Syllabus
M.Sc. (Chemistry) Programme
(SEMESTER – II)

Spectroscopy I
Programme Code- (MSCCH -21)
Course Code – (MSCCH -509)

Block 1: Atomic spectroscopy

Unit 1 Fundamentals of Spectroscopy

Recapitulation and role of Quantum Mechanics and its importance to the understanding of spectroscopy in chemistry. Characterization of electromagnetic radiation. Heisenberg's Uncertainty Principle and line width. Basic elements of spectroscopy. Einstein coefficients. Lambert-Beer's law. Integrated absorption coefficients. Oscillator strengths. Transition dipole moments and general selection rules based on symmetry ideas.

Unit 2: Atomic spectroscopy, XPS and UPS

Characterization of atomic states. Microstates and spin factoring methods. Hund's rules. Derivation of spin and orbital selection rules (based on recursion relations of Legendre polynomials). Spectra of complex atoms. Zeeman and Stark effects. Atomic photoelectron spectroscopy.

Block 2: Molecular Spectroscopy-I

Unit 3: Rotational Spectroscopy

Recapitulate Rotational spectra of diatomic molecules based on rigid rotator approximation. Determination of bond lengths and/or atomic masses from microwave data. Effect of isotopic substitution. Non-rigid rotator. Classification of polyatomic molecules. Energy levels and spectra of symmetric top molecules and asymmetric top molecules and applications.

Unit 4: Vibrational Spectroscopy-I : Diatomic Molecules

Basic principles of vibrational spectroscopy of homonuclear and heteronuclear diatomic molecules. Selection rules for diatomic molecules based on Harmonic oscillator approximation. Force constants and amplitudes. Anharmonic oscillator. Overtones and combination bands. Dissociation energies from Vibrational data. Vibration-rotation spectra, P, Q and R branches. Breakdown of the Born-Oppenheimner approximation, Nuclear spin effect.

Unit 5: Vibrational Spectroscopy-II : Polyatomic Molecules

Extension to polyatomic molecules, fingerprint region, Group frequencies, Interpretation IR spectra: IR region, molecular vibrations, the molecule spring analogy, Hookes law. Bond stretching frequencies effect of increasing atomic weight and bond energy, IR active and inactive frequencies, obtaining IR spectra, FTIR, Region of IR spectra, Compound comparison, and a general survey of different regions for detection of different functional groups. Factors influencing vibrational frequencies: Symmetry Conjugation lowering C=O and C=C frequencies, electronic effects

(inductive and mesmeric effects) Hydrogen bonding, Ring strain, Fermi resonance and coupled vibrations Interpretation of spectra of some classes of compounds.

Unit 6: Raman spectroscopy

Mechanism of Raman excitations, Stokes and anti-Stokes lines, Polari ability ellipsoids, Rotational and Vibrational Raman spectroscopy, Selection rules, Polarization of Raman lines, Rule of mutual exclusion.

Block 3: Molecular Spectroscopy-II

Unit 7: Electronic Spectroscopy : applications of UV-VIS Spectrometry

Diatomic molecules, Selection rules, Breakdown of selection rules. Franck-Condon principle. Coarse and Fine structure in electronic spectra of diatomic molecules. Dissociation energies. Transitions in simple polyatomic molecules, Photoelectron spectroscopy of diatomic (N2) and simple polyatomic molecules (H2O, formaldehyde). Adiabatic and vertical ionization energies, Use of Free Electron Model. Qualitative aspects of solvent effects- viscosity, polarity, hydrogen bonding. Absorption of UV- vis; electromagnetic radiation, electronic transitions and energy level; Isolated chromospheres (C=C and C=O), Beer-Lambert law; Effect of conjugation on UV Spectra; Terminology of UV Spectroscopy; Selection rules (allowed and for forbidden transitions) Solvent and their effect on different transitions. Measurement of UV spectra General application of spectroscopy (extent of conjugation, comparison of different compounds with the same chromophore, study of strain, study of geometrical isomerism and steric effects, study of tautomerism, effect of S-cis and S-trans conformations, effect of alkyl substitution and exocyclic double bond, Woodward Fieser rules for conjugated dienes and enones, identification of aromatic systems, Trans annular conjugation. Influence of constituents ring size and strain on UV Spectra.

Book Suggested:

1. Practical NMR Spectroscopy, M. L. Martin. J. J. Deepish and G. J. Martin, Heyden.
2. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley.
3. Introduction to NMR spectroscopy, R. J. Abraham, J. Fisher and P. Loftus, Wiley.
4. Application of Spectroscopy of Organic Compounds, J. R. Dyer Prentice Hall.
5. Spectroscopic Methods in Organic Chemistry D. H. Williams, I. Fleming, Tata McGraw-Hill.
6. W. Kemp, Organic Spectroscopy, 3rd edition, Wiley, 1995.
7. Introduction to Spectroscopy: Donald L. Pavia, Thompson, 2009.
8. Modern NMR techniques for Chemistry Research, A. E. Derome, Pergamon.
9. Physical Methods in Chemistry, R. S. Drago, Saunders College.
10. Chemical Applications of Group Theory, F. A. Cotton.