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Class 11 Chemistry

Chapter 4: Chemical Bonding and Molecular Structure

📚 Chapter Overview

Why Chemical Bonding?

Chemical bonding explains why atoms combine to form molecules and compounds. Understanding bonding helps predict molecular structure, properties, and reactivity. This chapter is fundamental to all chemistry!

Exam Importance:

- **CBSE Board:** 6-8 marks (4-5 questions including 1 long answer)
- **JEE Main:** 2-3 questions (high weightage from VSEPR and hybridization)
- **NEET:** 2-3 questions (Lewis structures and bonding concepts)

1. Introduction to Chemical Bonding

1.1 Why Atoms Combine?

Atoms combine to achieve **noble gas configuration** (octet rule) and attain lower energy, hence greater stability.

Kössel-Lewis Theory (1916)

- Atoms combine to complete their octet (8 electrons in valence shell)
- Noble gases are stable because they already have complete octets
- Other atoms achieve stability by gaining, losing, or sharing electrons
- Exception: Hydrogen and Helium follow duet rule (2 electrons)

1.2 Types of Chemical Bonds

Bond Type	Formation	Example	Nature
Ionic Bond	Transfer of electrons	NaCl, MgO, CaF_2	Electrostatic attraction between ions
Covalent Bond	Sharing of electrons	H_2, O_2, CH_4, H_2O	Sharing of electron pairs
Coordinate/Dative Bond	Donation of electron pair	$NH_3 \rightarrow BF_3$, H_3O^+, NH_4^+	One-sided electron pair donation
Metallic Bond	Delocalized electrons	Na, Cu, Fe, Al	Sea of electrons model
Hydrogen Bond	Dipole-dipole interaction	H_2O, HF, DNA strands	Weak intermolecular force

2. Ionic or Electrovalent Bond

2.1 Formation of Ionic Bond

Ionic bond forms by **complete transfer of electrons** from one atom to another. The atom that loses electrons becomes a **cation** (positive ion), and the atom that gains electrons becomes an **anion** (negative ion).

Example: Formation of NaCl

Step 1: Na loses 1 electron → Na^+

$Na\ (2, 8, 1) \rightarrow Na^+\ (2, 8) + e^-$

Step 2: Cl gains 1 electron → Cl^-

$Cl\ (2, 8, 7) + e^- \rightarrow Cl^-\ (2, 8, 8)$

Step 3: Electrostatic attraction

$Na^+ + Cl^- \rightarrow NaCl$ (ionic bond)

2.2 Lattice Energy

Lattice Energy: Energy released when gaseous ions combine to form one mole of ionic solid

$$M^+(g) + X^-(g) \rightarrow MX(s) + \text{Lattice Energy}$$

Factors affecting Lattice Energy:

- **Charge on ions:** Higher charge → Higher lattice energy (MgO > NaCl)

- **Size of ions:** Smaller ions → Higher lattice energy ($LiF > KBr$)

2.3 Born-Haber Cycle

Thermochemical cycle used to calculate lattice energy indirectly using Hess's law.

For NaCl:

$Na(s) + \frac{1}{2}Cl_2(g) \rightarrow NaCl(s)$ $\Delta H°f = -411$ kJ/mol

Steps involved:

1. Sublimation of Na: $Na(s) \rightarrow Na(g)$ $\Delta H°sub = +108$ kJ/mol
2. Ionization of Na: $Na(g) \rightarrow Na^+(g) + e^-$ $IE = +496$ kJ/mol
3. Dissociation of Cl_2: $\frac{1}{2}Cl_2(g) \rightarrow Cl(g)$ $\Delta H°dis = +121$ kJ/mol
4. Electron gain by Cl: $Cl(g) + e^- \rightarrow Cl^-(g)$ $EA = -349$ kJ/mol
5. Formation of lattice: $Na^+(g) + Cl^-(g) \rightarrow NaCl(s)$ $U = ?$

By Hess's law:

$\Delta H°f = \Delta H°sub + IE + \frac{1}{2}\Delta H°dis + EA + U$

$-411 = 108 + 496 + 121 - 349 + U$

$U = -787$ kJ/mol (Lattice Energy)

2.4 Characteristics of Ionic Compounds

Property	Explanation
High melting and boiling points	Strong electrostatic forces between ions require high energy to break
Crystalline solids	Ions arranged in regular 3D lattice structure
Conduct electricity in molten/aqueous state	Ions become free to move in liquid/solution state
Do not conduct electricity in solid state	Ions are fixed in lattice positions
Soluble in polar solvents	Polar solvents (like water) can break ionic bonds
Hard but brittle	Strong forces make them hard; displacement causes repulsion → brittleness

3. Covalent Bond

3.1 Formation of Covalent Bond

Covalent bond forms by **sharing of electrons** between atoms. Each atom contributes one or more electrons to form shared electron pairs.

