Name of the Programme: M. Sc -I (Organic Chemistry)

Course Code: CHO-501 **Title of the course:** Organic Spectroscopy

Number of Credits: 04

Effective from AY: 2022-23

Prerequisites for the course:	Students should have studied Organic chemistry courses at M.Sc. Chemistry in semester I	
Course Objective:	1. To study various theoretical concepts related to organic spectroscopic techniques. 2. To understand the introductory aspects of commonly used 2D NMR techniques. 3. To learn interpretational aspects of spectral data pertaining to UV, IR, PMR, CMR and MS.	
Content	**1. UV-Visible Spectroscopy** a. Introduction. Electronic transition and energy levels, the absorption laws. b. Measurement of the spectrum, chromophores, Effect of solvent, Conjugation on UV-spectra. c. Study of Tautomerism, Steric effect and geometrical isomerism in UV spectra. d. Woodward-Fieser rule for conjugated dienes and carbonyl compounds.	No of hours 04
	2. **Infrared Spectroscopy** a. IR spectroscopy in structural elucidation of organic compounds (various functional classes to be considered). b. Methods in IR-Spectroscopy, effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination and Fermi resonance bands. c. Factors influencing vibrational frequencies. d. Characteristic frequencies of organic molecules. e. Interpretation of spectra.	08
	3. **NMR Spectroscopy** a. Principles of NMR. b. Instrumentation. c. Chemical shift- (revision of the basic concepts) d. Interpretation of PMR spectra. i.Coupling constants and AB, A_2B_2/A_2X_2, AMX and ABX spin systems. ii. Double resonance and decoupling iii. Nuclear Overhauser Effect and its applications. iv. NMR Shift reagents v. Determination of Absolute and Relative configuration	14
	4. ^{13}C –NMR spectroscopy	8

	a. Introductionto ^{13}C –NMR spectroscopy. b. ^{13}C- chemical shifts effects (α-, ß-, γ-, δ-substituent effects, π-conjugation, heavy atom effect and ring size effects) c. Proton coupled and proton decoupled 13Cspectra. d. Off- resonance decoupling, APT & DEPT techniques.	
	5. ^{19}F- NMR and ^{31}P- NMR spectroscopy Principles and applications; heteronuclear coupling of carbon to ^{19}F and ^{31}P.	6
	6. Two-dimensional NMR spectroscopy Introduction to 2D NMR techniques and interpretation ofspectra of simple organic compounds using following 2d-NMR techniques-COSY, NOESY, HSQC, HMQC, HMBC, TOCSY and INADEQUATE	8
	7. Mass spectrometry a. Ionization Methods, Mass Analysis, Even and odd electron ions and fragmentation modes. b. Molecular Formulae Index (D.B.E), Molecular ion peak, base peak, metastable ions, Nitrogen rule, effect of isotopes. c.Prediction of molecular formulae based on relative abundance. Rules for fragmentation, McLafferty rearrangement, retro-Diels-Alder fragmentation, fragmentation associated with functional groups; rearrangement and mass spectra of some chemical classes. **Note: Problems involving combined use of different type of spectra, in line with course objective/ Course outcomes are to be emphasized.**	12
Pedagogy	Mainly lectures and tutorials. Seminars/term papers/assignments/presentations/self-study or a combination of some of these can be used. ICT mode should be preferred. Sessions should be interactive to enable peer group learning.	
References / Readings	1. P.S. Kalsi, Spectroscopy of Organic compounds, New Age International Pub. Ltd. & Wiley Eastern Ltd., 2nd Ed., 1995. 2. R.M. Silverstein, F. X. Webster, D.Kiemle, D. Bryce, S.Samant, V. S. Nadkarni,Spectrometric Identification of Organic compounds, An Indian Adaptation John Wiley & Sons Inc., 8th Ed., 2022. 3. D. L. Pavia, G. M. Lampman, G. S. Kriz, J. R. Vyvyan, Introduction to Spectroscopy, Brooks Cole, 5th Ed., 2015. 4. R.M. Silverstein, F. X. Webster, Spectrometric Identification of Organic compounds, John Wiley & Sons Inc., 7th Ed. (reprint), 2011. 5. V.M. Parikh, Absorption Spectroscopy of Organic Molecules, Addison Wesley Longman Publishing Co., 1974. 6. D.H Williams & I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata Mcgraw Hill Education, 6th Ed., 2011. 7. W. Kemp, Organic Spectroscopy, Palgrave Macmillan, 3rd Ed., 1991.	

	8. W. Kemp, NMR in Chemistry: A Multinuclear Introduction, Macmillan, 1986. 9. J. R. Dyer, Applications of Absorption Spectroscopy of Organic compounds, Prentice Hall of India, 1987. 10. L. D. Field, H. L. Li., A. M. Magill, Organic Structures from 2D NMR Spectra, Wiley, 2015.
Course outcomes:	1. Students will be in a position to understand how spectral techniques can be used in structure elucidation. 2. Students will be able to deduce structures of simple to moderately complex molecules by combining the spectral data obtained using two or more spectral techniques. 3. Students will be in a position to apply various concepts in organic spectroscopy (PMR, CMR, MS and 2D NMR) and analyse/ predict PMR, CMR, MS and 2D NMR spectral data based on given structures of simple molecules. 4. Students will understand the fundamental difference between various spectroscopic techniques.