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Chemical Bonding Introduction

Key Concepts

- Chemical bond: Attractive force holding atoms/ions together.
- Atoms interact due to energy decrease from net attractive forces & desire for noble gas configuration.

Solved Examples

- Ex 1: Why do atoms form bonds? To lower energy and achieve stable electron configuration.

Practice Set

- Q1: What is a chemical bond?
  A. Repulsive force
  B. Attractive force
  C. Neutral force
  D. None
- Q2: Atoms combine to achieve:
  A. Maximum energy
  B. Noble gas configuration
  C. Random state
  D. Unstable state
- Q3: Which factor drives atoms to bond?
  A. Increase in energy
  B. Decrease in energy
  C. No change
  D. None

Answer Key

- Q1: B - Chemical bond is an attractive force holding atoms together.

- Q2: B - Atoms combine to achieve noble gas configuration.
- Q3: B - Bonding decreases energy making the system stable.

Memory Aids

- Atoms bond to lower energy and mimic noble gases.
- Think "bond = attraction + stability".

Kössel—Lewis Approach

Key Concepts

- Atoms combine by transferring or sharing valence electrons to complete octet/duplet.
- Octet rule: Atoms tend to have 8 electrons in outer shell (2 for H).
- Two ways to achieve stable configuration:
  - Electrovalency: Complete electron transfer → ionic bond.
  - Sharing electrons → covalent or coordinate (dative) bond.
- Covalent bond: Equal sharing of electrons.
- Coordinate bond: One atom donates both electrons.

Solved Examples

- Ex 1: Identify bond type in NaCl. Answer: Ionic (electrovalent) bond by electron transfer.
- Ex 2: Identify bond in H_2. Answer: Covalent bond by equal sharing.

Practice Set

- Q1: What bond forms by electron transfer?
  A. Covalent
  B. Ionic
  C. Coordinate
  D. Metallic

- Q2: When electrons are shared equally, bond is:
  A. Ionic
  B. Covalent
  C. Coordinate
  D. Hydrogen
- Q3: Coordinate bond involves:
  A. Both atoms donating electrons
  B. One atom donating both electrons
  C. Electron transfer
  D. No electron sharing

Answer Key

- Q1: B - Ionic bond forms by electron transfer.
- Q2: B - Covalent bond involves equal sharing.
- Q3: B - Coordinate bond has one atom donating both electrons.

Memory Aids

- Octet rule: Complete 8 electrons (except H: 2).
- Ionic = transfer, Covalent = share equally, Coordinate = share unequally.

Covalent Bond

Key Concepts

- Formed by mutual sharing of electron pairs between atoms.
- Each atom contributes at least one electron to shared pair.
- Atoms attain noble gas configuration by sharing electrons.
- Types of covalent bonds:
  - Single bond: 1 shared pair
  - Double bond: 2 shared pairs
  - Triple bond: 3 shared pairs

Solved Examples

- Ex 1: Number of bonds in O_2? Answer: Double bond (2 pairs shared).
- Ex 2: Number of bonds in N_2? Answer: Triple bond (3 pairs shared).

Practice Set

- Q1: Covalent bond involves:
  A. Electron transfer
  B. Electron sharing
  C. No electron movement
  D. Ionic interaction
- Q2: A triple bond shares how many electron pairs?
  A. 1
  B. 2
  C. 3
  D. 4
- Q3: Which molecule has a double bond?
  A. H_2
  B. O_2
  C. N_2
  D. He

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Answer Key

- Q1: B - Covalent bond is electron sharing.
- Q2: C - Triple bond shares 3 pairs.
- Q3: B - O_2 has a double bond.

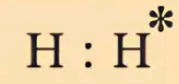
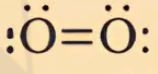
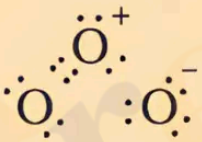
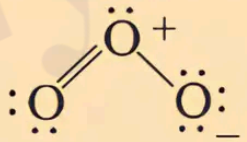
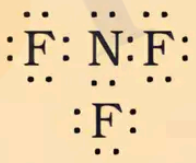
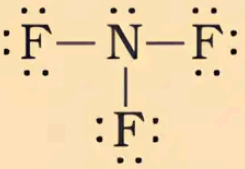
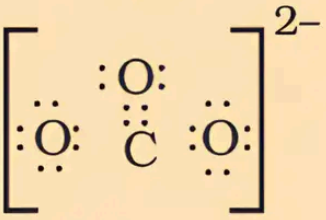
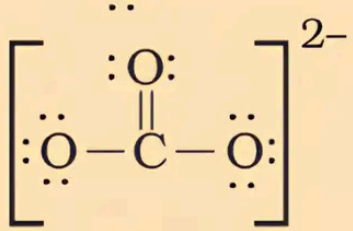
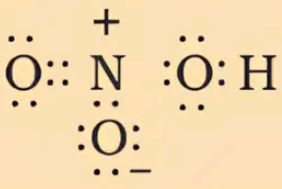
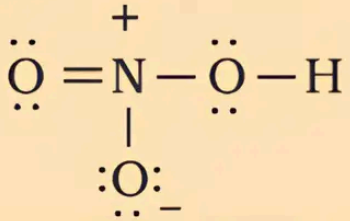
Memory Aids

- Single = 1 pair, Double = 2 pairs, Triple = 3 pairs shared.
- Remember: Covalent = share electrons.

Lewis Structures

Key Concepts

- Valence electrons shown as dots around atoms.
- Shared pairs shown as dots between atoms or lines.
- Lewis structures depict bonding and lone pairs.
- Octet rule visualized by electron pairs around atoms.
- For ions, brackets and charges indicate electron gain/loss.

Molecule/Ion	Lewis Representation	
H_2		
O_2		
O_3		
NF_3		
CO_3^{2-}		
HNO_3		

Solved Examples

- Ex 1: Draw Lewis structure of H_2O showing lone pairs and bonds.

Practice Set

- Q1: Lewis dots represent:
  A. Protons
  B. Valence electrons
  C. Neutrons
  D. Nucleus
- Q2: In Lewis structure, a line represents:
  A. Lone pair
  B. Bonding pair
  C. Proton
  D. Neutron
- Q3: What do brackets with charge indicate?
  A. Neutral molecule
  B. Ion with gained/lost electrons
  C. Isotope
  D. None

Answer Key

- Q1: B - Dots show valence electrons.
- Q2: B - Line represents bonding pair.
- Q3: B - Brackets with charge show ions.

