Course Code	Course Name	Credits
26CH513	ORGANIC SPECTROSCOPY	04

Course Objectives

- To develop a strong understanding of the fundamental principles, instrumentation, and theoretical aspects of modern spectroscopic techniques including UV–Visible, FT-IR, NMR, and Mass Spectroscopy.
- To enable students to interpret spectral data for structural elucidation and stereochemical assignments of organic compounds using various spectroscopic methods.
- To build problem-solving skills in the analysis of combined spectral data for the identification and characterization of organic molecules.

Learning Outcomes

Upon successful completion of this course, it is intended that a student will be able to:

- Understand the principles, instrumentation, and applications of UV–Visible and IR spectroscopy.
- Apply NMR techniques (^{1}H, ^{13}C, and 2D NMR) to analyze molecular structure and chemical environment.
- Analyze mass spectra to determine molecular weight, formula, and fragmentation patterns of compounds.
- Interpret combined spectroscopic data (UV, IR, NMR, MS) for structural elucidation of organic molecules.

Unit 1 - Electromagnetic radiation- UV-visible Spectroscopy (12 Hrs.)

Basic principles; absorption laws; instrumentation; theories of electronic spectroscopy; types of transitions; chromophore; auxochrome; absorption and intensity shifts; types of absorption bands; Woodward–Fieser rules for conjugated dienes, enones, and benzoyl derivatives; electronic transitions for charge transfer complexes; study of keto–enol tautomerism; applications of UV–Visible spectroscopy; octant rule; application of ORD and CD to stereochemical assignments.

Unit 2 – FT-IR spectroscopy (10 Hrs.)

Introduction; principle; instrumentation; sampling techniques; molecular vibrations; number of fundamental vibrations; selection rules; types of vibrations; interpretation of IR spectra for characterization of functional groups; factors influencing vibrational frequencies; fingerprint region; applications of infrared spectroscopy.

Unit 3 - 1H NMR Spectroscopy (14 Hrs.)

Introduction; theory of ^{1}H NMR spectroscopy; number of signals; chemical shift; integral value; spin–spin splitting; introduction to complex ^{1}H NMR spectra; shielding and deshielding; factors influencing chemical shift values; coupling constant.

^{13}C nucleus; proton-coupled ^{13}C spectra; spin–spin splitting of ^{13}C signals; proton-decoupled ^{13}C spectra; ^{13}C chemical shift; sample spectra and equivalent carbons; nuclear Overhauser effect (NOE); DEPT spectra; 2D NMR techniques including ^{1}H–^{1}H COSY and ^{1}H–^{13}C COSY spectra.

Unit 4 – Mass spectroscopy (10 Hrs.)

Basic principles; theory; instrumentation; ionization methods including Electron Ionization (EI), Chemical Ionization (CI), desorption ionization techniques (SIMS, FAB, MALDI), and Electrospray Ionization (ESI); mass analyzer; determination of molecular formula and molecular weight; nitrogen rule; structural analysis and fragmentation patterns of organic functional groups; Stevenson's rule; McLafferty rearrangement; other cleavage types; strategic approach to analysis of mass spectra and problem solving.

Unit 5 - Structural Elucidation using Spectroscopy (14 Hrs.)

Problem solving exercises involving UV, IR NMR & MS data

Reference Books:

1. Jag Mohan, Spectroscopy of Organic compounds, 2003, Narosa Publications, New Delhi.
2. Pavia, Lampman and Kriz, Introduction to Spectroscopy, 3rd Edn., 2009, Brooks/Cole Pubs. Co.
3. William Kemp, Organic Spectroscopy, 3rd Edn., 1994, MacMillon.
4. D.H Williams and Ian Fleming, Spectroscopic methods in organic chemistry, 1998, Tata McGraw Hill.
5. R.M. Silverstein and F. X. Webster, Spectrometric identification of organic compounds, 6th Edn., 1997, John Wiley and Sons.
6. Y.R. Sharma, Elementary Organic spectroscopy principles and chemical applications, 2013, S. Chand and Company Pvt. Ltd, New Delhi.
7. P.S. Kalsi, Spectroscopy of Organic compounds, 2005, New Age International Pvt. Ltd. New Delhi.

Websites and eLearning Sources:

1. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=13G8VouhmrFfuhs6rkiyTA==
2. https://www.pci.tu-bs.de/aggericke/PC4e_osv/Molecular-Spectroscopy.pdf
3. https://www.youtube.com/watch?v=VXvtkwubQQg
4. https://link.springer.com/chapter/10.1007/978-94-011-0727-3_1

COs and Bloom's Taxonomy Mapping – 26CH513		
Course Outcomes	**On completing U.G. program the students will be able to**	**BTL**
CO1	Recall and explain the fundamental principles, terminology and mechanisms associated with various spectroscopic techniques.	K1, K2
CO2	Apply spectroscopic techniques to determine the structure of simple organic compounds by interpreting their spectra.	K3
CO3	Analyze complex spectral data from multiple spectroscopic methods to elucidate the structure of unknown organic compounds.	K4
CO4	Critically evaluate the accuracy and reliability of spectroscopic data and the conclusions drawn from them in scientific literature.	K5
CO5	Design a systematic approach to solve problems using an integrated combination of spectroscopic techniques.	K6

BTL K1 and K2 – remembering and understanding, K3- Applying, K4 – Analyse, K5- Evaluate and K6- Create

Relationship Matrix – 26CH513												
Course Outcomes	**Programme Outcomes (POs)**						**Programme Specific Outcomes (PSOs)**					**Mean Score of Cos**
	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PSO1**	**PSO2**	**PSO3**	**PSO4**	**PSO5**	
CO1	3	3	3	1	1	3	3	2	3	3	3	2.3
CO2	3	3	3	1	1	3	3	3	3	3	3	2.4
CO3	3	3	3	1	1	2	3	3	3	3	3	2.3
CO4	3	3	3	1	1	3	3	2	3	3	3	2.3
CO5	3	3	3	1	1	3	3	3	3	3	3	2.4
											Total	2.34

Mean Score: 3- High, 2- Medium/Moderate, 1-Low