OC S 464: ORGANIC SPECTROSCOPY

Course Outcome

- Enable the students to understand the principle, theory, instrumentation and applications of UV/Electronic, IR, NMR (^{1}H, ^{13}C, ^{19}F, ^{31}P) and Mass spectroscopy.
- To solve the composite problems involving the applications of UV, IR, NMR (^{1}H &^{13}C) and Mass spectroscopic techniques.
- To develop the ability to analyse the spectrum and arrive at the correct structure of the compounds.
- Overall students can get confidence in solving spectroscopic problems.

UNIT-I **[12 hours]**

UV/Electronic Spectroscopy: Basic principles, chromophores, auxochromes, 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. Empirical rules to calculate $\lambda_{max.}$ Application of UV spectroscopy in the structural study of organic molecules.

IR Spectroscopy: Basic principles, Application of infrared spectroscopy in the structural study-identity by finger printing 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, anhydrides and acids). Factors affecting band positions and intensities such as effect of hydrogen bonding, phase and solvent on vibrational frequencies, overtones, combination bands and Fermi resonance.

UNIT-II Nuclear Magnetic Resonance Spectroscopy **[12 hours]**

Theory and principle, NMR spectrometer, FT NMR and its advantages. 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 (ABX, AMX, ABC, A_2B_2), spin decoupling, effects of chemical exchange, fluxional molecules, Hindered rotation through NMR spectrum, Karplus relationships (Karplus curve–variation of coupling constant with dihedral angle), double resonance techniques, NMR shift reagents, solvent effects and Nuclear Overhauser Effect. Applications of NMR spectroscopy in structure elucidation of simple organic and inorganic molecules. Use of NMR in Medical diagnostics.

NMR of nuclei other than proton: ^{13}C chemical shift & factors affecting it. Decoupling-Noise decoupling & Broad band decoupling. Off-resonance proton decoupling-some representative examples. Introduction to ^{19}F & ^{31}P NMR.

UNIT-III Mass Spectrometry **[12 hours]**

Basic principles, Instrumentation, interpretation of mass spectra, resolution, exact masses of nucleides, molecular ions, meta-stable ions and isotope ions. Fragmentation processes-representation of fragmentation, basic fragmentation types and rules. Factors influencing fragmentations and reaction pathways. McLafferty rearrangement. Fragmentations associated with functional groups- alkanes, alkenes, cycloalkanes, aromatic hydrocarbons, halides, alcohols, phenols, ethers, acetals, ketals, aldehydes, ketones, quinines, carboxylic acids, esters, amides, acid chlorides, nitro compounds and amines. Ion analysis, ion abundance, retro Diels-Alder fragmentation. Nitrogen rule. High resolution mass spectroscopy. Composite problems involving the applications of UV, IR, ^{1}H and ^{13}C NMR and mass spectroscopic techniques. Structural elucidation of organic molecules.

References

1. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Monnill, Wiley (1981).
2. Applications of Absorption Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall (1965).
3. Spectroscopy of Organic Compounds, 3rd edn., P. S. Kalsi, New Age, New Delhi (2000).
4. Spectroscopic Methods in Organic Chemistry, Williams and Fleming, TMH.
5. Introduction to Spectroscopy, D. L. Pavia, G. M. L. G. C. S. Kriz, 5th edn., Cengage Learning (2014).
6. Spectrometric Identification of Organic Compounds, 8th edn., R. M. Silverstein, F. X. Webster and D. J. Kiemle, Wiley (2014).
7. Organic Spectroscopy, 3rd edn., W. Kemp, Pagrave Publishers (1991).
8. Modern Spectroscopy, J. M. Hollas, 4th edn., John Wiley and sons (2004).
9. Organic Structures from Spectra, 5th edn., L. D. Field, S. Sternhell and J. R. Kalman, Wiley (2013).