SARDAR PATEL UNIVERSITY
Programme & Subject: M.Sc (Inorganic Chemistry)
Semester: IV
Syllabus with Effect from: June - 2013

Paper Code: PS04CINC01	**Total Credit: 4**
Title Of Paper: Spectroscopy - II	

Unit	Description in detail	Weightage (%)
I	**Infrared Spectroscopy:** Theory and principles, molecular vibrations and calculations of vibrational frequencies, characteristic group absorptions in hydrocarbons, aromatic compounds, alcohol and phenols, ethers, carbonyl compounds, amines, nitriles, nitro compounds, carboxylic acids and halide. **UV Spectroscopy:** Theory and principles of electronic transition and UV absorption, chromophores and auxochromes, Woodward-Fieser rules for dienes and enones, characteristic absorptions in alkenes and alkynes, alcohols, ethers, amines, carbonyl compounds. Effects of conjugation. Characteristic absorptions in aromatic compounds.	25%
II	**PMR Spectroscopy:** Proton resonance condition, aspects of PMR spectra – number of signals, chemical shifts, shielding and deshielding, diamagnetic anisotropy, factors affecting chemical shifts, peak area and integration, splitting of the signals – spin-spin coupling, coupling constants – vicinal, geminal, long range and virtual couplings, Pople notation and spin assignments, chemical shift equivalence and magnetic equivalence, first order and second order spectra, complex PMR spectra, simplification of the PMR spectra – high resolution spectra, use of shift reagents, spin-spin decoupling-double resonance, proton exchange, deuterium exchange, Nuclear Overhauser Effect. Use of PMR spectra in differentiation of stereoisomers.	25%
III	**13C-NMR Spectroscopy:** Difficulties and solution for recording 13C-NMR spectra, recording of 13C-NMR spectra – scale, solvents, solvent signals and their positions, multiplicity, 13C-1H coupling constant – proton coupled and decoupled 13C spectra, broad band decoupling, off resonance technique. Chemical shifts in 13C spectra – chemical shift calculation for alkanes, alkenes and alkynes, chemical shift calculation in internal and terminal substituted compounds, aromatic compounds. Use of 13C spectra in differentiating stereoisomers, Nuclear Overhauser Effect. 13C - DEPT spectra – differentiation in primary, secondary and tertiary carbons by DEPT – 45, DEPT – 90, DEPT – 135 spectra. **2D NMR Spectroscopy:** Theory and principles of 2D NMR spectroscopy, interpretation of 1H-1H COSY, 1H-13C HETCOR, HMQC, HMBC, INADEQUATE spectra.	25%
IV	**Mass Spectroscopy:** \Theory and principles of mass spectroscopy, Instrumentation, low and high resolution mass spectra, Ionization techniques – Electron Impact (EI) ionization, Chemical Ionization (CI), Field Desorption (FD), Fast Ion Bombardment (FAB), Electronspray Ionization (ESI) and Matrix Assisted Laser Desorption/Ionization (MALDI). Determination of molecular weight	25%

	and molecular formula, nitrogen rule, detection of molecular ion peak, metastable ion peak. Fragmentations – rules governing the fragmentations, McLafferty rearrangement. Interpretation of mass spectra of different class of 11 compounds – saturated and unsaturated hydrocarbons, aromatic hydrocarbons, alcohols, ethers, ketones, aldehydes, carboxylic acids, amines, amides, compounds containing halogens.	

Basic Text & Reference Books:-

- Spectroscopic Identification of Organic Compounds R. M. Silverstein and F. X. Webster, 6th edition (John Wiley & Sons).
- Introduction to Spectroscopy D. L. Pavia, G. M. Lampman and G. S. Kriz, 3rd edition (Thomson Brooks/Cole).
- Spectroscopic Methods in Organic Chemistry D. H. Williams and I. Fleming, 4th edition (Mcgraw – Hill Book Company).
- Organic Spectroscopy William Kemp, 3rd edition (Palgrave).
- Organic Spectroscopy – Principles and Applications Jag Mohan, 2nd edition (Narosa Publishing House).
- Spectroscopy of Organic Compounds P. S. Kalsi, 5th edition (New Age International Publishers).