SPECTROSCOPY

Semester	Subject Code	Category	Lecture hours		Theory hours		Practical hours		Credits
			Per week	Per sem.	Per week	Per sem.	Per week	Per sem.	
VI	21CCH6D	Elective-IV (Option-1)	3	45	3	45	-	-	3

COURSE OBJECTIVES:

The students will be able to

- Gain knowledge about the basic principles of UV, IR, Raman, Mass, NMR and ESR spectroscopy and their instrumentation techniques along with their applications.

COURSE OUTCOMES:

On the successful completion of the course, students will be able to

CO Number	CO Statement	Knowledge Level (K1-K4)
CO1	Gain knowledge about the basic principles of spectroscopy.	K4
CO2	Learn knowledge on the Instrumentation techniques of Visible and Ultraviolet Spectroscopy and to identify the simple organic molecules.	K3
CO3	Gain knowledge on the principles, instrumentation techniques and applications of IR and Raman spectroscopy.	K3
CO4	Know about the principles, instrumentation techniques and applications of NMR spectroscopy.	K3
CO5	Gain knowledge on the Instrumentation technique of mass spectroscopy and ESR and uses of MS to identify the simple organic molecules.	K2

*CO – Course Outcomes

Knowledge Level: K1 – Remember; K2 – Understand; K3 – Apply; K4 – Analyze.

MAPPING WITH PROGRAMME OUTCOMES:

COS	PO1	PO2	PO3	PO4	PO5	PO6
CO1	S	S	M	S	S	S
CO2	S	S	M	S	S	S
CO3	S	S	M	S	S	S
CO4	S	S	M	S	S	S
CO5	S	S	M	S	S	S

(S – Strong; M – Medium; L – Low)

UNIT-I: General Introduction of Spectral Methods of Analysis **9 Hours**

1.1 Introduction to spectroscopy – Definition of spectrum – Electromagnetic radiation − Types of spectroscopy − Atomic and molecular spectroscopy (elementary idea only), differences− Spectrum− Types of Spectrum− Absorption and emission spectrum (definition) − Absorption of radiation − Parameters of electromagnetic radiation (definition and formula only) − Wave length, wave number, frequency, velocity − Relation between wavelength, frequency and velocity − Energy.

1.2 Molecular Spectra – Quantisation of different forms of energy present in the molecules− Rotational, vibrational, electronic and translational energy – Born-Oppenheimer approximation – Conditions of Energy of Absorption of various types of spectra – Energy level diagram − Electromagnetic spectrum.

UNIT –II: Visible and Ultraviolet Spectroscopy **9 Hours**

2.1 Types of electrons involved in organic molecules − Modes of electronic transitions − Chromophore, chromogen and auxochrome − Definition, example and differences − Absorption bands and intensity − Bathochromic and hypsochromic shift - hyperchromic shift and hypochromic effects– Factors governing the absorption maximum and intensity −Solvent effect, conjugation effects, substituent effects andstereochemistry factors .

2.2 Frank-Condon principle – Absorption laws − Grotthus-Draper law – Calculations involving Beer-Lambertslaw − UV-Visible spectroscopy – Instrumentation – Block diagrams with description of components – Working – Applications of Ultraviolet Spectroscopy.

UNIT – III: IR and Raman Spectroscopy **9 Hours**

3.1 Infra red spectroscopy – Molecular vibrations – Hooke's law – Types of stretching (symmetric and asymmetric) and bending (in plane – scissoring, rocking and out plane – twisting ,wagging − deformation) vibrations − Vibrational frequencies – Factors affecting vibrational frequencies (bond strength, reduced mass, hydrogen bonding, bond angle and electronic effects – inductive effect, mesomeric effect and field effect) − Instrumentation, block diagram, source, monochromator, cell sampling techniques, detector and recorders – Solvent shift − Identification of simple organic molecules like aldehydes, ketones, alcohols and aromatic hydrocarbons.

3.2 Raman spectroscopy – Rayleigh and Raman scattering – Selection rules – Raman shift – Stokes and Anti-Stokes lines – Raman spectrophotometer – Instrumentation, block

diagram, components and their functions – Structural Elucidation in Inorganic and Organic compounds – Rotational − Raman spectra of non-centrosymmetric molecules – Advantages of using Laser in Raman spectroscopy – Differences between IR and Raman spectroscopy – Mutual exclusion principle (CO_2 and N_2O) – Applications – Structural diagnosis.

