

# In.M.Sc, Applied Chemistry (5 years)

## 8th Semester

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| FCYC-----803 | Spectroscopic identification of Molecules |  |  |
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### 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  $^1\text{H}$  and  $^{13}\text{C}$  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 Mc-Lafferty 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).

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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**

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