NCERT Chemical Bonding and Molecular Structure - Exercise Answer Key

Class 11 Chemistry - Unit 4

4.1 Explain the formation of a chemical bond.

Answer: A chemical bond is an attractive force that holds atoms together in molecules or compounds. Bonds form because:

- Atoms tend to achieve stable electronic configurations (usually octet)
- Bond formation releases energy, making the system more stable
- Two main types: **Ionic bonds** (electron transfer between atoms) and **Covalent bonds** (electron sharing between atoms)
- The driving force is the lowering of potential energy when atoms combine compared to isolated atoms

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4.2 Write Lewis dot symbols for atoms of the following elements: Mg, Na, B, O, N, Br.

Answer:

- **Na**: Na•
- **Mg**: Mg••
- **B**: •B•
- **N**: •N•••

- **O**: •O••••
- **Br**: •Br•••••••

Note: Dots represent valence electrons around the element symbol

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4.3 Write Lewis symbols for the following atoms and ions: S and S^{2-}; Al and Al^{3+}; H and H^-

Answer:

- **S**: •S•••••• (6 valence electrons)
- **S^{2-}**: $[$•S••••••$]^{2-}$ (8 electrons, octet complete)
- **Al**: •Al••• (3 valence electrons)
- **Al^{3+}**: Al^{3+} (no valence electrons, all removed)
- **H**: H• (1 valence electron)
- **H^-**: $[$H••$]^-$ (2 electrons, duplet complete)

4.4 Draw the Lewis structures for the following molecules and ions: H_2S, $SiCl_4$, BeF_2, CO_3^{2-}, HCOOH

Answer:

H_2S:

```
   H
   |
H : S :
   |
  (lone pairs on S)
```

Total valence electrons = 8, S has 2 bonding pairs and 2 lone pairs

SiCl$_4$:

```
  Cl
  |
Cl-Si-Cl
  |
  Cl
```

Tetrahedral structure, Si forms 4 single bonds with Cl atoms

BeF$_2$:

```
F-Be-F
```

Linear structure, Be has incomplete octet (4 electrons)

CO$_3^{2-}$:

```
   O⁻
  / \
 O=C=O⁻
```

Resonance hybrid with partial double bond character in all C-O bonds

HCOOH:

```
  O
  ||
H-C-OH
```

Formic acid with C forming double bond with one O and single bond with OH group

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4.5 Define octet rule. Write its significance and limitations.

Answer:

Definition: Atoms tend to gain, lose, or share electrons to achieve 8 electrons in their valence shell (noble gas configuration).

Significance:

- Explains formation of ionic and covalent bonds
- Helps predict chemical formulas and structures
- Basis for understanding chemical stability

Limitations:

1. **Incomplete octet**: Be, B, Al (less than 8 electrons)
2. **Expanded octet**: P, S, Cl in period 3+ (more than 8 electrons)
3. **Odd-electron molecules**: NO, NO_2
4. **Noble gases can form compounds**: XeF_4, XeF_6

4.6 Write the favourable factors for the formation of ionic bond.

Answer:

1. **Low ionization enthalpy** of metal (easy cation formation)
2. **High electron gain enthalpy** of non-metal (easy anion formation)
3. **High lattice enthalpy** (strong electrostatic attraction in crystal)
4. **Large size difference** between atoms
5. **Large electronegativity difference** (>1.7)
6. **Simple electron transfer** to achieve noble gas configuration

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4.7 Discuss the shape of the following molecules using the VSEPR model: $BeCl_2$, BCl_3, $SiCl_4$, AsF_5, H_2S, PH_3

Answer:

$BeCl_2$:

- Electron pairs around Be = 2
- Geometry = Linear, Bond angle = 180°

BCl_3:

- Electron pairs around B = 3
- Geometry = Trigonal planar, Bond angle = 120°

$SiCl_4$:

- Electron pairs around Si = 4
- Geometry = Tetrahedral, Bond angle = 109.5°

AsF_5:

- Electron pairs around As = 5
- Geometry = Trigonal bipyramidal, Bond angles = 90°, 120°

H_2S:

- Electron pairs around S = 4 (2 bonding + 2 lone pairs)
- Geometry = Bent, Bond angle $< 109.5°$ (~92°)

PH_3:

- Electron pairs around P = 4 (3 bonding + 1 lone pair)
- Geometry = Trigonal pyramidal, Bond angle $< 109.5°$ (~93.5°)

4.8 Although geometries of NH_3 and H_2O molecules are distorted tetrahedral, bond angle in water is less than that of ammonia. Discuss.

