

UNIVERSITY OF MADRAS
M.Sc. DEGREE PROGRAMME IN CHEMISTRY
 SYLLABUS WITH EFFECT FROM 2023-2024

Title of the Course	MOLECULAR SPECTROSCOPY						
Paper No.	Elective IV						
Category	Elective	Year	I	Credits	4	Course Code	424E2C
		Semester	II				
Instructional hours per week	Lecture	Tutorial	Lab Practice		Total		
	4	1	-		5		
Prerequisites	Basic knowledge of spectroscopy						
Objectives of the course	<p>To understand the influence of rotation and vibrations on the spectra of the polyatomic molecules.</p> <p>To study the principle of Raman spectroscopy, ESR spectroscopy, EPR spectroscopy and fragmentation patterns in Mass spectroscopy.</p> <p>To highlight the significance of Franck-Condon principle to interpret the selection rule, intensity and types of electronic transitions.</p> <p>To interpret the first and second order NMR spectra in terms of splitting and coupling patterns using correlation techniques such as COSY, HETCOR, NOESY.</p> <p>To carry out the structural elucidation of molecules using different spectral techniques.</p>						
Course Outline	<p>UNIT-I: Rotational and Raman Spectroscopy: Rotational spectra of diatomic and polyatomic molecules. Intensities of rotational spectral lines, effect of isotopic substitution. Non-rigid rotators. Classical theory of the Raman effect, polarizability as a tensor, polarizability ellipsoids, quantum theory of the Raman effect, Pure rotational Raman spectra of linear and asymmetric top molecules, Stokes and anti-Stokes lines. Vibrational Raman spectra, Raman activity of vibrations, rule of mutual exclusion, rotational fine structure-O and S branches, Polarization of Raman scattered photons.</p>						
	<p>UNIT-II: Vibrational Spectroscopy: Vibrations of molecules, harmonic and anharmonic oscillators- vibrational energy expression, energy level diagram, vibrational wave functions and their symmetry, selection rules, expression for the energies of spectral lines, computation of intensities, hot bands, effect of isotopic substitution. Diatomic vibrating rotor, vibrational-rotational spectra of diatomic molecules, P, R branches, breakdown of the Born-Oppenheimer approximation. Vibrations of polyatomic molecules – symmetry properties, overtone and combination frequencies. Influence of rotation on vibrational spectra of polyatomic molecule, P, Q, R branches, parallel and perpendicular vibrations of linear and symmetric top molecules.</p>						
	<p>UNIT-III: Electronic spectroscopy: Electronic Spectroscopy: Electronic spectroscopy of diatomic molecules, Frank-Condon principle, dissociation and predissociation spectra. $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transitions and their selection rules. Lasers: Laser action, population inversion, properties of laser radiation, examples of simple laser systems.</p>						

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	<p>UNIT-IV: NMR and ESR spectroscopy: Chemical shift, Factors influencing chemical shifts: electronegativity and electrostatic effects; Mechanism of shielding and deshielding. Spin systems: First order and second order coupling of AB systems, Simplification of complex spectra. Spin-spin interactions: Homonuclear coupling interactions - AX, AX₂, AB types. Vicinal, germinal and long-range coupling-spin decoupling. Nuclear Overhauser effect (NOE), Factors influencing coupling constants and Relative intensities. ¹³CNMR and structural correlations, Satellites. Brief introduction to 2D NMR – COSY, NOESY. Introduction to ³¹P, ¹⁹F NMR. ESR spectroscopy Characteristic features of ESR spectra, line shapes and line widths; ESR spectrometer. The g value and the hyperfine coupling parameter (A), origin of hyperfine interaction. Interpretation of ESR spectra and structure elucidation of organic radicals using ESR spectroscopy; Spin orbit coupling and significance of g-tensors, zero/non-zero field splitting, Kramer’s degeneracy, application to transition metal complexes (having one to five unpaired electrons) including biological molecules and inorganic free radicals. ESR spectra of magnetically dilute samples.</p>
	<p>UNIT-V: Mass Spectrometry, EPR and Mossbauer Spectroscopy: Ionization techniques- Electron ionization (EI), chemical ionization (CI), desorption ionization (FAB/MALDI), electrospray ionization (ESI), isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral fragmentation, high resolution. Effect of isotopes on the appearance of mass spectrum. EPR spectra of anisotropic systems - anisotropy in g-value, causes of anisotropy, anisotropy in hyperfine coupling, hyperfine splitting caused by quadrupole nuclei. Zero-field splitting (ZFS) and Kramer’s degeneracy. Applications of EPR to organic and inorganic systems. Structural elucidation of organic compounds by combined spectral techniques.</p>
<p>Extended Professional Component (is a part of internal component only, Not to be included in the external examination question paper)</p>	<p>Questions related to the above topics, from various competitive examinations UPSC / TRB / NET/ UGC-CSIR / GATE /TNPSC others to be solved (To be discussed during the Tutorial hours)</p>
<p>Skills acquired from this course</p>	<p>Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.</p>

