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Chemical Bonding and Molecular Structure Class 11 Notes | CBSE Chemistry Chapter 4

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Chemical Bonding and Molecular Structure Class 11 Notes | CBSE Chemistry Chapter 4

Chemical Bonding and Molecular Structure is Chapter 4 of CBSE Class 11 Chemistry — and one of the most rewarding chapters you will ever study. It answers a single big question: *why* do atoms join together at all, and once they do, what shape do the resulting molecules take? Master this chapter and a huge slice of NEET, JEE, and your board paper turns into easy marks.

By the end of these notes you will be able to draw a Lewis structure, decide whether a bond is ionic or covalent, predict molecular shapes using VSEPR, work out the hybridisation of any central atom, write molecular orbital diagrams, calculate bond order, and explain hydrogen bonding and dipole moment. This is a very high-weightage chapter carrying roughly 8–10 marks in boards and a guaranteed cluster of questions in every entrance exam.

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Key Concepts

1. Why Atoms Form Bonds — Kossel-Lewis Approach

Atoms combine to achieve a stable, lower-energy state — usually the stable electronic configuration of the nearest noble gas. A **chemical bond** is the attractive force that holds atoms or ions together in a molecule or compound.

Kossel and Lewis (1916) explained bonding in terms of the outer (valence) electrons. **Lewis symbols** show only the valence electrons as dots around the element symbol — for example, nitrogen is drawn with five dots.

The number of dots that pair up or are shared gives the **valence** of the element. Kossel went further: electron transfer gives ions (ionic bond), while Lewis proposed electron sharing (covalent bond).

2. The Octet Rule and Its Limitations

The **octet rule** states that atoms tend to gain, lose, or share electrons so as to have eight electrons in their valence shell — the stable octet of a noble gas (hydrogen aims for a duplet of 2).

It is a powerful guide, but it has clear **limitations**:

- **Incomplete octet:** central atom has fewer than 8 electrons, e.g. BeCl_2 (4), BF_3 (6), LiCl .
 - **Expanded octet:** central atom has more than 8 electrons using d-orbitals, e.g. PF_5 (10), SF_6 (12), H_2SO_4 .
 - **Odd-electron molecules:** NO (11 electrons) and NO_2 cannot satisfy the octet.
 - It does not explain the **shape** of molecules or the **relative stability** in terms of energy.
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3. The Ionic (Electrovalent) Bond

An **ionic bond** forms by the complete transfer of one or more electrons from a metal (low ionisation enthalpy) to a non-metal (high electron gain enthalpy), producing oppositely charged ions held by electrostatic attraction.

Example: Na (2,8,1) loses one electron to become Na^+ and Cl (2,8,7) gains it to become Cl^- ; the ions attract to give NaCl .

Favourable conditions: low ionisation enthalpy of the metal, high (more negative) electron gain enthalpy of the non-metal, and high lattice enthalpy of the compound formed.

4. Lattice Enthalpy

Lattice enthalpy is the energy released when one mole of an ionic crystal is formed from its gaseous ions (or the energy required to break one mole of the solid into gaseous ions). The larger the lattice enthalpy, the more stable the ionic compound.

It increases with higher ionic charge and smaller ionic size — that is why MgO (charges 2+, 2-) has a much larger lattice enthalpy than NaCl .

Lattice enthalpy is calculated indirectly using the **Born-Haber cycle**, which applies Hess's law to the steps of compound formation.

5. The Covalent Bond and Lewis Structures

A **covalent bond** forms when two atoms share one or more electron pairs, each contributing electrons so that both attain a stable octet. Sharing one pair gives a single bond (H-H), two pairs a double bond (O=O), three pairs a triple bond ($\text{N}\equiv\text{N}$).

A **Lewis (electron-dot) structure** shows bonding pairs and lone pairs. Steps: count total valence electrons, place the least electronegative atom in the centre, form single bonds, then distribute remaining electrons as lone pairs to complete octets, adding multiple bonds if needed.

In a **coordinate (dative) bond** both shared electrons come from the same atom, shown by an arrow — as in NH_4^+ and the formation of O_3 .

