CHEMISTRY
(Major)
(6th Semester)
Course No.:**CHM-DSC-352**
Spectroscopy
Theory and Applications
Contact Hours: 60; Credits: 04
Full Marks = 100[End Semester Exam (70) Internal Assessment (30)]
Pass Marks = 40 [End Semester Exam (28) Internal Assessment (12)]

Unit-1: Molecular Spectroscopy-I

Interaction of electromagnetic radiation with molecules and various types of spectra; Born Oppenheimer approximation.

Rotation spectroscopy: Rotational spectra of diatomic rigid rotator, Selection rules, intensities of spectral lines, determination of bond lengths of diatomic molecules, isotopic substitution,

Vibrational spectroscopy: Simple Harmonic Oscillator, computation of force constant, amplitude of diatomic molecular vibrations, anharmonicity, Morse potential energy curve, dissociation energies, fundamental frequencies, overtones, Selection rules, degrees of freedom for polyatomic molecules, modes of vibration, concept of group frequencies. Vibration-rotation spectroscopy: diatomic vibrating rotator, P, Q, R branches.

Unit-2: Molecular Spectroscopy-II

Raman Spectroscopy: Rayleigh scattering, Quantum theory of Raman Effect, Stoke and anti-stokes' lines, molecular polarizability, Qualitative treatment of Rotational Raman effect (linear molecule). Qualitative discussion on vibrational Raman spectra of H_2O & CO_2, mutual exclusion rule,

Electronic spectroscopy: Born-Oppenheimer approximation, Franc-Condon Principle, Beer-Lambert law and its application, electronic transitions, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation. Determination of composition of metal complexes using Job's method.

Unit 3: UV & IR Spectroscopy

UV Spectroscopy: Chromophores and Auxochromes; Application of Woodward Rules for calculation of λ-max for the following systems: α, β- unsaturated aldehydes, ketones, carboxylic acids and esters; Conjugated dienes: alicyclic, homoannular and heteroannular,

Extended conjugated systems (aldehydes, ketones and dienes); distinction between cis and trans isomers. Applications of UV for identification of simple organic molecules.
IR Spectroscopy: IR absorption positions of O, N and S containing functional groups; Fingerprint region and its significance; application in functional group analysis. Applications of IR for identification of alkanes, alkenes and simple alcohols (inter and intramolecular hydrogen bonding), aldehydes, ketones, carboxylic acids and their derivatives (effect of substitution on >C=O stretching absorptions).

Unit 4: NMR Spectroscopy
Basic principles of Proton Magnetic Resonance, shielding and deshielding of protons, TMS, chemical shift and factors influencing it; Spin – Spin coupling and coupling constant; Interpretation of NMR spectra of simple compounds (Ethyl bromide, toluene, o & p-nitrotoluene, anisole, ethyl alcohol, ethyl acetate, mesitylene, acids and carbonyl compounds). Applications of NMR for identification of simple organic molecules.

Unit 5: Mass Spectroscopy
Mass Spectroscopy: Basic principles, instrumentation, determination of m/e ratio, base peak, molecular ion, nitrogen rule, metastable ions, isotopic peak, daughter ions, Mc–Lafferty rearrangement, RDA, General rules for fragmentation pattern, fragmentation pattern of simple compounds of hydrocarbons, alcohols, amines, aldehyde, ketone, ether, acids, phenols, nitro compounds, alicyclic compounds.

Reference Books:

- Banwell, C. N. & McCash, E. M. Fundamentals of Molecular Spectroscopy 4th Ed. Tata McGraw-Hill: New Delhi (2006).
- B.K Sen , Quantum Chemistry including Spectroscopy 3rd edition, Kalyani Publishers.
- Kapoor K.L, Quantum Chemistry and Molecular spectroscopy vol-4, Laxmi Publications-New Delhi.
- Kemp William, Organic Spectroscopy, 3rd Edition, Palgrave Publisher, 1991.
- J Kalsi P. S., Spectroscopy of Organic Compounds, 5th Edition, New Age International Publishers, 2016.
- Sharma Y. R, Elementary Organic Spectroscopy, 5th Edition, S. Chand & Company, 2013.
- Jag Mohan, Organic Spectroscopy and Applications, Narosa Publishers, 2012.