Answer:

Both NH_3 and H_2O have **sp^3 hybridization** with distorted tetrahedral electron geometry.

Bond angles:

- NH_3: 107°
- H_2O: 104.5°

Reason: Lone pair-lone pair repulsion > Lone pair-bond pair repulsion > Bond pair-bond pair repulsion

- **NH_3** has 1 lone pair, so 3 lp-bp repulsions reduce angle from 109.5° to 107°

- **H_2O** has 2 lone pairs, so 1 lp-lp + 4 lp-bp repulsions reduce angle further to 104.5°

The additional lone pair in H_2O causes greater distortion.

4.9 How do you express the bond strength in terms of bond order?

Answer:

Bond Order = Number of bonds between two atoms

Relationship with bond strength:

- **Higher bond order = Stronger bond = Higher bond dissociation energy**
- **Higher bond order = Shorter bond length**

Examples:

- Single bond (C-C): Bond order = 1, Length = 154 pm
- Double bond (C=C): Bond order = 2, Length = 133 pm
- Triple bond (C≡C): Bond order = 3, Length = 120 pm

In MO theory: Bond Order = ½(Nb - Na) where Nb = bonding electrons, Na = antibonding electrons

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4.10 Define the bond length.

Answer:

Bond Length: The equilibrium distance between the nuclei of two bonded atoms in a molecule.

Key points:

- Measured by spectroscopic and X-ray diffraction techniques
- Sum of covalent radii of bonded atoms
- **Factors affecting bond length:**
  - Bond order (higher order = shorter length)
  - Atomic size (larger atoms = longer bonds)
  - Hybridization (more s-character = shorter bonds)

Examples:

- H-H = 74 pm
- C-C = 154 pm, C=C = 133 pm, C≡C = 120 pm

4.11 Explain the important aspects of resonance with reference to the CO_3^{2-} ion.

Answer:

Resonance in CO_3^{2-}:

Three canonical structures:

```
Structure I:   Structure II:   Structure III:
  O⁻             O               O⁻
 /              //              /
C=O    ↔     C-O⁻    ↔     C-O
 \              \               \\
  O⁻             O⁻              O
```

Important aspects:

1. **All C-O bonds are equivalent** (experimental bond length = 129 pm)
2. **Resonance hybrid** is more stable than any single structure
3. **Delocalization** of electrons over the entire ion
4. **Bond order** = 1.33 (between single and double bond)
5. **Charge distribution** spreads over all three oxygen atoms

Real structure: Average of all canonical forms, not switching between them.

4.12 H_3PO_3 can be represented by structures 1 and 2 shown below. Can these two structures be taken as the canonical forms of the resonance hybrid representing H_3PO_3? If not, give reasons for the same.

Answer:

No, these cannot be resonance structures.

Requirements for resonance:

1. Same molecular formula ✓
2. Same arrangement of atoms ✓
3. Only electrons should move, not atoms ✗

Reasons why not resonance:

- If the structures show different **atomic positions** (P-H vs P-OH arrangements), they represent **tautomers**, not resonance structures
- **Tautomers** involve movement of both electrons and atoms (usually hydrogen)
- **Resonance** only involves movement of electrons with fixed atomic positions

These would be **structural isomers** or **tautomers**, not canonical forms of resonance.

4.13 Write the resonance structures for SO_3, NO_2 and NO_3^-.

Answer:

SO_3 (three resonance structures):

```
 O     O⁻    O
//    /    //
S=O  ↔  S=O⁺  ↔  O-S⁺
\\    \\    /
 O     O    O⁻
```

NO_2 (two resonance structures):

```
 O     O⁻
//    /
N   ↔  N⁺
\     \\
 O⁻    O
```

NO_3^- (three resonance structures):

```
 O⁻     O     O⁻
/      //    /
N=O  ↔  N-O⁻  ↔  N-O
\\     \\    //
 O⁻     O⁻   O
```

4.14 Use Lewis symbols to show electron transfer between the following atoms to form cations and anions: (a) K and S (b) Ca and O (c) Al and N.