UNIT – IV: NMR Spectroscopy **9 Hours**

4.1 NMR spectroscopy – Principle of Nuclear magnetic Resonance – Basic instrumentation – Shielding and deshielding mechanism – Chemical shift − Definition, formula, importance – Ranges of chemical shift – Factors affecting chemical shift − Local diamagnetic shielding and diamagnetic anisotropic shielding −Inductive effect − Hydrogen bonding.

4. 2 Number of signals – Advantages of using TMS as reference − Number of signals – Spin-spin coupling and coupling constants – Splitting of signals – NMR spectrum of simple organic compounds such as ethyl bromide, 1,1,2-tribromo ethane, ethanol, acetaldehyde, ethyl acetate, toluene and acetophenone – Applications of NMR Spectroscopyin structural elucidation of organic compounds.

UNIT – V: ESR and Mass Spectroscopy **9 Hours**

5.1 ESR spectroscopy – Condition – Selection rule for transition – Theory of ESR spectra – Principle – Basic Instrumentation – ESR Spectrometer – Components and their functions – Radiation source, magnet, detector – Hyperfine splitting – ESR spectra of simple radicals – CH_3, CD_3, Naphthalene radical ions only – Applications of ESR spectra in structural elucidation.

5.2 Mass spectroscopy − Basic principles of mass spectrum – Instrumentation – Molecular ion peak – Base peak – Isotopic peak – Metastable peak – Fragmentation − Types of simple cleavage−Homolytic and heterolytic fission−Factors influencing the fragmentation – Nitrogen rule – Ring rule – McLafferty Rearrangement – Determination of molecular formulae with examples − Mass spectrum of simple organic compounds − Identification of isobutene, toluene, alkenes, alcohols, and aldehydes.

TEXT BOOKS:

S. No.	Authors	Title	Publishers	Year of publication
1.	R. Gopalan	Elements of Analytical Chemistry	Sultan Chand and Sons	2002
2.	V. Veeraiyan	Textbook of Analytical Chemistry	Highmount Publishing House	2006
3.	H. H. Willard, L. L. Merritt, J. Dean and F. A. Settle	Instrumental Methods of Analysis	Wadsworth Publishing Company Limited, Belmont, California	1988
4.	Gurdeep R. Chatwal, Sham K. Anand	Instrumental Methods of Chemical Analysis	Himalaya Publishing House	2000

REFERENCE BOOKS:

S. No.	Authors	Title	Publishers	Year of publication
1.	Douglas A. Skoog, Donald M. West ,Stanley R. Crouch and F. James Holler	Fundamentals of Analytical Chemistry	Thomson-Brooks/Cole	2004
2.	J. Mendham, R. C. Denney, J. D. Barnes and M. J. K. Thomas	Vogel's Textbook of quantitative Chemical Analysis	Pearson Education Limited	2008
3.	S. M. Khopkar	Basic Concepts of Analytical Chemistry	New Age International.	1998
4.	V. K. Srivastava and K. K. Srivastava	Introduction to Chromatography	S. Chand and Co. Ltd,	1990
5.	R. P. Budhiraja	Separation Chemistry	New Age International Publishers	2004
6.	John Kenkel	Analytical Chemistry for Technician	CRC Press	2014
7.	Frank A. Settle	Handbook of Instrumental Techniques for Analytical Chemistry	Prentice Hall PTR	1997
8.	S. M. Khopkar	Basic Concepts of Analytical Chemistry	New Academic Science	2008
9.	R. A. Day, and A. L.Underwood	Quantitative Analysis	Prentice Hall	1991
10.	S. A. Iqbal and M.	An Introduction to Analytical	Discovery Publishing	1994

	S. Setii	Chemistry	House	
11	J. R. Dyer	Application of Absorption Spectroscopy of Organic Compounds	Prentice-Hall of India Pvt. Ltd.	2010
12	Donald L. Pavia, Gray M. Lampman, George S. Kriz and James R. Vyvyan	Introduction to Spectroscopy	Cengage Learning India Private Limited	2015
13	B. R. Puri, L. R Sharma and M. S Pathania	Principles of Physical Chemistry	Vishal Publishing Company	2016
14	Samuel H. Maron, Jerome B. Lando and Carl R. Prutton,	Fundamentals of Physical Chemistry,	Macmillan, New York	1974

TEACHING METHODOLOGY:

- Conventional chalk and board teaching
- Power Point Presentations
- Assignments
- Animated videos
- Chalk and Board
- Interactive sessions
- Recent information through internet.

SYLLABUS DESIGNER:

- Dr. S. Sashikala, Assistant Professor of Chemistry