Chaper 1 [C]

VSEPR Theory

[Valence shell electron pair repulsion Theory]

- This theory was proposed by sidgwick and Nyholm in 1957.
- Accourding to this theory,

"The geometry of the molecule depends upon the number of binding and non-bonding electron pairs arround central atom, which arrange in such way that there is minimum repultion between them."

Rules of VSEPR Theory

Rule-1

If the central atom has only bond pairs of electron (in its valence shell) then the geometry of the molecule is regular

eg

No. of Bond pair	Molecule (A → central atom, B → Bonded atoms)	Geometry	Bond Angle	Examples
2	AB_2	Linear	180°	$BeCl_2$, BeF_2
3	AB_3	Trigonal Planar	120°	BF_3
4	AB_4	Tetrahedral	109° 28'	CH_4
5	AB_5	Trigonal bipyramidal	120° & 90°	PCl_5
6	AB_6	octahedral	90°	SF_6
7	AB_7	pentagonal	72° & 90°	IF_7

Bond angle = 360 / No. of bonds

Rule-2

If the molecule contain lone pair of electrons around central atom then, geometry of molecule gets disturbs and affects bond angle.

extra

Order of repultion → lone pair-lone pair > lone pair-Bond pair > B.P-B.P

The lone pair of electrons occupies more space than bond pair. Therefore repultion between lone pair is more than bond pair.

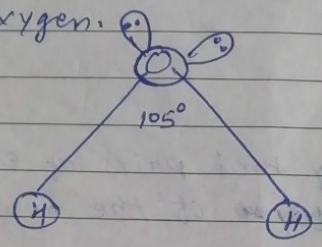
eg.

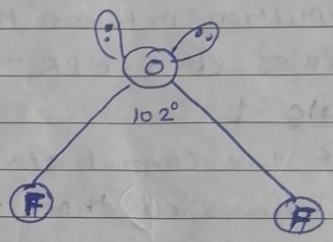
Molecule	No. of B.P.	No. of L.P.	Actual geometry	Bond angle
CH_4	4	0	Tetrahedral	109° 28'
NH_3	3	1	Pyramidal	107° 28'
H_2O	2	2	V-shaped	104° 28'

Rule - 3.

IF the electronegativity of bonded atom is more than, electron pairs are (attracted toward electronegative atom) pulled away from the central atom. Due to this repulsion between bond pairs decreases and also bond angle decreases.

eg In H_2O bond angle is 105° & in OF_2 bond angle is 102° because Fluorine is more electronegative than oxygen.





Rule - 4

The repulsion between electron pairs of completely filled valence shell is greater than the repulsion between electron pair of incompletely filled valence shells.

eg H_2O and H_2S

H_2O

$_8O \rightarrow 2 | 6$

$1s^2 | 2s^2 2p^4$

1s | 1s | 2p$_x$ | 2p$_y$ | 2p$_z$

↑↓ | ↑↓ | ↑↓ | ↑ | ↑

→ completely filled valence orbitals of oxygen.

→ ~~Bond angle = 105°~~ Extent of

→ Repulsion in electron pair is more & bond angle is more

→ Bond angle = 105°

H_2S

$_{16}S \rightarrow 2, 8 | 6$

$\rightarrow 1s^2 2s^2 2p^6 | 3s^2 3p^4 3d^0$

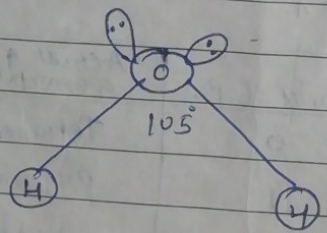
3s | 3p | 3d

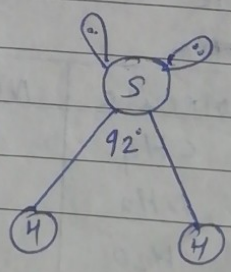
↑↓ | ↑↓ | ↑ | ↑

→ Incompletely filled valence orbitals of sulphur

→ Extent of repulsion bet^n electron pair is less & therefore bond angle is less.

