

Assignment for B.Sc. Sem VI Chemistry (Major 1 + Major 2) 2025-26

Paper: Quantum Mechanics and Spectroscopy

Assignment Submission Date: 25.03.2026

M.M. 25

S. No.	Topics	Roll No.
1	<p>Rotational Spectroscopy of Diatomic Molecules:</p> <ul style="list-style-type: none">• Energy level of a rigid rotor, selection rules, spectral intensity distribution, determination of bond length and isotope effect <p>Vibrational Spectrum-Infrared Spectrum:</p> <ul style="list-style-type: none">• Energy levels of simple harmonic oscillator, selection rules, pure vibrational spectrum, intensity, qualitative relation of force constant and bond energies, effect of anharmonic motion and isotope on the spectrum <p>Raman Spectrum:</p> <ul style="list-style-type: none">• Concept of polarizability, pure rotational and pure vibrational Raman spectra of diatomic molecules, selection rules	<p>Bio (2330014010006 — 4010058)</p> <p>Math (2330014020005 — 4020025)</p>
2	<p>Elementary Quantum Mechanics:</p> <ul style="list-style-type: none">• de Broglie's hypothesis, the Heisenberg's uncertainty principle, Hamiltonian operator. Statement of Born-oppenheimer approximation.• Schrodinger wave equation and its importance. Physical interpretation of wave function, postulates of quantum mechanics, particle in one dimensional box.• Schrodinger wave equation for H -atom and its separations into three equations (without derivation), quantum numbers, wave function, angular wave functions.	<p>Bio (2330014010065 — 4010129)</p> <p>Math (2330014020026 — 4020036)</p>

3	<p>Basic idea of molecular orbital theory:</p> <ul style="list-style-type: none"> • Criteria for forming molecular orbitals (M.O's) from atomic orbitals (A.O's), construction of M.O's by LCAO-H²⁺ ion, calculation of energy levels from wave functions, physical picture of bonding and antibonding wave functions • Hybrid Orbitals-sp, sp², sp³, calculation of coefficients of A.O's used in sp and sp² hybrid orbital only. • Introduction to valence bond model of H₂, comparison of M.O. and V.B. models. 	<p>Bio (2330014010130 — 4010184)</p> <p>Math (2330014020037 — 4020050)</p>
4	<p>Ultraviolet (UV) absorption spectroscopy:</p> <ul style="list-style-type: none"> • Absorption laws (Beer Lambert law), molar absorptivity, presentation and analysis of UV spectra, types of electronic transitions, effect of conjugation. • Concept of chromophore and auxochrome, bathochromic, hypsochromic, hyperchromic and hypochromic shifts. • U.V. spectra of conjugated enes and enones. • Woodward fieser rule. 	<p>Bio (2330014010186 — 4010231)</p> <p>Math (2330014020057 — 4020075)</p>
5	<p>Infrared (I.R.) absorption spectroscopy:</p> <ul style="list-style-type: none"> • Molecular vibrations, Hook's law, selection rules, intensity and position of I.R. bands. • Fingerprint region, characteristic absorptions of various functional groups. • Interpretation of I.R. spectra of simple organic compounds- hydrocarbons, aldehydes & ketones in IR spectrum (positions only) 	<p>Bio (2330014010232 — 4010275)</p> <p>Math (2330014020077 — 4020103)</p>

6	<p>Nuclear magnetic resonance (NMR):</p> <ul style="list-style-type: none"> • Spectroscopy, proton magnetic resonance (¹H NMR) spectroscopy, nuclear shielding and deshielding. Chemical shifts and molecular structure, spin-spin splitting and coupling constants, areas of signals. • Interpretation of ¹H NMR spectra of simple organic molecules such as ethyl bromide, ethanol, acetaldehyde, 1,1,2-tribromoethane, ethyl acetate, toluene and acetophenones. • Problems pertaining to the structure elucidation of simple organic compounds using ¹H NMR spectroscopy techniques. 	<p>Bio (2330014010277 — 4010327)</p> <p>Math (2330014020108 — 4020119)</p>
7	<p>Introduction to Mass Spectrometry:</p> <ul style="list-style-type: none"> • Principle of mass spectrometry, the mass spectrum, mass spectrometry diagram • Molecular ion, metastable ion, Nitrogen Rule, fragmentation process • McLafferty rearrangement 	<p>Bio (2330014010330 — 4010380)</p> <p>Math (2330014020120 — 4020141)</p>

- Note:**
- 1. Students have to select assignment topics as per their Roll No.**
 - 2. This assignment is common for Major 1 & Major 2 B.Sc. Sem VI chemistry students**
 - 3. Students are instructed to use a fair register copy for writing**
 - 4. Students must bring their previous semester marksheets at the time of assignment submission**
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