

Hybridization

Predicting type of hybridisation & The shape of the molecule :

Number of electron pairs in central atom = $\frac{\text{Group number of central atom} + \text{number of bonded pairs}}{2}$

BeCl ₂	number of e ⁻ pairs = $\frac{2+2}{2} = 2$	sp	linear
BCl ₃	number of e ⁻ pairs = $\frac{3+3}{2} = 3$	sp ²	Trigonal planar
SO ₂	number of e ⁻ pairs = $\frac{6+0}{2} = 3$	sp ² (2b.p + 1l.p)	Angular
SO ₃	number of e ⁻ pairs = $\frac{6+0}{2} = 3$	sp ² (3b.p + 0 l.p)	Trigonal planar
NH ₃	number of e ⁻ pairs = $\frac{5+3}{2} = 4$	sp ³ (3b.p + 1 l.p)	Pyramidal
H ₃ O ⁺	number of e ⁻ pairs = $\frac{6+3-1}{2} = 4$	sp ³	Pyramidal

No. of electron pairs	Bond pairs	lone pairs	Hybridisation	Shape	Angle	Examples
2	2	-	sp	Linear	180°	BeCl ₂ , CO ₂ , HCN
3	3	-	sp ²	Trigonal planar	120°	BCl ₃ , BF ₃ , SO ₂
	2	1	sp ²	Angular	-	SO ₂ , SnCl ₂
4	4	-	sp ³	Tetrahedral	109°	CH ₄ , CCl ₄ , CF ₄
	3	1	sp ³	Pyramidal	107°	NH ₃ , H ₃ O ⁺ (Hydronium ion)
	2	2	sp ³	Angular	-	H ₂ O, H ₂ S, Cl ₂ O, OF ₂
5	5	-	sp ³ d	Trigonal bipyramidal	90°, 120° 180°	PCl ₅ , PF ₅
	4	1	sp ³ d	Distorted tetrahedral	-	SCl ₄ , SF ₄
	3	2	sp ³ d	T	90°, 180°	ClF ₃ , BrF ₃ , ICl ₃
	2	3	sp ³ d	Linear	180°	XeF ₂ , ICl ₂ [⊖]
6	6	-	sp ³ d ²	Octahedral	90°	SF ₆
	5	1	sp ³ d ²	Distorted octahedral	-	ClF ₅ , IF ₅
	4	2	sp ³ d ²	Square planar	90°	XeF ₄
7	7	-	sp ³ d ³	Pentagonal bipyramidal	72°, 90°	IF ₇
	6	1	sp ³ d ³	Distorted octahedral	-	XeF ₆

CCl ₄	number of e ⁻ pairs = $\frac{4+4}{2} = 4$	tetrahedral	
PCl ₅	number of e ⁻ pairs = $\frac{5+5}{2} = 5$	sp ³ d	trigonal bipyramidal
SF ₆	number of e ⁻ pairs = $\frac{6+6}{2} = 6$	sp ³ d ²	octahedral
IF ₇	number of e ⁻ pairs = $\frac{7+7}{2} = 7$	sp ³ d ³	pentagonal bipyramidal

