

**Approval: 9<sup>th</sup> Senate Meeting**

**Course Name:** Organic Inorganic Spectroscopy

**Course Number:** CY 553

**Credits:** 3-0-0-3

**Prerequisites:** B.Sc in Sciences with Chemistry as main subject

**Intended for:** PG

**Distribution:** Elective for Master's in Chemistry

**Semester:** odd/even

***Preamble:***

Structural elucidation by spectroscopic techniques is one of the most significant aspects of synthetic chemistry. The course enables the students to learn the structural elucidation techniques for both organic and inorganic systems.

***Course Outline:***

Fundamentals of organic spectroscopy are a part of curriculum of Bachelor's degree in sciences with chemistry as a subject. This curriculum ensures the recapitulation of fundamentals of organic spectroscopy (UV IR, NMR and mass spectroscopy). The main focus of organic spectroscopy part will be on structural elucidation problems with joint application of UV, IR, NMR and mass spectroscopy. The inorganic spectroscopy includes fundamentals and application of Nuclear Quadrupole Resonance, Mossbauer Spectroscopy and Electron Paramagnetic Resonance Spectroscopy. In addition Circular Dichroism is also included.

***Modules:***

**Module 1-Recapitulation of UV, IR, NMR and Mass spectroscopy (In this module the elaborated syllabus has been included for a better idea of the topics to be covered)**

**UV includes:** Color and light absorption, the chromophore concept. Theory of electronic spectroscopy, orbitals involved and electronic transitions, effect of solvent and conjugation on  $\lambda_{\max}$ . Woodward Fieser rules e.t.c.

**IR –includes:** Molecular vibrations and modes of vibrations. Factors influencing vibrational frequencies vibrational coupling, hydrogen bonding, conjugation, inductive, mesomeric (resonance), field effects and bond angles, application to identify functional groups.

**NMR –includes:** Nuclear spins resonance, chemical shift and its measurement. Relaxation processes, factors influencing chemical shift. Shielding, deshielding and anisotropic effects. Effect of restricted rotation, concentration temperature and hydrogen bonding. Spin coupling (simple and complex), mechanism of coupling.

**Mass includes:** Introduction, Mass spectrum and Metastable ion peak, Determination of molecular formula and recognition of molecular ion peak and the Nitrogen rule, Molecular formula and index of

Hydrogen deficiency, General rules of fragmentation and the McLafferty rearrangement, Fragmentations associated with functional groups.

**Structure elucidation** of organic compounds by joint applications of IR, NMR and Mass spectroscopy.  
(12 lectures)

**Module 2: Circular Dichroism (This is a new module introduced on the suggestions of reviewers)**

Theory of polarized light, optical activity and optically active molecules, Cotton effects, CD, Octet Rule, Experimental Techniques, Applications. (6 lectures)

**Module 3-Nuclear Quadrupole Resonance Spectroscopy**

Introduction, energies of quadrupole transitions, effect of magnetic field on the spectra, relationship between electric field gradient and molecular structure, applications, interpretations of structural information from NQR spectra. (7 lectures)

**Module 4: Mossbauer Spectroscopy**

The Mossbauer effect, the Mossbauer active nuclei.. The chemical isomer shift. The quadrupole splitting, magnetic hyperfine interactions. Mossbauer spectroscopy applied to study nature of chemical bond, structural determination and analytical applications. (8 lectures)

**Module 5:Electron Paramagnetic Resonance Spectroscopy**

Introduction, Principles, Presentation of the spectrum, hyperfine splitting in isotropic systems involving more than one nucleus, Contributions to the hyperfine coupling constant in isotropic systems. Anisotropic Effects: Anisotropy in the g value, EPR of triplet states, nuclear quadrupole interaction, line widths, EPR applications. (9 lectures)

**Books Recommended**

1. NMR, NQR, EPR and MOSSBAUER SPECTROSCOPY IN INORGANIC CHEMISTRY by R. V. PARISH, *Publishers: ELIS HORWOOD LIMITED.*
2. Spectrometric Identification of Organic Compound, Robert M. Silverstein, Francis X. Webster, David J. Kiemle, David L. Bryce *Publishers John Wiley and Sons.*
3. Organic Spectroscopy by William Kemp, *Publishers: Macmillan*
4. Physical Methods in Inorganic Chemistry by Russell S. Drago, *Publishers Van Nostrand Reinhold.*
5. Fundamentals of Analytical Chemistry by Skoog, West and Holler, *Publishers: Saunders's College publishing.*
6. Organic structures from Spectra by Field, Sternhell & Kalman, *Publishers: John Wiley and Sons.*