Chemical Bonding

Hybridisation and Geometry

S.No.	Type of Orbital	No. of hybrid orbital	3D orientation	Example
1.	one s + on p	2; sp	Linear	BeH_2, $BeCl_2$
2.	one s + two p	3; sp^2	Triangular	BCl_3, BF_3
3.	one s + three p	4; sp^3	Tetrahedral	CH_4, CCl_4
4.	one s + three p + one d	5; sp^2d	Triangular bipyramidal	PCl_5
5.	one s + three p + two d	6; sp^3d^2	Octahedral	SF_6
6.	one s + three p + three d	7; sp^3d^3	Pentagonal bipyramidal	IF_7

VSEPR Theory & Geometry of Some Molecules/Ions :

No. of Electron pirs	No. of Lone pairs	No. of bonding pairs	Electron pair geometry	Molecular geometry	Examples
2	0	2	Linear	Linear	$BeBr_2$, CO_2
3	0	3	Trigonal planar	Trigonal planar	BF_3, BCl_3, BH_3
4	0	4	Tetrahedral	Tetrahedral	CH_4, NH_4^+, $SiCl_4$
5	0	5	Trigonal bipyramidal	Trigonal bipyramidal	PCl_5, SbF_5, AsF_5
6	0	6	Octahedral	Octahedral	SF_6, TeF_6, SeF_6
3	1	2	Trigonal planar	Bent	SO_2, O_3
4	1	3	Tetrahedral	Trigonal pyramidal	NH_3, PCl_3
4	2	2	Tetrahedral	Bent	H_2O, OF_2, H_2S, SCl_2
5	1	4	Trigonal bipyramidal	See-saw	SF_4
5	2	3	Trigonal bipyramidal	T-shaped	ClF_3, BrF_3, ICl_3
6	1	5	Octahedral	Square pyramidal	BrF_5, IF_5
6	2	4	Octahedral	Square planar	XeF_4

- **Molecular Orbital Theory**
  Formation of molecule or orbitals from atomic orbitals ($\psi_A \pm \psi_B$)
  $\psi_{MO} = \psi_A \pm \psi_B$

$\sigma = \psi_A + \psi_B$ (Bonding molecular orbital)
$\sigma^* = \psi_A - \psi_B$ (Antibonding molecular orbital)

Relative energies of M.O. having
Less than or equal to 14 electrons.
$\sigma 1s < \sigma^* 1s < \sigma 2s < \sigma^* 2s < \pi 2p_x = \pi 2p_y < \pi 2p_z < [\pi^* 2p_x = \pi^* 2p_y] < \sigma^* 2p_z$

For more than 14 electrons
$\sigma 1s < \sigma^* 1s < \sigma 2s < \sigma^* 2s < \pi 2p_z < [\pi^* 2p_x = \pi^* 2p_y] < [\pi^* 2p_x = \pi^* 2p_y] < \sigma^* 2p_z$

Bond order
Bond order = 1/2 [Number of bonding electrons – Number of antibonding electrons]
Or, $N_b - N_a/2$
B.O. ∝ B.E. ∝ 1/B.L ∝ Stability

•Dipole moments and geometry of some molecules:

Types of molecule	Examples	Dipole moment μ (D)	Geometry
Molecule AB	HG HCl HBr H_2	1.91 1.03 0.79 0	Linear Linear Linear Linear
Molecule AB_2	H_2O H_2S CO_2	1.85 0.95 0	Angular (Bent) Angular (Bent) Linear
Molecule AB_3	NH_3 NF_3 BF_3	1.47 0.23 0	Trigonal pyramidal Trigonal pyramidal Trigonal planar
Molecule AB_4	CH_4 $CHCl_4$ CCl_4	0 1.04 0	Tetrahedral Tetrahedral Tetrahedral

Formulae :

1. Formal charge, F.C. = V.E. – N.E. – (B.E./2)
   Where,
   V.E. = Total number of valence electrons in free atom.
   N.E. = Total number of non-bonding or lone pairs of electrons.
   B.E. = Total number of bonding or shared electrons.
2. Bond order = $\frac{N_b - N_a}{2}$
   Where,
   N_b = Number of electrons in bonding MOs.
   N_a = Number of electrons in antibonding MOs.