Memory Aids

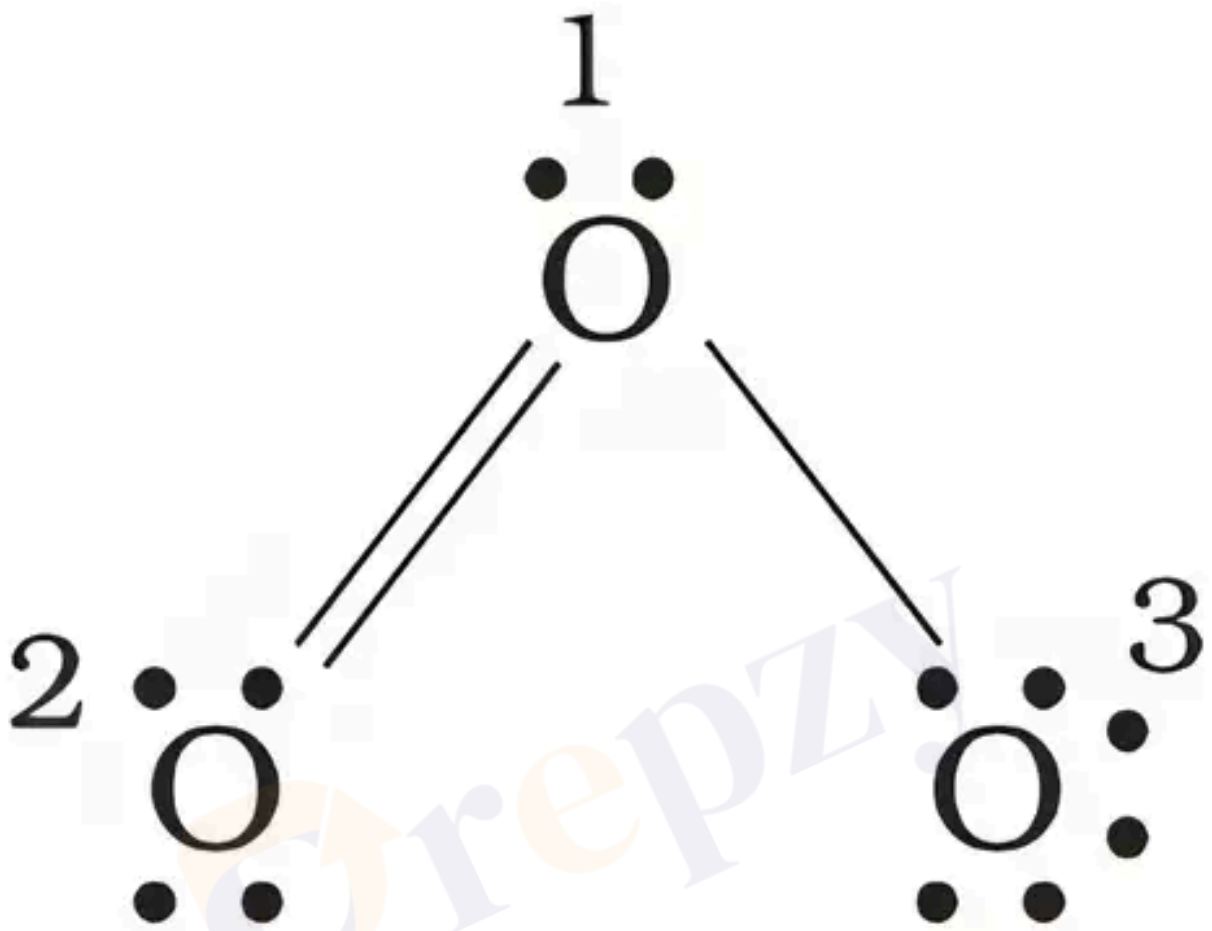
- Dots = valence electrons, Lines = bonds.
- Brackets + charge = ion.

Formal Charge

Key Concepts

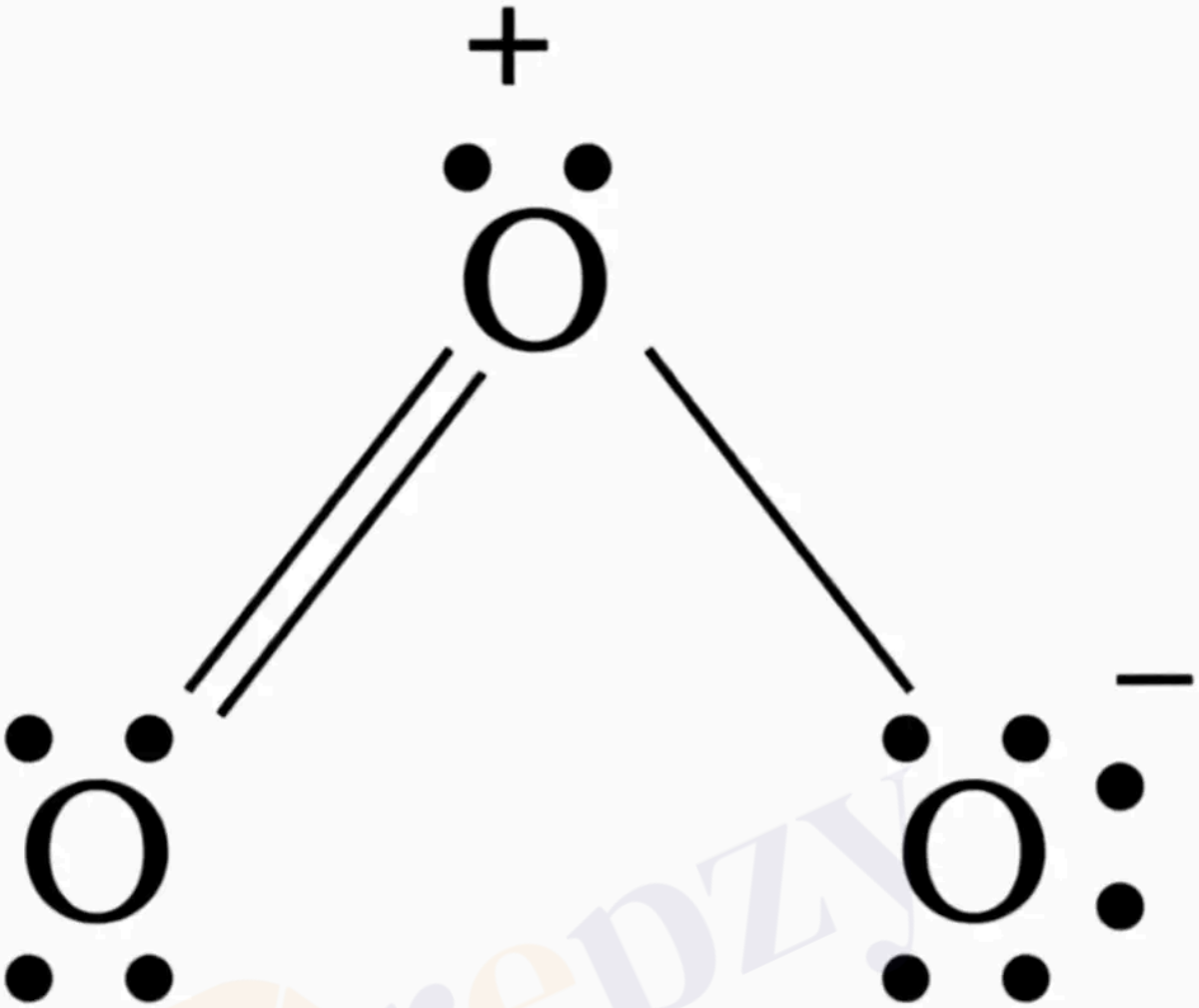
- Formal charge = Valence electrons - Non-bonding electrons - 1/2 Bonding electrons.

- Used to find most stable Lewis structure.
- Lowest energy structure has smallest formal charges.



Solved Examples

- Ex 1: Calculate formal charge on central O in O_3: 6 - 2 - 1/2(6) = +1.
- Ex 2: Calculate formal charge on end O in O_3: 6 - 4 - 1/2(4) = 0.