→ Bond angle = 92°





Rule -5

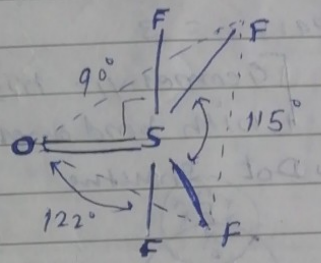
Bond angle in the molecule involving multiple bond is greater than that of single bond.

Extra shot ↗ Not written in exam

⇒ Multiple bonds behave like lone pair and occupy the position where there is minimum ~~repulsion~~ interaction with other electron pair

⇒ In Trigonal bipyramidal geometry, multiple bond will occupy equatorial site therefore bond angle is increased but does not change geometrical shape of molecule.

eg SOF_4 molecule



Rule -6

Repulsion is maximum when electron pairs are at 90° and it decreases sharply with increase in bond angle and minimum at 180°.

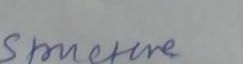
Applications of VSEPR Theory

(A) Structure of molecule with regular geometry.

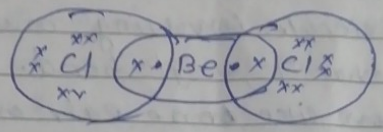
(1) Shape of $BeCl_2$ molecule [AB_2 Type]

- Central atom is Be
- Electronic configuration of Be is $1s^2 2s^2$
- Number of valence electrons is 2
- No. of $\bar{e}$s contributed by two chlorine atoms are 2
- Total no. of valence electrons = 2+2 = 4
- No. of valence electron pairs = 2
- No. of bond pairs = 2 [∵ geometry is linear with bond angle 180°]

- Dot & Structure



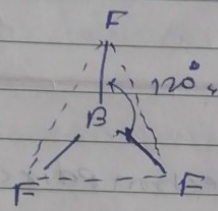
→ Lewis Structure



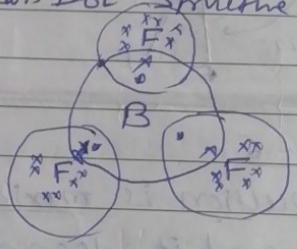
(2) Structure of BF_3 molecule [AB_3 Type]

- Central atom is B
- Electronic configuration of B is $1s^2 2s^2 2p^1$
- No. of valence electrons = 3
- No. of $\bar{e}$s contributed by Flumine atoms = 3
- Total no. of valence electrons = 3+3=6
- No. of valence electron pairs = 3
- No. of bond pairs = 3 [Geometry is trigylar planer with bond angle - 120°]

→ Dash structure



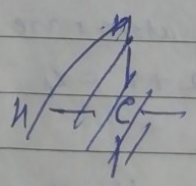
Lewis Dot Structure

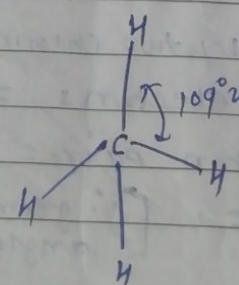


(3) Shape of methane molecule [AB_4 Type]

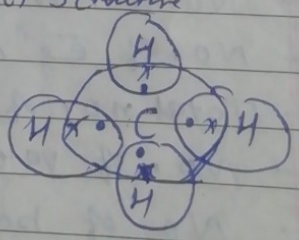
- Central atom is Carbon
- E.C. of Carbon is - $1s^2 2s^2 2p^2$
- No. of valence electron = 4
- No. of $\bar{e}$s contributed by 4-Hydrogen atoms = 4
- Total no. of valence electrons = 8
- No. of valence electron pairs = 4
- No. of bond pair = 4 [Geometry is tetrahedral with bond angle - 109°28']

→ Dash Structure





Dot structure



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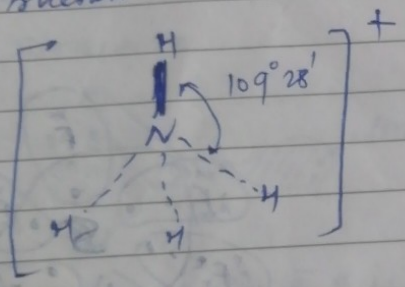
(4) Shape of NH_4^+ molecule [AB_4 Type]