Answer:

(a) K and S:

$2K\bullet + \bullet S\bullet\bullet\bullet\bullet\bullet\bullet \rightarrow 2K^{+} + [S\bullet\bullet\bullet\bullet\bullet\bullet]^{2-}$

K_2S formation: $2K^{+} + S^{2-}$

(b) Ca and O:

$Ca\bullet\bullet + \bullet O\bullet\bullet\bullet\bullet \rightarrow Ca^{2+} + [O\bullet\bullet\bullet\bullet\bullet\bullet]^{2-}$

CaO formation: $Ca^{2+} + O^{2-}$

(c) Al and N:

$2Al\bullet\bullet\bullet + N\bullet\bullet\bullet \rightarrow 2Al^{3+} + [N\bullet\bullet\bullet\bullet\bullet\bullet]^{3-}$

But: $4Al\bullet\bullet\bullet + 4N\bullet\bullet\bullet \rightarrow 4Al^{3+} + 4[N\bullet\bullet\bullet\bullet\bullet\bullet]^{3-}$

AlN formation: $Al^{3+} + N^{3-}$ (1:1 ratio in crystal)

Actually forms: $2Al^{3+} + 3N^{2-} \rightarrow Al_2N_3$

4.15 Although both CO_2 and H_2O are triatomic molecules, the shape of H_2O molecule is bent while that of CO_2 is linear. Explain this on the basis of dipole moment.

Answer:

CO_2: $\mu = 0$ D (Linear shape)

- C has no lone pairs, sp hybridization
- Two C=O dipoles are equal and opposite
- Vector sum = 0, hence linear

H_2O: $\mu = 1.85$ D (Bent shape)

- O has 2 lone pairs, sp^3 hybridization
- Two O-H dipoles don't cancel due to bent geometry
- Bond angle = 104.5°, resultant dipole exists

Conclusion:

- **Zero dipole moment** in CO_2 confirms linear shape
- **Non-zero dipole moment** in H_2O confirms bent shape

4.16 Write the significance/applications of dipole moment.

Answer:

Applications:

1. **Determining molecular shapes** (polar vs non-polar)
2. **Distinguishing between isomers** (cis-trans isomers)
3. **Predicting solubility** (like dissolves like principle)
4. **Understanding intermolecular forces** (dipole-dipole interactions)
5. **Calculating partial charges** on atoms
6. **Determining polarity of bonds** and molecules
7. **Explaining physical properties** (boiling point, melting point)

Examples:

- Trans-alkenes (μ = 0) vs Cis-alkenes (μ ≠ 0)
- Solubility of polar compounds in polar solvents

4.17 Define electronegativity. How does it differ from electron gain enthalpy?

Answer:

Electronegativity: The tendency of an atom to attract shared electron pairs in a covalent bond.

Electron Gain Enthalpy: Energy released when a gaseous atom gains an electron to form anion.

Differences:

Electronegativity	**Electron Gain Enthalpy**
Relative tendency	Actual energy change
No units (relative scale)	Units: kJ/mol
For bonded atoms	For isolated gaseous atoms
Predicts bond polarity	Measures tendency to form anions
Pauling, Mulliken scales	Measured experimentally

4.18 Explain with the help of suitable example polar covalent bond.

Answer:

Polar Covalent Bond: Covalent bond with unequal sharing of electron pair due to electronegativity difference.

Example: HCl molecule

- **Electronegativity:** H (2.1), Cl (3.0)
- **Difference:** 0.9 (significant but <1.7)
- **Result:** Cl attracts electron pair more strongly
- **Polarity:** H^δ+ — Cl^δ-
- **Dipole moment:** 1.07 D

Characteristics:

- Partial charges develop (δ+ and δ-)
- Electron density shifts toward more electronegative atom
- Results in dipole moment
- Bond has both ionic and covalent character

4.19 Arrange the bonds in order of increasing ionic character in the molecules: LiF, K_2O, N_2, SO_2 and ClF_3.

Answer:

Order of increasing ionic character: $N_2 < SO_2 < ClF_3 < LiF < K_2O$

Reasoning (based on electronegativity difference):

- **N_2:** $\Delta\chi = 0$ (purely covalent)
- **SO_2:** $\Delta\chi = 1.0$ (S=3.0, O=3.5) - polar covalent
- **ClF_3:** $\Delta\chi = 1.0$ (Cl=3.0, F=4.0) - polar covalent
- **LiF:** $\Delta\chi = 3.0$ (Li=1.0, F=4.0) - ionic

- **K_2O:** Δχ = 2.6 (K=0.8, O=3.5) - highly ionic

Rule: Higher electronegativity difference = More ionic character

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4.20 The skeletal structure of CH_3COOH as shown below is correct, but some of the bonds are shown incorrectly. Write the correct Lewis structure for acetic acid.

