FREE EDITION · NOTES + 3 SAMPLE MCQS

CUET · CHEMISTRY · CLASS XI · CODE 306

Chemical Bonding and Molecular Structure

CUET unit: Chemical Bonding and Molecular Structure

By **UniDrill** · NCERT-grounded study material

WWW.UNIDRILL.IN

📌 Snapshot

- Builds the conceptual core for "why atoms combine and what shape the resulting species takes" — covers Kossel–Lewis (ionic + Lewis dot), octet rule and its three exceptions, ionic bond energetics (lattice enthalpy, Fajans rules), bond parameters (length, angle, enthalpy, order, resonance, polarity), VSEPR shapes, valence bond / hybridisation, molecular orbital theory for second-row diatomics, and hydrogen bonding.
- One of the two most heavily examined Class XI chemistry units in CUET — hybridisation type, VSEPR shape, MOT bond order/magnetic behaviour, and H-bonding-driven anomalies appear almost every year.
- Tables 4.1–4.8 and Figs. 4.1–4.22 are dense with data; CUET stems are usually mined directly from these.
- Acts as a prerequisite for organic chemistry ($sp/sp^2/sp^3$ in C), coordination chemistry (hybridisation, geometry), and physical chemistry (bond enthalpy, dipole moment).

📖 Detailed Notes

2.1 Core concepts

- **Chemical bond** is the attractive force holding constituent atoms/ions together in a molecule; Kossel and Lewis (1916) gave the first satisfactory electronic explanation based on noble-gas inertness (NCERT §4.1, p. 101).
- **Lewis dot symbols** show the valence electrons of an atom; group valence equals either the number of dots or 8 minus the number of dots (NCERT §4.1, p. 101).
- **Kossel view of ionic bond:** the highly electronegative halogens and electropositive alkali metals are separated by noble gases; transfer of electrons gives ions with ns^2np^6 configuration that are stabilised by electrostatic attraction — e.g. NaCl, CaF_2 (NCERT §4.1, p. 101).
- **Octet rule** (Kossel–Lewis, 1916): atoms combine by transfer or sharing of valence electrons to attain an octet in their valence shell (NCERT §4.1.1, p. 102).
- **Covalent bond** (Langmuir 1919): formed by sharing of an electron pair; sharing 1, 2, 3 pairs gives single, double (e.g. CO_2, C_2H_4), triple (e.g. N_2, C_2H_2) bonds (NCERT §4.1.2, p. 102).

- **Writing Lewis structures:** sum valence electrons (add for anions, subtract for cations); least electronegative atom is central (e.g. N in NF_3, C in CO_3^{2-}); after single bonds, leftover electrons go as multiple bonds or lone pairs so every atom gets an octet (NCERT §4.1.3, p. 103).
- **Formal charge** = (valence e^- in free atom) – (non-bonding e^-) – ½(bonding e^-); used to pick the lowest-energy Lewis structure (smallest formal charges). For O_3, central O has F.C. = +1 and the terminal O atoms have 0 and –1 (NCERT §4.1.4, p. 104–105).
- **Limitations of octet rule:** (i) **incomplete octet** — LiCl, BeH_2, BCl_3, $AlCl_3$, BF_3; (ii) **odd-electron molecules** — NO, NO_2; (iii) **expanded octet** — PF_5, SF_6, H_2SO_4 (3d orbitals available from period 3 onwards). Octet rule is also silent on shape, molecular energy, and noble-gas compounds like XeF_2, KrF_2 (NCERT §4.1.5, p. 105–106).
- **Ionic bond formation** is favoured by low ionisation enthalpy of the metal, high (negative) electron gain enthalpy of the non-metal, and large lattice enthalpy. For NaCl, IE(Na) + $\Delta_e gH$(Cl) = +147.1 kJ mol⁻¹ but lattice enthalpy = –788 kJ mol⁻¹, so the crystal is stable (NCERT §4.2, p. 106).
- **Lattice enthalpy** is the energy required to separate one mole of a solid ionic compound into gaseous ions; NaCl lattice enthalpy = 788 kJ mol⁻¹. It is the true measure of ionic-compound stability, not mere octet completion (NCERT §4.2.1, p. 107).
- **Bond length** is the equilibrium internuclear distance; covalent radius is half the distance between two like atoms covalently bonded. Typical values: H–H 74 pm, Cl–Cl 199 pm, N≡N 109 pm, O=O 121 pm (Tables 4.2, 4.3) (NCERT §4.3.1, p. 107–108).
- **Bond angle** is the angle between bonding orbitals around the central atom (e.g. 104.5° in H_2O) (NCERT §4.3.2, p. 108).
- **Bond enthalpy** is the energy to break one mole of a bond in the gas phase: H–H = 435.8, O=O = 498, N≡N = 946 kJ mol⁻¹. For polyatomics like H_2O, mean bond enthalpy = (502 + 427)/2 = 464.5 kJ mol⁻¹ (NCERT §4.3.3, p. 108–109).
- **Bond order** in Lewis theory = number of bonds between two atoms: H_2 = 1, O_2 = 2, N_2 = 3, CO = 3. Isoelectronic species have the same bond order (F_2 and O_2^{2-} → 1; N_2, CO, NO^+ → 3). Higher bond order ⇒ higher bond enthalpy and shorter bond length (NCERT §4.3.4, p. 109).
- **Resonance:** when one Lewis structure cannot describe a species, several canonical forms with identical nuclear positions but different electron arrangements are drawn — their hybrid represents the real molecule. Examples: O_3 (both O–O bonds equal at 128 pm, between single 148 pm and double 121 pm), CO_3^{2-} (three equivalent C–O bonds), CO_2, benzene. The hybrid has lower energy than any canonical form; canonical forms have no real existence (NCERT §4.3.5, p. 109–110).
- **Polarity / dipole moment:** $\mu = Q \times r$, measured in Debye (1 D = 3.33564×10^{-30} C m). HF is polar ($\mu = 1.78$ D); H_2, BF_3, CO_2, CCl_4 have $\mu = 0$ because bond dipoles

