IV SEMESTER

PARVATHANENI BRAHMAYYA
SIDDHARTHA COLLEGE OF ARTS & SCIENCE
Autonomous
Siddhartha Nagar, Vijayawada–520010
Re-accredited at 'A+' by the NAAC

22CH4T1: ADVANCED ORGANIC SPECTROSCOPY

Course Code	22CH4T1	I A Marks	30
No. of Lecture Hours / Week	4	End Exam Marks	70
Total Number of Lecture Hours	60	Total Marks	100
Seminar	-	Exam Hours	03

Course: Advanced Organic Spectroscopy **(code CH4T1)**		
S.No	COURSE OUTCOMES	PO`s
	The student will be able to	
1	Memorize the basic concepts of advanced organic spectroscopy	2,7
2	Sumarize the principle, theory and advanced aspects of ^{1}HNMR, ^{13}C NMR, 2D NMR, ORD & CD spectroscopic techniques.	1,2,7
3	Display the knowledge gained in the areas of ^{1}HNMR, ^{13}C NMR, 2D NMR, ORD & CD spectroscopic techniques in chosen job role.	1, 6
4	Interpret the spectral data of ^{1}HNMR, ^{13}C NMR, 2D NMR, ORD & CD in elucidating the structure of the molecule.	1, 7
5	Assess that how far the spectral data of ^{1}HNMR, ^{13}C NMR, 2D NMR, ORD &CD are useful in establishing the structure of the molecule.	1, 7

CO-PO MATRIX								
COURSE CODE 22CH4T1	CO-PO	PO1	PO2	PO3	PO4	PO5	PO6	PO7
	CO1		H					M
	CO2	M	M					L
	CO3	H					H	
	CO4	H						M
	CO5	H						M

UNIT – I

Proton NMR Spectrscopy:

Determination of structure of organic compounds using PMR data. Spin system, Nomenclature of spin system, spin system of simple and complex PMR spectrum (Study of AB – A_2 – AB_2. ABX – ABC – AMX interactions)

Simplification of complex spectra- nuclear magnetic double resonance, chemical shift reagents, solvent effects on PMR Spectrum . Nuclear Overhauser Effect (NOE).

UNIT-II

13C-NMR spectroscopy:

Similarities and Difference between PMR and CMR-CMR recording techniques -BBC-BBD-SFORD-Gate pulse CMR spectrum.

General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonylcarbon), coupling constants.Typical examples of CMR spectroscopy – simple problems.

UNIT-III

ORD& CD Curves:

Optical rotatory dispersion : Theory of optical rotatory dispersion – Cotton effect –CD curves-types of ORD and CD curves-similarities and difference between ORD and CD curves. α- Halo keto rule, Octant rule – application in structural studies.

UNIT-IV

2D NMR spectroscopy:

Definitions and importance of COSY, DEPT, HOMCOR, HETCOR,INADEQUATE, INDOR, INEPT, NOESY, HOM2DJ, HET2DJ.

Study of COSY ,DEPT, HOMCOR, HETCOR, INADEQUATE INDOR INEPT ,NOESY HOM2DJ, HET2DJ, taking simple organic compounds as examples.

UNIT –V

Structural Elucidation of Organic compounds Using UV, IR, 1H-NMR, 13C-NMR and Mass spectroscopy.

References :

1. Introduction to Spectroscopy – D. L. Pavia, G.M. Lampman, G. S. Kriz, 3rd Ed. (Harcourt College publishers).
2. Spectrometric identification of organic compounds R. M. Silverstein, F. X. Webster, 6th Ed.John Wiley and Sons.
3. Spectroscopic methods in organic chemistry - D. H. Williams and I Flemming McGraw Hill
4. Absorption spectroscopy of organic molecules – V. M. Parikh
5. Nuclear Magnetic Resonance – Basic Principles- Atta-Ur-Rehman, Springer- Verlag (1986).
6. One and Two dimensional NMR Spectroscopy – Atta-Ur-Rehman, Elsevier (1989).
7. Organic structure Analysis- Phillip Crews, Rodriguez, Jaspars, Oxford University Press (1998)
8. Organic structural Spectroscopy- Joseph B.Lambert, Shurvell, Lightner, Cooks, Prentice-Hall (1998).
9. Organic structures from spectra –Field L.D., Kalman J.R. and Sternhell S. 4th Ed. John Wiley and sons Ltd.