Answer:

Correct Lewis structure for CH_3COOH:

```
  H   O
  |   ||
H—C—C—OH
  |
  H
```

Key corrections likely needed:

- C=O double bond in carboxyl group
- Single C-OH bond
- All atoms should satisfy octet rule (except H with duplet)
- Total valence electrons = 24
- Left carbon: sp^3 hybridized (tetrahedral)
- Right carbon: sp^2 hybridized (trigonal planar)

4.21 Apart from tetrahedral geometry, another possible geometry for CH_4 is square planar with the four H atoms at the corners of the square and the C atom at its centre. Explain why CH_4 is not square planar?

Answer:

Reasons why CH_4 is tetrahedral, not square planar:

1. **Orbital hybridization:** C undergoes sp^3 hybridization (not dsp^2)
2. **d-orbital availability:** Carbon (Period 2) has no d-orbitals for dsp^2 hybridization
3. **VSEPR theory:** 4 bonding pairs arrange to minimize repulsion → tetrahedral
4. **Energy considerations:** Tetrahedral geometry has lower energy than square planar
5. **Bond angles:** Tetrahedral (109.5°) vs Square planar (90°, 180°)
6. **Experimental evidence:** X-ray diffraction confirms tetrahedral structure

Square planar geometry requires d-orbitals (like in $[PtCl_4]^{2-}$ with dsp^2 hybridization).

4.22 Explain why BeH_2 molecule has a zero dipole moment although the Be–H bonds are polar.

Answer:

Reasons for zero dipole moment in BeH_2:

1. **Linear geometry:** H-Be-H bond angle = 180°
2. **Symmetrical structure:** Two Be-H bonds are identical
3. **Vector cancellation:** The two polar bonds have equal magnitude but opposite directions
4. **Net dipole = 0:** Individual bond dipoles cancel each other

Be-H bond polarity:

- Electronegativity difference exists (H = 2.1, Be = 1.5)
- Each bond is polar (Be^δ+ — H^δ-)
- But molecular geometry causes cancellation

Similar examples: CO_2, BF_3 (polar bonds, zero molecular dipole)

4.23 Which out of NH_3 and NF_3 has higher dipole moment and why?

Answer:

NH_3 has higher dipole moment than NF_3.

Dipole moments:

- NH_3: $\mu = 1.47$ D
- NF_3: $\mu = 0.23$ D

Explanation:

In NH_3:

- N is more electronegative than H
- Bond dipoles point toward N
- Lone pair dipole also points away from N
- Both effects add up → Higher net dipole

In NF_3:

- F is more electronegative than N

- Bond dipoles point toward F atoms (away from N)
- Lone pair dipole points away from N
- Bond dipoles and lone pair dipole oppose each other → Lower net dipole

Result: Despite F being more electronegative, NH_3 has higher dipole moment due to constructive addition of bond and lone pair dipoles.

4.24 What is meant by hybridisation of atomic orbitals? Describe the shapes of sp, sp^2, sp^3 hybrid orbitals.

Answer:

Hybridization: Process of mixing atomic orbitals of similar energies to form new equivalent hybrid orbitals.

Shapes of hybrid orbitals:

sp Hybridization:

- **Orbitals mixed:** 1s + 1p
- **Shape:** Linear with two lobes of unequal size
- **Angle:** 180°
- **Example:** BeF_2, C_2H_2

sp^2 Hybridization:

- **Orbitals mixed:** 1s + 2p
- **Shape:** Trigonal planar arrangement
- **Angle:** 120°
- **Example:** BF_3, C_2H_4

sp^3 Hybridization:

- **Orbitals mixed:** 1s + 3p
- **Shape:** Tetrahedral arrangement
- **Angle:** 109.5°
- **Example:** CH_4, NH_3, H_2O

Each hybrid orbital has one large lobe (for bonding) and one small lobe.