Practice Set

- Q1: Formal charge formula is:
  A. Valence - Lone pairs - 1/2 bonding
  B. Valence + Lone pairs + bonding
  C. Valence only
  D. None
- Q2: Formal charge helps to:
  A. Find highest energy structure
  B. Find lowest energy structure
  C. Ignore structure stability
  D. None
- Q3: Formal charge on O with 6 valence, 6 lone electrons, 2 bonding electrons is:
  A. -1
  B. 0
  C. +1
  D. +2

Answer Key

- Q1: A - Correct formula for formal charge.
- Q2: B - Helps find lowest energy structure.
- Q3: A - Calculation: 6 - 6 - 1/2(2) = -1.

Memory Aids

- Formal charge = valence - lone pairs - half bonding.
- Lowest formal charge = most stable structure.

Limitations of Octet Rule

Key Concepts

- Fails for atoms with less than 4 valence electrons (e.g., $BeCl_2$, BF_3).
- Fails for atoms with d-orbitals available (e.g., PF_5).
- Fails for molecules with odd electrons (e.g., NO, ClO_2).
- Does not explain paramagnetism of O_2.
- Noble gases can form compounds, contradicting inertness assumption.
- Does not explain molecular shape, stability, or energy.
- Electron deficient molecules act as Lewis acids.

Solved Examples

- Ex 1: PF_3 obeys octet, PF_5 does not due to d-orbitals.
- Ex 2: $BeCl_2$ has incomplete octet, acts as Lewis acid.

Practice Set

- Q1: Octet rule fails for:
  A. Atoms with <4 valence electrons
  B. Atoms with d-orbitals
  C. Molecules with odd electrons
  D. All above
- Q2: Molecules with incomplete octet are:
  A. Lewis bases
  B. Lewis acids
  C. Inert gases
  D. None
- Q3: Octet rule does not explain:
  A. Molecular shape
  B. Stability
  C. Paramagnetism
  D. All above

Answer Key

- Q1: D - All listed cases fail octet rule.
- Q2: B - Electron deficient molecules are Lewis acids.
- Q3: D - Octet rule fails to explain shape, stability, paramagnetism.

Memory Aids

- Octet rule exceptions: <4 valence, d-orbitals, odd electrons.
- Electron deficient molecules = Lewis acids.

Ionic or Electrovalent Bond

Definition and Formation

- An ionic bond is the electrostatic attraction between cations and anions formed by complete electron transfer to achieve noble gas configuration.
- Forms easily between elements with low ionization energy and high negative electron gain enthalpy.
- Stability depends on lattice enthalpy, not just octet completion in gaseous ions.

Solved Examples

- **Ex 1:** Formation of NaCl
  - Na ($1s^2 2s^2 2p^6 3s^1$) loses 1 electron → Na^+
  - Cl ($1s^2 2s^2 2p^6 3s^2 3p^5$) gains 1 electron → Cl^-
  - Na^+ and Cl^- attract to form NaCl ionic bond.

Practice Set

- Q1: Which pair is most likely to form an ionic bond?
  - A. Na and Cl
  - B. H and O
  - C. C and H
  - D. N and O
- Q2: Ionic bonds form due to
  - A. Sharing of electrons
  - B. Complete transfer of electrons
  - C. Metallic bonding
  - D. Hydrogen bonding
- Q3: Which factor favors ionic bond formation?
  - A. High ionization energy of metal
  - B. Low electron gain enthalpy of non-metal
  - C. Low ionization energy of metal and high negative electron gain enthalpy of non-metal
  - D. Similar electronegativities

Answer Key

- Q1: A - Na and Cl form ionic bond due to electron transfer.
- Q2: B - Ionic bonds form by complete electron transfer.
- Q3: C - Low ionization energy metal and high negative electron gain enthalpy non-metal favor ionic bond.

Memory Aids

- Low I.E. metal + high negative EGE non-metal = ionic bond.
- NaCl is classic ionic compound example.
- Stability depends on lattice enthalpy, not just octet.

Lattice Enthalpy

Definition

- Energy required to separate 1 mole of ionic solid into gaseous ions completely.

Factors Affecting Lattice Enthalpy

- **Charge on ions:** Higher charge → stronger attraction → higher lattice enthalpy.
  - Order: bi-bivalent > uni-bi or bi-uni > uni-univalent ions.
- **Size of ions:** Smaller ions → stronger attraction → higher lattice enthalpy.
  - Lattice enthalpy $\propto$ 1 / size of ions.

Solved Examples

- **Ex 1:** Compare lattice enthalpy of MgO and NaCl
  - Mg^{2+} and O^{2-} have higher charges than Na^{+} and Cl^{-}.
  - MgO has higher lattice enthalpy due to higher ionic charges and smaller ion sizes.

Practice Set

- Q1: Lattice enthalpy increases with
  - A. Decreasing ionic charge
  - B. Increasing ionic charge
  - C. Increasing ionic size
  - D. Decreasing ionic charge and size
- Q2: Which ionic compound has highest lattice enthalpy?
  - A. NaCl
  - B. KBr
  - C. MgO
  - D. CsI
- Q3: Lattice enthalpy is directly proportional to
  - A. Size of ions
  - B. Charge on ions
  - C. Number of ions
  - D. Atomic mass

Answer Key

- Q1: B - Higher ionic charge increases lattice enthalpy.
- Q2: C - MgO has highest lattice enthalpy due to 2+ and 2− ions.
- Q3: B - Lattice enthalpy ∝ charge on ions.

Memory Aids

- Charge ↑ → lattice enthalpy ↑
- Size ↑ → lattice enthalpy ↓
- MgO > NaCl in lattice enthalpy due to charge and size.

Valence Shell Electron Pair Repulsion Theory

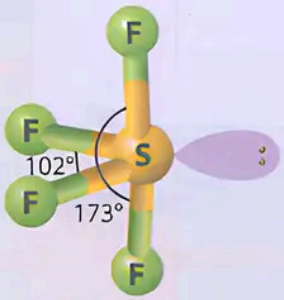
Key Concepts

- Developed by Nyholm and Gillespie in 1957.
- Molecules adopt shapes that keep bonded atoms as far apart as possible around the central atom.
- Shape depends on the number of valence shell electron pairs (bonded and lone pairs) around the central atom.
- Electron pairs repel each other in the order: lone pair-lone pair (lp-lp) > lone pair-bond pair (lp-bp) > bond pair-bond pair (bp-bp).
- Electron pairs arrange themselves to minimize repulsion and maximize distance.
- Applicable to molecules with resonance structures.

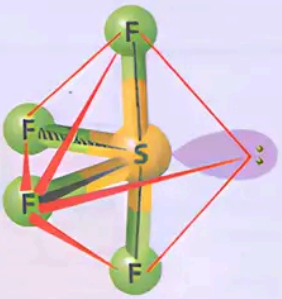
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VSEPR Theory

SF_4 (Sulphur Tetrafluoride)

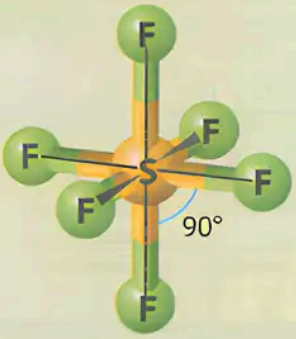


The F—S—F angle involving the axial F atoms is **173°**.

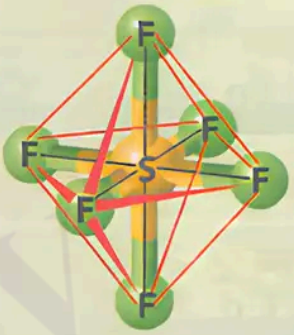


The red lines outline a **trigonal bipyramid**.
Black lines show the electron pairs.