H ₂ O	number of e ⁻ pairs =	$\frac{6+2}{2} = 4$	(2 b.p + 2 l.p) sp ³	Angular
NH ₃	number of e ⁻ pairs	$= \frac{5+3}{2} = 4$	(3 b.p + 1 l.p) sp ³	Pyramidal
NF ₃	number of e ⁻ pairs	$= \frac{5+3}{2} = 4$	sp ³ (3b.p + 1l.p)	Pyramidal
PCl ₃	number of e ⁻ pairs	$= \frac{5+3}{2} = 4$	sp ³ (3b.p + 1 l.p)	Pyramidal
POCl ₃	number of e ⁻ pairs	$= \frac{5+3}{2} = 4$	sp ³ (4b.p + o l.p)	Tetrahedral
SOCl ₂	number of e ⁻ pairs	$= \frac{6+2}{2} = 4$	sp ³ (3b.p + 1 l.p)	Pyramidal
XeF ₂	number of e ⁻ pairs	$= \frac{8+2}{2} = 5$	sp ³ d (2b.p + 3 l.p)	Linear
XeF ₄	number of e ⁻ pairs	$= \frac{8+4}{2} = 6$	sp ³ d ² (4b.p + 2 l.p)	Square planar
XeF ₆	number of e ⁻ pairs	$= \frac{8+6}{2} = 7$	sp ³ d ³ (6b.p + 1 l.p)	distorted octahedral
ClF ₃	number of e ⁻ pairs	$= \frac{7+3}{2} = 5$	sp ³ d (3b.p + 2 l.p)	T shape
ICl ₃	number of e ⁻ pairs	$= \frac{7+3}{2} = 5$	sp ³ d (3 b.p + 2 l.p)	T shape
ICl ₅	number of e ⁻ pairs	$= \frac{7+5}{2} = 6$	sp ³ d ² (5 b.p + 1 l.p)	Square pyramidd
NO ₂ ⁻	number of e ⁻ pairs	$= \frac{5+1}{2} = 3$	sp ² (2 b.p + 1l.p)	Angular
NO ₃ ⁻	number of e ⁻ pairs	$= \frac{5+1}{2} = 3$	sp ² (3 b.p + 0 l.p)	Triagonal planar
BrF ₅	number of e ⁻ pairs	$= \frac{7+5}{2} = 6$	sp ³ d ² (5 b.p + 1l.p)	Square pyramidal
SO ₃ ²⁻	number of e ⁻ pairs	$= \frac{6+2}{2} = 4$	sp ³ (3 b.p + 1l.p)	Pyramidal
SO ₄ ²⁻	number of e ⁻ pairs	$= \frac{6+0+2}{2} = 4$	sp ³ (4 b.p + 0 l.p)	Tetrahedral
ClO ⁻	number of e ⁻ pairs	$= \frac{7+1}{2} = 4$	sp ³ (1b.p + 3l.p)	Linear
ClO ₂ ⁻	number of e ⁻ pairs	$= \frac{7+1}{2} = 4$	sp ³ (2 b.p + 2l.p)	Angular
ClO ₃ ⁻	number of e ⁻ pairs	$= \frac{7+1}{2} = 4$	sp ³ (3 b.p + 1l.p)	Pyramidal
ClO ₄ ⁻	number of e ⁻ pairs	$= \frac{7+1}{2} = 4$	sp ³ (4 b.p + 0l.p)	Tetrahedral
NH ₄ ⁺	number of e ⁻ pairs	$= \frac{5+4-1}{2} = 4$	sp ³ (4 b.p + 0l.p)	Tetrahedral
CH ₃ ⁺	number of e ⁻ pairs	$= \frac{4+3-1}{2} = 3$	sp ² (3 b.p + 0l.p)	Trigonal planar
NH ₂ ⁻	number of e ⁻ pairs	$= \frac{5+2+1}{2} = 4$	sp ³ (2 b.p + 2l.p)	Angular
I ₃ ⁻	number of e ⁻ pairs	$= \frac{7+2+1}{2} = 5$	sp ³ d (2 b.p + 3l.p)	Linear
OF ₂	number of e ⁻ pairs	$= \frac{6+2}{2} = 4$	sp ³ (2b.p + 2l.p)	Angular
Cl ₂ O	number of e ⁻ pairs	$= \frac{6+2}{2} = 4$	sp ³ (2b.p + 2l.p)	Angular
SnCl ₂	number of e ⁻ pairs	$= \frac{4+2}{2} = 3$	sp ² (2b.p + 1l.p)	Angular
SnCl ₄	number of e ⁻ pairs	$= \frac{4+4}{2} = 4$	sp ³ (4 b.p + 0l.p)	Tetrahedral
SnCl ₂	number of e ⁻ pairs	$= \frac{6+2}{2} = 4$	sp ³ (2b.p + 2l.p)	Angular
SnCl ₄	number of e ⁻ pairs	$= \frac{6+4}{2} = 5$	sp ³ d (4b.p + 1l.p)	Distorted tetrahedral

SF_4 number of e^- pairs $= \frac{6+4}{2} = 5$ sp^3d (4b.p + 1l.p) Distorted tetrahedral

The above formula to calculate e^- pairs is applicable only for simple molecules or ions mentioned above.

It is not applicable for

- Polycentred molecules like C_2H_6 , C_2H_4 , C_2H_2 , etc
- Polymeric substances like diamond (SP^3) graphite (SP^2); polyethene (SP^2); SiC (SP^3),

It is also not applicable for odd electronic species like NO, NO_2 , ClO_2 , etc.