cancel. H_2O is bent so μ = 1.85 D. NH_3 (1.47 D) > NF_3 (0.23 D) because in NH_3 the lone-pair dipole adds to the N–H bond dipoles whereas in NF_3 it opposes them (NCERT §4.3.6, p. 110–112).

- **Fajans rules for partial covalent character of ionic bonds:** small cation, large anion, high cation charge, and $(n-1)d^n ns^0$ configuration all increase covalent character (NCERT §4.3.6, p. 112).
- **VSEPR theory** (Sidgwick–Powell 1940; Nyholm–Gillespie 1957): valence-shell electron pairs (bonded + lone) arrange to minimise repulsion. Repulsion order: lp–lp > lp–bp > bp–bp. A multiple bond is treated as one super-pair. Basic geometries: AB_2 linear, AB_3 trigonal planar, AB_4 tetrahedral, AB_5 trigonal bipyramidal, AB_6 octahedral (NCERT §4.4, Table 4.6, p. 112–114).
- **With lone pairs** (Tables 4.7, 4.8): AB_2E bent (e.g. SO_2, 119.5°), AB_3E trigonal pyramidal (NH_3, 107°), AB_2E_2 bent (H_2O, 104.5°), AB_4E see-saw (SF_4, lp at equatorial position), AB_3E_2 T-shape (ClF_3), AB_4E_2 square planar (XeF_4), AB_5E square pyramidal (BrF_5) (NCERT §4.4, Tables 4.7–4.8, p. 115–117).
- **Valence Bond (VB) theory** (Heitler–London 1927, Pauling): covalent bond forms when half-filled atomic orbitals with opposite-spin electrons overlap; greater overlap ⇒ stronger bond. For H_2, the potential-energy curve has a minimum at 74 pm corresponding to 435.8 kJ mol^{-1} of bond enthalpy (NCERT §4.5, p. 117–118).
- **σ vs π bond:** σ bond by head-on (axial) overlap of s–s, s–p, p–p along internuclear axis; π bond by sidewise overlap of parallel p-orbitals, giving two electron clouds above and below the molecular plane. σ is stronger because of greater overlap. Multiple bonds = 1 σ + 1 (or 2) π (NCERT §4.5.4–4.5.5, p. 120).
- **Hybridisation** (Pauling): mixing of orbitals of slightly different energies to give equivalent hybrid orbitals. Types: sp (linear, 180°; $BeCl_2$), sp^2 (trigonal planar, 120°; BCl_3, C in C_2H_4), sp^3 (tetrahedral, 109.5°; CH_4; also explains NH_3 at 107° and H_2O at 104.5° because of lone-pair repulsion), sp^3d (trigonal bipyramidal; PCl_5), sp^3d^2 (octahedral; SF_6), dsp^2 (square planar; $[Ni(CN)_4]^{2-}$), sp^3d^2 also gives square pyramidal BrF_5 (NCERT §4.6, p. 120–125).
- **PCl_5 geometry:** three equatorial P–Cl bonds at 120°, two axial at 90° to the equatorial plane; axial bonds are longer/weaker due to greater repulsion from equatorial pairs, making PCl_5 reactive (NCERT §4.6.3, p. 125).
- **Molecular Orbital (MO) theory** (Hund–Mulliken 1932): atomic orbitals of comparable energy and same symmetry combine by LCAO to give equal numbers of bonding (lower energy, electron density between nuclei) and antibonding (higher energy, node between nuclei) MOs. Filling follows aufbau, Pauli, Hund (NCERT §4.7.1, p. 126).
- **MO energy order:** for O_2, F_2 — $\sigma 1s$ < **$\sigma 1s$ < $\sigma 2s$ < σ**$2s$ < $\sigma 2p\_z$ < ($\pi 2p\_x$ = $\pi 2p\_y$) < (π**$2p\_x$ = π**$2p\_y$) < σ^*2p_z. For Li_2, Be_2, B_2, C_2, N_2 — $\sigma 2p\_z$ lies above ($\pi 2p\_x$ = $\pi 2p\_y$) (NCERT §4.7.4, p. 128–129).

