Programme: M. Sc. Part-II (Analytical Chemistry)

Course Code: ACO-505
Title of the Course: Problems on combined 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:** basic concepts; Application of electronic and IR spectroscopy in structural elucidation of organic compounds **2. NMR Spectroscopy:** Theory of Nuclear magnetic resonance, quantum description of NMR, classical description of NMR, Types of NMR spectra, environmental effects of NMR Spectra, the chemical shift, Applications of proton NMR in qualitative and quantitative analysis (in general). **3. ^{13}C –NMR spectroscopy:** Introduction, proton coupled and proton decoupled ^{13}C- spectra. Off- resonance decoupling, APT & DEPT techniques; 13C chemical shifts – factors affecting the chemical shifts – Homonuclear (^{13}C -^{13}CJ) and heteronuclear (^{13}C – ^{1}H, ^{13}C – ^{2}HJ) couplings. **4. Two-dimensional NMR spectroscopy:** Introduction to 2D-NMR, Classification of 2D experiments- 2DJ resolved spectroscopy; interpretation of spectra of simple organic compounds using following 2D-NMR techniques-COSY, NOESY, HSQC, HMQC, HMBC, TOCSY and INADEQUATE **5. Identification of organic compounds** using combined spectral methods: UV, IR, PMR, CMR, 2D NMR, Mass *(Note: More emphasis shall be given for solving combined spectroscopic data for structural elucidation*)	04 hrs 05 hrs 06 hrs 07 hrs 14 hrs
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. D. L. Pavia, G. M. Lampman, G. S. Kriz, J. R. Vyvyan, *Introduction to Spectroscopy*, Brooks Cole, 2009, 4th Ed, 2. J. R. Dyer, *Applications of Absorption Spectroscopy of Organic compounds*, Prentice Hall of India, 1987 3. W. Kemp, *NMR in Chemistry: A Multinuclear Introduction*, Macmillan, 1986. 4. R.M. Silverstein, F. X. Webster, *Spectrometric Identification of Organic compounds*, John Wiley & Sons Inc., 2011, 7th Ed. 4. D.H Williams & I. Fleming, *Spectroscopic methods in organic chemistry*, Tata Mcgraw Hill Education, 2011, 6th Ed. 6. W. Kemp, *Organic spectroscopy*, Palgrave Macmillan, 1991, 3rd Ed. 7. P.S. Kalsi, *Spectroscopy of Organic compounds*, New Age International Pub. Ltd. & Wiley Eastern Ltd., 1995, 2nd Ed. 8. L. D. Field, H. L. Li, A. M. Magill, *Organic Structures from 2D NMR Spectra*, Wiley, 2015.	