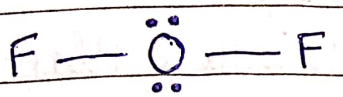
E·G = Trigonal bipyramidal

M·G = T-shaped

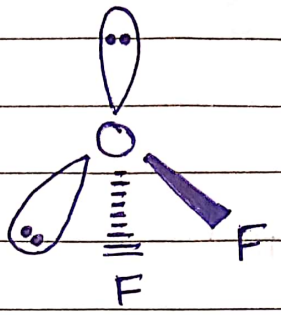


• Planar

(12) OF_2

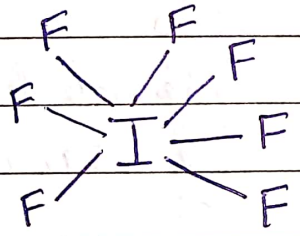


n = 4, sp^3
E·G = Tetrahedral
M·G = Bent

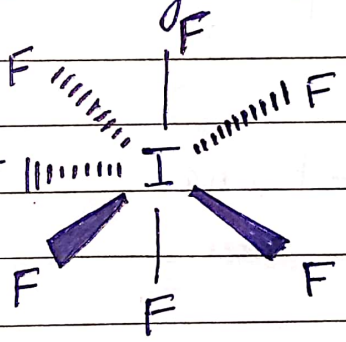


• Planar

(11) IF_7

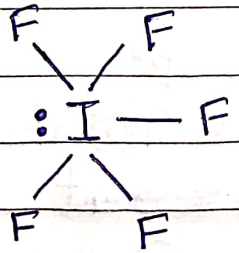


n = 7, sp^3d^3
E·G = Pentagonal bipyramidal
M·G = Pentagonal bipyramidal

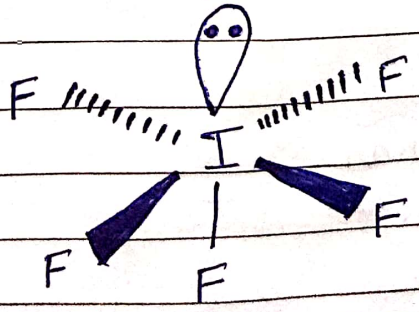


• Non-Planar

(10) IF_5

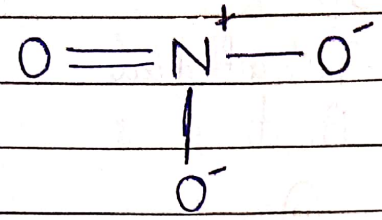


n = 6, sp^3d^2
E·G = Octahedral
M·G = Square pyramidal



• Non-Planar

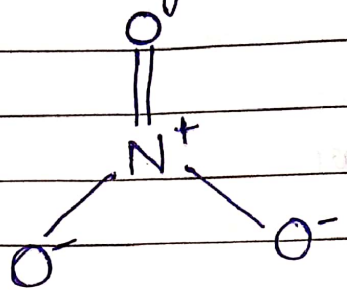
(13) NO_3^-



$n = 3$, sp^2

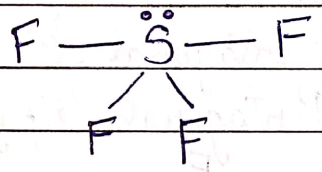
E·G = Trigonal Planar

M·G = Trigonal Planer



- Planar
- $(2p_\pi - 2p_\pi)1$

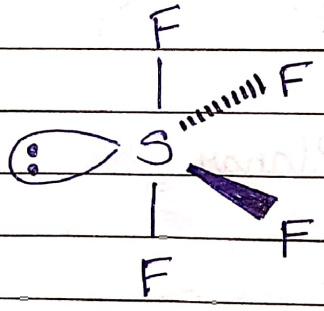
(14) SF_4



$n = 5$, sp^3d

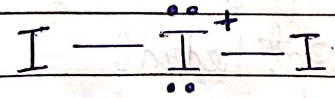
E·G = Trigonal bipyramidal

M·G = See-saw



- Non-Planar.

