FREE NOTES · NCERT + JEE/NEET LEVEL

Chemical Bonding & Molecular Structure

Octet rule, Lewis structures, formal charge, ionic bond and lattice enthalpy, bond parameters, resonance, polarity and dipole moment, Fajans' rule, VSEPR shapes, valence bond theory, hybridisation, molecular orbital theory and hydrogen bonding.

01 Octet rule & Lewis structures
02 Ionic bond & lattice enthalpy
03 Bond parameters & resonance
04 Polarity, dipole moment & Fajans' rule
05 VSEPR theory & shapes
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01 Octet rule & Lewis structures

Atoms combine to get 8 electrons in the outer shell (Kossel-Lewis). Covalent bonds share electron pairs; ionic bonds transfer electrons.

$$\text{Formal charge} = V - L - \tfrac{1}{2}B$$

V = valence electrons, L = non-bonding (lone pair) electrons, B = bonding electrons. The best Lewis structure has the smallest formal charges. O_3: central O +1, single-bonded O -1.

OCTET RULE FAILS FOR

- Incomplete octet: $BeCl_2$ (4), BCl_3 (6), LiCl.
- Odd electrons: NO, NO_2.
- Expanded octet (period 3+): PCl_5 (10), SF_6 (12), H_2SO_4.
- Noble gas compounds (XeF_2, XeF_4); can't explain shape or energy.

02 Ionic bond & lattice enthalpy

Formed easily when: low ionisation enthalpy of metal, high negative electron gain enthalpy of non-metal, high **lattice enthalpy** (energy released when gaseous ions form 1 mol of solid). Higher charge and smaller ions ⇒ larger lattice enthalpy. Calculated by the Born-Haber cycle.

03 Bond parameters & resonance

- **Bond length:** C–C 154 pm > C=C 134 pm > C≡C 120 pm.
- **Bond order** ↑ ⇒ bond enthalpy ↑, bond length ↓.
- **Bond angle**: angle between orbitals around the central atom (H_2O 104.5°).
- **Resonance:** when one Lewis structure can't describe a molecule, the real structure is a hybrid of several (O_3, CO_3^{2-}, benzene). In CO_3^{2-} all C–O bonds are equal (bond order 1.33). The hybrid is more stable than any single structure.

04 Polarity, dipole moment & Fajans' rule

$$\mu = q \times d$$

Unit: debye (1 D = 3.336 × 10^{-30} C m). Vector: points from + to − (chemists' arrow from + to −).

- μ = 0 for symmetrical molecules: CO_2, BF_3, CH_4, CCl_4, BeF_2.
- H_2O (1.85 D) is bent so μ ≠ 0. NH_3 (1.47 D) > NF_3 (0.23 D): in NH_3 the lone pair moment adds to bond moments; in NF_3 it opposes them.
- cis-isomer usually polar, trans non-polar; p-dichlorobenzene μ = 0.

FAJANS' RULE (COVALENT CHARACTER IN IONIC BONDS)

More covalent when: **small cation, large anion, high charges**, cation with pseudo-noble-gas (18 e^-) configuration. LiCl more covalent than NaCl; $AlCl_3$ covalent.

05 VSEPR theory & shapes

Electron pairs around the central atom repel and stay as far apart as possible. Repulsion: **lp–lp > lp–bp > bp–bp**.

bp + lp	Shape	Example, angle
2 + 0	Linear	$BeCl_2$, CO_2 180°
3 + 0	Trigonal planar	BF_3 120°
2 + 1	Bent	SO_2 ~119°
4 + 0	Tetrahedral	CH_4 109.5°
3 + 1	Trigonal pyramidal	NH_3 107°
2 + 2	Bent	H_2O 104.5°
5 + 0	Trigonal bipyramidal	PCl_5 120°, 90°
4 + 1	See-saw	SF_4
3 + 2	T-shaped	ClF_3
2 + 3	Linear	XeF_2, I_3^-
6 + 0	Octahedral	SF_6 90°
5 + 1	Square pyramidal	BrF_5
4 + 2	Square planar	XeF_4

06 Valence bond theory & hybridisation

A bond forms by **overlap** of half-filled orbitals. Head-on overlap ⇒ **σ bond** (stronger); sideways p–p overlap ⇒ **π bond**. A double bond = 1σ + 1π; triple = 1σ + 2π.

HYBRIDISATION SHORTCUT

$$H = \tfrac{1}{2}(V + M - C + A)$$

V = valence e^- of central atom, M = monovalent atoms, C = cation charge, A = anion charge. 2 = sp, 3 = sp^2, 4 = sp^3, 5 = sp^3d, 6 = sp^3d^2.

Hybrid	Geometry	Examples
sp	Linear 180°	$BeCl_2$, C_2H_2
sp^2	Trigonal planar 120°	BCl_3, C_2H_4
sp^3	Tetrahedral 109.5°	CH_4, NH_3, H_2O
sp^3d	Trigonal bipyramidal	PCl_5 (axial bonds longer)
sp^3d^2	Octahedral	SF_6

% s character: sp 50 > sp^2 33 > sp^3 25 ⇒ more s character, smaller and more electronegative orbital.