4.25 Describe the change in hybridisation (if any) of the Al atom in the following reaction: $AlCl_3 + Cl^- \rightarrow AlCl_4^-$

Answer:

Hybridization change:

- **$AlCl_3$:** sp^2 hybridization → Trigonal planar geometry
- **$AlCl_4^-$:** sp^3 hybridization → Tetrahedral geometry

Details:

In $AlCl_3$:

- Al has 3 bonding pairs, 0 lone pairs
- Uses 1s + 2p orbitals → sp^2 hybridization
- Planar triangular structure
- Bond angle = 120°

In $AlCl_4^-$:

- Al has 4 bonding pairs, 0 lone pairs
- Uses 1s + 3p orbitals → sp^3 hybridization
- Tetrahedral structure
- Bond angle = 109.5°

Mechanism: Cl^- ion donates electron pair to empty p-orbital of Al, forming coordinate bond.

4.26 Is there any change in the hybridisation of B and N atoms as a result of the following reaction? $BF_3 + NH_3 \rightarrow F_3B \leftarrow NH_3$

Answer:

Hybridization changes:

Boron (B):

- **Before (BF_3):** sp^2 hybridization (trigonal planar)
- **After ($F_3B \leftarrow NH_3$):** sp^3 hybridization (tetrahedral)
- **Change:** $sp^2 \rightarrow sp^3$

Nitrogen (N):

- **Before (NH_3):** sp^3 hybridization (trigonal pyramidal)
- **After ($F_3B \leftarrow NH_3$):** sp^3 hybridization (tetrahedral)
- **Change:** No change in hybridization, but geometry becomes more regular

Reason:

- NH_3 donates lone pair to empty p-orbital of B
- B now has 4 bonding pairs instead of 3

- N still has 4 electron pairs (3 bonding + 1 bonding through coordinate bond)

4.27 Draw diagrams showing the formation of a double bond and a triple bond between carbon atoms in C_2H_4 and C_2H_2 molecules.

Answer:

C_2H_4 (Ethene) - Double bond formation:

Hybridization: Both carbons sp^2 hybridized

```
σ-bond: sp²-sp² overlap (head-on)
π-bond: 2p-2p overlap (sidewise)

H   H
 \ /
  C=C   ← One σ + One π bond
 / \
H   H
```

C_2H_2 (Ethyne) - Triple bond formation:

Hybridization: Both carbons sp hybridized

```
σ-bond: sp-sp overlap (head-on)
π-bonds: 2p-2p overlap (two sidewise overlaps)

H-C≡C-H  ← One σ + Two π bonds
```

Key points:

- σ bonds are stronger and formed first
- π bonds are weaker and form after σ bond
- Multiple bonds restrict rotation

4.28 What is the total number of sigma and pi bonds in the following molecules? (a) C_2H_2 (b) C_2H_4

Answer:

(a) C_2H_2 (Ethyne):

- **Structure:** H-C≡C-H
- **σ bonds:** 2 C-H + 1 C-C = **3 σ bonds**
- **π bonds:** 2 (from triple bond) = **2 π bonds**
- **Total:** 3σ + 2π = 5 bonds

(b) C_2H_4 (Ethene):

- **Structure:** $H_2C=CH_2$
- **σ bonds:** 4 C-H + 1 C-C = **5 σ bonds**
- **π bonds:** 1 (from double bond) = **1 π bond**
- **Total:** 5σ + 1π = 6 bonds

Remember:

- Single bond = 1σ
- Double bond = 1σ + 1π
- Triple bond = 1σ + 2π

4.29 Considering x-axis as the internuclear axis which out of the following will not form a sigma bond and why? (a) 1s and 1s (b) 1s and $2p_x$; (c) $2p_y$ and $2p_y$ (d) 1s and 2s.

Answer:

(c) $2p_y$ and $2p_y$ will NOT form a sigma bond.

Explanation:

Sigma bond requirements:

- Head-on (end-to-end) overlap along internuclear axis
- Cylindrical symmetry around bond axis

Analysis:

- **(a) 1s and 1s:** ✓ Forms σ bond (spherical, head-on overlap)
- **(b) 1s and $2p_x$:** ✓ Forms σ bond (s overlaps with lobe of p_x along x-axis)
- **(c) $2p_y$ and $2p_y$:** ✗ Forms π bond (sidewise overlap, perpendicular to x-axis)
- **(d) 1s and 2s:** ✓ Forms σ bond (spherical orbitals, head-on overlap)

Reason for (c): $2p_y$ orbitals are perpendicular to x-axis, so they overlap sideways, forming a π bond, not σ bond.

