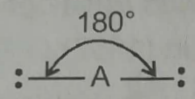
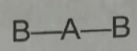
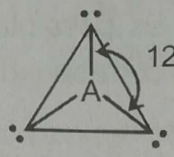
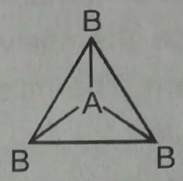
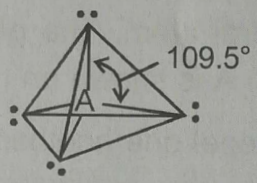
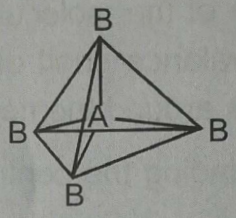
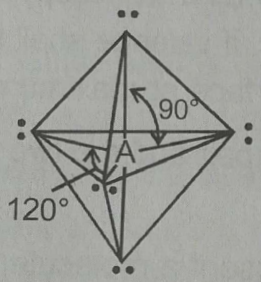
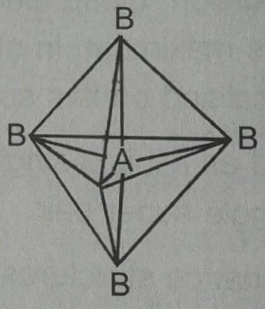
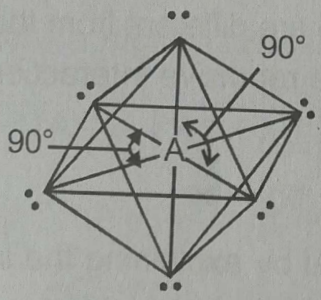
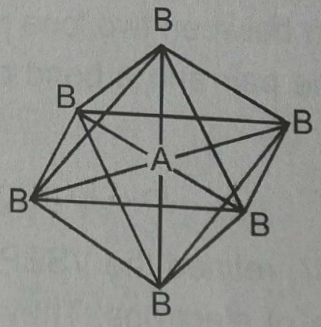
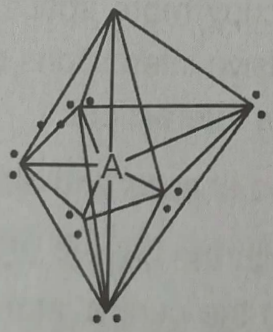
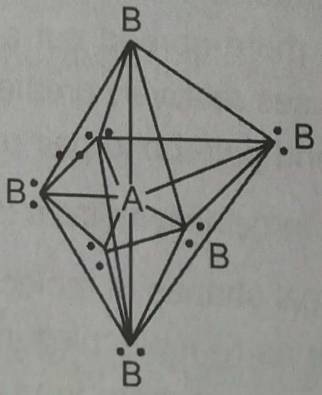
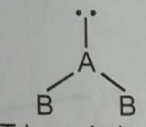
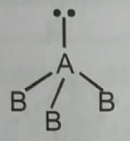
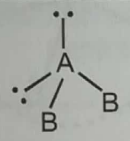
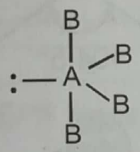
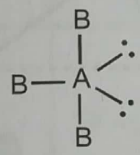
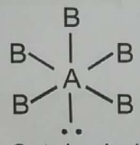
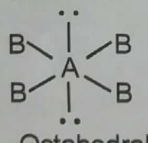
Geometry of Molecules in which the Central Atom has No Lone Pair of Electrons

Number of electron pairs	Arrangement of electron pairs	Molecular geometry	Examples
2	 Linear	 Linear	$BeCl_2$, $HgCl_2$
3	 Trigonal planar	 Trigonal planar	BF_3
4	 Tetrahedral	 Tetrahedral	CH_4, NH_4^+
5	 Trigonal bipyramidal	 Trigonal bipyramidal	PCl_5
6	 Octahedral	 Octahedral	SF_6
7	 Pentagonal Bipyramidal	 Pentagonal Bipyramidal	IF_7

r the table shown as above in compounds of AB_2, AB_3, AB_4, AB_5 and AB_6 the arrangement of

Some Simple Molecules/Ions with Central Ions having One or More Lone Pairs of Electrons(E)

Molecule type	No. of bonding pairs	No. of lone pairs	Arrangement of electron pairs	Shape	Examples
AB_2E	2	1	 Trigonal planar	Bent	SO_2, O_3
AB_3E	3	1	 Tetrahedral	Trigonal pyramidal	NH_3
AB_2E_2	2	2	 Tetrahedral	Bent (V-shaped)	H_2O
AB_4E	4	1	 Trigonal bi-pyramidal	See-saw	SF_4
AB_3E_2	3	2	 Trigonal bi-pyramidal	Distorted T-shape	ClF_3
AB_5E	5	1	 Octahedral	Square pyramid	BrF_5
AB_4E_2	4	2	 Octahedral	Square planar	XeF_4