SF_6 (Sulphur Hexafluoride)

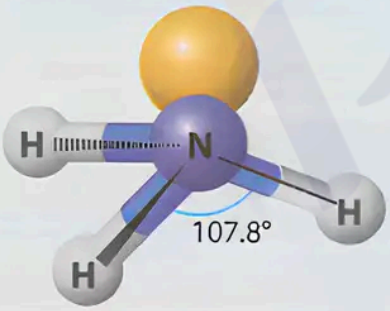


All F—S—F angles are **90°**.

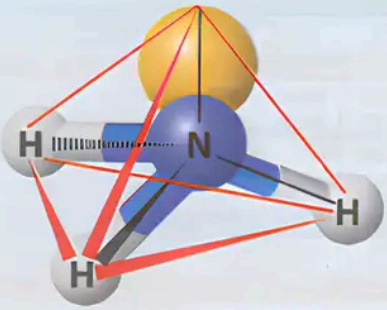


The red lines outline an **octahedron**.
Black lines show the covalent bonds.

NH_3 (Ammonia)

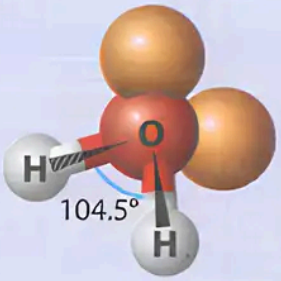


The H—N—H bond angle is **107.8°.**

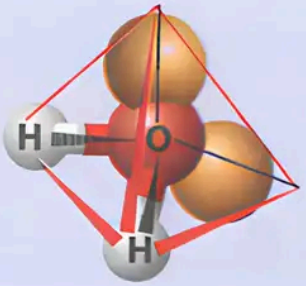


The red lines outline an **tetrahedron**.
Black lines show the electron pairs.

H_2O (Water)



The H—O—H bond angle is **104.5°**.



The red lines outline a **tetrahedron**.
Black lines show the electron pairs.

Solved Examples

- **Ex 1:** Predict the shape of SF_4.
- SF_4 has 5 electron pairs (4 bonding, 1 lone pair) around S.
- Shape: Trigonal bipyramidal with one lone pair causing distortion.
- Bond angle between axial fluorines is 173° (almost linear).

Practice Set

- Q1: What is the bond angle in NH_3?
  - A. 109.5°
  - B. 107.8°
  - C. 104.5°
  - D. 90°
- Q2: Which molecule has an octahedral shape?
  - A. SF_4
  - B. SF_6
  - C. NH_3
  - D. H_2O
- Q3: Arrange the repulsion strength in decreasing order.
  - A. bp-bp > lp-bp > lp-lp
  - B. lp-lp > lp-bp > bp-bp
  - C. lp-bp > lp-lp > bp-bp
  - D. bp-bp > lp-lp > lp-bp

Answer Key

- Q1: B - NH_3 has a bond angle of 107.8° due to one lone pair reducing the ideal tetrahedral angle.
- Q2: B - SF_6 has an octahedral shape with 6 bonding pairs and 90° bond angles.
- Q3: B - Lone pair-lone pair repulsion is strongest, followed by lone pair-bond pair, then bond pair-bond pair.

Memory Aids

- Remember: "lp-lp > lp-bp > bp-bp" for repulsion strength.
- Trigonal bipyramidal shape has 5 electron pairs; lone pairs occupy equatorial positions.
- Octahedral shape has 6 bonding pairs with 90° angles.

Geometry Based on VSEPR Theory

Key Concepts

- Molecular shape depends on total electron pairs around the central atom (bonded + lone pairs).
- Electron pairs arrange to minimize repulsion, defining molecular geometry.
- Common geometries include linear, trigonal planar, tetrahedral, trigonal bipyramidal, and octahedral.
- Formulas like AX_2, AX_3E indicate bonded atoms (X) and lone pairs (E) around central atom (A).
- Examples: $BeCl_2$ (linear), CH_4 (tetrahedral), NH_3 (trigonal pyramidal), H_2O (bent).

Total number of electron pairs	Molecular formula	Geometry	Example
2	AX_2	Linear	$BeCl_2$
3	AX_3 AX_2E	Triangular planar Bent (V-shape)	BF_3 SO_2
4	AX_4 AX_3E AX_2E_2	Tetrahedral Trigonal pyramidal Bent	CH_4 NH_3 H_2O
5	AX_5 AX_4E AX_3E_2 AX_2E_3	Trigonal bipyramidal Irregular tetrahedral (See saw) T-shaped Linear	PCl_5 SF_4 ClF_3 I_3^-
6	AX_6 AX_5E AX_4E_2	Octahedral Square pyramidal Square planar	SF_6 BrF_5 XeF_4
7	AX_7	Pentagonal bipyramidal	IF_7

Solved Examples

- **Ex 1:** Determine the shape of NH_3 using AX_3E notation.
- NH_3 has 3 bonded atoms and 1 lone pair (AX_3E).
- Shape: Trigonal pyramidal with bond angle 107.8°.

Practice Set

- Q1: What is the shape of a molecule with formula AX_2E_2?
  - A. Linear
  - B. Bent
  - C. Trigonal planar
  - D. Tetrahedral
- Q2: Which molecule is tetrahedral?
  - A. CO_2
  - B. CH_4
  - C. NH_3
  - D. SO_2
- Q3: For AX_5E, what is the molecular shape?
  - A. Trigonal bipyramidal
  - B. Square pyramidal
  - C. See-saw
  - D. Octahedral

Answer Key

- Q1: B - AX_2E_2 corresponds to bent shape (e.g., H_2O).
- Q2: B - CH_4 is tetrahedral with 4 bonded atoms and no lone pairs.
- Q3: C - AX_5E has see-saw shape due to one lone pair in trigonal bipyramidal arrangement.

Memory Aids

- AX_nE_m notation helps predict shape: A = central atom, X = bonded atoms, E = lone pairs.
- More lone pairs reduce bond angles from ideal geometry.