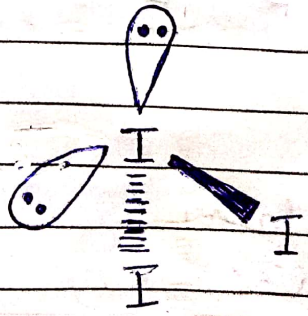
(15) I_3^+



$n = 4$, sp^3

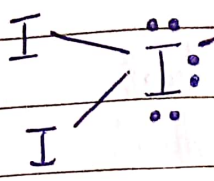
E·G = Tetrahedral

M·G = Bent



- Planar

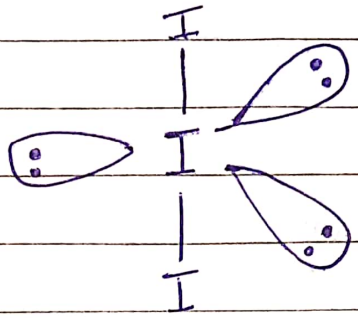
(16) I_3^-



n = 5, sp^3d

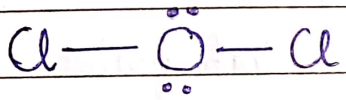
E·G = Trigonal bipyramidal

M·G = Linear



• Planar

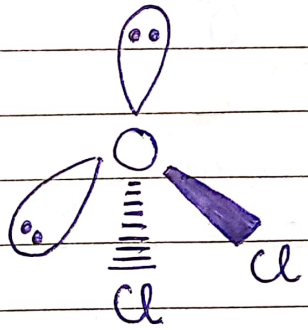
(17) OCl_2



n = 4, sp^3

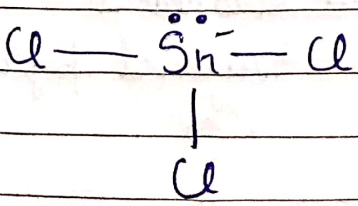
E·G = Tetrahedral

M·G = Bent



• Planar

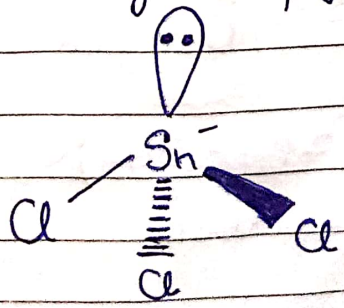
(18) $SnCl_3^-$



n = 4, sp^3

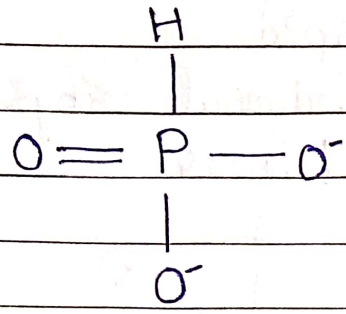
E·G = Tetrahedral

M·G = Trigonal pyramidal

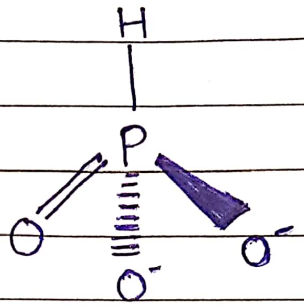


• Non-Planar

(19) HPO_3^{2-}

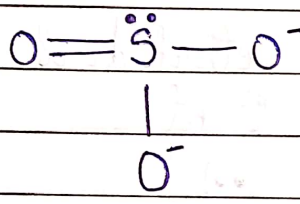


n = 4, sp^3
E.G = Tetrahedral
M.G = Tetrahedral

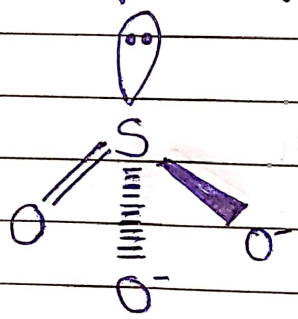


- 1 ($2p_\pi - 3d_\pi$)
- Non-Planar

(20) SO_3^{2-}

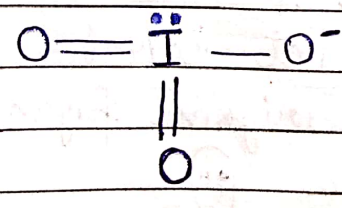


n = 4, sp^3
E.G = Tetrahedral
M.G = Trigonal pyramidal

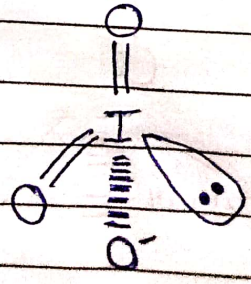


- Non-Planar
- 1 ($2p_\pi - 3d_\pi$)