4.30 Which hybrid orbitals are used by carbon atoms in the following molecules? (a) $CH_3–CH_3$; (b) $CH_3–CH=CH_2$; (c) CH_3-CH_2-OH; (d) CH_3-CHO (e) CH_3COOH

Answer:

(a) CH_3–CH_3 (Ethane):

- Both C atoms: **sp^3 hybridization**

(b) CH_3–CH=CH_2 (Propene):

- CH_3 carbon: **sp^3 hybridization**
- CH= carbon: **sp^2 hybridization**
- =CH_2 carbon: **sp^2 hybridization**

(c) CH_3-CH_2-OH (Ethanol):

- Both C atoms: **sp^3 hybridization**

(d) CH_3-CHO (Acetaldehyde):

- CH_3 carbon: **sp^3 hybridization**
- CHO carbon: **sp^2 hybridization** (C=O double bond)

(e) CH_3COOH (Acetic acid):

- CH_3 carbon: **sp^3 hybridization**
- COOH carbon: **sp^2 hybridization** (C=O double bond)

Rule: sp^3 (4 σ bonds), sp^2 (3 σ bonds + π bonds), sp (2 σ bonds + π bonds)

4.31 What do you understand by bond pairs and lone pairs of electrons? Illustrate by giving one example of each type.

Answer:

Bond Pairs (Bonding Pairs):

- Electron pairs shared between two atoms
- Participate in chemical bonding
- Located between atomic nuclei

Lone Pairs (Non-bonding Pairs):

- Electron pairs localized on a single atom
- Do not participate in bonding
- Affect molecular geometry through repulsion

Examples:

NH_3 (Ammonia):

```
   H
   |
H : N : H
   |
  (lone pair)
```

- **Bond pairs:** 3 (N-H bonds)
- **Lone pairs:** 1 (on N atom)
- **Total:** 4 electron pairs around N

Effect: Lone pair causes trigonal pyramidal geometry instead of trigonal planar.

4.32 Distinguish between a sigma and a pi bond.

Answer:

Property	**Sigma (σ) Bond**	**Pi (π) Bond**
Formation	Head-on overlap	Sidewise overlap
Overlap type	End-to-end	Lateral
Symmetry	Cylindrical around bond axis	Not cylindrical
Strength	Stronger	Weaker
Bond energy	Higher	Lower
Free rotation	Allows rotation	Restricts rotation
Electron density	Along internuclear axis	Above and below bond axis
Examples	C-C, C-H bonds	C=C, C≡C (additional bonds)
Number	One per bond	Additional to σ bond

Key point: Every covalent bond has one σ bond. Multiple bonds have additional π bonds.

4.33 Explain the formation of H_2 molecule on the basis of valence bond theory.

Answer:

H_2 molecule formation:

Step 1: Approaching hydrogen atoms

- Two H atoms with $1s^1$ electronic configuration
- Each has one unpaired electron

Step 2: Orbital overlap

- 1s orbitals of both atoms overlap head-on
- Overlap region has increased electron density

- Electrons pair up with opposite spins

Step 3: Bond formation

- Maximum overlap occurs at internuclear distance = 74 pm
- System achieves minimum energy (most stable state)
- Bond energy = 435.8 kJ/mol released

Step 4: Stabilization

- Electron density between nuclei increases
- Nuclear-electron attraction > electron-electron and nuclear-nuclear repulsions
- Net attractive force holds atoms together

VB theory explains: Bond strength depends on extent of orbital overlap.

4.34 Write the important conditions required for the linear combination of atomic orbitals to form molecular orbitals.

Answer:

Conditions for LCAO (Linear Combination of Atomic Orbitals):

1. **Energy condition:**
    - Combining atomic orbitals must have similar energies
    - Large energy difference prevents effective combination
2. **Symmetry condition:**
    - Orbitals must have proper symmetry about molecular axis
    - Same symmetry elements required for overlap

3. **Overlap condition:**
    - Atomic orbitals must overlap significantly
    - Greater overlap → better MO formation
4. **Orientation condition:**
    - Proper spatial orientation for maximum overlap
    - Correct directional alignment needed

Examples:

- ✓ 2s + 2s (same energy, symmetry)
- ✓ 2pz + 2pz (along internuclear axis)
- ✗ 1s + 2p (large energy difference)
- ✗ 2px + 2py (wrong symmetry)

