BACHELORS WITH CHEMISTRY AS MAJOR

8th SEMESTER

CHM822J2 CHEMISTRY _ SPECTROSCOPY OF ORGANIC COMPOUNDS

CREDITS: THEORY-4, TUTORIALS-2

THEORY (4 CREDITS: 60 HOURS)

Course Objectives:

To familiarize the students with the organic structure determination methods involving spectroscopy.

Learning Outcomes:

The students will acquire knowledge of:

1. IR range for functional groups, λmax for polyenes and α, β-unsaturated carbonyl compounds which are helpful in structural elucidation of organic compounds.

2. Fragmentation pattern in Mass spectrometry and its application in structural elucidation.

3.Chemical shift values and their significance in NMR.

4. 2D NMR Techniques and applications.

5. Solving structural problems based on UV-Vis, IR, ^{1}HNMR, ^{13}CNMR and mass spectral data.

UNIT I: Infrared And Ultra Violet Spectroscopy (15 hours)

Principles of Ultra Violet Spectroscopy, Electronic transitions in organic molecules, Woodward-Fieser rules for calculation of λ_{max} of organic compounds. Applications of Ultra Violet Spectroscopy in structural elucidation of organic compounds.

Principles of Infrared spectroscopy, The Infrared spectrum, The functional group and fingerprint regions, Characteristic IR absorption bands, Intensity and position of absorption bands. Structural features that affect vibrational frequency. Application of IR spectroscopy in structural elucidation of organic compounds.

UNIT II: Mass Spectrometry (15 hours)

Introduction, Instrumentation, Determination of molecular formula, Role of Isotopes, Nitrogen Rule. Fragmentation pattern like Stevenson rule, initial ionization event, α-cleavage, inductive cleavage, two bond cleavage, Retro-Diels Alder cleavage, McLaffertey Rearrangements. Fragmentation pattern of alkanes, alkenes, alcohols, phenols, aldehydes, ketones, Carboxylic acids, Amines. Application of Mass Spectrometry in structural elucidation of organic compounds.

UNIT III: Proton NMR Spectroscopy (15 hours)

Basic concepts, Mechanism of Measurements, Chemical shift values for various classes of compounds. Fourier Transform (FT), Techniques and advantages. One bond coupling, two bond coupling, three bond coupling, second order spectra A_2, AB, AX, AB_2, ABX, AX_2, A_2B_2. Proton exchange, deuterium exchange, Peak broadening exchange. Nuclear overhouser effect (NOE).

Applications of ^{1}H NMR in structural elucidation of simple and complex compounds.

UNIT IV: Carbon 13 spectroscopy (15 hours)

Carbon 13-chemical shifts, proton coupled and decoupled spectra. Off-Resonance De-coupling. DEPT-45, DEPT-90, DEPT-135. NOE signal enhancement.

Applications of ^{13}CNMR in structural elucidation of simple and complex compounds.

Structure elucidation of organic compounds using combined (UV, IR, Mass and NMR) spectroscopic methods.

Books Recommended:

1. *Spectrometric Identification of Organic Compounds. 5th Ed., R. M. Silverstein, G. C. Bassler and T. C. Morill. (Jhon Wiley-1991).*
2. *Introduction to NMR Spectroscopy, R. J. Abraham. J. Fisher and P. Loftus (Wiley-1991)*
3. *Applications of absorption spectroscopy of Organic Compounds, J. R. Dyer (Prentice Hall-1991).*
4. *Spectroscopic Methods in organic Chemistry, D. H. Williams; I. Fleming (Tata- McGraw Hill, 1988).*
5. *Introduction to Spectroscopy. 5th Edition. Donald L. Pavia, Gary M. Lampman, George S. Kriz and James R. Vyvyan. 2015.*
1. *Advanced Organic Chemistry; Dr. Jagdamba Singh and LDS Yadav; Pragati edition,2017.*
2. *Principles of Physical Chemistry; B.R. Puri, L.R. Sharma and L.S. Pathania; 47th Edn., Vishal Pubs & Co, 2017.*
3. *Physical Chemistry; T. Engel, P. Reid, 3rd Edn., Pearson India, 2013.*

TUTORIALS (2 CREDITS: 60 HOURS)

1. Recording of IR, UV and NMR spectra wherever possible for simple molecules and their interpretation.
2. Elucidation of the structure of different types of compounds using UV, IR, Mass and NMR spectra (Spectra to be provided).
3. Videos showing working of UV, IR, Mass and NMR spectrometers.

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1. *Spectrometric Identification of Organic Compounds. 5th Ed., R. M. Silverstein, G. C. Bassler and T. C. Morill. (Jhon Wiley-1991).*
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