- **Bond order = ½(N_b − N_a):** positive ⇒ stable, zero/negative ⇒ unstable. H_2 b.o. = 1 (stable, diamagnetic); He_2 b.o. = 0 (does not exist); Li_2 b.o. = 1 (diamagnetic); C_2 b.o. = 2 (both bonds are π; diamagnetic); N_2 b.o. = 3; O_2 b.o. = 2 and is **paramagnetic** because of two unpaired electrons in π2p_x, π2p_y — a landmark success of MOT (NCERT §4.8, p. 129–131).
- **Magnetic nature:** all electrons paired ⇒ diamagnetic; one or more unpaired ⇒ paramagnetic (e.g. O_2, B_2) (NCERT §4.7.5, p. 129).
- **Hydrogen bond:** the attractive force between a hydrogen covalently bonded to a highly electronegative atom (F, O, N) of one molecule and an electronegative atom of another molecule; weaker than a covalent bond but stronger than van der Waals forces. Represented by a dotted line (NCERT §4.9, p. 131).
- **Types of H-bond:** (i) **intermolecular** — HF, H_2O, alcohols, ice; (ii) **intramolecular** — within the same molecule, e.g. o-nitrophenol where H sits between two oxygen atoms. H-bonding strongly affects structure and properties (e.g. anomalously high boiling point of water, lower density of ice than water) (NCERT §4.9.2, p. 132).

2.2 Definitions to memorise

Term	Definition	Page
Chemical bond	Attractive force holding constituent atoms/ions together in a chemical species	100
Octet rule	Atoms combine by transfer/sharing of valence electrons to attain 8 electrons in the valence shell	102
Electrovalent (ionic) bond	Bond formed by electrostatic attraction between oppositely charged ions formed by electron transfer	101–102
Formal charge	(Valence e^- in free atom) – (lone-pair e^-) – ½(bonding e^-)	104
Lattice enthalpy	Energy required to completely separate one mole of a solid ionic compound into gaseous ions	107
Bond length	Equilibrium distance between the nuclei of two bonded atoms	107
Bond angle	Angle between orbitals containing bonding electron pairs around the central atom	108
Bond enthalpy	Energy required to break one mole of a particular type of bond in the gaseous state	108
Bond order (Lewis)	Number of bonds between two atoms in a molecule	109
Bond order (MOT)	½ (N_b – N_a), where N_b, N_a are bonding and antibonding electrons	129
Resonance	Representation of a species by two or more canonical Lewis structures whose hybrid describes the actual species	109
		110

Term	Definition	Page
Dipole moment (μ)	Product of magnitude of charge and distance between centres of positive and negative charge; $\mu = Q \times r$, unit Debye (1 D = 3.33564×10^{-30} C m)	
VSEPR theory	Shape determined by repulsion among valence-shell electron pairs (lp–lp > lp–bp > bp–bp)	113
Hybridisation	Intermixing of orbitals of slightly different energies to give a new set of equivalent orbitals	120
σ bond	Bond by head-on (axial) overlap along the internuclear axis	120
π bond	Bond by sidewise overlap of parallel p-orbitals; cloud lies above and below the molecular plane	120
Bonding MO	LCAO $\psi\_A + \psi\_B$; electron density between nuclei; lower energy than parent AO	126
Antibonding MO	LCAO $\psi\_A - \psi\_B$; nodal plane between nuclei; higher energy than parent AO	126
Hydrogen bond	Attractive force between H atom of one molecule and an F, O or N atom of another molecule	131