4.35 Use molecular orbital theory to explain why the Be$_2$ molecule does not exist.

Answer:

Be$_2$ molecular orbital analysis:

Electronic configuration of Be: 1s^2 2s^2 **Total electrons in Be$_2$:** 8 electrons

MO configuration: Be$_2$: (σ1s)^2 (σ*1s)^2 (σ2s)^2 (σ*2s)^2

Bond order calculation:

- **Bonding electrons (Nb):** 4 (in σ1s and σ2s orbitals)
- **Antibonding electrons (Na):** 4 (in σ*1s and σ*2s orbitals)

- **Bond order = ½(Nb - Na) = ½(4 - 4) = 0**

Conclusion:

- Bond order = 0 means **no net bonding**
- Be_2 molecule is **thermodynamically unstable**
- **Does not exist** under normal conditions

Reason: Equal number of bonding and antibonding electrons cancel each other's effect.

4.36 Compare the relative stability of the following species and indicate their magnetic properties: O_2^+, O_2, O_2^-, O_2^{2-}

Answer:

Electronic configurations and analysis:

O_2^+ (15 electrons):

- Configuration: $(\sigma 1s)^2(\sigma 1s)^2(\sigma 2s)^2(\sigma 2s)^2(\sigma 2pz)^2(\pi 2px)^2(\pi 2py)^2(\pi^* 2px)^1$
- Bond order = ½(10-5) = 2.5
- **Magnetic nature:** Paramagnetic (1 unpaired electron)

O_2 (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 = ½(10-6) = 2
- **Magnetic nature:** Paramagnetic (2 unpaired electrons)

O_2^- (17 electrons):

- Configuration: $(\sigma 1s)^2(\sigma 1s)^2(\sigma 2s)^2(\sigma 2s)^2(\sigma 2pz)^2(\pi 2px)^2(\pi 2py)^2(\pi 2px)^2(\pi 2py)^1$
- Bond order = ½(10-7) = 1.5
- **Magnetic nature:** Paramagnetic (1 unpaired electron)

O_2^{2-} (18 electrons):

- Configuration: $(\sigma 1s)^2(\sigma 1s)^2(\sigma 2s)^2(\sigma 2s)^2(\sigma 2pz)^2(\pi 2px)^2(\pi 2py)^2(\pi 2px)^2(\pi 2py)^2$
- Bond order = ½(10-8) = 1
- **Magnetic nature:** Diamagnetic (all electrons paired)

Stability order: $O_2^+ > O_2 > O_2^- > O_2^{2-}$ (Higher bond order = Greater stability)

4.37 Write the significance of a plus and a minus sign shown in representing the orbitals.

Answer:

Significance of + and - signs in orbitals:

1. **Phase of wave function:**
   - Represent different phases (not electric charges)
   - Mathematical signs of orbital wave function
   - Similar to wave crests (+) and troughs (-)
2. **Orbital overlap:**
   - **Same signs overlap:** Constructive interference → Bonding MO
   - **Opposite signs overlap:** Destructive interference → Antibonding MO
   - **Different signs, no overlap:** Zero overlap
3. **Electron probability:**

    - Signs don't affect electron density ($|\psi|^2$ is always positive)
    - Only relative phases matter for bonding
4. **Bonding implications:**
    - Proper phase matching required for effective bonding
    - Determines whether MO is bonding or antibonding

Example: In H_2 formation:

- (+) + (+) → Bonding MO (constructive)
- (+) + (-) → Antibonding MO (destructive)

4.38 Describe the hybridisation in case of PCl_5. Why are the axial bonds longer as compared to equatorial bonds?

Answer:

Hybridization in PCl_5:

Ground state P: [Ne] $3s^2$ $3p^3$ **Excited state P:** [Ne] $3s^1$ $3p^3$ $3d^1$ **Hybridization:** sp^3d (1s + 3p + 1d orbitals)

Geometry: Trigonal bipyramidal

- **3 equatorial bonds:** 120° angles in horizontal plane
- **2 axial bonds:** 90° to equatorial plane, 180° to each other

Why axial bonds are longer:

1. **Greater repulsion:** Axial bonds experience repulsion from 3 equatorial bonds at 90°

2. **Less repulsion:** Equatorial bonds experience repulsion from only 2 other equatorial bonds at 120°
3. **Electron density:** Lower electron density in axial bonds due to more repulsion
4. **Orbital character:** Different s and p character in axial vs equatorial bonds

Result:

- **Axial P-Cl bonds:** Longer and weaker
- **Equatorial P-Cl bonds:** Shorter and stronger
- This makes PCl_5 **more reactive** (axial bonds break first)

4.39 Define hydrogen bond. Is it weaker or stronger than the van der Waals forces?

Answer:

Hydrogen Bond Definition: Attractive interaction between a hydrogen atom (bonded to highly electronegative atom F, O, or N) and another electronegative atom with lone pairs.

