

Applications of Spectroscopic Techniques (02 Credits)

Max. Marks: 50

Duration: 32 Contact hours

Continuous Internal Assessment: 10 Marks

End Semester: 40 Marks

Unit-I UV, IR and Nuclear Magnetic Resonance Spectroscopy

(16 Contact hours)

Recapitulation of UV, IR Spectroscopy, Woodward-Fieser rules, characteristic absorptions of various functional groups. Interpretation of IR Spectra.

Basic concepts, chemical shift values for various classes of compounds. Fourier Transform (FT) techniques and advantages, nuclear overhauser effect (NOE). Two bond, three bond and long range coupling. Second order spectra; A₂, AB, AX, AB₂, AX₂, A₂B₂. Proton exchange, deuterium exchange, peak broadening exchange.

C-13 NMR: Carbon 13-chemical shifts, proton coupled and decoupled spectra. Nuclear overhauser effect, off-resonance decoupling, overview of DEPT techniques. Introduction to two-dimensional spectroscopic methods, Cosy, HETCOR and NOESY techniques, combined structure problems.

Unit-II Mass Spectrometry:

(16 Contact hours)

Introduction, instrumentation, Ionization methods like EI, CI, SIMS, FAB, MALDI, ESI, MS/MS. Mass analyzers like magnetic sector mass analyzer, double focusing mass analyzer, quadrupole mass analyzer, time-of-flight mass analyzer. Determination of molecular formula, role of Isotopes, Nitrogen rule, metastable peak. Fragmentation pattern like Stevenson rule, initial ionization event, α -cleavage, inductive cleavage, two bond cleavage, retro-Diels-Alder cleavage, McLafferty rearrangements. Fragmentation pattern of alkanes, alkenes, alcohols, phenols, aldehydes, ketones, carboxylic acids, amines. Problems based on Mass Spectroscopy. Some specific examples from natural products like flavonoids, terpenes, steroids, alkaloids.

Books recommended

1. Spectroscopy of Organic Compounds; 6th edn.; P. S. Kalsi; New Age Publishers; 2006

2. Spectrometric identification of Organic Compounds; 5th edn.; R. M. Silverstein, G. C. Bassler and T. C. Morill; John Wiley; 1991
3. Introduction to NMR Spectroscopy; R. J. Abraham. J. Fisher and P. Loftus; Wiley; 1991
4. Applications of absorption spectroscopy of Organic Compounds, J. R. Dyer (Prentice Hall-1991)
5. Spectroscopic Methods in organic Chemistry; D. H. Williams, I. Fleming; Tata McGraw Hill; 1988
6. NMR Spectroscopy Explained; Neil Jacobsen, Wiley Interscience 2007
7. Understanding NMR Spectroscopy, James Keeler, John Wiley & Sons 2005
8. Spin Dynamics, Malcom H. Levitt, John Wiley & Sons 2008
9. Basic One and Two Dimensional NMR Spectroscopy, Horst Friebolin, Wiley-VCH-Germany 1998
10. Introduction to Spectroscopy, 5th Ed., Donald L. Pavia, Gary M. Lampman, George S. Kriz and James A. Vyvyan, Cengage Learning India Pvt. Ltd.