

Q1. The principal quantum number (n) describes which of the following?

c) The energy level of the electron

Q2. The Aufbau principle states that electrons will fill:

b) Orbitals in order of increasing energy

Q3. The magnetic quantum number (m) gives information about:

d) The orientation of the orbital in space

Q4. The Pauli Exclusion Principle states that:

b) Electrons in the same orbital must have opposite spins

Q5. In the IR spectrum, the C=O stretching vibration typically appears around:

b) 1700–1750 cm^{-1}

Q6. Which of the following bonds would absorb IR radiation at the highest frequency?

a) $\text{C}\equiv\text{C}$

(Triple bonds absorb at higher frequencies than double and single bonds.)

Q7. Which of the following nuclei is commonly used in carbon-13 NMR spectroscopy?

c) ^{13}C

Q8. The region of the electromagnetic spectrum used in UV-Vis spectroscopy typically ranges from:

b) 200–800 nm

Q9. In UV-Vis spectroscopy, the intensity of absorption is proportional to:

a) The concentration of the absorbing species

Q10. Which of the following trends is observed as you move across a period in the periodic table?

b) Atomic size decreases

Q11. Which of the following elements has the highest first ionization energy?

c) Neon (Ne)

(Noble gases have the highest ionization energies in their periods.)

Q12. Which of the following elements has the highest electronegativity?

b) Fluorine (F)

(Fluorine is the most electronegative element.)

Q13. Electronegativity generally increases as you move:

d) From left to right in a group (This is likely a typo in the options; it should be "From left to right in a period")

Most correct based on logic: b) Across a period from left to right

Q14. Which of the following is the strongest type of intermolecular force?

c) Hydrogen bonding

Q15. Which of the following is true about entropy (S)?

a) Entropy is a measure of the disorder of a system.

Q16. Explain the forms of hydrogen atom wave functions and their plots.

The hydrogen atom wave functions are solutions to the Schrödinger equation. These are called orbitals and are defined by three quantum numbers:

Principal quantum number (n) – defines energy level and size

Azimuthal quantum number (l) – defines shape (s, p, d, f)

Magnetic quantum number (m) – defines orientation

The wave function ψ depends on both radial and angular parts. For example:

1s orbital is spherical and non-directional.

2p orbital has a dumbbell shape and is directional.

The radial distribution function shows the probability of finding an electron at a particular distance from the nucleus. Plots of ψ^2 give us visual representations of electron clouds.

Q17. Explain the π -molecular orbitals of butadiene.

Butadiene ($\text{CH}=\text{CH}-\text{CH}=\text{CH}$) is a conjugated diene with four π electrons. According to Molecular Orbital Theory:

The 4 p-orbitals (from the 4 carbon atoms) combine to form 4 π molecular orbitals: Ψ , Ψ (bonding), Ψ^* , Ψ^* (antibonding).

Electrons fill the lowest energy orbitals first (Ψ and Ψ).

Key points:

Delocalization: The π electrons are spread across the molecule, increasing stability.

HOMO and LUMO: Highest Occupied Molecular Orbital (Ψ), Lowest Unoccupied (Ψ^*) are critical in reactivity and UV-Vis absorption.

The energy diagram and phase diagrams illustrate constructive and destructive overlaps.

Q18. Explain bending vibrations in IR spectroscopy.

Bending vibrations (also called deformation vibrations) occur when bond angles change. There are two main types:

In-plane bending:

Scissoring – atoms move toward each other like scissors.

Rocking – atoms move in the same direction.

Out-of-plane bending:

Wagging – atoms move up and down together.

Twisting – one atom moves up while the other moves down.

These vibrations usually occur at lower frequencies than stretching vibrations. They are useful in identifying functional groups in IR spectroscopy.

Q19. Explain applications of IR Spectroscopy.

IR spectroscopy is widely used in both qualitative and quantitative analysis:

Identification of functional groups (e.g., OH, C=O, NH):

Each bond has a characteristic absorption frequency.

Structure determination:

Helps confirm the presence of specific linkages.

Quality control in pharmaceuticals and polymer industries.

Environmental monitoring:

Detects pollutants like CO , SO .

Forensic analysis:

Fiber and drug identification.

Food industry:

Tests adulterants, moisture content.

Q20. Discuss in detail electronegativity.

Electronegativity is the ability of an atom to attract shared electrons in a bond.

Pauling scale is the most common, where fluorine is assigned 4.0.

Other scales: Mulliken, Allred-Rochow.

Trends in the periodic table:

Increases across a period (more nuclear charge)

Decreases down a group (more shielding)

Applications:

Predicting bond polarity

Determining ionic or covalent character

Influences acid/base behavior and reactivity

Example: In HCl, Cl is more electronegative and pulls the electron density, making the bond polar.

Q21. Discuss in detail ionization energy and electron affinity.

Ionization Energy (IE):

The energy required to remove an electron from a gaseous atom.

First IE < Second IE < Third IE (due to increasing nuclear attraction)

Electron Affinity (EA):

Energy released when an atom gains an electron.

High EA: Halogens

Low or negative EA: Noble gases, some alkaline earth metals

Trends:

IE increases across a period and decreases down a group.

EA becomes more negative across a period.

Applications:

Determines reactivity (e.g., alkali metals vs. halogens)

Helps explain formation of cations and anions.

Q22. Write a short note on entropy and how we can estimate it.

Entropy (S) is a measure of randomness or disorder in a system.

