ACHARYA NAGARJUNA UNIVERSITY
DEPARTMENT OF CHEMISTRY

M.Sc. ORGANIC CHEMISTRY:: SEMESTER–IV

PAPER–I: ORGANIC SPECTROSCOPY-II (R22OC41)

(*For the students admitted from the A.Y. 2022-2023 onwards*)

Max. Marks: 100   **(Internal-30M & External-70M)**

SYLLABUS

Learning Objectives:

- ✓ To learn about the basics of ^{13}C NMR, Mass, and 2D NMR spectroscopic techniques.
- ✓ To understand the instrumentation of Mass, types of ionizations, types of analyzers in Mass spectroscopic techniques.
- ✓ To apply the spectroscopy knowledge for the structural elucidation of natural products and stereochemistry of organic compounds.
- ✓ To learn about the structural elucidation of natural products.
- ✓ To know the spectral problems – UV; ^1H, ^{13}C, Mass spectrometry.

UNIT-I   **12H**

^{13}C NMR Spectroscopy:

Types of 13C NMR spectra, Undecoupled, proton- decoupled, single frequency off-resonance decoupled (SFORD) and selectively decoupled spectra. Signal enhancement by Nuclear OVER HAUSER effect. ^{13}C chemical shifts, factors affecting the chemical shifts. Noise decoupled and off-resonance spectra of simple Compounds. Calculation of chemical shifts of alkanes, alkenes, alkynes, and aromatic compounds. Typical examples of CMR spectroscopy –problems.

UNIT-II   **12H**

Mass Spectroscopy:

Introduction, Principles of Ionization Methods: EI, CI, FDI, PDI, LDI, FAB, TSI and ESI, Types of mass analyzers; Types of fragments-odd electron and even electron containing neutral and charged species (even electron rule), nitrogen rule, molecular-ion peak, base peak, metastable ion, isotopic abundance. High Resolution-MS (HRMS), index of hydrogen deficiency (IHD). Fragmentation of typical organic compounds-hydrocarbons, aromatics, alcohols, alkyl halides, ethers, Carbonyls, carboxylic acids, esters, amines, amides, nitro compounds. General methods of mass spectral fragmentation-β-cleavage, Mclafferty rearrangement, retro Diels-Alder fragmentation and ortho effect. Factors affecting fragmentation-Mass spectra related problems.

UNIT-III   **12H**

2D NMR Techniques:

Principles of 2D NMR, classification of 2D-experiments, 2D-J-resolved spectroscopy. Correlation spectroscopy (COSY), HOMO COSY (^1H-^1H COSY), COSY of *m*-dinitrobenzene, isopentyl acetate, Hetero COSY (1H, ^{13}C COSY) Hetero COSY of isopentyl acetate and 4-methyl-2-pentanol, HMQC, HMQC of codeine, long range ^1H, ^{13}C COSY (HMBC), HMBC of codeine and NOESY, NOESY of 9-benzylanthracene, 2-D INADEQUATE experiments.

UNIT-IV   **12H**

Spectral Characteristics of Natural Products involving all Spectral Data: Use of spectroscopic methods UV, IR, ^{1}H and ^{13}C NMR and Mass spectra in the structure elucidation of natural products. Illustration with suitable compounds like Apigenin (Flavone), Kaempferol (flavonol), Umbelliferone (coumarin), Camphor (Terpenoid), Lawsone (Naphthoquinone), Papaverine (Alkaloid), and Equilenine (steroid).

UNIT-V   **12H**

Spectral Problems:

Applications of ^{13}C NMR spectroscopy: Stereochemistry, and reaction mechanisms.

Applications of ^{1}H NMR spectroscopy: Stereochemistry-Geometrical and optical isomerism.

Spectral Problems involving all spectral data UV-Vis. ^{1}H NMR, ^{13}C NMR, Mass spectrometry & 2D NMR techniques.

Reference Books:
1) Spectrometric identification of organic compounds by R.N.Silverstein & G.C.Bassier (John Willey)
2) Spectroscopic methods in Organic Chemistry by Williams and Fleming (McGraw Hill).
3) Organic photochemistry by R.O.Kan (Mc Graw Hill)
4) Advanced organic Chemistry Reaction Mechanisms and Structure by J March (Mc Graw Hill & Kogshusha).
5) Carbon-13 NMR Spectroscopy by J.B. Stothers.

Learning Outcomes:
- ✓ Students can understand the fundamentals of ^{13}C NMR and Mass spectroscopic techniques and apply to investigate the structural information of molecules.
- ✓ It can provide ability to apply the spectroscopy knowledge for the structural elucidation of natural products and stereochemistry of organic compounds.
- ✓ It also provides platform for awareness towards ^{13}C NMR and Mass Spectrometry which aims to apply these knowledge towards research.
- ✓ Students can understand the spectral characterstics of natural products involving all spectral data.
- ✓ Students can understand the spectral problems involving all spectral data UV-Vis. ^{1}H NMR, ^{13}C NMR, Mass spectrometry & 2D NMR techniques.

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