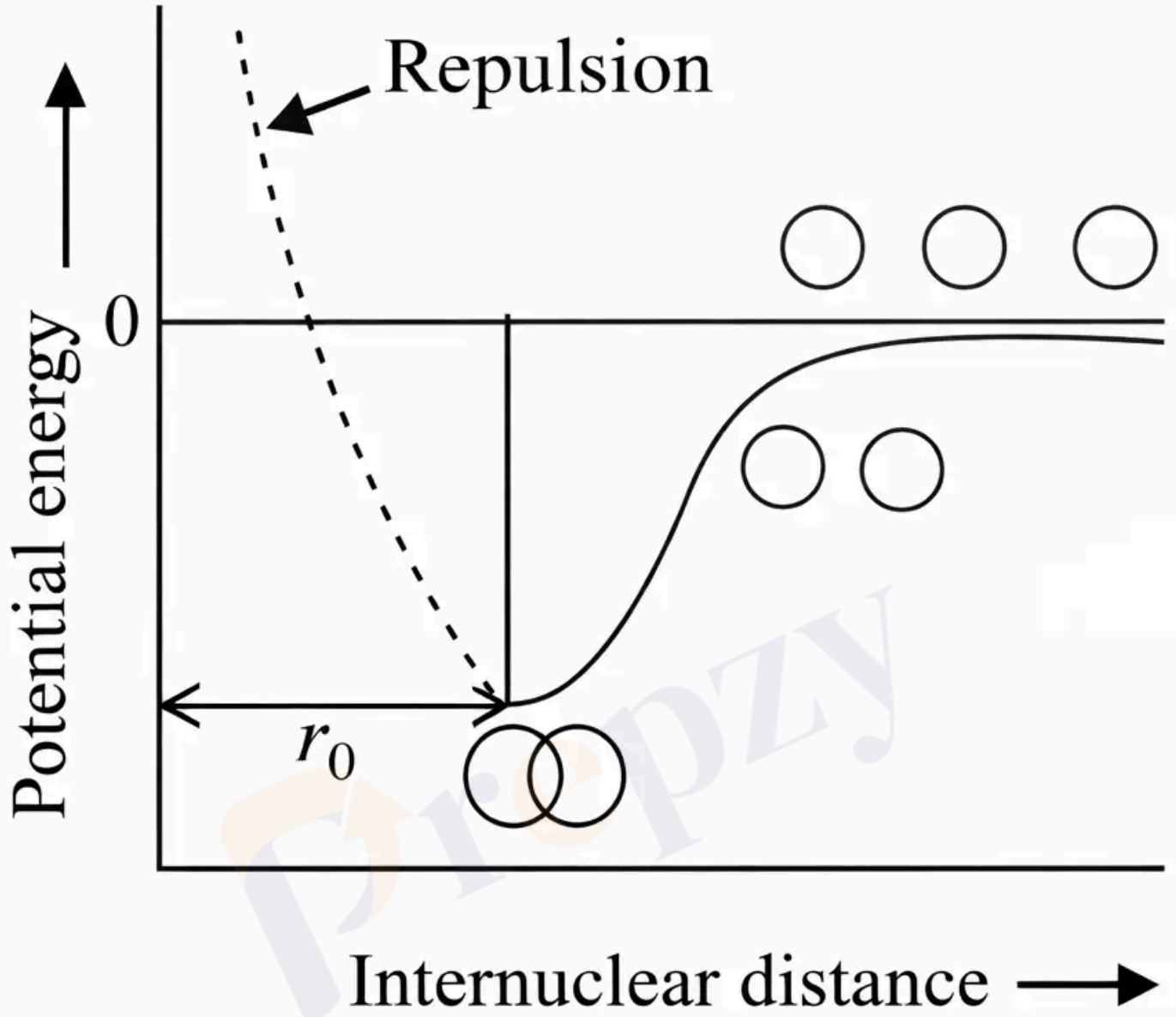
- Common shapes: linear (2 pairs), trigonal planar (3 pairs), tetrahedral (4 pairs), trigonal bipyramidal (5 pairs), octahedral (6 pairs).

Valence Bond Theory

Main Postulates

- Bond forms by interaction of valence electrons; core electrons do not participate.
- Only valence electrons lose their identity during bond formation.
- Bond formation releases energy, providing bond stability.
- Molecule has minimum energy at equilibrium (intermolecular) distance; greater energy decrease means stronger bond.

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Energy vs Internuclear Distance

- Graph shows potential energy changes as atomic nuclei distance varies.
- Close nuclei cause steep energy rise due to repulsion.
- Minimum energy at optimal distance r_0 indicates stable molecule formation.
- Energy increases if nuclei separate beyond r_0, atoms stop interacting.
- Minimum point balances attraction and repulsion forces.

Solved Examples

- **Ex 1:** Explain why bond formation releases energy.
  - Valence electrons overlap, lowering system energy.
  - Energy release stabilizes the molecule.

Practice Set

- Q1: Which electrons participate in bond formation?
  A. Core electrons
  B. Valence electrons
  C. Both
  D. None
- Q2: What happens to energy at equilibrium bond distance?
  A. Maximum
  B. Minimum
  C. Zero
  D. Infinite
- Q3: Why is bond formation stable?
  A. Energy absorption
  B. Energy release
  C. No energy change
  D. Electron loss

Answer Key

- Q1: B - Only valence electrons form bonds.
- Q2: B - Energy is minimum at equilibrium distance.
- Q3: B - Bond formation releases energy, stabilizing molecule.

Memory Aids

- Valence electrons = Bond makers, core electrons = spectators.
- Energy minimum = stable bond distance.

Types of Overlapping and Nature of Covalent Bond

Orbital Overlapping

- Atomic orbitals overlap to form molecular orbitals when atoms approach.
- Overlap can be positive, negative, or zero based on orbital phase and orientation.
- **Sigma (σ) bond:** Head-on overlap along internuclear axis (s-s, s-p, p-p).
- **Pi (π) bond:** Lateral overlap perpendicular to internuclear axis, only p-orbitals.

Strength of Sigma and Pi Bonds

- Sigma bonds have greater overlap extent; stronger than pi bonds.
- Multiple bonds include one sigma and one or more pi bonds.
- Bond energy order: Single < Double < Triple.
- Bond length order: Triple < Double < Single.
- Reactivity order: Single < Double < Triple.

Additional Points

- Maximum covalent bonds between two atoms = 3.
- Pi bond never forms alone; always with sigma bond.
- Head-on overlap stronger than lateral overlap.
- Free rotation possible about sigma bond, not pi bond.

Solved Examples

- **Ex 1:** Identify bond types in ethene (C_2H_4).
  - C-C double bond = 1 sigma + 1 pi bond.
  - C-H bonds = sigma bonds.

Practice Set

- Q1: Sigma bond forms by:
  A. Lateral overlap
  B. Head-on overlap
  C. No overlap
  D. Random overlap
- Q2: Which bond is stronger?
  A. Pi bond
  B. Sigma bond
  C. Both equal
  D. None
- Q3: Which is true about pi bonds?
  A. Form alone
  B. Form with sigma bond
  C. Allow free rotation
  D. Stronger than sigma

Answer Key

- Q1: B - Sigma bonds form by head-on overlap.
- Q2: B - Sigma bonds are stronger due to greater overlap.
- Q3: B - Pi bonds always accompany sigma bonds.

Memory Aids

- Sigma = Straight (head-on), Pi = Parallel (sideways).
- Max 3 bonds between atoms.
- Rotation allowed only about sigma bonds.

Hybridisation

Definition and Features

- Atomic orbitals of similar energy mix to form new hybrid orbitals of equivalent energy.
- Number of hybrid orbitals = number of atomic orbitals mixed.
- Hybrid orbitals are equivalent in shape and energy.
- They orient in space to minimize electron pair repulsion.

Hybridisation Formula

$H = 1/2 (V + M - C + A)$

- H = number of hybrid orbitals (2 to 7) corresponding to sp, sp^2, sp^3, sp^3d, sp^3d^2, sp^3d^3
- V = valence electrons of central atom
- M = monovalent atoms attached
- C = charge on cation
- A = charge on anion

Conditions for Hybridisation

- Only valence shell orbitals hybridise.
- Orbitals must have nearly equal energies.
- Electron promotion before hybridisation is not necessary.
- Both half-filled and filled orbitals can hybridise.

Solved Examples

Ex 1: Calculate hybridisation of central atom in BF_3.