Types of Covalent Bonds:

- **Single Bond:** Sharing of 1 electron pair (e.g., H-H, Cl-Cl, C-C)
- **Double Bond:** Sharing of 2 electron pairs (e.g., O=O, C=C, C=O)
- **Triple Bond:** Sharing of 3 electron pairs (e.g., N≡N, C≡C, C≡N)

3.2 Lewis Dot Structures

Lewis structures represent valence electrons as dots around atomic symbols and shared electron pairs as lines.

Examples of Lewis Structures:

1. Water (H_2O):

H-O-H with 2 lone pairs on O

Total electrons: 2(1) + 6 = 8 electrons = 4 pairs

2 bonding pairs + 2 lone pairs on O

2. Ammonia (NH_3):

Pyramidal structure with N at center

Total electrons: 3(1) + 5 = 8 electrons = 4 pairs

3 bonding pairs + 1 lone pair on N

3. Carbon dioxide (CO_2):

$O=C=O$ (linear)

Total electrons: 6 + 4 + 6 = 16 electrons = 8 pairs

4 bonding pairs (2 double bonds) + 4 lone pairs on O atoms

4. Nitrogen molecule (N_2):

$N\equiv N$ with 1 lone pair on each N

Total electrons: 5 + 5 = 10 electrons = 5 pairs

3 bonding pairs (triple bond) + 2 lone pairs

3.3 Formal Charge

Formal Charge = $V - N - B/2$

V = Valence electrons of free atom
N = Non-bonding electrons (lone pairs)
B = Bonding electrons (shared electrons)

Rules for Stable Lewis Structure:

- Sum of formal charges = charge on molecule/ion
- Formal charges should be as close to zero as possible
- Negative formal charge should be on more electronegative atom
- Like charges should not be on adjacent atoms

Example: Formal Charge Calculation for CO_2

Structure: O=C=O

For Carbon:

V = 4, N = 0, B = 8

Formal Charge = 4 - 0 - 8/2 = 4 - 0 - 4 = 0

For each Oxygen:

V = 6, N = 4, B = 4

Formal Charge = 6 - 4 - 4/2 = 6 - 4 - 2 = 0

Total formal charge = 0 + 0 + 0 = 0 ✓

3.4 Resonance

Resonance occurs when a molecule cannot be represented by a single Lewis structure. The actual structure is a **resonance hybrid** of all contributing structures.

Important Points about Resonance:

- Resonance structures differ only in electron arrangement, not atom positions
- Actual molecule is more stable than any single resonance structure
- All resonance structures must have same number of paired/unpaired electrons
- Greater number of resonance structures → Greater stability

Examples of Resonance:

1. Ozone (O_3):

Two equivalent structures with double bond on either side

O=O-O ↔ O-O=O

Actual: Both O-O bonds are equivalent (1.5 bond order)

2. Carbonate ion (CO_3^{2-}):

Three equivalent structures

All C-O bonds are equivalent with bond order 1.33

3. Benzene (C_6H_6):

Two Kekulé structures with alternating single and double bonds

Actual: All C-C bonds are equivalent (bond order 1.5)

3.5 Exceptions to Octet Rule

Type of Exception	Description	Examples
Incomplete Octet	Central atom has less than 8 electrons	BF_3 ($6e^-$), BCl_3 ($6e^-$), BeH_2 ($4e^-$), BH_3 ($6e^-$)
Expanded Octet	Central atom has more than 8 electrons (Period 3 onwards)	PCl_5 ($10e^-$), SF_6 ($12e^-$), IF_7 ($14e^-$), H_2SO_4 ($12e^-$)
Odd Electron Molecules	Total number of valence electrons is odd	NO ($11e^-$), NO_2 ($17e^-$), ClO_2 ($19e^-$)

⚠ Common Mistake:

Wrong: Period 2 elements (N, O, F) can have expanded octet

Right: Only Period 3 onwards (P, S, Cl, etc.) can have expanded octet because they have vacant d-orbitals

3.6 Characteristics of Covalent Compounds

Property	Explanation
Low melting and boiling points	Weak van der Waals forces between molecules
Do not conduct electricity	No free ions or electrons present
Exist as gases or liquids	Weak intermolecular forces at room temperature
Soluble in non-polar solvents	"Like dissolves like" - polar in polar, non-polar in non-polar
Directional bonds	Covalent bonds have specific directions → definite shape

4. Bond Parameters

4.1 Bond Length

Bond length is the equilibrium distance between the nuclei of two bonded atoms.