- Central atom is Nitrogen
- E.C. of Nitrogen - $1s^2 2s^2 2p^3$
- No. of valence electrons = 5
- No. of electrons contributed by 4-H-atoms = 4
- Total no. of valence electrons = 5+4-1 = 8
- No. of bond pairs = 4 [Therefore geometry is tetrahedral with bond angle $109^\circ 28'$]

- Structure

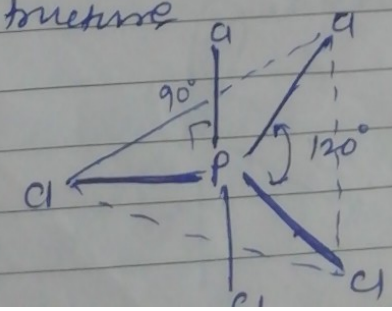


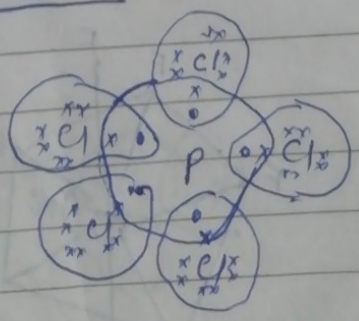
(5) Shape of PCl_5 molecule [AB_5 Type]

- Central atom is Phosphorous
- E.C. of Phosphorous = $1s^2 2s^2 2p^6 3s^2 3p^3$
- No. of valence electrons = 5
- No. of electrons contributed by five chlorine atoms = 5
- Total no. valence electrons = 10
- Total no. valence electron pair = 5
- Geometry - Trigonal bipyramidal.
- Bond angle - $120^\circ, 90^\circ$

extra [In TBP, Three bonds are present along trigonal plane called as equatorial bonds and two bonds are perpendicular to the plane called as axial bonds

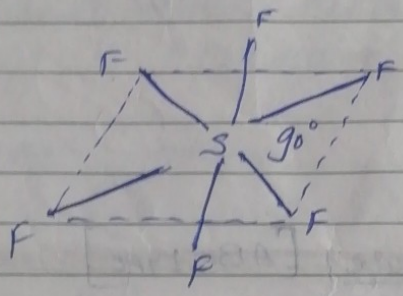
- Structure

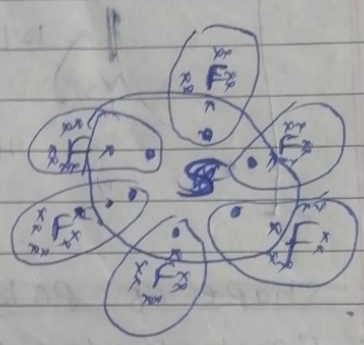




(6) Shape of SF_6 molecules [AB_6 TYPE]

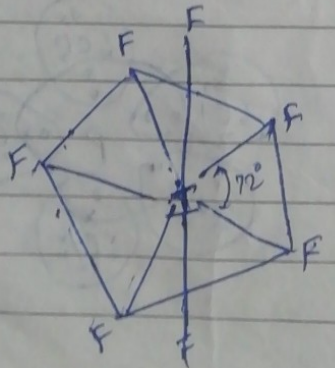
- Central atom is Sulphur
- E.C. of Sulphur - $1s^2 2s^2 2p^6 3s^2 3p^4$
- No. of valence electron = 6
- No. of electrons contributed by six fluorine atoms = 6
- Total no. of valence electrons = 6+6 = 12
- No. of valence shell electron pairs = 6
- No. of bond pairs = 6
- Geometry = Octahedral
- Bond angle = 90°
- Structure





(7) Shape of IF_7 molecule [AB_7]

- Central atom - Iodine
- Valence shell E.C. of iodine = $5s^2 5p^5$
- No. of valence electron = 7
- No. of Es contributed by 7 fluorine atom = 7
- Total no. of valence electrons = 7+7 = 14
- No. of valence electron pairs = 7
- No. of bond pairs = 7
- Geometry - Pentagonal bipyramidal
- Bond angle - 72°, 90°



