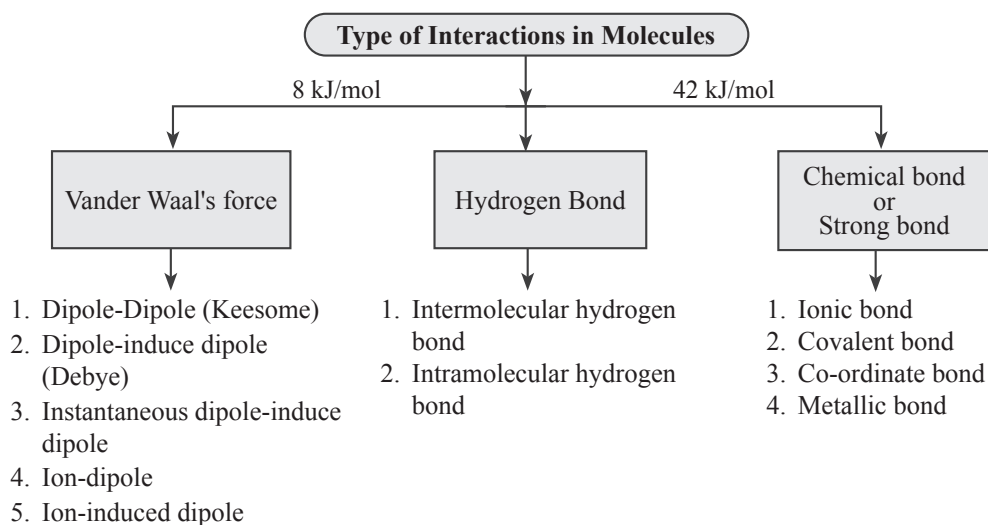


Chemical Bonding and Molecular Structure

Chemical Bond

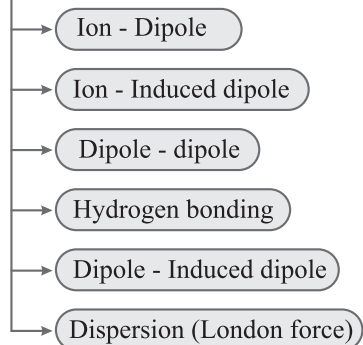
The force of attraction which hold atoms together, molecule or ions within chemical species.

It is always exothermic process.



Types of Intermolecular Forces

Types of Intermolecular Forces



Force

Table: Relative strength of forces

Force	Relative strength	Interaction energy
Ion-ion (Cation-anion)	Very strong	Interaction energy $\propto r^{-1}$
Covalent bonds	Strong, (140–523 kJ/mole)	Interaction energy $\propto r^{-1}$
Ion-dipole	Moderate	Interaction energy $\propto r^{-2}$
Hydrogen bond	Moderate to weak (10–100 kJ/mol)	Interaction energy $\propto r^{-1}$
Dipole-dipole	Weak (5–25 kJ/mol)	Interaction energy $\propto r^{-3}$ (for stationary polar molecules) Interaction energy $\propto r^{-6}$ (for rotating polar molecules)
London force or dispersion force	Very weak (0.05–20 kJ/mol)	Interaction energy $\propto r^{-6}$

Hybridisation

Table : Hybridisation and geometry

S.No.	Type or orbital	No. of hybrid orbital	3D orientation	Example
1.	one s + one 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 ³ d	Triangular bipyramidal	PCl ₅
5.	one s + three p + two d	6; sp ³ d ²	Octahedral	SF ₆
6.	one s + three p + three d	7; sp ³ d ³	Pentagonal bipyramidal	IF ₇

Type of Hybridisation & Possible Structure

Table : Hybridisation and Shape

Type of Hybridisation	No. of B.P.	No. of L.P.	Shape	Examples
1. sp-hybridisation	2	-	Linear	BeF ₂ , CO ₂ , CS ₂ , BeCl ₂
2. (a) sp ² -hybridisation	3	-	Trigonal planar	BF ₃ , AlCl ₃ , BeF ₃ ⁻
(b) sp ² -hybridisation	2	1	V-shape, Angular	NO ₂ ⁻ , SO ₂ , O ₃
3. (a) sp ³ -hybridisation	4	0	Tetrahedral	CH ₄ , CCl ₄ , PCl ₄ ⁺ , ClO ₄ ⁻ , NH ₄ ⁺ , BF ₄ ⁻ , SO ₄ ⁻² , AlCl ₄ ⁻
(b) sp ³ -hybridisation	3	1	Pyramidal	NH ₃ , PF ₃ , ClO ₃ ⁻ , H ₃ O ⁺ , PCl ₃ , XeO ₃ , N(CH ₃) ₃ , CH ₃ ⁻
(c) sp ³ -hybridisation	2	2	V-shape Angular	H ₂ O, H ₂ S, NH ₂ ⁻ , OF ₂ , Cl ₂ O ₂ , SF ₂ , I ₃ ⁺
4. (a) sp ³ d-hybridisation	5	—	Trigonal bipyramidal	PCl ₅ , SOF ₄ , AsF ₅
(b) sp ³ d-hybridisation	4	1	See-Saw, folded square distorted tetrahedral almost T-shape	SF ₄ , PF ₄ ⁻ , AsF ₄ ⁻ SbF ₄ ⁻ , XeO ₂ F ₂
(c) sp ³ d-hybridisation	3	2	Linear	ClF ₃ , ICl ₃
(d) sp ³ d-hybridisation	2	3		I ₃ ⁻ , Br ₃ ⁻ , ICl ₂ ⁻ , XeF ₂

