ST.JOSEPH'S COLLEGE FOR WOMEN (AUTONOMOUS), VISAKHAPATNAM

VII SEMESTER B.Sc. HONOURS CHEMISTRY Time: 4Hrs/Week

Code CH7202(3) Revised Syllabus Under CBCS 2020-21 Marks: 100

Spectroscopy of Organic Compounds

I.

Course Objective: To enable students to understand and apply the theoretical principles of different spectroscopic techniques in the determination of molecular structure

Course Outcomes: By the end of the course, the students will be able to:

- Gain insight into the basic fundamental principles of IR and UV-Vis spectroscopic techniques.
- Use basic theoretical principles underlying UV-visible and IR spectroscopy as a tool for functional group identification in organic molecules.
- Interpret of IR, UV-visible spectra and their applications.
- Interpret of NMR, Mass spectra and their applications.
- Interpret the spectra in identifying the organic compounds.

II. Syllabus

Unit-I 12 hours

UV Spectroscopy: a) Energy transitions – Simple chromophores – UV absorption of Alkenes – polyenes unsaturated cyclic systems – Carbonyl compounds, α, β-unsaturated carbonyl systems - Woodward Fisher rules – aromatic systems – solvent effects – geometrical isomerism – acidand base effects – typical examples –calculation of λmax values using Woodward - Fisher rules.

b) **ORD:** Theory of optical rotatory dispersion, α-Axial halo ketone rule and octant rule – Application of these rules in the determination of absolute configuration of cyclohexanones, decalones and cholestanones.

c) **Circular Dichroism:** Principle – positive and negative cotton effects –
Absolute configuration.

Unit-II 12 hours

Infrared Spectroscopy (FT-IR): Fundamental modes of vibrations – Stretchingand bending vibrations – overtones, combination bands and Fermi resonance, factors influencing vibrational frequencies, hydrogen bonding – fingerprint region and its importance – Study of

typical group frequencies for – CH, -OH, -NH, -CO-NH_2, -CC, -CHO, -CO and aromatic systems. Application in structural determination –Simple problems.

Unit-III **12 hours**

1H NMR spectroscopy:

a) Magnetic properties of Nuclei, Nuclear resonance, Fourier Transformation and its importance in NMR. Equivalent and non-equivalent protons, The chemical shift and it's importance, calculation of chemical shift, factors affecting the chemical shifts such as electronegativity and anisotropy, effect of deuteration, Signal integration, Spin-spin coupling: vicinal (Karplus relationships), germinal and long range. Coupling constants (*J*) and factors affecting coupling constants. –Shielding and deshielding mechanisms in acetylene carbonyl and Benzene, anisotropy –Spin-Spin Interactions related to first order and higher order spectra (AB, A_2; AB_2, ABX, ABC, AMX) –temperature dependence spectra, Hydrogen bonding. Nuclear Overhauser effect (NOE).

Unit-IV **12 hours**

Electron Spin Resonance Spectroscopy (**ESR**):

Basic Principles, Comparison of NMR & ESR. Determination of 'g' value, Factors affecting the 'g' value. Isotropic and Anisotropic constants. Splitting, hyperfine splitting coupling constants. Line width, Zero field splitting, and Kramer degeneracy. Crystal field splitting, Crystal field effects.

Applications: Detection of free radicals; ESR spectra of(a) Methyl radical (CH_3·), (b) Benzene anion (C_6H_6-).

UNIT-V

MASS SPECTROMETRY **12 hours**

Introduction, ion production, type of ionization, 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, Mac Lafferty rearrangement. Nitrogen rule, isotope labeling.High resolution mass spectrometry, Examples of mass spectral Fragmentation of organic compounds with respect to their structure determination.

III. Suggested Co-Curricular Activities

1. Training of students by related industrial experts.

2. Assignments, Seminars and Quiz (on related topics), collection of relevant videos and material.
3. Visits of abilities, firms, research organizations etc.
4. Invited lectures and presentations on related topics by field/industrial experts.

IV. Suggested Text Books:

1. Organic spectroscopy, W. Kemp 5th Ed, ELBS
2. Spectroscopy of organic compounds, RM Silversteen and others, 5th Ed, John Wiley
3. Spectroscopy of organic compounds, P.S. Kalsi, Wiley, 1993.

V. References:

1. NMR in chemistry-A multi nuclear introduction, William Kemp, McMillan, 1986.
2. Spectroscopic methods in Organic chemistry, DH Williams & I Flemmi.