C Si Ge Sn Pb (OR) C Si Ge Sn Pb
कोरशी गमे शिव पार्वती — पंडुओं सिनाटल अर्जुन पंजाबमध्ये दिल्ली

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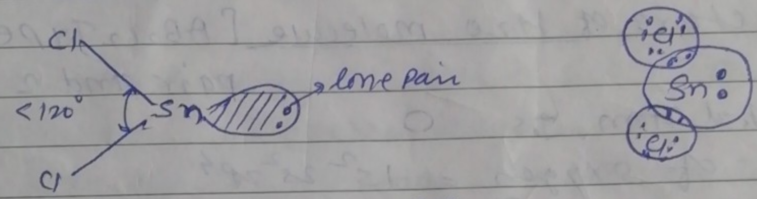
(14) **Structure of molecules with distorted geometry [Containing lone pair]**

C-6
Si-14
Ge-32
Sn-50
Pb-82
FI-114

(1) **Structure of $SnCl_2$ molecule [AB_2L Type - 2 bond pair & 1 lone pair]**

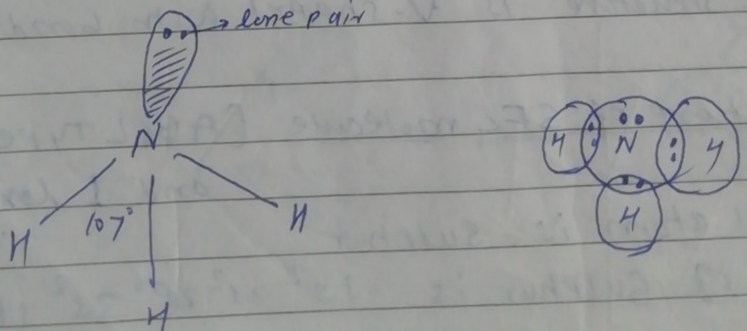
- Central atom is tin (Sn)
- Valence shell E.C. of Sn - $5s^2 5p^2$
- No. of valence electrons = 4
- No. of $\bar{e}$s contributed by two chlorine atoms = 2
- Total no. of valence electrons = 4+2 = 6
- Total no. of valence electrons pairs = 3
- Structure



As total no. of $\bar{e}$ pairs are three therefore expected geometry is trigonal planar but due to the presence of lone pair, geometry is distorted and actual structure is V-shaped or angular or bent. and bond angle is less than 120°.

(2) **Structure of NH_3 molecule [AB_3L Type - 3 bond pair and 1 lone pair]**

- Central atom is nitrogen
- E.C. of nitrogen is $1s^2 2s^2 2p^3$
- No. of valence electron is 5
- No. of $\bar{e}$s contributed by three Hydrogen atoms = 3
- Total no. of valence electrons = 5+3 = 8
- Total no. of valence electrons pair = 4



Total no: of electron pairs are 4. Therefore excepted geometry is tetrahedral but due to presence of lone pair of e^-, geometry is destorted ~~tetrahedral~~ and actual structure is pyramidal and bond angle decreases to 107°

(3) Structure of PCl_3 molecule [AB_3L type - 3 bond pairs and 1 lone pair]

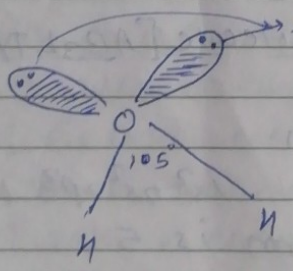
same as that of NH_3

(4) Structure of H_2O molecule [AB_2L_2 Type - 2 bond pair and 2 lone pair]

Central atom is O

E. C. of oxygen = $1s^2 2s^2 2p^4$

- No. of valence $\bar{e}$s = 6
- No. of $\bar{e}$s contributed by two Hydrogen atoms = 2
- Total no. of valence shell electrons = 6 + 2 = 8
- Total no. of valence shell $\bar{e}$s pairs = 4