Bond Length = $r_A + r_B$
(Sum of covalent radii of bonded atoms)

Factors Affecting Bond Length:

- **Size of atoms:** Larger atoms → Longer bond (C-C > C-N > C-O)
- **Bond order:** Higher bond order → Shorter bond (C≡C < C=C < C-C)
- **Hybridization:** More s-character → Shorter bond ($sp < sp^2 < sp^3$)

Typical Bond Lengths:

- C-C: 154 pm | C=C: 134 pm | C≡C: 120 pm
- C-N: 147 pm | C=N: 129 pm | C≡N: 116 pm
- C-O: 143 pm | C=O: 120 pm

4.2 Bond Energy

Bond energy (Bond enthalpy) is the energy required to break one mole of bonds in gaseous state.

Key Points:

- Higher bond energy → Stronger bond → More stable molecule
- Triple bond > Double bond > Single bond (in terms of strength)
- N≡N (946 kJ/mol) > O=O (498 kJ/mol) > F-F (158 kJ/mol)

Bond	Bond Energy (kJ/mol)	Bond	Bond Energy (kJ/mol)
H-H	436	C-H	414
C-C	347	C=C	611
C≡C	837	O-H	464
N-H	389	N≡N	946
O=O	498	Cl-Cl	243

4.3 Bond Angle

Bond angle is the angle between two adjacent bonds at an atom.

Common Bond Angles:

- **Linear:** 180° (CO_2, BeF_2, C_2H_2)
- **Trigonal planar:** 120° (BF_3, BCl_3, C_2H_4)
- **Tetrahedral:** 109.5° (CH_4, CCl_4)
- **Trigonal pyramidal:** 107° (NH_3)
- **Bent:** 104.5° (H_2O)

4.4 Bond Order

Bond Order = (Number of bonding electrons - Number of antibonding electrons) / 2

OR

Bond Order = Number of electron pairs shared between two atoms

Examples:

- **Single bond:** Bond order = 1 (H_2, Cl_2, C-C)
- **Double bond:** Bond order = 2 (O_2, C=C)
- **Triple bond:** Bond order = 3 (N_2, C≡C)
- **Resonance:** Bond order can be fractional (Benzene = 1.5, O_3 = 1.5)

💡 Relationship:

Bond Order $\propto$ Bond Strength $\propto$ Bond Energy

Bond Order $\propto$ 1/Bond Length

Higher bond order → Stronger, shorter, more stable bond

5. VSEPR Theory

Valence Shell Electron Pair Repulsion Theory predicts molecular geometry based on repulsion between electron pairs.

Postulates of VSEPR Theory:

1. Electron pairs arrange themselves to minimize repulsion
2. Order of repulsion: **lp-lp > lp-bp > bp-bp**
3. Lone pairs occupy more space than bonding pairs
4. Multiple bonds treated as single electron pair for geometry
5. The shape is determined by positions of atoms only (not lone pairs)

5.1 Molecular Shapes

Formula	BP	LP	Geometry	Shape	Bond Angle	Examples
AB_2	2	0	Linear	Linear	180°	$BeCl_2$, CO_2, C_2H_2
AB_3	3	0	Trigonal planar	Trigonal planar	120°	BF_3, BCl_3, $AlCl_3$
AB_2E	2	1	Trigonal planar	Bent/V-shaped	<120°	SO_2, $SnCl_2$
AB_4	4	0	Tetrahedral	Tetrahedral	109.5°	CH_4, CCl_4, NH_4^+
AB_3E	3	1	Tetrahedral	Trigonal pyramidal	107°	NH_3, PCl_3, H_3O^+
AB_2E_2	2	2	Tetrahedral	Bent/V-shaped	104.5°	H_2O, H_2S, OF_2
AB_5	5	0	Trigonal bipyramidal	Trigonal bipyramidal	90°, 120°	PCl_5, PF_5
AB_4E	4	1	Trigonal bipyramidal	See-saw	<90°, <120°	SF_4, IF_4^+
AB_3E_2	3	2	Trigonal bipyramidal	T-shaped	<90°	ClF_3, BrF_3
AB_2E_3	2	3	Trigonal bipyramidal	Linear	180°	XeF_2, I_3^-
AB_6	6	0	Octahedral	Octahedral	90°	SF_6, $[Co(NH_3)_6]^{3+}$

AB_5E	5	1	Octahedral	Square pyramidal	<90°	BrF_5, IF_5
AB_4E_2	4	2	Octahedral	Square planar	90°	XeF_4, ICl_4^-

💡 Quick Formula:

Total electron pairs = (V + M - C + A) / 2

V = Valence electrons of central atom

M = Monovalent atoms attached

C = Cationic charge (subtract)

A = Anionic charge (add)

Lone pairs = Total pairs - Bonding pairs

Example: Predicting Shape of NH_3

Step 1: Calculate total electron pairs

V = 5 (N), M = 3 (H atoms)

Total pairs = (5 + 3) / 2 = 4 pairs

Step 2: Identify bonding and lone pairs

Bonding pairs = 3 (N-H bonds)

