Syllabus
M.Sc. (Chemistry) Programme
(SEMESTER – III)

Spectroscopy II
Programme Code- (MSCCH -21)
Course Code – (MSCCH -602)

Block I Spin Resonance Spectroscopy-I

Unit 1: ^{1}H NMR Spectroscopy-I

Introduction to NMR; isotope ratios, nuclear spin; chemical shifts, coupling constants and integration; Fourier transform technique. Chemical shifts, coupling constants and correlation with structure and stereochemistry. Long range coupling; magnetic and chemical shift equivalence; first and second order spectra; dynamic process; simplification of spectra by shift reagents and decoupling experiments; stereochemistry by NOE measurements.

Unit 2: ^{1}H NMR Spectroscopy-II

Nuclear Spin states and Larmor precession, spin-spin and spin-lattice relaxations Selection rules and relative intensities of lines Treatment of Chemical Shift and spin-spin coupling in AX, AMX and AB proton NMR, Multinuclei NMR with special reference to C-13 and relative abundances and intensities, Spin-decoupling methods, Origin of NMR chemical shift, and spin-spin coupling. Factors Affection Chemical Shifts, Chemical exchange, Pulsed FT-NMR- Time and Frequency Domain Spectra.

Unit 3: Carbon -13 NMR Spectroscopy:

General considerations, chemical shift (aliphatic, olefinic, alkyne and aromatic hetero aromatic and carbonyl carbon). Coupling constants.

Unit 4: 2D NMR Spectroscopy

Two dimensional NMR spectroscopy – principles; DEPT, APT, COSY, HETCOR, NOESY, INADEQUATE techniques for structure of small molecules.

Block II Spin Resonance Spectroscopy-II

Unit 5 Basic Priciples of ESR spectroscopy

Electron Spin and its Characteristics, Treatment of ESR of hydrogen atom with spin levels, g-value and hyperfine interaction in hydrogen atom and free radicals, Mechanism of proton splitting in organic molecules; McConnel Equation. Basic introduction to anisotropic g- and A-tensors from transition ions, Energy levels in many electron spin systems and zero-field splitting.

Unit 6 Basic Principles of Mossbauer spectroscopy

Mossbauer effect and Mossbauer Spectroscopy and Mossbauer energy levels with isomer shift, Qudrupole splitting and hyperfine interaction with special reference to Fe57, and Sn119.

Block III Mass Spectrometry

Unit 7 Mass Spectrometry-I

Introduction, ion production-EI, CI, FD and FAB, factors affecting fragmentation , ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule, example of Mass fragmentation of organic compounds with respect to their structure determination. Problems based on spectroscopic techniques.

Unit 8: Mass Spectrometry-II

Mass spectral fragmentation of organic compounds with common functional groups; molecular ion peak; metastable peaks, Mc Lafferty rearrangement; nitrogen rule. High resolution mass spectrometry – ESIMS and MALDI-TOF. Examples of mass spectral fragmentation of organic compounds.

Books Suggested:

1. Practical NMR Spectroscopy, M. L. Martin. J. J. Deepish and G. J. Martin, Heyden.
2. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C. Bassler and T. C. Morrill, John Wiley.
3. Introduction to NMR spectroscopy, R. J. Abraham, J. Fisher and P. Loftus, Wiley.
4. Application of Spectroscopy of Organic Compounds, J. R. Dyer Prentice Hall.
5. Spectroscopic Methods in Organic Chemistry D. H. Williams, I. Fleming, Tata McGraw-Hill.
6. W. Kemp, Organic Spectroscopy, 3rd edition, Wiley, 1995.
7. Introduction to Spectroscopy: Donald L. Pavia, Thompson, 2009.

8. Modern NMR techniques for Chemistry Research, A. E. Derome, Pergamon.
9. Physical Methods in Chemistry, R. S. Drago, Saunders College.
10. Chemical Applications of Group Theory, F. A. Cotton