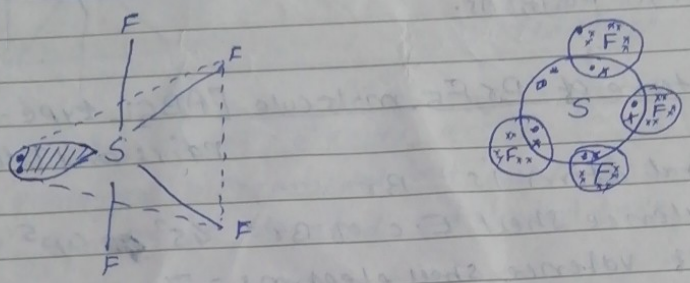
Total no. of electron pairs are 4. Therefore expected geometry is tetrahedral but due to the presence of two lone pairs of $\bar{e}$, geometry is distorted and actual structure is V-shaped with bond angle 105°.

(5) Structure of SF_4 molecule [AB_4L Type - 4 bond pairs and 1 lone pair]

Central atom is Sulphur

E. C. of Sulphur is $1s^2 2s^2 2p^6 3s^2 3p^4$

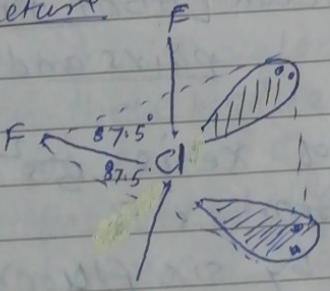
- NO. of valence $\bar{e}s$ = 6
- NO. of $\bar{e}s$ contributed by Four Flourine atoms = 4
- Total no. of valence shell electrons = 6+4=10
- Total no. of valence shell $\bar{e}s$ pairs = 5
- Structure:

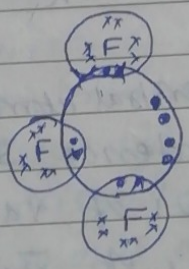


Total no. of valence $\bar{e}s$ pairs are 5 Therefore expected geometry is Trigonal bipyramidal but due to presence of lone pair of electrons, The geometry is distorted. The lone pair occupy equatorial position in TBP geometry. and actual geometry is See-saw type OR distorted tetrahedral type.

⑥ Structure of ClF_3 molecule [AB_3L_2 type - 3 bond pairs and 2 lone pairs]

Central atom is chlorine [Cl]
E.C. of chlorine is $1s^2 2s^2 2p^6 3s^2 3p^5$
NO. of Valence shell electrons = 7
NO. of $\bar{e}s$ contributed by three fluorine atoms = 3
Total NO. of valence shell electrons = 7+3=10
- Total no. Valence sheel electron pairs = 5
- Structure





Total no. of valence electrons pairs are 5. out of these three are bond pairs and two are lone pairs. Because of two lone pairs, geometry is distorted and shape of molecule is T-shaped and bond angle is 87.5°. Two lone pairs are present at equatorial positions.

⑦ Structure of BrF_5 molecule [AB_5L type - 5 bond pairs and 1 lone pair]

Central atom is Br

The valence shell E.C. of Br = $4s^2 4p^5$

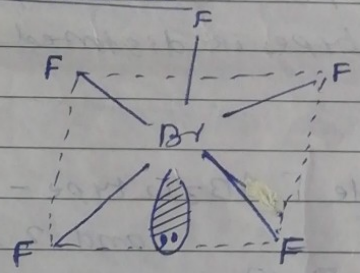
NO. of valence shell electrons = 7

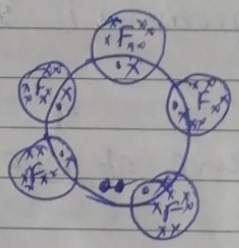
NO. of $\bar{e}$s contributed by five fluorine atoms = 5

NO. of valence shell electrons = 7 + 5 = 12

NO. of valence shell electrons pairs = 6

Structure





Total no. of valence $\bar{e}$s pairs are 6, Therefore expected geometry is octahedral but due to the presence of one lone pair, the geometry is distorted and actual shape of molecule is square pyramidal.

⑧ Structure of XeF_6 molecule [AB_6L TYPE - 6 bond pairs and 1 L.P.]