- V = 3 (Boron valence electrons)
- M = 3 (three F atoms)

- C = 0, A = 0 (neutral molecule)
- H = 1/2 (3 + 3 - 0 + 0) = 3 → sp^2 hybridisation

Practice Set

- Q1: Hybridisation of carbon in CH_4 is?
  - A. sp
  - B. sp^2
  - C. sp^3
  - D. sp^3d
- Q2: Number of hybrid orbitals formed in sp^3d hybridisation?
  - A. 3
  - B. 4
  - C. 5
  - D. 6
- Q3: Hybridisation of central atom in SF_6 is?
  - A. sp^3d
  - B. sp^3d^2
  - C. sp^3d^3
  - D. sp^2

Answer Key

- Q1: C (sp^3) - Carbon forms 4 bonds, so 4 hybrid orbitals.
- Q2: C (5) - sp^3d involves 5 hybrid orbitals.
- Q3: B (sp^3d^2) - SF_6 has 6 bonds, requiring 6 orbitals.

Memory Aids

- sp: 2 orbitals, linear, 180°
- sp^2: 3 orbitals, trigonal planar, 120°
- sp^3: 4 orbitals, tetrahedral, 109.5°
- sp^3d: 5 orbitals, trigonal bipyramidal, 90° & 120°

- sp^3d^2: 6 orbitals, octahedral, 90°

Hybridisation in Molecules with Bond Pairs Only

Types and Structures

Type of hybridisation	No. of hybrid orbitals	Shape of molecule	Bond angle	Examples
sp	2	Linear	180°	$BeCl_2$, BeF_2, CO_2, CS_2, C_2H_2, $[Ag(CN)_2]^-$, $HgCl_2$, HCN
sp^2	3	Triangular planar	120°	BF_3, BCl_3, C_2H_4, NO_3^-, CO_3^{2-}, SO_3, CH_3^+
sp^3	4	Tetrahedral	109°28′	CH_4, CCl_4, $SnCl_4$, SiF_4, NH_4^+
dsp^2	4	Square planar	90°	$[PtCl_4]^{2-}$, $[Ni(CN)_4]^{2-}$
dsp^3 or sp^3d	5	Trigonal bipyramidal	120° and 90°	PCl_5, PF_5, SbF_5
d^2sp^3 or sp^3d^2	6	Octahedral	90°	SF_6, TeF_6,$[CrF_6]^{3-}$, $[Co(NH_3)_6]^{3+}$
d^3sp^3 or sp^3d^3	7	Pentagonal bipyramidal	72° and 90°	IF_7

- sp: 2 orbitals, linear shape, 180° bond angle (e.g., CO_2).
- sp^2: 3 orbitals, trigonal planar, 120° (e.g., BF_3).
- sp^3: 4 orbitals, tetrahedral, 109.5° (e.g., CH_4).
- sp^3d: 5 orbitals, trigonal bipyramidal, 90° & 120° (e.g., PCl_5).
- sp^3d^2: 6 orbitals, octahedral, 90° (e.g., SF_6).

Solved Examples

Ex 1: Determine shape and bond angle of $BeCl_2$.

- Hybridisation: sp (2 orbitals)
- Shape: Linear
- Bond angle: 180°

Practice Set

- Q1: Bond angle in sp^3 hybridised molecule?
  - A. 90°
  - B. 109.5°
  - C. 120°
  - D. 180°
- Q2: Shape of PCl_5 molecule?
  - A. Tetrahedral
  - B. Trigonal bipyramidal
  - C. Octahedral
  - D. Linear
- Q3: Hybridisation of CO_2?
  - A. sp
  - B. sp^2
  - C. sp^3
  - D. sp^3d

Answer Key

- Q1: B (109.5°) - Tetrahedral bond angle for sp^3.
- Q2: B (Trigonal bipyramidal) - PCl_5 has 5 bonds.
- Q3: A (sp) - CO_2 is linear with sp hybridisation.

Memory Aids

- Linear = 2 bonds, sp
- Tetrahedral = 4 bonds, sp^3
- Trigonal bipyramidal = 5 bonds, sp^3d

Hybridisation in Molecules with Lone and Bond Pairs

Structures and Effects

Types of molecules	No. of bond pair(s)	No. of lone pair(s)	Hybridisation	Bond angle	Expected geometry	Actual geometry	Examples
AX_2E	2	1	sp^2	<120°	Trigonal planar	V-shape or Bent	SO_2, $SnCl_2$, $PbCl_2$, O_3
AX_2E_2	2	2	sp^3	<109°28′	Tetrahedral	V-shape or Bent	H_2O, H_2S, NH_2^-, SCl_2, OF_2, Cl_2O, ClO_2^-, ClOF
AX_2E_3	2	3	sp^3d	180°	Trigonal bipyramidal	Linear	XeF_2, I_3^-, ICl_2^-
AX_3E_2	3	2	sp^3d	90°	Trigonal bipyramidal	T-shape	ClF_3, IF_3, BrF_3, $XeOF_2$
AX_3E	3	1	sp^3	<109°28′	Tetrahedral	Pyramidal	NH_3, PH_3, PCl_3, $BiCl_3$, $AsCl_3$, XeO_3, ClO_3^-, SO_3^{2-}
AX_4E	4	1	sp^3d	120°, 90°	Trigonal bipyramidal	See saw or Distorted tetrahedron	SF_4, SCl_4, $TeCl_4$, XeO_2F_2
AX_4E_2	4	2	sp^3d^2	—	Octahedral	Square planar	XeF_4, ICl_4^-
AX_5E	5	1	sp^3d^2	<90°	Octahedral	Square pyramidal	IF_5, BrF_5, SbF_5^{2-}, $XeOF_4$
AX_6E	6	1	sp^3d^3	–	Pentagonal bipyramidal	Distorted octahedral	XeF_6

- Count bond pairs (X) and lone pairs (E) around central atom (AX_nE_m notation).
- Predict hybridisation from total electron pairs.
- Lone pairs affect bond angles and molecular shape.
- Shapes include bent, T-shaped, seesaw, square pyramidal, etc.
- Examples: NH_3 (sp^3, trigonal pyramidal), H_2O (sp^3, bent).

Solved Examples

Ex 1: Hybridisation of NH_3.

- 3 bond pairs + 1 lone pair = 4 electron pairs
- Hybridisation: sp^3

- Shape: Trigonal pyramidal
- Bond angle: ~107°

Practice Set

- Q1: Shape of H_2O molecule?
  - A. Linear
  - B. Bent
  - C. Trigonal planar
  - D. T-shaped
- Q2: Hybridisation of central atom in SF_4?
  - A. sp^3
  - B. sp^3d
  - C. sp^3d^2
  - D. sp^2
- Q3: Bond angle in NH_3?
  - A. 109.5°
  - B. 107°
  - C. 120°
  - D. 90°

Answer Key

- Q1: B (Bent) - Due to 2 bond pairs and 2 lone pairs in H_2O.
- Q2: B (sp^3d) - SF_4 has 4 bonds + 1 lone pair.
- Q3: B (107°) - Slightly less than tetrahedral due to lone pair repulsion.

Memory Aids

- Lone pairs reduce bond angles.
- AX_2E_2 = bent shape.
- AX_3E = trigonal pyramidal.
- d orbitals involved: $d_{x^2-y^2}$ in dsp^2, d_{z^2} in sp^3d, $d_{x^2-y^2}$ and d_{z^2} in sp^3d^2, d_{xy}, d_{yz}, d_{xz} in sp^3d^3.

