UNIVERSITY OF MADRAS

B.Sc. DEGREE PROGRAMME IN CHEMISTRY

SYLLABUS WITH EFFECT FROM 2023-2024

<table>
<tr><td>Title of the Course</td><td colspan="7">FUNDAMENTALS OF SPECTROSCOPY</td></tr>
<tr><td>Paper No.</td><td colspan="7">EC VII (EC-7)</td></tr>
<tr><td rowspan="2">Category</td><td>Elective Course</td><td>Year</td><td>III</td><td>Credits</td><td>2</td><td>Course Code</td><td>324E6A</td></tr>
<tr><td></td><td>Semester</td><td>VI</td><td colspan="4"></td></tr>
<tr><td rowspan="2">Instructional hours per week</td><td>Lecture</td><td>Tutorial</td><td colspan="2">Lab Practice</td><td colspan="2">Total</td></tr>
<tr><td>4</td><td></td><td colspan="2">-</td><td colspan="2">4</td></tr>
<tr><td>Prerequisites</td><td colspan="7">General Chemistry I,II,III and IV</td></tr>
<tr><td>Objectives of the course</td><td colspan="7">This course is designed to provide knowledge on
electrical and magnetic properties of organic and inorganic compounds
basic principles of microwave, UV-Visible, infrared, Raman, NMR and Mass spectrometry
instrumentation of microwave, UV-Visible, infrared, Raman, NMR and Mass spectrometry
applications of various spectral techniques in structural elucidation
solving combined spectral problems</td></tr>
<tr><td>Course Outline</td><td colspan="7">UNIT I
Electrical and Magnetic properties of molecules
Dipole moment – polar and nonpolar molecules – polarisability of molecules. Application of dipole moments in the study of organic and inorganic molecules.
Magnetic permeability, volume susceptibility, mass susceptibility and molar susceptibility; diamagnetism, paramagnetism – determination of magnetic susceptibility using Guoy balance, ferromagnetism, anti-ferromagnetism
Microwave spectroscopy
Rotation spectra - diatomic molecules (rigid rotator approximation) selection rules – determination of bond length, effect of isotopic substitution – instrumentation and applications</td></tr>
</table>

UNIT II

Ultraviolet and Visible spectroscopy

Electronic spectra of diatomic molecules (Born Oppenheimer approximation) - vibrational coarse structure – rotational fine structure of electronic vibration transitions – Frank Condon principle – dissociation in electronic transitions – BirgeSponer method of evaluation of dissociation energy – pre-dissociation transition - σ -σ *, π-π*, n-σ*, n-π*transitions.

Applications of UV-Woodward – Fieser rules as applied to conjugated dienes and α, β - unsaturated ketones. Elementary Problems.

Colorimetry - principle and applications (estimation of Fe^{3+})

UNIT III

Infrared spectroscopy

Vibration spectra –diatomic molecules – harmonic oscillator and anharmonic oscillator; Vibration – rotation spectra – diatomic molecule as rigid rotator and anharmonic oscillator (Born-Oppenheimer approximation oscillator) - selection rules, vibrations of polyatomic molecules – stretching and bending vibrations – applications – determination of force constant, moment of inertia and internuclear distance – isotopic shift – application of IR spectra to simple organic and inorganic molecules – (group frequencies)

Raman Spectroscopy

Rayleigh scattering and Raman scattering of light – Raman shift – classical theory of Raman effect – quantum theory of Raman effect – Vibrational Raman spectrum – selection rules – mutual exclusion principle – instrumentation (block diagram) – applications.

UNIT IV

Nuclear magnetic resonance spectroscopy:

PMR – theory of PMR – instrumentation - number of signals – chemical shift – peak areas and proton counting – spin-spin coupling – applications. Problems related to shielding and deshielding of protons, chemical shifts of protons in hydrocarbons, and in simple monofunctional organic compounds; spin-spin splitting of neighboring protons in vinyl and allyl systems.

UNIT V

Mass spectrometry

Principle – different kinds of ionisation – instrumentation – the mass spectrum – types of ions – determination of molecular formula-fragmentation and structural elucidation – McLafferty rearrangement; Retro Diels Alder reaction - illustrations with simple organic molecules.

	Solving structure elucidation problems using multiple spectroscopic data (NMR, MS, IR and UV-Vis).
Extended Professional Component (is a part of internal component only, Not to be included in the external examination question paper)	Questions related to the above topics, from various competitive examinations UPSC/ JAM /TNPSC others to be solved (To be discussed during the Tutorial hours)
Skills acquired from this course	Knowledge, Problem solving, Analytical ability, Professional Competency, Professional Communication and Transferable skills.

Recommended Text	1. Gopalan, R.; Subramaniam, P. S.; Rengarajan, K. Elements of Analytical Chemistry; S Chand: New Delhi,2003. 2. Usharani, S. Analytical Chemistry, 1st ed.; Macmillan: India,2002. 3. Banwell, C.N.; Mc Cash, E. M. Fundamentals of Molecular Spectroscopy, 4th ed.; Tata McGraw Hill, New Delhi,2017. 4. U.N.Dash, Analytical Chemistry Theory and Practice, Sultan Chand &Sons,2nd Ed.,2005 5. B.K.Sharma, Spectroscopy,22nd ed., Goel Publishing House,2011.
Reference Books	1. Srivastava, A. K.; Jain, P. C. Chemical Analysis an Instrumental Approach, 3rd ed.; S.Chand, New Delhi,1997. 2. Robert D Braun. Introduction to Instrumental Analysis; Mc.Graw Hill: New York,1987. 3. Skoog, D. A.; Crouch, S. R.; Holler, F.J.; West, D. M. Fundamentals of Analytical Chemistry, 9th ed.; Harcourt college Publishers: USA, 2013. 4. Madan, R. L.; Tuli, G. D. Physical Chemistry, 2nd ed.; S.Chand: New Delhi,2005. 5. Puri, B. R.; Sharma, L. R.; Pathania, M.S. Principles of Physical Chemistry, 43rd ed.; Vishal Publishing: Delhi,2008.
Website and e-learning source	1. http://vallance.chem.ox.ac.uk/pdfs/SymmetryLectureNotes2004.pdf 2.http://chemistry.rutgers.edu/undergrad/chem207/SymmetryGroupTheory.html 3. www.epgpathshala.nic.in 4. www.nptel.ac.in 5..http:/swayam.gov.in

Course Learning Outcomes (for Mapping with POs and PSOs)

On completion of the course the students should be able to

CO1: explain electrical and magnetic properties of materials and microwave spectroscopy

CO2: explain theory, instrumentation and applications of Infrared and Raman spectroscopy

CO3: apply selection rules to understand spectral transitions, explain Woodward – Fieser's rule for the calculation of wavelength maximum of conjugated dienes

CO4: explain theory, instrumentation and applications of NMR spectroscopy

CO5: explain theory, instrumentation and applications of Mass spectrometry

UNIVERSITY OF MADRAS

B.Sc. DEGREE PROGRAMME IN CHEMISTRY

SYLLABUS WITH EFFECT FROM 2023-2024

	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10
CO1	S	S	S	S	S	S	S	M	S	M
CO2	M	S	S	S	M	S	S	M	M	M
CO3	S	S	S	M	S	S	S	M	S	M
CO4	S	S	S	S	S	S	S	M	M	M
CO5	S	M	S	S	S	S	S	M	M	S

CO-PO Mapping (Course Articulation Matrix)

CO /PSO	PSO 1	PSO 2	PSO 3	PSO 4	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

Level of Correlation between PSO's and CO's