Central atom is Xe

Valence shell E.C. of Xe is $5s^2 5p^6$

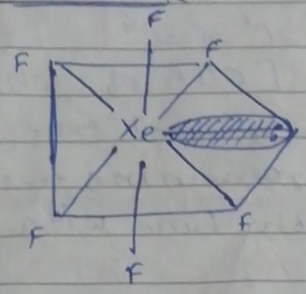
NO. of valence electrons is 8

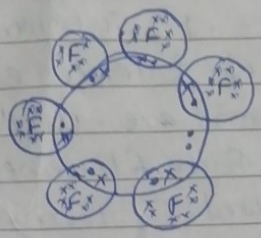
NO. of $\bar{e}$s contributed by six fluorine atoms = 6

Total no. of valence electrons = 8 + 6 = 14

Total no. of valence shell electron pairs = 7

Structure





The total no. of $\bar{e}$ pairs are 7. Therefore expected geometry is pentagonal bipyramidal but due to the presence of one lp. geometry is distorted octahedral type.

Structure of molecules with multiple bonds (double / triple bonds)

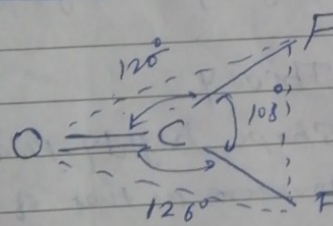
① Structure of COF_2 molecule

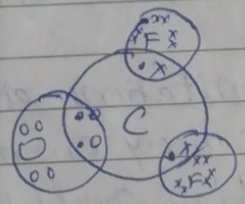
Central atom is carbon

E.C. of carbon is $1s^2 2s^2 2p^2$

NO. of valence electrons = 4 [out of four electrons, two electrons are used for formation of two bonds with two fluorine atoms and remaining two $\bar{e}$s are used for double bond with oxygen atom.]

Structure





from Fluorine ↓ 2 + 2 ← oxygen

Total no. of valence shell $\bar{e}$s are = 4 + 2 + 2 = 8

Total no. of valence shell $\bar{e}$s pairs = 4. [out of which three bond pairs are used for formation of σ-bonds and one pair of $\bar{e}$ is used for π-bond]

Therefore expected geometry is trigonal planar and bond angle is 120°. but due to the presence of double bond, bond angles are slightly changed and they are 126° and 108°.

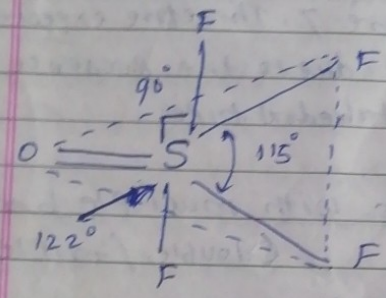
(2) Structure of SOF_4 molecule

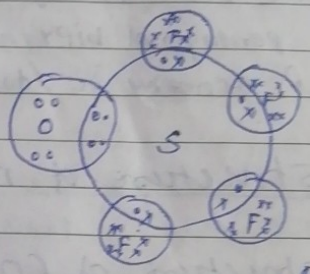
Central atom is sulphur (S)

E.C. of sulphur is $1s^2 2s^2 2p^6 3s^2 3p^4$

No. of valence electrons = 6 [Out of which four electrons are used for the formation of four bonds with four flourine atoms and remaining two electrons are used for formation of double bond with oxygen atom]

Structure





Total no. of valence shell electrons are $= 6 + 4 + 2 = 12$

Total no. of valence shell $\bar{e}$ pairs = 6 [out of which five bond pairs are used for formation of 5 σ-bonds and one pair of electrons is used for double bond.]

Therefore expected geometry is Trigonal bipyramidal but due to the presence of one double bond at equatorial position, the bond angle is slightly changed.

Limitations of VSEPR Theory

(1) This theory can not explain shape highly polar molecules eg Li_2O should have same structure as that of water (V-shape) but actually Li_2O is linear.

(2) This theory can not explain shape of molecules with extensive delocalised electron system.

(3) This theory cannot explain shape of molecule containing inert pair of electrons.

(4) This theory can not explain shape of some transition metal complexes.

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