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Recommended Text	<ol style="list-style-type: none"> 1. C. N. Banwell and E. M. McCash, <i>Fundamentals of Molecular Spectroscopy</i>, 4th Ed., Tata McGraw Hill, New Delhi, 2000. 2. R. M. Silverstein and F. X. Webster, <i>Spectroscopic Identification of Organic Compounds</i>, 6th Ed., John Wiley & Sons, New York, 2003. 3. W. Kemp, <i>Applications of Spectroscopy</i>, English Language Book Society, 1987. 4. D. H. Williams and I. Fleming, <i>Spectroscopic Methods in Organic Chemistry</i>, 4th Ed., Tata McGraw-Hill Publishing Company, New Delhi, 1988. 5. R. S. Drago, <i>Physical Methods in Chemistry</i>; Saunders: Philadelphia, 1992.
Reference Books	<ol style="list-style-type: none"> 1. P.W. Atkins and J. de Paula, <i>Physical Chemistry</i>, 7th Ed., Oxford University Press, Oxford, 2002. 2. I. N. Levine, <i>Molecular Spectroscopy</i>, John Wiley & Sons, New York, 1974. 3. A. Rahman, <i>Nuclear Magnetic Resonance-Basic Principles</i>, Springer-Verlag, New York, 1986. 4. K. Nakamoto, <i>Infrared and Raman Spectra of Inorganic and coordination Compounds</i>, PartB: 5th ed., John Wiley & Sons Inc., New York, 1997. 5. J. A. Weil, J. R. Bolton and J. E. Wertz, <i>Electron Paramagnetic Resonance</i>; Wiley Interscience, 1994.
Website and e-learning source	<ol style="list-style-type: none"> 1. https://onlinecourses.nptel.ac.in/noc20_cy08/preview 2. https://www.digimat.in/nptel/courses/video/104106122/L14.html
Course Learning Outcomes (for Mapping with POs and PSOs)	
<p>Students will be able:</p> <p>CO1: To understand the importance of rotational and Raman spectroscopy.</p> <p>CO2: To apply the vibrational spectroscopic techniques to diatomic and polyatomic molecules.</p> <p>CO3: To evaluate different electronic spectra of simple molecules using electronic spectroscopy.</p> <p>CO4: To outline the NMR, ¹³C NMR, 2D NMR – COSY, NOESY, Introduction to ³¹P, ¹⁹F NMR and ESR spectroscopic techniques.</p> <p>CO5: To develop the knowledge on principle, instrumentation and structural elucidation of simple molecules using Mass Spectrometry, EPR and Mossbauer Spectroscopy techniques.</p>	

CO-PO Mapping (Course Articulation Matrix)

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO 1	S	S	S	S	M	S	S	S	S	M
CO 2	M	S	S	S	S	M	S	S	S	S
CO 3	S	S	M	S	S	S	S	M	S	S
CO 4	M	S	S	S	S	M	S	S	S	S
CO 5	M	S	M	S	S	M	S	M	S	S

3 – Strong, 2 – Medium, 1 - Low

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Level of Correlation between PSO's and CO's

CO /PO	PSO1	PSO2	PSO3	PSO4	PSO5
CO1	3	3	3	3	3
CO2	3	3	3	3	3
CO3	3	3	3	3	3
CO4	3	3	3	3	3
CO5	3	3	3	3	3
Weightage	15	15	15	15	15
Weighted percentage of Course Contribution to Pos	3.0	3.0	3.0	3.0	3.0

3 – Strong, 2 – Medium, 1 – Low