



GAYATRI VIDYA PARISHAD
COLLEGE FOR DEGREE AND PG COURSES (AUTONOMOUS)
Affiliated to Andhra University || Accredited by NAAC and NBA
VISAKHAPATNAM

DEPARTMENT OF ORGANIC CHEMISTRY

M.Sc. (Final) CHEMISTRY
SEMESTER-IV SYLLABUS
PAPER II- ORGANIC SPECTROSCOPY AND PRINCIPLES OF
INSTRUMENTATION
(Effective from the admitted batch of 2022-2023)

Credits: 4		Theory: 4 Hours
Max Marks: 100	External: 80	Internal: 20

Course Outcomes (COs)/Course Specific Outcomes (CSOs):

- CO 1: Acquire the knowledge of ^{13}C NMR Spectroscopy
- CO 2: Understand ^{13}C and Heteronuclear, 2D NMR and Instrumentation, learn FT NMR spectroscopy, 2D-NMR, COSY and HETCOR and their applications in molecular structure determination
- CO 3: Develop interest in the areas, ORD and CD spectroscopy and structural determination of natural products by spectroscopy
- CO 4: Acquire interest in solving structures of organic molecules using 2D NMR, COSY, HETCOR, ORD and CD spectroscopy and structural determination of natural products by spectroscopy
- CO 5: know the various chromatographic separation techniques. Principle and instrumentation of GC, HPLC and XRD

Course learning outcome (LOs):

Upon completion of the course the students should be able to:

- LO 1: Explain theory and values of ^{13}C NMR Spectroscopy
- LO 2: Analyze and apply the concept of 2D NMR and Instrumentation, learn FT NMR spectroscopy, 2D-NMR, COSY and HETCOR in molecular structure determination
- LO 3: Apply the concept of ORD and CD spectroscopy and structural determination of natural products by spectroscopy
- LO 4: Interpret, Analyze and solve the structure of organic compounds using ^{13}C NMR, HNMR, 2D NMR, COSY and HETCOR.
- LO 5: Explain various chromatographic separation techniques. Principle and instrumentation of GC, HPLC and XRD

UNIT-I: ^{13}C NMR spectroscopy [12 Hours]

Introduction, ^{13}C -chemical shifts, factors affecting the chemical shifts, chemical shifts of organic compounds. Calculation of chemical shifts of alkanes, alkenes and aromatic compounds. Types of ^{13}C NMR spectra: Proton-coupled, proton-decoupled and OFF-resonance decoupled (ORD) spectra, DEPT. ^{13}C -NMR solvents:

UNIT-II: NMR Instrumentation, 2D-NMR techniques [12 Hours]

NMR Instrumentation: Types of NMR Spectrometers-Continuous Wave (CW)-NMR, Fourier Transform (FT)-NMR, NMR solvents, sample preparation.

2D-NMR techniques: Principles of 2D NMR, Correlation spectroscopy (COSY) HOMO COSY (^1H - ^1H COSY), Hetero COSY (^1H , ^{13}C COSY, HMQC), long range ^1H , ^{13}C COSY (HMBC), NOESY and 2D-INADEQUATE experiments and their applications.

UNIT-III: Optical Rotatory Dispersion (ORD) and CD Spectroscopy: [12 Hours]



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Optical rotation, circular birefringence, and circular dichroism and Cotton effect. Plain curves and anomalous curves. Empirical and semiempirical rules-The axial haloketone rule, the octant rule, Application of the rules to the study of absolute configuration and conformations of organic molecules.

UNIT-IV: Structure Determination of Natural Products by Spectral Methods

[12 Hours]

Structure elucidation - Spectroscopic techniques IR, UV, ^1H -NMR, ^{13}C -NMR, COSY, HETEROCOSY, and MS- natural products - Examples, flavones - Apigenin, flavanones-Hesperetin, isoflavones - Genistein, coumarins-7-hydroxycoumarin, alkaloids - morphine, quinine, terpenoids - (-)-Menthol, Steroids - stigmasterol, Glycosides - salicin (Alcoholic β -glucoside)

UNIT-V: Heteronuclear NMR spectroscopy and Principles of Instrumentation techniques

[12 Hours]

Heteronuclear couplings: ^{13}C - ^1H , ^{13}C -D, ^{13}C - ^{19}F , ^{13}C - ^{31}P , ^1H -D, ^1H - ^{19}F , ^1H - ^{31}P ,
Instrumentation - Gas Chromatography - High Performance Liquid Chromatography - X - Ray Diffraction (XRD).

Text books:

1. Spectroscopy, fourth edition, D. L Pavia, G. M Lampman CENGAGE Learning, 2012
2. Spectroscopic Methods in Organic Chemistry. Fourth Edition D.M. Williams and I. Fleming Tata - McGraw Hill, New Delhi, 1990. For all spectral methods except ORD and CD and ESR.
3. Organic Spectroscopy, Second Edition, W.Kemp, ELBS Macmillan, 1987 for ORD and CD and ESR.
4. Chemistry of natural products, S. V. Bhat, Narosa Publishing House, 6th reprint 2010
(For IVth unit)
5. Applications of absorption spectroscopy of Organic Compounds J.R.Dyer, Prentice Hall of India, New Delhi, 1984.
6. Spectrometric identification of Organic Compounds, Fourth Edition, R.M. Silverstein: G.C.Vassillir and T.C. Merill, John Wiley, Singapore, 1981.
7. For ORD and CD "Applications of Optical rotation and Circular Dichroism", G.C. Barret, in "Elucidation of Organic structures by Physical and Chemical Methods" Part I (Eds)
8. K.W. Bentley and G.W.Kirty John Wiley, 1972, Chapter VIII (only those aspects mentioned in the syllabus).

Purna den
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