Course Code	Course Name	Credits
26CH605	MOLECULAR SPECTROSCOPY	04

Course Objectives

- To develop a fundamental understanding of the principles and theoretical basis of molecular spectroscopy, including rotational, vibrational, electronic, and spin resonance techniques.
- To enable students to interpret spectroscopic data for molecular structure determination, bonding analysis, and energy transition studies in simple and complex chemical systems.
- To provide knowledge of modern spectroscopic instrumentation and applications in chemical analysis, structural elucidation, and materials characterization.

Learning Outcomes

Upon successful completion of this course it is intended that a student will be able to:

- Understand the interaction light with matter and the key concepts spectroscopy to probe the structure of molecules.
- Apply quantum mechanics and group theory principles to understand molecular spectra Identify the relationship between molecular spectra and molecular properties
- Analyses and explain the structure of atoms and molecules using various spectral data.

Unit 1 - Introduction To Spectroscopy (12 Hrs.)

Origin of different spectra; intensity of absorption; signal-to-noise ratio; natural line width; factors influencing spectral intensity and transition probability; Maxwell–Boltzmann distribution; contributing factors including Doppler broadening; Lamb dip spectrum; Beer–Lambert law; Born–Oppenheimer approximation; energy dissipation from excited states; relaxation time

Unit 2 – Microwave spectroscopy (12 Hrs.)

Rotation of molecules; rotational spectra; diatomic molecules; polyatomic molecules; techniques and instrumentation; chemical analysis by microwave spectroscopy; vibrational spectroscopy; vibrations of molecules; transitions; vibrational Raman spectra of diatomic molecules; vibrations of polyatomic molecules; vibrational Raman spectra of polyatomic molecules.

Unit 3 - Electronic Spectroscopy (10 Hrs.)

Term symbols and electronic spectra of diatomic molecules; selection rules; Franck–Condon principle; predissociation; calculation of heat of dissociation by the Birge–Sponer method; Fortrat diagram; electronic spectra of polyatomic molecules; radiative and non-radiative decay; Jablonski diagram; different types of lasers including solid-state, continuous wave, gas, and chemical lasers; frequency doubling.

Unit 4 – NMR Spectroscopy (14 Hrs.)

Nuclear spin interaction with magnetic field; nuclear energy levels and population; Larmor precession; relaxation methods; factors affecting nuclear relaxation; chemical shift; exchange phenomenon; factors influencing coupling; Karplus relationship; variation of coupling constant with dihedral angle.

FT-NMR; second-order effects on spectra; spin systems (AB, AB_2); simplification of second-order spectra using shift reagents; contact and pseudocontact shifts.

^{13}C NMR chemical shift and structure correlation; ^{13}C coupling constants; solid-state NMR; magic angle spinning.

Unit 5 - Spin Resonance Spectroscopy (12 Hrs.)

Spin and an applied field; Nuclear Magnetic Resonance spectroscopy of hydrogen nuclei; NMR spectroscopy of nuclei other than hydrogen; techniques and instrumentation; Electron Spin Resonance spectroscopy; Mössbauer spectroscopy including basic principles, Doppler effect, chemical shift, and applications to metal complexes.

Reference Books:

1. C.N. Banwell, E.M. McCash, Fundamentals of Molecular Spectroscopy, 4th Edn., 1994, Tata McGraw Hill.
2. G. Aruldhas, Molecular Structure and Spectroscopy, 2001, Prentice Hall of India.
3. H. Kaur, Spectroscopy, 6th Edn., 2011, Pragati Prakashan.
4. R.S. Drago, Physical Methods in Chemistry, 1992, Saunders College.
5. K.J. Laidler, J.H. Meiser, Physical Chemistry, 2nd Edn., 1999, CBS.
6. D.N. Sathyanarayana, Electronic Absorption Spectroscopy and Related Techniques, 2001, Universities Press.

Websites and eLearning Sources:

1. https://sist.sathyabama.ac.in/sist_coursematerial/uploads/SCYA7301.pdf
2. https://link.springer.com/chapter/10.1007/978-1-4020-2575-4_1
3. https://www.youtube.com/watch?v=RZLew6Ff-JE

COs and Bloom's Taxonomy Mapping – 26CH605		
Course Outcomes	**On completing P.G. program the students will be able to**	**BTL**
CO1	Recall and explain the principles and applications of various spectroscopic techniques and factors affecting spectral intensity.	K1, K2
CO2	Apply physical principles to enhance spectroscopic techniques and interpret molecular behavior.	K3
CO3	Analyze spectroscopic techniques to interpret molecular and metal complex structures and their applications.	K4
CO4	Evaluate the effect of signal-to-noise ratio and assess the applications of key spectroscopic techniques.	K5
CO5	Design and develop analytical methods using advanced spectroscopic techniques for molecular and structural analysis.	K6

BTL K1 and K2 – remembering and understanding, K3- Applying, K4 – Analyse, K5- Evaluate and K6-Create

Relationship Matrix – 26CH605												
Course Outcomes	**Programme Outcomes (POs)**						**Programme Specific Outcomes (PSOs)**					**Mean Score of Cos**
	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PSO1**	**PSO2**	**PSO3**	**PSO4**	**PSO5**	
CO1	3	2	1.5	1	2	2.5	2	3	3	2	2	2.1
CO2	2	3	3	2	3	2	2	2	1.5	1.5	2.5	2.2
CO3	2.5	2	2	2	2.5	1	3	2	2	3	2	2.1
CO4	2	2	3	2	2	3	1	3	3	2	3	2.3
CO5	3	3	3	2	3	3	2	3	3	3	3	2.8
											Total	2.3

Mean Score: 3- High, 2- Medium/Moderate, 1-Low