2.3 Diagrams / processes to remember

- Fig. 4.1 — Bond length R = r_A + r_B (p. 107).
- Fig. 4.2 — Covalent radius (99 pm) vs van der Waals radius (180 pm) in Cl_2 (p. 107).
- Fig. 4.3 — Resonance hybrid of O_3 from two canonical forms (p. 109).
- Fig. 4.4 — Three canonical structures of CO_3^{2-} (p. 110); Fig. 4.5 — three canonical forms of CO_2 (p. 110).
- Table 4.5 — Dipole moments and geometries: HF 1.78 D linear, H_2O 1.85 D bent, NH_3 1.47 D trigonal pyramidal, BF_3 0 D trigonal planar, CO_2 0 D linear, CCl_4 0 D tetrahedral (p. 112).
- Tables 4.6–4.8 — VSEPR geometries (p. 114–117).
- Fig. 4.7 / 4.8 — Forces and potential-energy curve in H_2 formation (p. 118).
- Fig. 4.10–4.16 — Hybridisation diagrams for $BeCl_2$ (sp), BCl_3 (sp^2), CH_4 (sp^3), NH_3 and H_2O (sp^3 with lone pairs), C_2H_4, C_2H_2 (p. 121–124).
- Fig. 4.17 — Trigonal bipyramidal PCl_5 (sp^3d) with axial vs equatorial bonds (p. 125).
- Fig. 4.18 — Octahedral SF_6 (sp^3d^2) (p. 125).
- Fig. 4.20 — Bonding/antibonding MOs from 1s, 2p_z, 2p_x AOs (p. 128).
- Fig. 4.21 — MO occupancy table for B_2 through Ne_2 with bond order and magnetic property (p. 131).
- Fig. 4.22 — Intramolecular H-bond in o-nitrophenol (p. 132).

2.4 Common confusions / NTA trap points

- **MOT energy order changes at O_2:** for B_2, C_2, N_2 the (π2p) lies below σ2p_z; for O_2, F_2, Ne_2 the σ2p_z lies below (π2p). NTA often inverts this in distractors.
- **NH_3 vs NF_3 dipole moments:** N is more electronegative than H but less than F. Yet $\mu(NH_3) > \mu(NF_3)$ because the lone-pair dipole **adds** in NH_3 but **subtracts** in NF_3. Easy trap.
- **H_2O bent ≠ $BeCl_2$ linear** even though both are AB_2 — H_2O has 2 lone pairs on O (AB_2E_2 → sp^3 → bent), $BeCl_2$ has none (AB_2 → sp → linear).
- **C_2 double bond is two π bonds** (no σ from 2p_z because σ2p_z is empty in the $(\pi 2p)^4$ configuration), unlike most double bonds which are $1\sigma + 1\pi$.
- **Formal charge ≠ oxidation state ≠ real charge.** It only helps in picking the best Lewis structure.
- **Hybridisation does not require half-filled orbitals** — even filled orbitals can hybridise (e.g. the lone-pair-bearing sp^3 orbitals of O in H_2O).
- **Bond order in resonance hybrid is fractional** — in CO_3^{2-} each C–O bond order = 4/3 (1 σ + delocalised π over 3 oxygens).
- **Ice less dense than water** because tetrahedral H-bonding in ice creates empty cages; this is an H-bonding consequence often asked through MCQs on density/boiling-point anomalies.

🎯 Practice MCQs

Q1. Which of the following pairs of molecules together contain examples of all three exceptions to the octet rule — incomplete octet, odd-electron, and expanded octet?

A. BF_3, NH_3, SF_6

B. BCl_3, NO, SF_6

C. CH_4, NO_2, PCl_5

D. BeH_2, H_2O, XeF_2

Q2. The formal charges on the central oxygen atom and the two terminal oxygen atoms in the conventional Lewis structure of the ozone molecule are, respectively:

A. 0, +1, −1

B. +1, 0, −1

C. −1, 0, +1

D. +1, +1, −2

Q3. Among the following, the molecule with the **largest** dipole moment is:

A. CO_2

B. BF_3

C. H_2O

D. CCl_4

📊 PYQ Alignment

This chapter is among the highest-yielding for CUET Chemistry, contributing 10–14 MCQs per paper across CUET 2022–2025. Hybridisation type (especially sp^3d, sp^3d^2 involving d orbitals), VSEPR shape with lone pairs (SF_4, ClF_3, XeF_4, BrF_5), MOT bond order / paramagnetism of O_2 and ions like O_2^+/O_2^-, dipole moment comparisons (NH_3 vs NF_3, H_2O vs CO_2), formal-charge calculation on O_3/CO_3^{2-}, and the consequences of hydrogen bonding (HF boiling point, ice density, intramolecular H-bond in o-nitrophenol) are recurring question types.

CUET 2023 — Actual PYQs from this chapter

Q.9 (CUET 2023) Chemical formula of laughing gas is:

- A) NO B) N_2O C) N_2O_3 D) N_2O_4

Tests: p-block oxides — N2O (closest module: bonding/molecular structure) **Answer:** Not in extracted key

Q.20 (CUET 2023) The oxoacid of sulphur which has one lone pair on sulphur is:

- A) H_2SO_4 B) H_2SO_3 C) $H_2S_2O_8$ D) $H_2S_2O_7$

Tests: Oxoacids of sulphur — lone pair on central atom (bonding/structure) **Answer:** Not in extracted key