Lone pairs = 4 - 3 = 1

Step 3: Determine geometry and shape

Geometry: Tetrahedral (4 pairs)

Shape: Trigonal pyramidal (3 BP + 1 LP)

Bond angle: ~107° (less than 109.5° due to lp-bp repulsion)

⚠ Common Mistakes:

- Confusing **geometry** with **shape** - Geometry considers all electron pairs; Shape considers only bonded atoms
- Forgetting that lone pairs reduce bond angles due to greater repulsion
- Not placing lone pairs in equatorial positions in trigonal bipyramidal geometry

6. Valence Bond Theory (VBT)

Postulates of VBT:

1. Covalent bond forms by **overlapping of atomic orbitals**
2. Overlapping orbitals must have **opposite spins**
3. Greater the overlap → Stronger the bond
4. Only **half-filled orbitals** participate in bonding
5. Bond formation releases energy and system becomes more stable

6.1 Types of Orbital Overlap

A. Sigma (σ) Bond

Formed by **head-on (axial) overlap** of orbitals along the internuclear axis.

- s-s overlap: H_2 molecule
- s-p overlap: HCl molecule
- p-p overlap: Cl_2, F_2 molecules

Characteristics: Stronger bond, cylindrically symmetric, allows free rotation

B. Pi (π) Bond

Formed by **lateral (sideways) overlap** of p-orbitals perpendicular to internuclear axis.

- Only p-p overlap can form π bonds
- Present in double and triple bonds

Characteristics: Weaker than σ bond, electron density above and below axis, restricts rotation

💡 Bond Composition:

- **Single bond:** 1σ
- **Double bond:** 1σ + 1π
- **Triple bond:** 1σ + 2π

6.2 Hybridization

Hybridization is the mixing of atomic orbitals to form new equivalent hybrid orbitals suitable for bonding.

Key Concepts:

- Only atomic orbitals of similar energy can hybridize
- Number of hybrid orbitals = Number of atomic orbitals mixed
- Hybrid orbitals are equivalent in energy and shape
- Hybrid orbitals are more directional → stronger bonding

6.3 Types of Hybridization

A. sp Hybridization

Mixing: 1s + 1p → 2 sp hybrid orbitals

Geometry: Linear

Bond angle: 180°

% s-character: 50%

Examples: BeF_2, $BeCl_2$, C_2H_2 (acetylene), CO_2

Example: BeF_2

Be ground state: $1s^2 2s^2$

Be excited state: $1s^2 2s^1 2p^1$

Hybridization: 2s + 2p → 2 sp orbitals

Structure: F-Be-F (linear, 180°)

Each sp orbital forms σ bond with F atom

B. sp^2 Hybridization

Mixing: 1s + 2p → 3 sp^2 hybrid orbitals

Geometry: Trigonal planar

Bond angle: 120°

% s-character: 33.3%

Examples: BF_3, BCl_3, C_2H_4 (ethylene), $CH_2=CH_2$

Example: BF_3

B ground state: $1s^2\ 2s^2\ 2p^1$

B excited state: $1s^2\ 2s^1\ 2p^2$

Hybridization: $2s + 2p^2 \rightarrow 3\ sp^2$ orbitals

Structure: Trigonal planar with F atoms at 120°

Each sp^2 orbital forms σ bond with F atom

C. sp^3 Hybridization

Mixing: $1s + 3p \rightarrow 4\ sp^3$ hybrid orbitals

Geometry: Tetrahedral

Bond angle: 109.5°

% s-character: 25%

Examples: CH_4, CCl_4, NH_3, H_2O, C_2H_6

Example: CH_4 (Methane)

C ground state: $1s^2 2s^2 2p^2$

C excited state: $1s^2 2s^1 2p^3$

Hybridization: $2s + 2p^3 \rightarrow 4\ sp^3$ orbitals

Structure: Tetrahedral with H atoms at 109.5°

Each sp^3 orbital forms σ bond with H atom

D. sp^3d Hybridization

Mixing: $1s + 3p + 1d \rightarrow 5\ sp^3d$ hybrid orbitals

Geometry: Trigonal bipyramidal

Bond angles: 90° and 120°

Examples: PCl_5, PF_5

E. sp^3d^2 Hybridization

Mixing: $1s + 3p + 2d \rightarrow 6\ sp^3d^2$ hybrid orbitals

Geometry: Octahedral

Bond angle: 90°

Examples: SF_6, $[Co(NH_3)_6]^{3+}$

6.4 Determining Hybridization

💡 Quick Method:

Hybridization = Number of σ bonds + Lone pairs on central atom

Steric Number	Hybridization	Geometry
2	sp	Linear
3	sp^2	Trigonal planar
4	sp^3	Tetrahedral
5	sp^3d	Trigonal bipyramidal
6	sp^3d^2	Octahedral

