Programme: M. Sc. (Chemistry, Part-II)
Course Code: OCC-501
Title of the Course: Organic Spectroscopy
Number of Credits: 3 **Effective from AY:** 2019-20

Prerequisites for the course:	Should have studied the spectroscopy topics at T Y B Sc (Chemistry) and M Sc part-I (Chemistry) levels.	
Course Objective:	1. Study of various theoretical concepts related to organic spectroscopic techniques. 2. Introduction of commonly used 2D NMR techniques. 3. Learning interpretational aspects of spectral data pertaining to IR, PMR, CMR and MS.	
Course Outcome	1. Students should be in a position to deduce structures of simple to moderately complex molecules by combining the spectral data obtained using two or more spectral techniques. 2. Students should be in a position to apply various concepts in organic spectroscopy (PMR, CMR, MS and 2D NMR) and generate/ predict PMR, CMR, MS and 2D NMR spectral data based on given structures of simple molecules.	
Content:	**1. Electronic and Infrared Spectroscopy:** Theory of electronic and IR spectroscopy (revision of the basic concepts/solving problems). Application of electronic and IR spectroscopy in structural elucidation of organic compounds (various functional classes to be considered). **2. NMR Spectroscopy** Principles of NMR, instrumentation, chemical shift- (revision of the basic concepts); Interpretation of PMR spectra. a) Coupling constants and AB, A_2B_2/A_2X_2, AMX and ABX spin systems. b) Double resonance and decoupling c) Nuclear Overhauser Effect and its applications. d) NMR Shift reagents **3. ^{13}C –NMR spectroscopy:** Introduction, 13C- chemical shifts effects (α-, ß-, γ-, δ-substituent effects, π-conjugation, heavy atom effect and ring size effects), proton coupled and proton decoupled 13C-spectra. Off- resonance decoupling, APT & DEPT techniques. **4. ^{19}F- NMR and ^{31}P- NMR spectroscopy:** Principles and applications; heteronuclear coupling of carbon to ^{19}F and ^{31}P.	04 hours 07 hours 07 hours 04 hours

	5. Two-dimensional NMR spectroscopy: Introduction to 2D NMR techniques and interpretation of spectra of simple organic compounds using following 2d-NMR techniques- COSY, NOESY, HSQC, HMQC, HMBC, TOCSY and INADEQUATE **6. Mass spectrometry** Even and odd electron ions and fragmentation modes a) McLafferty rearrangement and retro-Diels-Alder fragmentation. b) Mass spectra of compounds like alcohols, amines, ethers carbonyl compounds, hydrocarbons, halogen compounds, nitro compounds and cyanides. Note: Problems involving combined use of different type of spectra, in line with course objective/ learning outcome are to be emphasized.	08 hours 06 hours
Pedagogy:	lectures/ tutorials/ seminars/ term papers/assignments/ presentations/ self-study/ Case Studies etc. or a combination of some of these. Sessions shall be interactive in nature to enable peer group learning.	
References/Readings	1. P.S. Kalsi, *Spectroscopy of Organic compounds*, New Age International Pub. Ltd. & Wiley Eastern Ltd., 1995, 2nd Ed. 2. J. R. Dyer, *Applications of Absorption Spectroscopy of Organic compounds*, Prentice Hall of India, 1987. 3. R.M. Silverstein, F. X. Webster, *Spectrometric Identification of Organic compounds*, John Wiley & Sons Inc., 2011, 7th Ed. (reprint). 4. V.M. Parikh, *Absorption Spectroscopy of Organic Molecules*, Addison Wesley Longman Publishing Co., 1974. 5. D.H Williams & I. Fleming, *Spectroscopic Methods in Organic Chemistry*, Tata Mcgraw Hill Education, 2011, 6th Ed. 6. William Kemp, *Organic Spectroscopy*, Palgrave Macmillan, 1991, 3rd Ed. 7. William Kemp, *NMR in Chemistry: A Multinuclear Introduction*, Macmillan, 1986. 8. Donald L. Pavia, Gary M. Lampman, George S. Kriz, James R. Vyvyan, *Introduction to Spectroscopy*, Brooks Cole, 2009, 4th Ed. 9. L. D. Field, H. L. Li & A. M. Magill, *Organic Structures from 2D NMR Spectra*, Wiley, 2015.	