Approval: 43rd BoA Meeting

Course Title	**: Organic Spectroscopy**
Course Number	**: CY 556**
Credits	**: 3-0-0-3**
Prerequisites	**:**
Intended for	**: MSc Chemistry and PhD (any discipline)**
Distribution	**: Elective Course**
Semester	**: Even / Odd**

Preamble:

The main objective of this course is to teach fundamental principles of various spectroscopic techniques used for structural elucidation of organic compounds. Along with the fundamental aspects, the focus will be given on problem solving which can help students from research perspective.

Modules:

1. UV Spectroscopy (4 Lectures)

Introduction, Principle of UV spectroscopy, Concept of chromophore, Solvent effect, Fluorescence and phosphorescence, Characteristic absorption of organic compounds, Woodward-Fieser rules for dienes and enones, Substituent effects, Model compound studies.

3. Infra-red (IR) Spectroscopy (4 Lectures)

Introduction, Molecular vibrations, factors influencing molecular frequencies, Infrared spectrometer, application of IR spectroscopy for identification of functional groups.

2. Mass Spectroscopy (4 Lectures)

Basic principle, Ionization methods, Determination of molecular weight and molecular formula, Molecular ion and its recognition, Fragmentation and rearrangements, Examples of organic compounds from different classes such as hydrocarbon, hydroxy compounds, ketones, aldehydes, carboxylic acids and esters, lactones, amines and amides, nitro compounds, nitriles and heteroaromatic compounds

4. ^{1}H NMR Spectroscopy (12 Lectures)

The NMR Phenomenon, Theory of nuclear magnetic resonance, Chemical shift and factors affecting chemical shift, integral and integration in proton NMR, Chemical equivalence and magnetic equivalence, First order and second order

spectra, Spin-spin coupling, Pascal's triangle, Coupling constant, Factors influencing coupling constant, A_2, AB, and AX spin systems, AMX, ABX and ABC spin system with three coupling constants, D_2O exchange, Shift reagents, Effect of chiral center, ^{19}F and ^{31}P NMR, Structure elucidation of organic compound using ^{1}H NMR.

4. ^{13}C NMR Spectroscopy and 2-D NMR spectroscopy (10 Lectures)

Introduction, Correlation chart for ^{13}C chemical shift, Proton-coupled ^{13}C spectra, Proton-decoupled ^{13}C spectra, carbon-deuterium coupling, NOE effects, Structural applications of ^{13}C NMR, Fundamentals and applications of DEPT technique in NMR spectroscopy, Application of 2-D NMR spectroscopic techniques such as ^{1}H-^{1}H COSY, ^{1}H-^{13}C COSY, HMBC and HSQC for structure determination of complex organic compounds.

5. Structural Elucidation of Organic Compounds (8 Lectures)

Interpretation of spectroscopic data of unknown compounds, Application of UV-Vis, MS, IR and NMR spectroscopic techniques for solving structure of organic molecules

Textbooks:

1. NMR Spectroscopy 2nd Edition, Harald Gunther, Wiley Publishers.

2. Modern NMR Spectroscopy: A workbook of Chemical Problems 2nd Edition, Jeremy K.M. Sanders, Edwin C. Constable, Brian K. Hunter and Clive M. Pearce Oxford University Press.

3. Organic Structure Determination, using 2-D NMR Spectroscopy, a problem-based approach, Jeffrey H. Simpson

References:

1. Structure Determination of Organic Compounds, Tables of Spectral Data, Erno Pretsch, Philippe Buhlmann, Martin Badertscher, Springer.

2. Spectrometric Identification of Organic Compounds, Robert M. Silverstein, Francis X. Webster, David Kiemle, John Wiley & Sons; 7th Edition edition.

3. Organic Spectroscopy 3rd Edition, William Kemp, Palgrave Publishers Ltd