Examples:

1. **NH_3:** 3 σ bonds + 1 LP = 4 → sp^3

2. **H_2O:** 2 σ bonds + 2 LP = 4 → sp^3

3. **C_2H_4:** Each C has 3 σ bonds + 0 LP = 3 → sp^2

4. **C_2H_2:** Each C has 2 σ bonds + 0 LP = 2 → sp

5. **SF_4:** 4 σ bonds + 1 LP = 5 → sp^3d

7. Molecular Orbital Theory (MOT)

Postulates of MOT:

1. Atomic orbitals combine to form **molecular orbitals** (MOs)
2. Number of MOs formed = Number of atomic orbitals combined
3. Combining atomic orbitals must have comparable energy and proper symmetry
4. MOs extend over entire molecule
5. Electrons in MOs belong to molecule, not individual atoms

7.1 Types of Molecular Orbitals

A. Bonding Molecular Orbitals (BMO)

- Formed by **constructive interference** of atomic orbitals
- **Lower energy** than original atomic orbitals
- Electron density increases between nuclei
- Stabilizes the molecule
- Notation: σ, π

B. Antibonding Molecular Orbitals (ABMO)

- Formed by **destructive interference** of atomic orbitals
- **Higher energy** than original atomic orbitals
- Electron density decreases between nuclei (node)
- Destabilizes the molecule
- Notation: σ*, π*

💡 Energy Order of MOs:

For O_2, F_2, Ne_2 ($Z \geq 8$):

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

For B_2, C_2, N_2 ($Z < 8$):

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

7.2 Electronic Configuration of Molecules

Examples:

1. H_2 molecule (2 electrons):

Configuration: $(\sigma 1s)^2$

Bond order = (2-0)/2 = 1

2. He_2 molecule (4 electrons):

Configuration: $(\sigma 1s)^2$ $(\sigma^* 1s)^2$

Bond order = (2-2)/2 = 0 (unstable, doesn't exist)

3. O_2 molecule (16 electrons):

Configuration: $(\sigma 1s)^2$ $(\sigma^* 1s)^2$ $(\sigma 2s)^2$ $(\sigma^* 2s)^2$ $(\sigma 2pz)^2$ $(\pi 2px)^2$ $(\pi 2py)^2$ $(\pi^* 2px)^1$ $(\pi^* 2py)^1$

Bond order = (10-6)/2 = 2

Paramagnetic (2 unpaired electrons)

4. N_2 molecule (14 electrons):

Configuration: $(\sigma 1s)^2$ $(\sigma^* 1s)^2$ $(\sigma 2s)^2$ $(\sigma^* 2s)^2$ $(\pi 2px)^2$ $(\pi 2py)^2$ $(\sigma 2pz)^2$

Bond order = (10-4)/2 = 3

Diamagnetic (all paired)

7.3 Bond Order in MOT

Bond Order = (Nb - Na) / 2

Nb = Number of electrons in bonding MOs
Na = Number of electrons in antibonding MOs

Molecule	Total Electrons	Nb	Na	Bond Order	Magnetic Nature
H_2	2	2	0	1	Diamagnetic
He_2	4	2	2	0	Does not exist
Li_2	6	4	2	1	Diamagnetic
B_2	10	6	4	1	Paramagnetic
C_2	12	8	4	2	Diamagnetic
N_2	14	10	4	3	Diamagnetic
O_2	16	10	6	2	Paramagnetic
F_2	18	10	8	1	Diamagnetic

💡 Key Observations:

- Bond order 0 → Molecule does not exist
- Higher bond order → Stronger, shorter bond
- Unpaired electrons → Paramagnetic
- All paired electrons → Diamagnetic
- O_2 is paramagnetic (VBT fails to explain this; MOT succeeds)

8. Hydrogen Bonding

8.1 What is Hydrogen Bonding?

Hydrogen bonding is an electrostatic attraction between a hydrogen atom bonded to highly electronegative atom (F, O, N) and another electronegative atom.

X-H····Y

X, Y = F, O, or N
(—) = Covalent bond
(····) = Hydrogen bond

8.2 Types of Hydrogen Bonding

A. Intermolecular Hydrogen Bonding

Hydrogen bonding between **different molecules** of same or different compounds.

- **Examples:** H_2O, HF, NH_3, alcohols (R-OH), carboxylic acids (R-COOH)
- **Effects:** Increases boiling point, increases solubility in water, association of molecules

Example: Water (H_2O)

Each water molecule forms hydrogen bonds with up to 4 other water molecules

H-O-H····O-H····O-H

This extensive hydrogen bonding explains:

- High boiling point of water (100°C vs -60°C for H_2S)
- High heat of vaporization
- Lower density of ice than liquid water

B. Intramolecular Hydrogen Bonding

Hydrogen bonding **within the same molecule**.

