III SEMESTER

ICH 501: SPECTROSCOPIC TECHNIQUES

Course Objectives:

1. To understand molecular spectroscopy techniques namely vibrational and Raman spectroscopy.
2. To learn the theory and application UV, IR, NMR and mass spectroscopy in structure determination of organic molecule.
3. To learn structure elucidation by solving composite spectral problems.

UNITI **14 hr**

Introduction to spectroscopic techniques, intensity of spectral lines, natural line width and line broadening. Rotational, vibrational and electronic energy levels and selection rules. **Microwave Spectroscopy:** The rotation and classification of molecules, rotation spectra of diatomic and polyatomic molecules. Rigid and non-rigid rotator models. Determination of bond lengths, isotope effect on rotation spectra. Stark effect, nuclear and electron spin interaction. Microwave Spectrometer.

Vibrational Spectroscopy: Vibration spectra of diatomic molecules - linear harmonic oscillator, vibrational energies, zero point energy, force constants & bond strengths; anharmonicity of molecular vibrations- Morse PE diagram, selection rules, fundamental, overtones and hot bands. Vibrations of polyatomic molecules- normal modes of vibrations & nature of molecular vibrations (Ex-CO_2 & H_2O). **Vibration-rotation spectra** of diatomic and polyatomic molecules, selection rules, PQR branches.

Raman spectroscopy: Introduction, theory and applications of Raman spectra, mutual exclusion principles and its applications.

UNIT II **14 hr**

Application of infrared spectroscopy in the structural study-identity by fingerprinting and identification of functional groups. Characteristic vibrational frequencies of common functional groups (alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines). Study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides and acids). Factors affecting band positions and intensities-hydrogen bonding, phase and solvent.

UV/Electronic Spectroscopy: Basic principles, Beer-Lambert law, molar absorptivity, energy levels, types of electronic transitions. Franck - Condon principles, ground and excited electronic states of diatomic molecules. Chromophores, auxochromes, electronic spectra of polyatomic molecules. Emission spectra, spectra of transition metal complexes, charge transfer spectra. Instrumentation and application. Factors affecting the positions of UV bands. Electronic transitions and empirical correlations of predicting λ_{max} of organic compounds. Woodward–Fieser rules. UV absorption of aromatic compounds - effect of substituents and solvent effects. Emperical rules to calculate $\lambda_{max.}$ Application of UV spectroscopy in the structural study of organic molecules.

UNIT III **14 hr**

Nuclear Magnetic Resonance Spectroscopy: Magnetic properties of nuclei, theory and measurement techniques, NMR spectrometer, solvents used, chemical shift and its measurements, factors affecting chemical shift. Integration of NMR signals, spin-spin coupling, coupling constant. Shielding and deshielding. Chemical shift assignment of major functional groups, Classification (AX, AMX, ABX), spin decoupling; effects of chemical exchange, fluxional molecules, Hindered rotation through NMR spectrum, Karplus relationships (Karplus curve), double resonance techniques, solvent effects and Nuclear Overhauser Effect.

NMR of nuclei other than proton: ^{13}C chemical shift & factors affecting it, Coupling constants. Decoupling-Noise decoupling & broad band decoupling. Off-resonance proton decoupling-some representative examples. 2D NMR techniques.

UNIT IV: 14 hr

Mass Spectrometry: Basic principles, interpretation of mass spectra, molecular ions, meta- stable ions and isotope ions, ion abundance. Fragmentation processes-representation of fragmentation, basic fragmentation types and rules. McLafferty rearrangement. Fragmentations (fragmentation of organic compounds with respect to their structure determination) associated with functional groups-alkanes, alkenes, cycloalkanes, aromatic hydrocarbons, halides, alcohols, phenols, ethers, aldehydes, ketones, carboxylic acids, esters, amides, acid chlorides, nitrocompounds and amines, retro Diels-Alder fragmentation and Nitrogen rule.

Composite problems involving the applications of UV, IR, ^{1}H and ^{13}C NMR and mass spectroscopic techniques.

Course Outcomes:

The course will make a student well versed in

- Molecular spectroscopy technique namely vibrational and Raman spectroscopy.
- Applications of UV, IR,NMR and mass spectroscopy in structure determination of organic molecule.
- Application of spectroscopy by solving composite problems.

References

1. Organic spectroscopy, William Kemp, 3rd Edn.,PALGRAVE, 1991.
2. Organic spectroscopy: Principles and applications, Jagmohan, 2nd Edn.,Narosa,2007.
3. I.L.Finar Organic Chemistry Vol I 6th edition ELBS Longman 1973
4. Fundamentals of Molecular Spectroscopy IV ed., C. N. Banwell & E. M. McCash Tata McGrraw- Hill Publishing Company Ltd.,1994.
5. Organic Analytical Chemistry Theory and Practice, Jag Mohan, Narosa Publishing House2003
6. Spectrophotometric Identification of Organic Compounds, R.M.Silverstein, F.X. Webster, 6th Ed., John Wiley &Sons,Inc, Newyork, 2004.