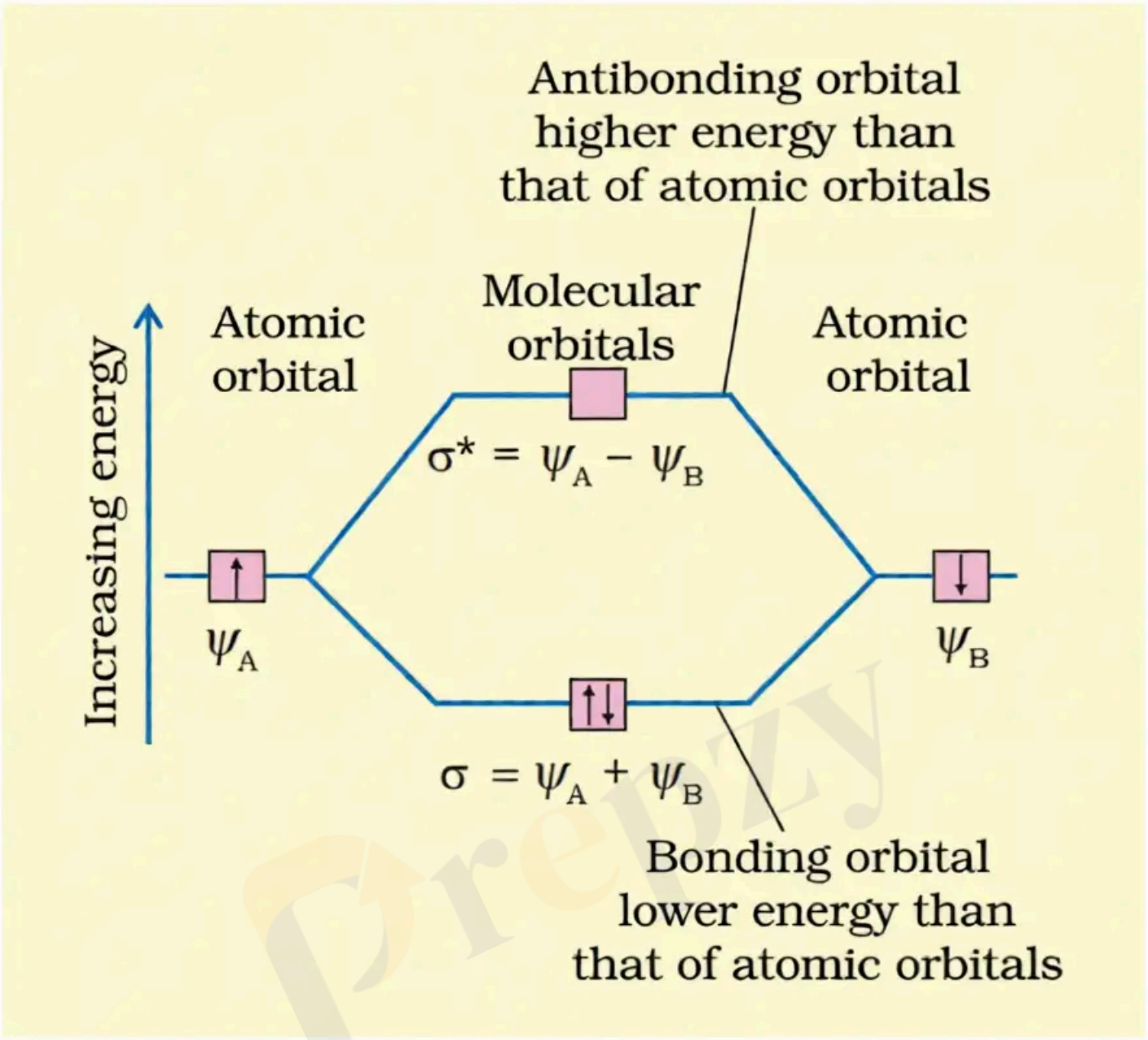
Molecular Orbital Theory

Key Features

- Electrons in molecules occupy molecular orbitals (MOs).
- Atomic orbitals (AOs) of similar energy and symmetry combine to form MOs.
- MOs are polycentric, influenced by multiple nuclei.
- Number of MOs formed equals number of combining AOs.
- Two AOs combine to form one bonding MO and one antibonding MO.
- Bonding MO has lower energy and greater stability than antibonding MO.
- MOs represent electron probability distribution around nuclei.
- MOs fill according to Aufbau principle, Pauli's exclusion, and Hund's rule.

Formation of MOs (LCAO)

- MOs form by addition or subtraction of AO wave functions.
- Addition forms bonding MOs (σ or π) with lower energy.
- Subtraction forms antibonding MOs (σ* or π*) with higher energy.



Formation of bonding (σ) and antibonding (σ) molecular orbitals by the linear combination of atomic orbitals ψ_A and ψ_B centered on two atoms A and B respectively.*

Solved Examples

- **Ex 1:** Combine 1s orbitals of two H atoms: □91s + 1s□9 forms bonding □c3 MO; □91s - 1s□9 forms antibonding □c3* MO.

Practice Set

- **Q1:** What is formed when two atomic orbitals combine?
  A. One bonding MO
  B. One antibonding MO
  C. One bonding and one antibonding MO
  D. No MO formed
- **Q2:** Which principle is NOT followed in filling molecular orbitals?
  A. Aufbau principle
  B. Hund's rule
  C. Pauli’s exclusion principle
  D. Le Chatelier's principle
- **Q3:** What type of MO is formed by subtraction of wave functions?
  A. Bonding MO
  B. Antibonding MO
  C. Non-bonding MO
  D. Hybrid MO

Answer Key

- **Q1:** C - Two MOs form: one bonding and one antibonding.
- **Q2:** D - Le Chatelier's principle is unrelated to MO filling.
- **Q3:** B - Subtraction forms antibonding MOs with higher energy.

Memory Aids

- MO formation: Addition = Bonding (lower energy), Subtraction = Antibonding (higher energy).
- Bonding MOs stabilize molecule; antibonding MOs destabilize.
- Follow Aufbau, Pauli, Hund for electron filling.

Molecular Orbital Energy Order

Energy Order for Homonuclear Diatomic Molecules (O_2, F_2, Ne_2)

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

Energy Order for Lighter Diatomic Molecules (B_2, C_2, N_2)

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

Solved Examples

- **Ex 1:** Arrange MOs for O_2: $\sigma 1s < \sigma^* 1s < \sigma 2s < \sigma^* 2s < \sigma 2p_z < \sigma 2p_x = \sigma 2p_y < \sigma^* 2p_x = \sigma^* 2p_y < \sigma^* 2p_z$.

Practice Set

- **Q1:** Which MO has the lowest energy in O_2?
  A. $\sigma^* 1s$
  B. $\sigma 1s$
  C. $\sigma 2p_z$
  D. $\sigma^* 2p_z$
- **Q2:** In B_2, which MO comes just after $\sigma^* 2s$?
  A. $\sigma 2p_z$
  B. $\sigma 2p_x = \sigma 2p_y$
  C. $\sigma^* 2p_x$
  D. $\sigma^* 2p_z$
- **Q3:** Which molecule follows the MO order with $\sigma 2p_x = \sigma 2p_y$ before $\sigma 2p_z$?
  A. O_2
  B. F_2

C. N_2

D. B_2

Answer Key

- **Q1:** B - □c31s is the lowest energy MO.
- **Q2:** B - □c32p_x = □c32p_y come after □c3*2s in lighter diatomics.
- **Q3:** D - B_2 shows this MO energy order.

Memory Aids

- O_2, F_2, Ne_2: □c32p_z before □c32p_x, □c32p_y.
- B_2, C_2, N_2: □c32p_x, □c32p_y before □c32p_z.
- Remember by atomic number: lighter elements have different MO order.