- **Examples:** o-nitrophenol, o-hydroxybenzaldehyde, salicylaldehyde
- **Effects:** Decreases boiling point, decreases solubility in water, no association

Example: o-Nitrophenol vs p-Nitrophenol

o-Nitrophenol:

- Forms intramolecular H-bond
- Lower boiling point
- Less soluble in water

p-Nitrophenol:

- Forms intermolecular H-bonds
- Higher boiling point
- More soluble in water

8.3 Effects of Hydrogen Bonding

Property	Effect	Examples
Boiling Point	Increases significantly	H_2O (100°C) >> H_2S (-60°C) HF (20°C) >> HCl (-85°C)
Solubility	Increases in polar solvents	Alcohols, sugars, proteins soluble in water
Viscosity	Increases	Glycerol is highly viscous
Density	Ice < water (anomalous)	Ice floats on water
DNA Structure	Stabilizes double helix	Base pairing: A-T, G-C

Order of Boiling Points:

Group 16 hydrides: $H_2O > H_2S > H_2Se > H_2Te$

Group 17 hydrides: $HF > HCl > HBr > HI$

Group 15 hydrides: $NH_3 > PH_3 > AsH_3 > SbH_3$

In each group, the first member (H_2O, HF, NH_3) has abnormally high boiling point due to **hydrogen bonding**

9. Solved Numerical Examples

Example 1: Calculate formal charges in CO

Given: Carbon monoxide (CO)

Solution:

Lewis structure: :C≡O: (triple bond with lone pair on each)

For Carbon:

$V = 4, N = 2, B = 6$

$FC = 4 - 2 - 6/2 = 4 - 2 - 3 = -1$

For Oxygen:

$V = 6, N = 2, B = 6$

$FC = 6 - 2 - 6/2 = 6 - 2 - 3 = +1$

Answer: C has -1, O has +1 formal charge

Example 2: Predict geometry of XeF_4

Given: XeF_4

Solution:

Valence electrons of Xe = 8

Total pairs = (8 + 4)/2 = 6 pairs

Bonding pairs = 4 (Xe-F bonds)

Lone pairs = 6 - 4 = 2

Geometry: Octahedral (6 pairs)

Shape: Square planar (4 BP + 2 LP)

Bond angle: 90°

Answer: Square planar with 90° bond angles

Example 3: Determine hybridization in C_2H_4

Given: Ethylene (C_2H_4)

Solution:

Structure: $H_2C=CH_2$ (double bond between carbons)

For each carbon:

σ bonds = 3 (2 C-H + 1 C-C)

Lone pairs = 0

Steric number = 3 + 0 = 3

Hybridization: sp^2

Geometry: Trigonal planar around each C

Bond angles: ~120°

Bonding: 1 σ bond + 1 π bond between carbons

Example 4: Calculate bond order of O_2^+

Given: O_2^+ ion

Solution:

Total electrons in O_2^+ = 16 - 1 = 15 electrons

Electronic configuration:

$(\sigma 1s)^2 (\sigma^*1s)^2 (\sigma 2s)^2 (\sigma^*2s)^2 (\sigma 2p_z)^2 (\pi 2p_x)^2 (\pi 2p_y)^2 (\pi^*2p_x)^1$

$N_b = 10$

$N_a = 5$

Bond order = (10-5)/2 = 2.5

Answer: Bond order = 2.5

Paramagnetic (1 unpaired electron)

Example 5: Why is O_2 paramagnetic?

Given: Explain paramagnetism of O_2

Solution:

O_2 has 16 electrons

Electronic configuration:

$(\sigma1s)^2\ (\sigma^*1s)^2\ (\sigma2s)^2\ (\sigma^*2s)^2\ (\sigma2pz)^2\ (\pi2px)^2\ (\pi2py)^2\ (\pi^*2px)^1\ (\pi^*2py)^1$

Analysis:

Last two electrons occupy π^*2px and π^*2py orbitals separately (Hund's rule)

Two unpaired electrons present

Answer: O_2 is paramagnetic due to 2 unpaired electrons in antibonding π^* orbitals

VBT cannot explain this; MOT successfully explains it

10. Practice Questions

10.1 Multiple Choice Questions (MCQs)

Q1. Which of the following has the highest lattice energy?

(a) NaCl

(b) MgO

(c) CaO

(d) KCl

Q2. The shape of NH_3 molecule is:

(a) Tetrahedral

(b) Trigonal pyramidal

(c) Trigonal planar

(d) Bent

Q3. Which molecule has zero dipole moment?

(a) H_2O

(b) NH_3

(c) CO_2

(d) HCl

Q4. The hybridization of carbon in CH_4 is:

(a) sp

(b) sp^2

(c) sp^3

(d) sp^3d

Q5. Which of the following is paramagnetic?

