

MCYC204 Spectroscopic Identification of Molecules (3-1-0)

(4 credits)

Module I

(12 hours)

Introduction to spectroscopic techniques of structure elucidation. Electromagnetic radiation, energy and electromagnetic spectrum, units, absorption of energy by organic compounds, types of spectroscopic methods to organic structure elucidation.

IR – Spectroscopy – Basic principles, characteristic frequencies of common functional groups.

UV – Visible Spectroscopy: Basic principles, application of UV – Visible spectroscopy to organic structure elucidation, Woodward – Fisher rules.

Module II

(12 hours)

Nuclear Magnetic Resonance Spectroscopy: Application of ^1H and ^{13}C NMR spectroscopy including COSY, NOESY, NOE techniques in the structural determination of complex organic systems and NMR of common heteroatoms present in organic compounds (N, F, O, P, S and D). Applications in conformational analysis. Multinuclear NMR of various inorganic and organometallic compounds.

Electron Spin Resonance Spectroscopy: Analysis of ESR spectra of systems in liquid phase, radicals containing single set, multiple sets of protons, triplet ground states. Transition metal ions.

Double resonance techniques: ENDOR in liquid solution, ENDOR in powders and non-oriented solids. EPR of triplet states, zero field splitting, Kramer's rule, survey of EPR spectra of first row transition metal ion complexes.

Module III

(8 hours)

Mass spectroscopy: Experimental arrangements and presentation of spectra, molecular ions, appearance and ionization potential, fragmentation, ion reactions and their interpretation, effect of isotopes on the appearance of a mass spectrum, molecular weight determination, thermodynamic data. Application of mass spectroscopy to inorganic compounds.

Fragmentation and rearrangements (including McLafferty rearrangement) of different classes of organic molecules. Isotope effects and basics of HRMS, and its necessity in organic synthetic chemistry field.

Module IV

(8 hours)

Problem solving exercises involving UV, IR, NMR & MS data: Problems involving interpretation of spectral details of organic compounds.

Text Books:

1. Ebsworth, E. A. O. Structural Methods in Inorganic Chemistry Blackwell Scientific Publications (1991).
 2. Drago, R. S. Physical Methods in Chemistry W. B. Saunders Co.: U.K. (1977).
 3. Carrington, A. & McLachlan, A. D. Introduction to Magnetic Resonance Chapman & Hall: N.Y. (1983).
 4. Mabbs, F. E. & Machin, D. J. Magnetism and Transition Metal Complexes Chapman and Hall: U.K. (1973).
- R. M. Silverstein and F. X. Webster, Spectrometric identification of organic compounds., John Wiley and Sons.Inc., Sixth edition (1997).

Reference Books

- W. Kemp, Organic Spectroscopy, Third Edition, MacMillan (1994).
- Pavia, Lampman and Kriz, Introduction to Spectroscopy, 3rd Edn., Brooks/Cole Pubs. Co.
- D. H Williams and Ian Fleming, Spectroscopic methods in organic chemistry, Tata McGraw Hill, (1998).
- William Kemp, Introduction to multinuclear NMR.