(21) IO_3^-

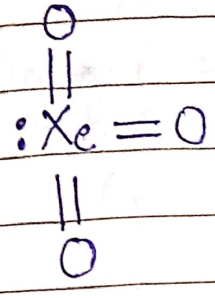


n = 4, sp^3
E.G = Tetrahedral
M.G = Trigonal pyramidal

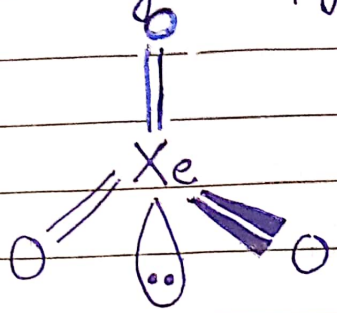


- 2 ($2p_\pi - 5d_\pi$)
- Non-Planar

(22) XeO_3

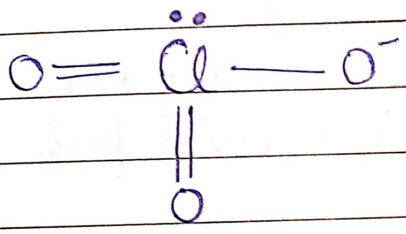


$n = 4, sp^3$
E.G = Tetrahedral
M.G = Trigonal pyramidal

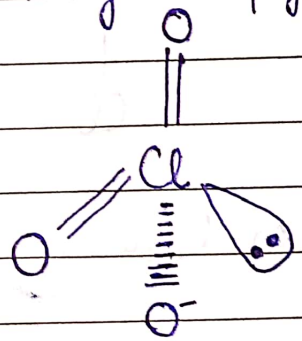


- $3(2p_\pi - 5d_\pi)$
- Non-Planar

(23) ClO_3^-

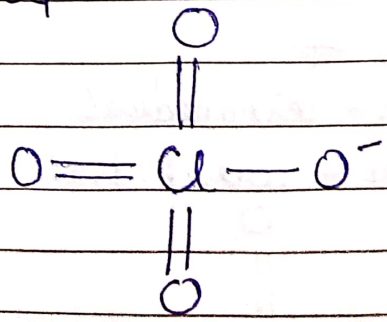


$n = 4, sp^3$
E.G = Tetrahedral
M.G = Trigonal pyramidal

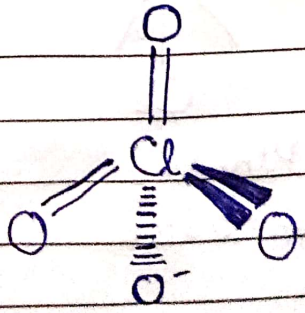


- Non-Planar
- $2(2p_\pi - 3d_\pi)$

(24) ClO_4^-



$n = 4, sp^3$
E.G = Tetrahedral
M.G = Tetrahedral



- Non-Planar
- $3(2p_\pi - 3d_\pi)$

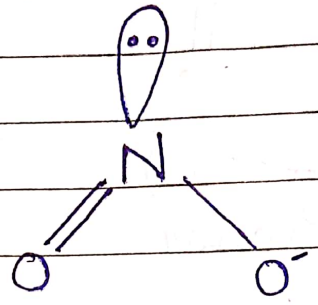
(25) NO_2^-

$O = \ddot{N} - O^-$

$n = 3, sp^2$

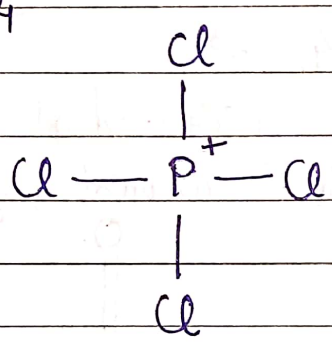
E·G = Trigonal Planar

M·G = Bent



- Planar
- $1(2p_\pi - 2p_\pi)$

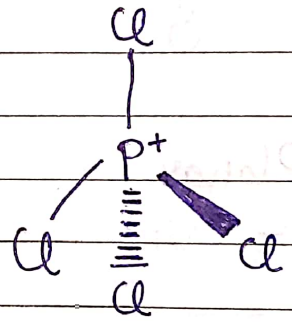