Representation: X-H···Y (where X, Y = F, O, N)

Strength Comparison: Hydrogen bonds are STRONGER than van der Waals forces

Typical energies:

- **Hydrogen bonds:** 10-40 kJ/mol
- **van der Waals forces:** 0.4-4 kJ/mol
- **Covalent bonds:** 200-800 kJ/mol

Characteristics:

- **Directional** (unlike van der Waals)
- **Specific** (requires H and electronegative atoms)
- **Longer than covalent bonds** but shorter than van der Waals
- **Partially covalent character**

Examples:

- HF molecules: H-F···H-F
- Water molecules: $H_2O \cdots H_2O$
- DNA base pairing: A-T, G-C

4.40 What is meant by the term bond order? Calculate the bond order of: N_2, O_2, O_2^+ and O_2^-.

Answer:

Bond Order Definition:

- **Classical:** Number of bonds between two atoms
- **MO Theory:** ½(Number of bonding electrons - Number of antibonding electrons)
- **Formula:** Bond Order = ½(Nb - Na)

Calculations:

N_2 (14 electrons):

- Configuration: $(\sigma 1s)^2(\sigma\mathit{1s)^2(\sigma 2s)^2(\sigma}2s)^2(\pi 2px)^2(\pi 2py)^2(\sigma 2pz)^2$
- Nb = 10, Na = 4
- **Bond order = ½(10-4) = 3** (Triple bond)

O_2 (16 electrons):

- Configuration: $(\sigma 1s)^2(\sigma 1s)^2(\sigma 2s)^2(\sigma 2s)^2(\sigma 2pz)^2(\pi 2px)^2(\pi 2py)^2(\pi 2px)^1(\pi 2py)^1$
- Nb = 10, Na = 6
- **Bond order = ½(10-6) = 2** (Double bond)

O_2^+ (15 electrons):

- Configuration: $(\sigma 1s)^2(\sigma 1s)^2(\sigma 2s)^2(\sigma 2s)^2(\sigma 2pz)^2(\pi 2px)^2(\pi 2py)^2(\pi^* 2px)^1$
- Nb = 10, Na = 5
- **Bond order = ½(10-5) = 2.5**

O_2^- (17 electrons):

- Configuration: $(\sigma 1s)^2(\sigma 1s)^2(\sigma 2s)^2(\sigma 2s)^2(\sigma 2pz)^2(\pi 2px)^2(\pi 2py)^2(\pi 2px)^2(\pi 2py)^1$
- Nb = 10, Na = 7
- **Bond order = ½(10-7) = 1.5**

Bond strength order: N_2 (3) > O_2^+ (2.5) > O_2 (2) > O_2^- (1.5)

Summary Table - Key Answers

Question	Key Point	Answer
4.2	Lewis symbols	Na•, Mg••, •B•, •N•••, •O••••, •Br•••••••
4.8	Bond angles	H_2O (104.5°) < NH_3 (107°) due to more lone pairs
4.9	Bond strength	Higher bond order = Stronger bond = Shorter length
4.15	Molecular shapes	CO_2 linear ($\mu=0$), H_2O bent ($\mu \neq 0$)
4.19	Ionic character	N_2 < SO_2 < ClF_3 < LiF < K_2O
4.23	Dipole moments	NH_3 (1.47 D) > NF_3 (0.23 D)

Question	Key Point	Answer
4.28	Sigma/Pi bonds	C_2H_2: 3σ + 2π, C_2H_4: 5σ + 1π
4.35	Be_2 existence	Bond order = 0, does not exist
4.40	Bond orders	N_2(3), O_2^+(2.5), O_2(2), O_2^-(1.5)

Note: All answers provide medium-level detail suitable for NEET preparation, focusing on key concepts and calculations without excessive elaboration.