Gerade and Ungerade Molecular Orbitals

Symmetry and Notation

- Gerade (g): Symmetrical MOs about center; symbol ‘g’.
- Ungerade (u): Unsymmetrical MOs; symbol ‘u’.
- All σ bonding MOs are gerade.
- All σ antibonding MOs (σ*) are ungerade.
- All π antibonding MOs (π*) are gerade.
- All π bonding MOs are ungerade.

Solved Examples

- **Ex 1:** σ bonding MO in H_2 is gerade.
- **Ex 2:** σ* antibonding MO in H_2 is ungerade.

Practice Set

- **Q1:** What does gerade (g) indicate?
  A. Unsymmetrical MO
  B. Symmetrical MO
  C. Antibonding MO
  D. Non-bonding MO
- **Q2:** Which MO is ungerade?
  A. σ bonding
  B. σ* antibonding
  C. π* bonding
  D. π bonding
- **Q3:** π* MOs are generally?
  A. Gerade
  B. Ungerade
  C. Non-bonding
  D. Hybrid

Answer Key

- **Q1:** B - Gerade means symmetrical MO.
- **Q2:** B - σ* antibonding MOs are ungerade.
- **Q3:** A - π* antibonding MOs are gerade.

Memory Aids

- Gerade = g = symmetrical; Ungerade = u = unsymmetrical.
- σ bonding = gerade; σ* antibonding = ungerade.
- π bonding = ungerade; π* antibonding = gerade.

Bond Order and Stability

Bond Order Calculation

- Bond order (B.O.) = 1/2 (N_b - N_a)
- N_b = Number of bonding electrons.
- N_a = Number of antibonding electrons.
- If B.O. > 0, molecule is stable.
- If B.O. = 0 or < 0, molecule is unstable.
- Bond order ∝ Bond energy ∝ Stability ∝ 1 / Bond length.
- Higher bond order means higher bond dissociation energy and shorter bond length.
- Molecule is diamagnetic if all electrons are paired; paramagnetic if unpaired electrons present.

Solved Examples

- **Ex 1:** Calculate B.O. for O_2: N_b=10, N_a=6; B.O. = 1/2(10-6) = 2 (stable).

Practice Set

- **Q1:** What is bond order if N_b = 8 and N_a = 4?
  A. 1
  B. 2
  C. 3
  D. 4
- **Q2:** If bond order is zero, molecule is:
  A. Stable
  B. Unstable
  C. Paramagnetic
  D. Diamagnetic
- **Q3:** Which property increases with bond order?
  A. Bond length
  B. Bond dissociation energy
  C. Number of antibonding electrons
  D. Paramagnetism

Answer Key

- **Q1:** B - B.O. = 1/2(8-4) = 2.
- **Q2:** B - B.O. = 0 means unstable molecule.
- **Q3:** B - Bond dissociation energy increases with bond order.

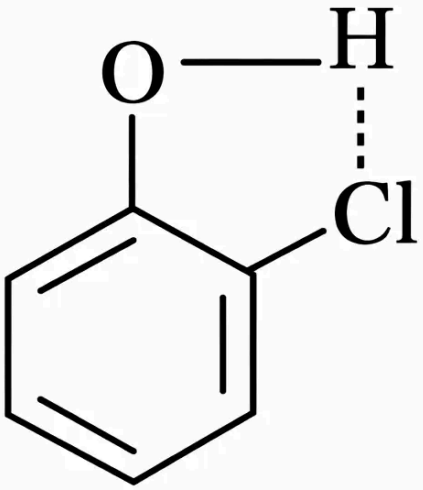
Memory Aids

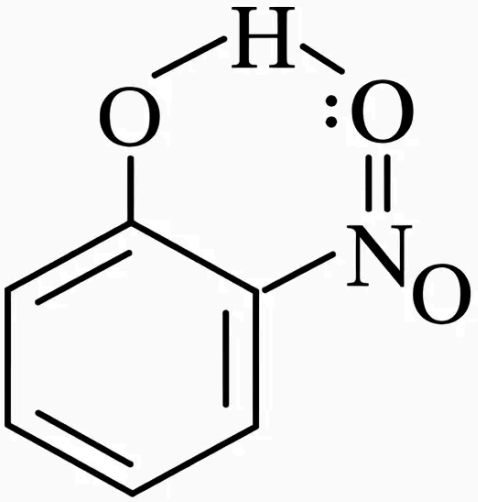
- Bond order formula: 1/2 (bonding electrons - antibonding electrons).
- Higher bond order = stronger, shorter bond.
- Diamagnetic = all paired; paramagnetic = unpaired electrons.

Hydrogen Bonding

Concept and Types

- **Hydrogen bond**: Attractive force between hydrogen atom of one molecule and electronegative atom (F, O, N) of another molecule.
- **Intermolecular hydrogen bonding**: Occurs between two different molecules (e.g., HF, H_2O, ROH).
- $$- - - H^{\delta+}-F^{\delta-} - - -H^{\delta+} - F^{\delta-} - - - H^{\delta+} - F^{\delta-}$$
  - H in HF has partial positive charge ($H^{\delta+}$), F has partial negative ($F^{\delta-}$).
  - Hydrogen bond shown as dashed line between H and F of different molecules.
  - Hydrogen bonding increases boiling point and reduces volatility.
- **Intramolecular hydrogen bonding**: Bond formed within the same molecule (e.g., o-nitrophenol), causing cyclization and preventing association.





o-Chlorophenol *o*-Nitrophenol

-
    - o-Chlorophenol and o-Nitrophenol have -OH and substituent groups at ortho positions.
    - Dashed lines show intramolecular hydrogen bonding in o-nitrophenol.
- Double bonds count as one electron pair in molecular geometry prediction.
- Intermolecular H-bonding ∝ Solubility ∝ Boiling point ∝ 1/Volatility.
- Intramolecular H-bonding ∝ 1/Solubility ∝ 1/Boiling point ∝ Volatility.

Solved Examples

- **Ex 1:** Explain hydrogen bonding in HF.
    - HF has polar covalent bond ($H^{\delta+}$-$F^{\delta-}$).
    - Positive H attracts negative F of another molecule forming H-bond.
    - H-bonds shown as dashed lines increase boiling point.
- **Ex 2:** Identify intramolecular H-bond in o-nitrophenol.
    - H of -OH forms bond with O of NO_2 group within same molecule.
    - This cyclization reduces intermolecular association.

Practice Set

- Q1: Which atom does hydrogen bond with?
    - A. Carbon

    - B. Fluorine
    - C. Hydrogen
    - D. Sodium
- Q2: Intramolecular hydrogen bonding occurs in:
    - A. HF
    - B. o-Nitrophenol
    - C. Water
    - D. Ethanol
- Q3: Which property increases due to intermolecular hydrogen bonding?
    - A. Volatility
    - B. Boiling point
    - C. Solubility decreases
    - D. Molecular weight

Answer Key

- Q1: B - Hydrogen bonds with electronegative atoms like fluorine, oxygen, or nitrogen.
- Q2: B - Intramolecular hydrogen bonding occurs within the same molecule, e.g., o-nitrophenol.
- Q3: B - Intermolecular hydrogen bonding increases boiling point by stronger molecular attraction.

Memory Aids

- H-bond forms only with F, O, N atoms.
- Intermolecular H-bonding ↑ solubility, boiling point; ↓ volatility.
- Intramolecular H-bonding ↓ solubility, boiling point; ↑ volatility.
- Double bonds count as one electron pair in shape prediction.