Type of Hybridisation	No. of B.P.	No. of L.P.	Shape	Examples
5. (a) sp^3d^2 -hybridisation	6	—	Square bipyramidal/octahedral	PCl_6^- , SF_6
(b) sp^3d^2 -hybridisation	5	1	Square pyramidal/distorted octahedral	$XeOF_4$, ClF_5 , SF_5^- ,
(c) sp^3d^2 -hybridisation	4	2	Square planar	XeF_5^+ , XeF_4
6. (a) sp^3d^3 -hybridisation	7	—	Pentagonal bipyramidal	IF_7
(b) sp^3d^3 -hybridisation	6	1	Pentagonal pyramidal/ distorted octahedral/capped octahedral	XeF_6
(c) sp^3d^3 -hybridisation	5	2	Pentagonal planar	XeF_5^-

Molecular Orbital Theory

Formation of molecule or orbitals from atomic orbitals ($\psi_A \pm \psi_B$)

$$\psi_{MO} = \psi_A \pm \psi_B$$

$$\sigma = \psi_A + \psi_B \text{ (Bonding molecular orbital)}$$

$$\sigma^* = \psi_A - \psi_B \text{ (Antibonding molecular orbital)}$$

Relative energies of M.O having

Less than or equal to 14 electrons.

$$\sigma 1s < \sigma^* 1s < \sigma 2s < \sigma^* 2s < \pi 2p_x = \pi 2p_y < \sigma 2p_z < [\pi^* 2p_x = \pi^* 2p_y] < \sigma^* 2p_z$$

For more than 14 electrons

$$\sigma 1s < \sigma^* 1s < \sigma 2s < \sigma^* 2s < \sigma 2p_z < [\pi 2p_x = \pi 2p_y] < [\pi^* 2p_x = \pi^* 2p_y] < \sigma^* 2p_z$$

Bond order

$$\text{Bond order} = \frac{1}{2} [\text{Number of bonding electrons} - \text{Number of antibonding electrons}]$$

$$\text{or, } = \frac{N_b - N_a}{2}$$

$$\text{B.O} \propto \text{B.E} \propto \frac{1}{\text{B.L}} \propto \text{Stability}$$

Properties of Ionic Salt

General Properties

Hard, Solid, Brittle (strong electrostatic attraction between ions)

Non directional nature (ionic compound do not exhibit stereo isomerism)

Higher Melting Point / Boiling Point

Isomorphism: $MgSO_4 \cdot 7H_2O$; $ZnSO_4 \cdot 7H_2O$; $FeSO_4 \cdot 7H_2O$

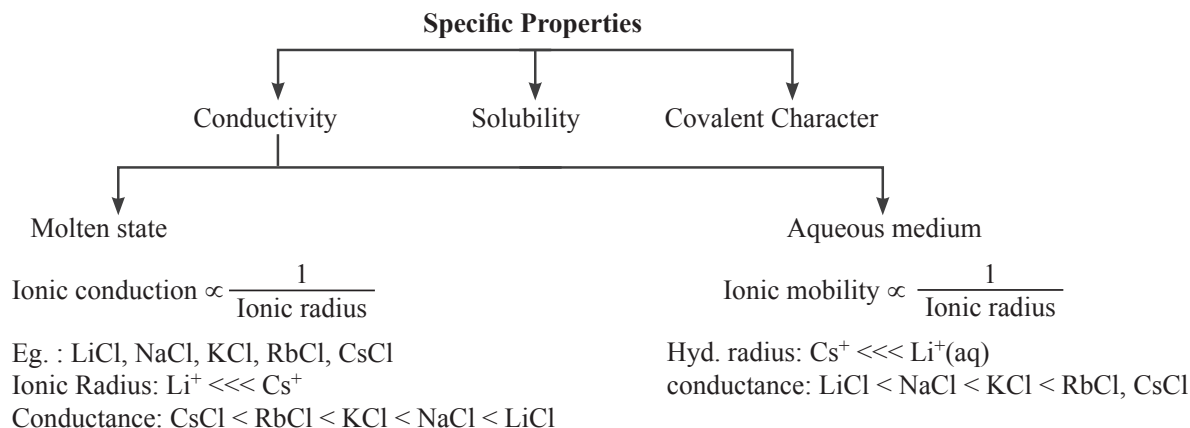


Table: Hybridisation of following species in specified state

Species	Cationic part	Anionic part
PCl_5	$\text{PCl}_4^+ (\text{sp}^3)$	$\text{PCl}_6^- (\text{sp}^3\text{d}^2)$
PBr_5	$\text{PBr}_4^+ (\text{sp}^3)$	Br^-
XeF_6	$\text{XeF}_5^+ (\text{sp}^3\text{d}^2)$	F^-
N_2O_5	$\text{NO}_2^+ (\text{sp})$	$\text{NO}_3^- (\text{sp}^2)$
I_2Cl_6 (liquid)	$\text{ICl}_2^+ (\text{sp}^3)$	$\text{ICl}_4^- (\text{sp}^3\text{d}^2)$
Cl_2O_6	$\text{ClO}_2^+ (\text{sp}^2)$	$\text{ClO}_4^- (\text{sp}^3)$
I_2 (molten state)	$\text{I}_3^+ (\text{sp}^3)$	$\text{I}_3^- (\text{sp}^3\text{d})$

Table: Magnetic behaviour of odd electron species

	Hybridisation	Shape	Magnetic behaviour
NO_2	sp^2	V shape	Para
ClO_2	sp^2	V shape	Para
ClO_3	sp^3	Pyramidal	Para
$\cdot\text{CH}_3$	sp^2	Trigonal planar	Para
$\cdot\text{CH}_3/\cdot\text{CHF}_2/\text{CH}_2\text{F}$	sp^3	Pyramidal	Para

Odd e^- species: Total number of electron or valence electron in odd number.