6. Formal Charge and Resonance

Formal charge on an atom = (valence electrons) – (lone-pair electrons) – $\frac{1}{2}$ (bonding electrons). It helps choose the most plausible Lewis structure — the best one has formal charges closest to zero.

Resonance is used when a single Lewis structure cannot describe a molecule. The real molecule is a **resonance hybrid** of two or more contributing structures, and it is more stable (lower in energy) than any single one.

Classic examples are O_3 , CO_3^{2-} , and the carbonate/nitrate ions, where all bonds are found experimentally to be of equal length — exactly what a hybrid predicts.

7. Bond Parameters

Bond parameters describe a covalent bond numerically.

- **Bond length:** the equilibrium distance between the nuclei of two bonded atoms. It decreases as bond order increases ($\text{C}-\text{C} > \text{C}=\text{C} > \text{C}\equiv\text{C}$).
 - **Bond enthalpy:** the energy required to break one mole of a particular bond in the gas phase; it increases with bond order.
 - **Bond angle:** the angle between two bonds at the central atom (e.g. 104.5° in H_2O).
 - **Bond order:** the number of bonds between two atoms (1 for single, 2 for double, 3 for triple).
-

8. Dipole Moment

When bonded atoms differ in electronegativity, the shared pair shifts and the bond becomes **polar**. The **dipole moment** (μ) measures this polarity: $\mu = q \times d$, where q is the charge and d the distance. SI unit: coulomb-metre; commonly measured in **debye (D)**.

Dipole moment is a **vector**. A molecule may have polar bonds yet a net zero dipole moment if the bond dipoles cancel by symmetry.

That is why CO_2 (linear, $\mu = 0$) is non-polar but H_2O (bent, $\mu = 1.85 \text{ D}$) is polar; likewise BF_3 ($\mu = 0$) versus NH_3 ($\mu = 1.47 \text{ D}$).

9. VSEPR Theory and Molecular Geometry

The **Valence Shell Electron Pair Repulsion (VSEPR)** theory predicts molecular shape: electron pairs around the central atom arrange themselves as far apart as possible to minimise repulsion.

Repulsion order: lone pair–lone pair > lone pair–bond pair > bond pair–bond pair. Lone pairs therefore reduce bond angles.

[DIAGRAM: CH₄ tetrahedral (109.5°), NH₃ pyramidal (107°) with one lone pair, H₂O bent (104.5°) with two lone pairs — angle shrinks as lone pairs increase.]

Bond pairs + lone pairs	Geometry	Example
2 + 0	Linear (180°)	BeCl ₂ , CO ₂
3 + 0	Trigonal planar (120°)	BF ₃
4 + 0	Tetrahedral (109.5°)	CH ₄
3 + 1	Trigonal pyramidal (107°)	NH ₃
2 + 2	Bent (104.5°)	H ₂ O
5 + 0	Trigonal bipyramidal	PCl ₅
6 + 0	Octahedral (90°)	SF ₆

10. Valence Bond Theory (VBT)

Valence Bond Theory says a covalent bond forms by the **overlap** of half-filled atomic orbitals of two atoms; greater overlap means a stronger bond. The shared pair has opposite spins.

- **Sigma (σ) bond:** head-on (axial) overlap of orbitals (s-s, s-p, p-p); stronger.
- **Pi (π) bond:** sideways (lateral) overlap of p-orbitals; weaker, formed only after a σ bond.

A single bond is one σ ; a double bond is one σ + one π ; a triple bond is one σ + two π .

11. Hybridisation

Hybridisation is the intermixing of atomic orbitals of nearly equal energy to form an equal number of new, identical **hybrid orbitals** that explain the actual shape of molecules.

Hybridisation	Geometry	Bond angle	Example
sp	Linear	180°	BeCl ₂ , C ₂ H ₂
sp ²	Trigonal planar	120°	BF ₃ , C ₂ H ₄
sp ³	Tetrahedral	109.5°	CH ₄ , NH ₃ , H ₂ O
sp ³ d	Trigonal bipyramidal	90°, 120°	PCl ₅
sp ³ d ²	Octahedral	90°	SF ₆

Quick rule to find hybridisation: number of hybrid orbitals = number of σ bonds + number of lone pairs on the central atom.