(a) N_2

(b) O_2

(c) F_2

(d) H_2

Q6. Bond angle in H_2O is approximately:

(a) 109.5°

(b) 107°

(c) 104.5°

(d) 120°

Q7. Which of the following has expanded octet?

(a) BF_3

(b) SF_6

(c) NH_3

(d) H_2O

Q8. The geometry of PCl_5 is:

(a) Tetrahedral

(b) Square pyramidal

(c) Trigonal bipyramidal

(d) Octahedral

Q9. Which has the shortest C-C bond length?

(a) C_2H_6

(b) C_2H_4

(c) C_2H_2

(d) C_6H_6

Q10. The bond order of N_2 is:

(a) 1

(b) 2

(c) 3

(d) 2.5

Q11. Which molecule shows intramolecular hydrogen bonding?

(a) H_2O

(b) HF

(c) o-Nitrophenol

(d) p-Nitrophenol

Q12. In VSEPR theory, the order of repulsion is:

(a) lp-lp > lp-bp > bp-bp

(b) bp-bp > lp-bp > lp-lp

(c) lp-bp > lp-lp > bp-bp

(d) bp-bp > lp-lp > lp-bp

Q13. The type of bond present in NH_4^+ ion is:

(a) Only ionic bond

(b) Only covalent bond

(c) Covalent and coordinate bond

(d) Only coordinate bond

Q14. The molecule with square planar geometry is:

(a) SF_4

(b) XeF_4

(c) BF_4^-

(d) NH_4^+

Q15. Which has maximum covalent character?

(a) NaCl

(b) $MgCl_2$

(c) $AlCl_3$

(d) $SiCl_4$

Q16. The hybridization of central atom in SF_6 is:

(a) sp^3
(b) sp^3d
(c) sp^3d^2
(d) dsp^2

Q17. Which of the following is isoelectronic with CO_2?

(a) NO_2
(b) N_2O
(c) SO_2
(d) CO

Q18. The bond with highest bond energy is:

(a) C-C
(b) C=C
(c) C≡C
(d) All equal

Q19. Sigma bond is formed by:

(a) Lateral overlap
(b) Head-on overlap
(c) Both
(d) None

Q20. Which molecule has highest boiling point?

(a) H_2O

(b) H_2S

(c) H_2Se

(d) H_2Te

Answer Key:

1.(b) 2.(b) 3.(c) 4.(c) 5.(b) 6.(c) 7.(b) 8.(c) 9.(c) 10.(c)

11.(c) 12.(a) 13.(c) 14.(b) 15.(d) 16.(c) 17.(b) 18.(c) 19.(b) 20.(a)

10.2 Case-Based Questions

Case Study 1: VSEPR Theory and Molecular Shapes

VSEPR theory helps predict molecular geometry based on electron pair repulsion. The shape depends on the number of bonding pairs and lone pairs around the central atom. Lone pairs occupy more space than bonding pairs, leading to variations in bond angles.

(i) The shape of SF_4 molecule is:

(a) Tetrahedral (b) Square planar (c) See-saw (d) T-shaped

(ii) In which molecule is the bond angle exactly 90°?

(a) NH_3 (b) H_2O (c) SF_6 (d) BF_3

(iii) The geometry of XeF_2 is:

(a) Linear (b) Bent (c) T-shaped (d) Trigonal planar

(iv) Which has the smallest bond angle?

(a) NH_3 (b) H_2O (c) CH_4 (d) BF_3

Answers: (i) c, (ii) c, (iii) a, (iv) b

Case Study 2: Hybridization and Bonding

Hybridization involves mixing of atomic orbitals to form equivalent hybrid orbitals suitable for bonding. The type of hybridization determines the geometry and bond angles in molecules. Carbon shows sp, sp^2, and sp^3 hybridization in different compounds.

(i) The hybridization of carbon atoms in C_2H_6 is:

(a) sp (b) sp^2 (c) sp^3 (d) sp^3d

(ii) In C_2H_2, the number of sigma and pi bonds are:

(a) $3\sigma, 2\pi$ (b) $4\sigma, 1\pi$ (c) $5\sigma, 2\pi$ (d) $3\sigma, 1\pi$

(iii) Which carbon compound has sp^2 hybridization?

(a) CH_4 (b) C_2H_4 (c) C_2H_2 (d) C_2H_6

(iv) The % s-character in sp^3 hybrid orbital is:

(a) 25% (b) 33.3% (c) 50% (d) 75%

Answers: (i) c, (ii) a, (iii) b, (iv) a

Case Study 3: Molecular Orbital Theory

Molecular Orbital Theory explains bonding in terms of molecular orbitals formed by combination of atomic orbitals. It successfully explains the paramagnetic nature of O_2 and provides accurate bond order calculations. The stability of molecules can be predicted using bond order.