(26) PCl_4^+



$n = 4, sp^3$

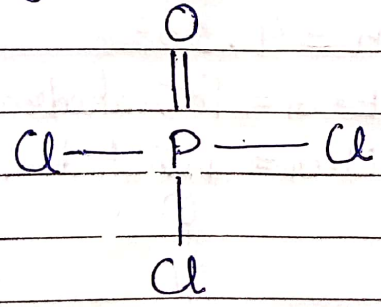
E·G = Tetrahedral

M·G = Tetrahedral



- Non-Planar

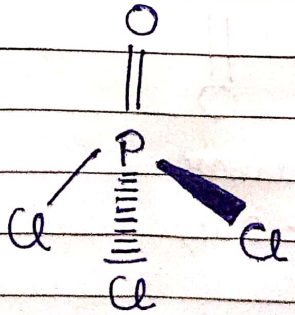
(27) $POCl_3$



$n = 4, sp^3$

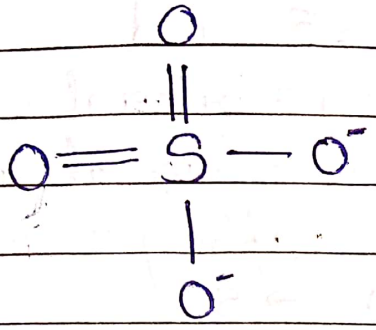
E·G = Tetrahedral

M·G = Tetrahedral



- Non-Planar
- $1(2p_\pi - 3d_\pi)$

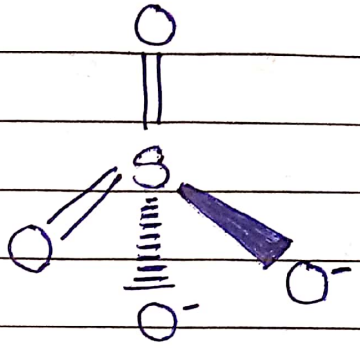
(28) SO_4^{2-}



$n = 4, sp^3$

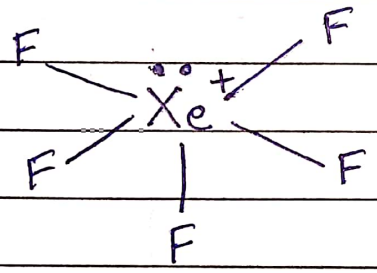
E.G = Tetrahedral

M.G = Tetrahedral



- Non-Planar
- $2(2p_\pi - 3d_\pi)$

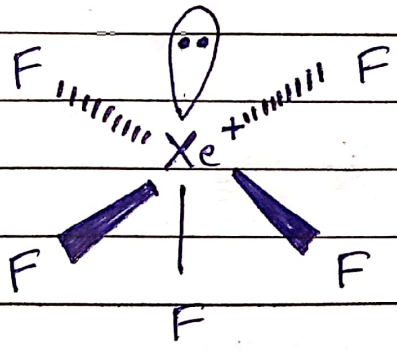
(29) XeF_5^+



$n = 6, sp^3d^2$

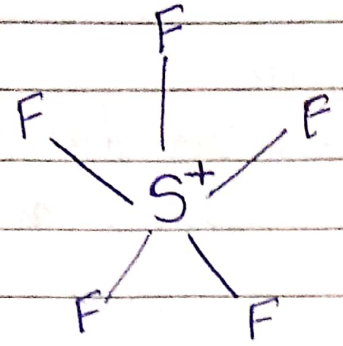
E.G = Octahedral

M.G = Square pyramidal



- Non-Planar

Q- SF_5^+



h = 5, sp^3d

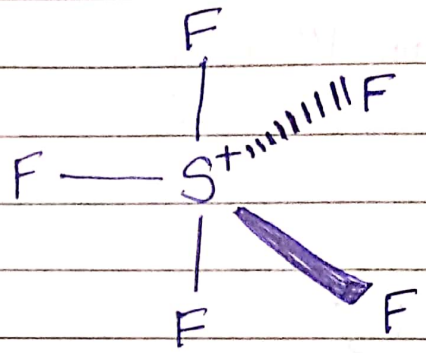
E·G = Trigonal bipyramidal

M·G = Trigonal bipyramidal

Overlapping = $sp^3d - 2p$

$\sigma \rightarrow 5$,

$\pi \rightarrow 0$



• Non-Planar