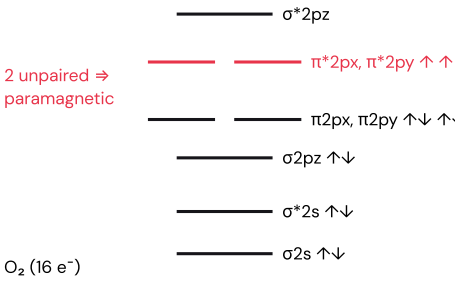
07 Molecular orbital theory

Atomic orbitals combine (LCAO) to give **bonding** (lower energy) and **antibonding** (higher, *) MOs.

$$\text{Bond order} = \tfrac{1}{2}(N_b - N_a)$$

BO = 0 ⇒ molecule doesn't exist (He_2). Higher BO ⇒ more stable, shorter bond. Unpaired electrons ⇒ paramagnetic.

Order up to N_2 ($14\ e^-$): σ1s σ*1s σ2s σ*2s ($\pi 2p_x = \pi 2p_y$) $\sigma 2p_z$ (π*) σ*.
O_2 onward: $\sigma 2p_z$ comes before the π2p pair.



MO filling for O_2: BO = 2, paramagnetic

Species	BO	Magnetic
H_2	1	Dia
N_2	3	Dia
O_2 / O_2^+ / O_2^- / O_2^{2-}	2 / 2.5 / 1.5 / 1	Para / para / para / dia
B_2 / C_2	1 / 2	Para / dia

08 Hydrogen bonding

H attached to a small, highly electronegative atom (F, O, N) is attracted to another such atom. Strength: ~10–40 kJ/mol (weaker than covalent).

- **Intermolecular** (between molecules): H_2O, HF, NH_3 ⇒ high b.p.; ice is less dense than water (open cage structure).
- **Intramolecular** (within one molecule): o-nitrophenol, salicylaldehyde ⇒ lower b.p., steam volatile.

09 JEE Extra + Tricks

JEE LEVEL

- Hybridisation shortcut: $H = \frac{1}{2}(V + M - C + A)$ (V = valence e^- of central atom, M = monovalent atoms, C = cation charge, A = anion charge). H = 2 sp, 3 sp^2, 4 sp^3, 5 sp^3d, 6 sp^3d^2.
- Shapes with lone pairs: SF_4 see-saw, ClF_3 T-shaped, XeF_2 linear, XeF_4 square planar, BrF_5 square pyramidal, XeF_6 distorted octahedral.
- Bond order from MOT: $\frac{1}{2}(N_b - N_a)$. O_2 (BO 2) is paramagnetic; N_2 BO 3; for up to 14 electrons $\sigma 2p_z$ is above $\pi 2p$ (s–p mixing).
- Bond length $\propto$ 1/bond order; bond energy $\propto$ bond order.
- Dipole moment zero for symmetric molecules: CO_2, BF_3, CH_4, CCl_4, PCl_5, SF_6; NH_3 (1.47 D) > NF_3 (0.23 D).
- Fajans' rules: covalent character increases with small cation, large anion, high charge; pseudo noble gas cations (Cu^+, Ag^+) more covalent.

10 Solved questions

Q1. Shape and hybridisation of XeF_4?

Xe: 8 valence e^-, 4 F ⇒ H = ½(8 + 4) = 6 ⇒ sp^3d^2, 4 bp + 2 lp ⇒ **square planar**.

Q2. Why does BF_3 have zero dipole moment but NH_3 doesn't?

BF_3 is trigonal planar; three bond moments cancel. NH_3 is pyramidal with a lone pair; they add up.

Q3. Bond order and magnetism of N_2^+.

13 e^-: N_b = 9, N_a = 4 ⇒ BO = 2.5; one unpaired ⇒ paramagnetic.

Q4. σ and π bonds in $CH_2{=}CH{-}C{\equiv}N$?

σ: 3 C–H + C=C(1) + C–C + C≡N(1) = **6σ**; π: 1 + 2 = **3π**.

11 Mistakes & practice

- Counting lone pairs in the shape name (shape = arrangement of atoms only).
- Using the N_2 MO order for O_2 and F_2.
- Saying CO_2 is polar because C=O is polar (moments cancel).
- Thinking π bonds can exist without a σ bond.

1. Shape of ClF_3?
2. Which has higher dipole moment: NH_3 or NF_3?
3. Hybridisation of C in CO_2?
4. Bond order of He_2^+?
5. Why is ice lighter than water?

ANSWERS

1) T-shaped · 2) NH_3 · 3) sp · 4) 0.5 · 5) H-bonding gives an open cage structure with empty space

12 Quick revision: 5 minutes before the exam

BASICS

- FC = V − L − ½B.
- Fajans: small cation, big anion ⇒ covalent.
- μ = q × d; symmetric ⇒ 0.

VSEPR

- lp–lp > lp–bp > bp–bp.
- NH_3 107°, H_2O 104.5°.
- XeF_2 linear, XeF_4 square planar.

HYBRIDISATION

- H = ½(V + M − C + A).
- sp 180°, sp^2 120°, sp^3 109.5°.
- Double = σ + π.

MOT

- BO = ½(N_b − N_a).
- O_2: BO 2, paramagnetic.
- N_2: BO 3, diamagnetic.

Have a doubt? Ask the AI Doubt Solver at padhaiadda.netlify.app, or take the mock test on this chapter.