Higher entropy → more disorder

Gases have more entropy than liquids, which have more than solids.

Mathematically,

$$\Delta S = q_{\text{rev}} / T$$

$$\Delta S = T q_{\text{rev}}$$

where q_{rev} is reversible heat and T is temperature.

Standard molar entropy (S°) is tabulated for various substances at 298 K.

Estimation:

From calorimetry data

Using statistical mechanics: $S = k \ln W$

Entropy increases in spontaneous processes (Second Law of Thermodynamics).

Q23. Write a short note on Nernst equation and applications.

Nernst Equation relates cell potential to ion concentrations:

$$E = E^\circ - \frac{RT}{nF} \ln Q$$

$$E = E^\circ - \frac{nFRT}{n} \ln Q$$

At 25°C:

$$E = E^\circ - 0.0591 \log Q$$

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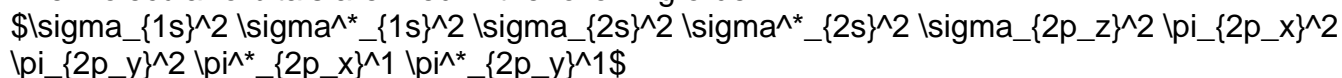
Where:

E° : Standard

Q.24: Molecular Orbital Theory of O₂ molecule

According to Molecular Orbital Theory (MOT), atomic orbitals from two atoms combine to form bonding and antibonding molecular orbitals (MOs), which extend over the entire molecule. Oxygen molecule (O₂) consists of 16 total electrons (8 from each oxygen atom).

The molecular orbitals are filled in the following order:



* The π_{2p_x} and π_{2p_y} orbitals are degenerate.

* The antibonding π^* orbitals each hold one unpaired electron.

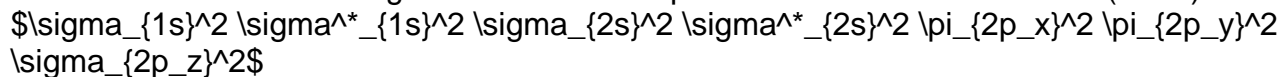
$$\text{Bond order} = \frac{(\text{Bonding electrons}) - (\text{Antibonding electrons})}{2} = \frac{10 - 6}{2} = 2$$

This gives O₂ a **double bond**. The presence of unpaired electrons in degenerate π^* orbitals explains why oxygen is **paramagnetic**, a fact that cannot be explained by classical Lewis structures. MOT correctly predicts the magnetic behavior and delocalization of electrons.

Q.25: Construction of MO diagram for N₂ and calculation of bond order

In the nitrogen molecule (N₂), each nitrogen atom has 7 electrons, giving a total of 14 electrons.

The molecular orbital configuration for second-period homonuclear diatomics (Z < 8) is:



* The π orbitals ($2p_x$ and $2p_y$) are filled before σ_{2p_z} due to their lower energy.

$$\text{Bond order} = \frac{(10 - 4)}{2} = 3$$

This indicates a **triple bond** in N₂. All electrons are paired, making the molecule **diamagnetic**. The high bond order is consistent with the molecule's stability and high bond dissociation energy.

Q.26: Comparison of bond strength and bond length

Bond strength and bond length are inversely related properties. As bond order increases:

* **Bond strength increases** (stronger overlap and greater electron sharing)

* **Bond length decreases** (nuclei pulled closer together)

Examples:

* **N₂**: Bond order = 3 → very strong triple bond → shortest bond length (~110 pm)

* **O₂**: Bond order = 2 → double bond → intermediate bond length (~121 pm)

* **F₂**: Bond order = 1 → single bond → weakest and longest (~142 pm)

Factors affecting bond length and strength:

* **Bond Order**: More shared electrons → stronger and shorter bond

* **Atomic Size**: Larger atoms form longer bonds

* **Electronegativity**: High electronegativity difference can lead to partial ionic character

* **Hybridization**: Greater s-character (e.g., $sp > sp^2 > sp^3$) results in shorter bonds

This comparison helps understand molecular stability, reactivity, and spectroscopic properties.

Q.27: Shapes of simple molecules using VSEPR theory

Valence Shell Electron Pair Repulsion (VSEPR) theory predicts molecular geometry based on repulsion between electron pairs (bonding and lone pairs) around the central atom. Electron pairs arrange themselves to minimize repulsion.

Examples:

1. **BeCl**: Linear geometry

- * Central atom: Be
- * Electron pairs: 2 bonding, 0 lone pairs
- * Bond angle: 180°

2. **BF**: Trigonal planar

- * Central atom: B
- * Electron pairs: 3 bonding, 0 lone pairs
- * Bond angle: 120°

3. **CH**: Tetrahedral

- * Central atom: C
- * Electron pairs: 4 bonding, 0 lone pairs
- * Bond angle: 109.5°

4. **NH**: Trigonal pyramidal

- * Central atom: N
- * Electron pairs: 3 bonding, 1 lone pair
- * Bond angle: $\sim 107^\circ$ (slightly less due to lone pair repulsion)

5. **H O**: Bent (angular)

- * Central atom: O
- * Electron pairs: 2 bonding, 2 lone pairs
- * Bond angle: $\sim 104.5^\circ$

VSEPR theory helps explain molecular shapes, polarities, and reactivity. Lone pairs exert more repulsion than bonding pairs, leading to distortions in ideal bond angles.