Type of Hybridisation	Atomic orbitals Involved	Spatial orientation of hybrid orbitals	Examples
sp^3d	$s + \underbrace{p_x + p_y + p_z}_{} + \underbrace{d_{z^2}}_{\text{outer}}$	Trigonal bipyramidal	PF_5, PCl_5
dsp^3	$\underbrace{d_{z^2}}_{\text{inner}} + s + \underbrace{p_x + p_y + p_z}_{}$	Trigonal bipyramidal	$[Fe(CO)_5]$
sp^3d^2	$s + \underbrace{p_x + p_y + p_z}_{} + \underbrace{d_{z^2} + d_{x^2-y^2}}_{\text{outer}}$	Octahedral	SF_6, $[CrF_6]^{3-}$
d^2sp^3	$\underbrace{d_{z^2} + d_{x^2-y^2}}_{\text{inner}} + s + \underbrace{p_x + p_y + p_z}_{}$	Octahedral	$[Co(NH_3)_6]^{3+}$
dsp^2	$\underbrace{d_{x^2-y^2}}_{\text{inner}} + s + \underbrace{p_x + p_y}_{}$	Square planar	$[Ni(CN)_4]^{2-}$, $[Cu(NH_3)_4]^{+2}$ $[Pt(Cl)_4]^{2-}$
sp^3d^3	$s + p_x + p_y + p_z + d_{xy} + d_{yz} + d_{zx}$	Pentagonal bipyramidal	IF_7

anion, the charge on the ion is represented by (a) whereas as if it is cation, the charge on it represented by c.

Calculate the number of hybrid orbitals (X) from the knowledge of SA, G, V as:

$X = SA + \frac{1}{2}(G\text{-}V)$ or $X = SA + \frac{1}{2}(G\text{-}V + a)$ or $X = SA + \frac{1}{2}(G\text{-}V - c)$

(For simple molecule) (For polyatomic anion) (For polyatomic cation)

Alternatively, the value of X can also be calculated by taking the sum of number of sigma bonds, number of co-ordinate bonds, number of lone pairs and number of odd electrons around the central atom in a species.

Now, hybrid state, shape, etc., can be predicted from the following table:

Value of X	*Hybrid state of central atom*	*Number of SA*	*Number of LP*	*Arrangement of SA and LP (geometry)*	*Shape*	*Type of molecule and Examples* **A** = *Central atom* **B** = *SA* **L** = *Lone pair*	
2	*sp*	2	0	Linear	Linear	AB_2	BeF_2, CO_2, CS_2, NO_2^+
3	sp^2	3	0	Trigonal Planar	Trigonal Planar	AB_3	BF_3, $AlCl_3$, SO_3, NO_3^-, CO_3^{2-}
		2	1	Do	Bent	AB_2L	SO_2, $PbCl_2$, $SnCl_2$, NO_2^-
4	sp^3	4	0	Tetrahedral	Tetrahedral	AB_4	CH_4, $SiCl_4$, SO_4^{2-}, ClO_4^-
		3	1	Do	Pyramidal	AB_3L	NH_3, NF_3, PH_3, PCl_3, H_3O^+
		2	2	Do	Bent	AB_2L_2	H_2O, NH_2^-
5	sp^3d	5	0	Trigonal bipyramidal	Trigonal bipyramidal	AB_5	PCl_5, PF_5, $SbCl_5$
		4	1	Do	See-saw	AB_4L	SF_4, TeF_4
		3	2	Do	T-shape	AB_3L_2	ClF_3, BrF_3
		2	3	Do	Linear	AB_2L_3	XeF_2, I_3^-, Br_3^-
6	sp^3d^2	6	0	Octahedral	Octahedral	AB_6	SF_6, SeF_6
		5	1	Do	Square pyramidal	AB_5L	IF_5, BrF_5
		4	2	Do	Square planar	AB_4L_2	XeF_4

If the value of X is 7, the hybrid state is sp^3d^3 and the geometry is pentagonal bipyramidal.

ILLUSTRATIONS : Let us find the hybrid state of some atoms :

(i) **S in SO_3 :** Here, SA = 3, G = 6, V = 6

$\therefore \quad X = 3 + \frac{1}{2}(6-6) = 3$ $\quad \therefore$ Hybrid state of S is sp^2

(ii) **S in SO_4^{2-} :** Here, SA = 4, G = 6, V = 8, a = 2

$\therefore \quad X = 4 + \frac{1}{2}(6-8+2) = 4$ $\quad \therefore$ Hybrid state of S is sp^3

(iii) **S in SF_4 :** Here, SA = 4, G = 6, V = 4

$\therefore \quad X = 4 + \frac{1}{2}(6-4) = 5$ $\quad \therefore$ Hybrid state of S is sp^3d

(iv) **Cl in ClO_3^- :** Here, SA = 3, G = 7, V = 6, a = 1

$\therefore \quad X = 3 + \frac{1}{2}(7-6+1) = 4$ $\quad \therefore$ Hybrid state of Cl is sp^3