12. Molecular Orbital Theory (MOT)

Molecular Orbital Theory says atomic orbitals combine to form **molecular orbitals** that belong to the whole molecule. Two atomic orbitals give one lower-energy **bonding** MO and one higher-energy **antibonding** MO (marked with *).

Electrons fill MOs following the Aufbau principle, Pauli's principle, and Hund's rule. The order for O_2 , F_2 is: $\sigma 1s$, $\sigma^* 1s$, $\sigma 2s$, $\sigma^* 2s$, $\sigma 2p_z$, ($\pi 2p_x = \pi 2p_y$), ($\pi^* 2p_x = \pi^* 2p_y$), $\sigma^* 2p_z$. For B_2 , C_2 , N_2 the $\sigma 2p_z$ lies above the π orbitals.

Bond order = $\frac{1}{2}(N_b - N_a)$, where N_b and N_a are electrons in bonding and antibonding MOs. A positive bond order means the molecule exists; higher bond order means greater stability and shorter bond length.

13. Bonding in Homonuclear Diatomic Molecules

- **H_2** : bond order = $\frac{1}{2}(2 - 0) = 1$; diamagnetic, stable.
- **He_2** : bond order = $\frac{1}{2}(2 - 2) = 0$; does not exist.
- **N_2** : bond order = $\frac{1}{2}(10 - 4) = 3$; very stable, diamagnetic.
- **O_2** : bond order = $\frac{1}{2}(10 - 6) = 2$; **paramagnetic** because of two unpaired electrons in π^* — a famous success of MOT that VBT could not explain.

14. Hydrogen Bonding

A **hydrogen bond** is the attraction between a hydrogen atom bonded to a highly electronegative atom (F, O, N) and a lone pair on another electronegative atom. It is weaker than a covalent bond but stronger than ordinary dipole forces.

- **Intermolecular H-bond**: between molecules — e.g. in H_2O , HF, NH_3 — raising boiling points. This is why water is liquid and ice floats.
- **Intramolecular H-bond**: within the same molecule, e.g. o-nitrophenol, which lowers its boiling point relative to the para isomer.

Weightage in Board & Entrance Exams

Exam	Typical Weightage	Most-Tested Areas
CBSE Board (Class 11)	8–10 marks	VSEPR shapes, hybridisation, dipole moment, hydrogen bonding
JEE Main / Advanced	2–4 questions	MOT & bond order, hybridisation, formal charge, back bonding
NEET	2–3 questions	Molecular shapes, paramagnetism of O_2 , bond order comparisons

[TABLE: Question-type split — VSA (1 mark): definitions, shapes, bond order; SA (2–3 marks): VSEPR shapes, hybridisation, dipole-moment comparison; LA (5 marks): MOT diagrams of N₂/O₂, octet limitations, hydrogen bonding.]

Important Definitions

Term	Definition
Chemical bond	Attractive force holding atoms together in a molecule or compound
Octet rule	Atoms gain, lose, or share electrons to attain 8 valence electrons
Ionic bond	Bond formed by complete transfer of electrons from metal to non-metal
Lattice enthalpy	Energy released when 1 mole of an ionic solid forms from its gaseous ions
Covalent bond	Bond formed by sharing of one or more electron pairs between atoms
Coordinate bond	Covalent bond in which both shared electrons come from one atom
Formal charge	$V - L - \frac{1}{2}B$; charge an atom appears to carry in a Lewis structure
Resonance	Representation of a real molecule as a hybrid of several Lewis structures
Dipole moment	Measure of bond/molecular polarity: $\mu = q \times d$ (in debye)
Hybridisation	Mixing of atomic orbitals of similar energy to form equivalent hybrid orbitals
Bond order	$\frac{1}{2}(N_b - N_a)$ in MOT; number of bonds between two atoms
Hydrogen bond	Attraction between H bonded to F/O/N and a lone pair on F/O/N

Solved Examples

Example 1

Predict the shape and bond angle of the water molecule (H₂O) using VSEPR theory.

Answer: Oxygen has 2 bond pairs and 2 lone pairs (4 electron pairs → sp³). The two lone pairs repel strongly, so the shape is **bent (angular)** with a bond angle of **104.5°**, less than the ideal 109.5°.

