P.B.SIDDHARTHA COLLEGE OF ARTS & SCIENCE
DEPARTMENT OF CHEMISTRY
M.Sc – CHEMISTRY (ORGANIC CHEMISTRY)
III SEMESTER

Paper Code & Title: 22CH3T1:ORGANIC SPECTROSCOPY

No. of hours per week: 04 **Total credits: 04**
Total marks: 100 **(Internal: 30 M & External: 70M)**

Course: Organic Spectroscopy (code 22CH3T1)		
S.No	COURSE OUTCOMES	PO`S
	The graduate will be able to	
1	Memorize the basic principles and theory involved in molecular absorption spectroscopy.	2,7
2	Comprehend the advanced concepts of molecular absorption spectroscopy.	1,2,5
3	Apply the knowledge of spectroscopy in establishing the structure of organic molecules.	1,5,7
4	Analyze the spectral data to ascertain the structure of unknown molecules.	1,4,2

UNIT- I

UV- Visible Spectroscopy:
Mechanics of measurement – Energy transitions – Simple chromophores – Auxochrome, Absorption shifts (Bathochromic shifts, Hypsocromic shift, Hyper chromic shift, Hypo chromic shift). UV absorption of Alkenes – polyenes, unsaturated cyclic systems .
UV absorption of Carbonyl compounds α,β-unsaturated carbonyl systems - UV absorption aromatic systems – solvent effects – geometrical isomerism – acid and base effects – typical examples – calculation of λmax values for simple molecules using Woodward -Fieser rules.

UNIT – II

IR Spectroscopy:
Mechanics of measurement – Fundamental modes of vibrations -Stretching and bending vibrations – Factors effecting vibrational frequency-hydrogen bonding.
Finger print region and its importance. Typical group frequencies for – CH,
-OH, -NH, -CC, -CO and aromatic systems - Application in structural determination Examples – simple problems.

UNIT – III

Nuclear Magnetic Resonance Spectroscopy (1HNMR – First Order PMR):
Introduction:Nuclear spin-Basic principle of -NMR - nuclear resonance –saturation-Larmor's frequency-Relaxation- Instrumentation(Cw and FT) shielding and de shielding of magnetic nuclei-chemical shift and its measurements, factors influencing chemical shift, spin–spin interactions and factors influencing spin -spin coupling- Dynamic NMR- coupling constant J. and factors effecting J value.

UNIT – IV

Mass Spectrometry I
Introduction- ionization methods-EI, CI, ES, MALDI and FAB – advantages and disadvantages-molecular ion peak and its importance, meta stable peak, Nitrogen rule and extension of nitrogen rule. Determination of Molecular weight and determination of molecular formulae- Isotopic Peaks-Identification of single chlorine atom and double chlorine atom single bromine atom and double bromine atoms in organic compounds. Instrumentation.

UNIT – V

Mass Spectrometry II

Fundamental fragmentation process- Stevenson's rule- radical site initiated cleavage-charge site initiated cleavage- two bond cleavage- Retrodielalder cleavage- Mc-Lafferty rearrangement and other cleavages. Mass spectral fragmentation of alkanes, cycloalkanes, alkenes, alkynes, aromatic hydrocarbons, alcohols, phenols, thiols, ethers, carbonyl containing compounds (Aldehydes, ketones, esters and carboxylic acids), nitrogen compounds, alkyl chlorides and alkyl bromides, Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

Text books/ Reference books:

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. FlemmingMc.Graw 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.