(i) The bond order of O_2 molecule is:

(a) 1 (b) 1.5 (c) 2 (d) 3

(ii) Which molecule does not exist according to MOT?

(a) H_2 (b) He_2 (c) Li_2 (d) O_2

(iii) O_2 molecule is paramagnetic because:

(a) It has 2 unpaired electrons (b) It has 2 lone pairs
(c) Bond order is 2 (d) It has double bond

(iv) The molecule with highest bond order is:

(a) O_2 (b) N_2 (c) F_2 (d) B_2

Answers: (i) c, (ii) b, (iii) a, (iv) b

11. Memory Tricks & Tips

🎯 Memorizing Hybridization:

"SPLIT"

- **S**teric number 2 → **SP**
- **P**yramidal/Planar (3) → **SP^2**
- **L**one pairs important
- **I**nclude sigma bonds
- **T**etrahedral (4) → **SP^3**

🎯 VSEPR Repulsion Order:

"Lonely Loners Push Bondmakers Back, But Partners Push Partners"

lp-lp > lp-bp > bp-bp

🎯 Bond Order Memory:

"NBC - NEWS"

Nb (bonding) **B**ring **C**elebration

Na (antibonding) **E**nd **W**ith **S**ubtraction

Bond Order = $(N_b - N_a) / 2$

🎯 Exceptions to Octet:

"BEN Incomplete, PIFS Expanded"

- **B**e, **B** (BeH_2, BF_3) - Incomplete octet
- **N**O, NO_2, ClO_2 - Odd electron molecules
- **P**, **S**, **Cl**, **I**, **F** (Period 3+) - Expanded octet (PCl_5, SF_6, IF_7)

12. Common Mistakes to Avoid

❌ Mistake 1: Confusing Geometry with Shape

Wrong: "H_2O has tetrahedral shape"

Right: "H_2O has tetrahedral geometry but bent/V-shaped molecular shape"

Remember: Geometry considers all electron pairs; Shape considers only bonded atoms

❌ Mistake 2: Formal Charge Calculation

Wrong: FC = V - N - B

Right: FC = V - N - B/2

Remember: Divide bonding electrons by 2 because they're shared

❌ Mistake 3: Expanded Octet in Period 2

Wrong: "N can form 5 bonds (expanded octet)"

Right: "Only Period 3+ elements can have expanded octet (d-orbitals available)"

Remember: N, O, F cannot exceed octet; P, S, Cl can

❌ Mistake 4: Bond Order from Structure

Wrong: "Benzene has alternating bond orders 1 and 2"

Right: "Benzene has resonance → all C-C bonds have bond order 1.5"

Remember: Resonance gives fractional bond orders

❌ Mistake 5: MO Energy Order

Wrong: "Same energy order for all diatomic molecules"

Right: "Different order for $Z<8$ (B_2, C_2, N_2) vs $Z\geq 8$ (O_2, F_2)"

Remember: σ2pz and π2p orbitals switch positions at $Z=8$

13. Exam Strategy & Preparation

📝 Topic-wise Priority for Board Exams:

Topic	Priority	Marks Weightage
VSEPR Theory & Shapes	⭐⭐⭐ HIGH	2-3 marks
Hybridization	⭐⭐⭐ HIGH	2-3 marks
Lewis Structures & Formal Charge	⭐⭐⭐ HIGH	2 marks
Hydrogen Bonding	⭐⭐ MEDIUM	1-2 marks
Molecular Orbital Theory	⭐⭐ MEDIUM	2 marks
Ionic Bonding & Lattice Energy	⭐ LOW	1 mark

⏰ Last Minute Revision Checklist:

- ✅ VSEPR table with all shapes and bond angles
- ✅ Hybridization determination formula
- ✅ MO energy level diagram for O_2 and N_2
- ✅ Bond order formula and calculations
- ✅ Formal charge formula
- ✅ Exceptions to octet rule (BF_3, SF_6, NO_2)
- ✅ Hydrogen bonding examples and effects
- ✅ Bond parameters relationships

✍️ Writing Tips for Long Answers:

- **For VSEPR:** Always mention total pairs → BP + LP → geometry → shape → bond angle
- **For Hybridization:** Write electronic configuration → excited state → mixing → hybrid orbitals
- **For MOT:** Write complete electronic configuration → calculate Nb and Na → bond order
- **For Structures:** Draw Lewis structure → calculate formal charges → show resonance if any

⚡ Quick Revision Table:

Concept	Key Formula/Rule
Steric Number	σ bonds + Lone pairs
Formal Charge	V - N - B/2
Bond Order (MOT)	(Nb - Na)/2
VSEPR Repulsion	lp-lp > lp-bp > bp-bp
Bond Strength	Triple > Double > Single
Bond Length	Triple < Double < Single
Paramagnetic	Unpaired electrons present
Diamagnetic	All electrons paired

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