St. Xavier's College (Autonomous), Ahmedabad-09

Syllabus of Semester – V of the following departments under Faculty of Science based on Under Graduate Curriculum Framework - 2023 to be implemented from the Academic Year 2025-26.

FACULTY OF SCIENCE

DEPARTMENT OF CHEMISTRY

BSc. (Hons.) Chemistry
Category – V

Discipline specific Minor Course –Spectroscopic techniques

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course Title & Code	Credit Distribution of The Course			Eligibility Criteria	Pre-requisite(s) of the Course (if any)
	Lecture	Tutorial	Practical / Practice		
CHMN551C: Spectroscopic techniques	3	0	1	10 + 2 from a recognized board in any stream	Foundation of organic chemistry-functional groups, symmetry of molecules

LEARNING OBJECTIVES (LO)	
LO-1	To learn fundamentals of ultraviolet spectroscopy and problems on UV Spectroscopy. To identify and quantify substances in solution, understand the principles of UV-Vis spectroscopy, choice of solvent and effects on wavelength.
LO-2	To understand its principles, identify functional groups in molecules based on IR spectra, and interpret the information gained to understand molecular structure and composition.
LO-3	To understand its theoretical foundations, relate NMR parameters to molecular structure, and apply NMR techniques for structural elucidation and analysis of molecules, including preparing samples, choosing experiments, and interpreting results.
LO-4	to interpret NMR spectra, correlate spectral data with molecular structure, and identify functional groups and chemical environments within molecules, to analyze the number of peaks, their chemical shifts (δ), and splitting patterns (singlet, doublet, triplet, etc.)

	to understand the structure of a molecule.
COURSE OUTCOMES (CO)	
On Completion of this course, the student will be able to	
CO-1	They should understand how to use Beer's Law to determine the concentration of a substance based on its absorbance, Students should know how to prepare samples for UV-Vis analysis, including choosing appropriate solvents and concentrations, Students should be aware of the various applications of UV-Vis spectroscopy, such as in chemical analysis, pharmaceutical analysis
CO-2	They'll learn to identify common functional groups (e.g., C=O, C-H, O-H) based on their characteristic absorption frequencies in IR spectra. They will understand how IR spectroscopy can be used for quantitative analysis, determining the concentration of specific molecules in a sample
CO-3	Students will be able to analyze NMR data, draw conclusions about molecular structure, and report their findings in a scientific manner.
CO-4	Students will be able to use UV IR and NMR spectra to deduce structural information about unknown organic molecules, Students should be able to analyze spectra using software and interpret them.

Unit-1 ULTRAVIOLET-VISIBLE SPECTROSCOPY (15L)

A Ultraviolet Spectroscopy

Origin of UV Spectra, Principle, Electronic transition (σ-σ*, n-σ*, π-π* and n-π*), relative positions of λ max considering conjugative effect, steric effect, solvent effect, red shift,

(bathochromic shift), blue shift (hypsochromic shift), hyperchromic effect, hypochromic effect (typical examples). Aromatic and Polynuclear aromatic hydrocarbons.

B Visible Spectroscopy

Introduction, Beer Lambert's law, instrumentation (light source, optical system, wavelength selector, light sensitive device), Accuracy and error of Spectrophotometry,

Problems of Dienes and enones using Woodward-Fieser rules.Problems of aromatic ketones, aldehydes and esters using empirical rules

Unit-2 INFRARED SPECTROSCOPY (15L)

Introduction, principle of IR spectroscopy, instrumentation, sampling technique, selection rules, types of bonds, absorption of common functional groups. Factors affecting frequencies, applications. Application of Hooke's law, characteristic stretching frequencies of O-H, N-H, C-H, C-D, C=C, C=N, C=O functions; factors affecting stretching frequencies (H-bonding, mass effect, electronic factors, bond multiplicity, ring size), Simple problems on infrared spectroscopy.

Unit-3 NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY (15L)

Principle, Magnetic and nonmagnetic nuclei, absorption of radio frequency. Equivalent and nonequivalent protons, Shielding and de-shielding effect, chemical shifts, anisotropic effect, relative strength of signals, spin-spin coupling, long range coupling, coupling constant, Deuterium labelling, applications to simple structural problems.

Unit-4 STRUCTURAL ELUCIDATION

Structural elucidation of Organic Compounds based on combined data UV, IR, and PMR

Suggestive Reading:

1. Introduction to Spectroscopy: Donald L. Pavia, Gary M. Lampman, George S. Kriz Cengage Learning; 4th Edition
2. Spectrometric Identification of Organic Compounds: Robert M. Silverstein, Francis X. Webster, David Kiemle Wiley; 7th Edition.
3. Infrared spectra of Complex molecules: J. Bellamy, John Wiley & Sons, Inc., 3rd Edition
4. Spectroscopic Method in Organic Chemistry: Dudley Williams, Ian Fleming McGraw-Hill Education; 6th Edition
5. Applications of spectroscopic techniques in Organic Chemistry: P.S. Kalsi, New Age International; 6th Edition
6. Elementary Organic Spectroscopy; Principles And Chemical Applications: Y. R. Sharma, S. Chand & Co Pvt Ltd
7. Fundamentals of Molecular Spectroscopy: C. M. Banwell and E. McCash, Tata McGraw Hill, 4th Edition
8. Modern Raman Spectroscopy: A Practical Approach; Ewen Smith, Geoffrey Dent., Wiley; 1st Edition