Example 2

Calculate the bond order of the O₂ molecule and state whether it is paramagnetic.

Answer: O_2 has 16 electrons: $N_b = 10$, $N_a = 6$. Bond order = $\frac{1}{2}(10 - 6) = 2$. It has two unpaired electrons in the π^* orbitals, so O_2 is **paramagnetic**.

Example 3

Find the hybridisation of the central atom in NH_3 .

Answer: Nitrogen forms 3 σ bonds and has 1 lone pair $\rightarrow 3 + 1 = 4$ hybrid orbitals $\rightarrow sp^3$ hybridisation, giving a trigonal pyramidal shape (107°).

Example 4

Why is the dipole moment of BF_3 zero while that of NH_3 is 1.47 D, even though both have polar bonds?

Answer: BF_3 is symmetrical (trigonal planar), so the three B–F bond dipoles cancel $\rightarrow \mu = 0$. NH_3 is pyramidal with a lone pair; the N–H dipoles and the lone-pair dipole add up to a **net dipole moment**, so NH_3 is polar.

Example 5

Calculate the formal charge on each oxygen atom in the ozone molecule (O_3).

Answer: Central O (1 lone pair, 3 bonds): $6 - 2 - 3 = +1$. Doubly bonded terminal O: $6 - 4 - 2 = 0$. Singly bonded terminal O: $6 - 6 - 1 = -1$. Net charge = 0, consistent with neutral O_3 .

Example 6

Arrange the bonds C–C, C=C, and C $\equiv$ C in increasing order of bond length and bond enthalpy.

Answer: Bond length: C $\equiv$ C < C=C < C–C. Bond enthalpy: C–C < C=C < C $\equiv$ C. As bond order rises, bonds become shorter and stronger.

Important Questions for Board Exams

1-Mark Questions (VSA)

1. Define a hydrogen bond and give one example.
2. What is the shape of the CO_2 molecule and why is its dipole moment zero?
3. Write the bond order of the N_2 molecule.
4. State the type of hybridisation of carbon in ethyne (C_2H_2).
5. Why does ice float on water?

2–3-Mark Questions (SA)

1. State the postulates of VSEPR theory and use them to explain the shape of NH_3 .

2. Explain the limitations of the octet rule with suitable examples.
3. Define lattice enthalpy. How does it depend on ionic charge and size?
4. Distinguish between sigma and pi bonds with examples.

5-Mark Questions (LA)

1. Draw the molecular orbital diagram of the O_2 molecule. Calculate its bond order and explain its paramagnetic behaviour.
 2. What is hybridisation? Explain sp , sp^2 , and sp^3 hybridisation with one example and the geometry of each.
 3. Explain hydrogen bonding, its types, and its effect on the physical properties of water.
-

Quick Revision Points

- Atoms bond to attain the stable noble-gas (octet) configuration and lower energy
 - Octet rule fails for incomplete (BF_3), expanded (SF_6), and odd-electron (NO) molecules
 - Ionic bond = electron transfer; favoured by low IE, high ΔH_{eg} , high lattice enthalpy
 - Covalent bond = electron sharing; coordinate bond = both electrons from one atom
 - Formal charge = $V - L - \frac{1}{2}B$; resonance hybrid is more stable than any single form
 - Bond order $\uparrow \Rightarrow$ bond length $\downarrow$ and bond enthalpy $\uparrow$
 - $\mu = q \times d$ (debye); CO_2 and BF_3 are non-polar by symmetry, H_2O and NH_3 are polar
 - VSEPR repulsion: $lp-lp > lp-bp > bp-bp$; lone pairs shrink bond angles
 - Hybrid orbitals = σ bonds + lone pairs: sp (180°), sp^2 (120°), sp^3 (109.5°), sp^3d , sp^3d^2
 - MOT bond order = $\frac{1}{2}(N_b - N_a)$; O_2 is paramagnetic (2 unpaired e^- in π^*)
 - N_2 bond order 3, O_2 2, He_2 0 (does not exist)
 - Hydrogen bonding (F, O, N) raises boiling points and explains water's anomalies
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Next Chapter: Chapter 5 — Thermodynamics



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