Name of the Programme: M. Sc -I (Physical Chemistry)

Course Code: CHP-502 **Title of the course:** Group Theory and Molecular Spectroscopy

Number of Credits: 04

Effective from AY: 2022-23

Prerequisites for the course:	Students should have studied physical chemistry courses at M.Sc. Chemistry in semester I	
Course Objective:	1. To introduce concepts in Group Theory and it applications to chemistry. 2. To introduce some advance topics in spectroscopy.	
Content	**1. Group Theory for Chemistry** a. Symmetry elements and symmetry operations, Concept of group and group multiplication tables, order of the group, classes and subgroups in a group, Different types of groups (cyclic, abelian and non-abelian groups). b. Point groups, Matrix representations of a group, Reducible and Irreducible representations groups, Great Orthogonality Theorem, Properties of Irreducible representations, Mulliken symbols for Irreducible representations, Character tables. c. Standard reduction formula, Direct products of representations and it applications Quantum Chemistry and spectroscopy: Vanishing of integrals, Selection rules. Applications of group theory for hybridization of atomic orbitals. Projection operator and Symmetry adapted linear combinations (SALCs), MO treatment (within Huckel Molecular Orbital Theory) of large molecules with symmetry. Applications of group theory to Infra-red and Raman spectroscopy. d. Space Groups**:** Symmetry elements, Schoenflies, and Hermann Mauguin notation, Representation of point groups and space groups, point symmetry, space symmetry, glide plane, helical screw axis	No of hours 30
	2. Microwave, IR and Raman Spectroscopy a. Theoretical treatment of Rotational and Vibrational spectroscopy. b. Principle of Fourier Transform (FT) spectroscopy, FTIR spectroscopy: Theory, instrumentation and applications. c. Quantum theory of Raman effect, Raman shift, Instrumentation, Resonance Raman spectroscopy, Complimentary nature of IR and Raman spectroscopy in structure determination, Applications.	12
	3. NMR Spectroscopy a. Basic principles of NMR b. Theory of pulse NMR and Fourier analysis, FT-NMR.	10

	c. Solid state NMR, magic angle spinning (MAS), dipolar decoupling and cross polarization, applications of solid-state NMR. d. Double resonance, NOE, Spin tickling, Solvent and shift reagents, Structure determination by NMR.	
	4. ESR Spectroscopy a. Theory and experimental techniques, Identification of odd-electron species (methyl and ethyl free radicals) and radicals containing hetero atoms. b. Spin trapping and isotopic substitution, Spin densities and McConell relationship, Double resonance techniques.	8
Pedagogy	Mainly lectures and tutorials. Seminars / term papers /assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.	
References / Readings	1. P. W. Atkins and J. D. Paula, Physical Chemistry, 8th Ed., Oxford University Press, New Delhi, 2007. 2. F.A. Cotton, Chemical Applications of Group Theory, 3rd Ed., John Wiley & Sons-Asia, New Delhi, 1999 3. K. V. Raman, Group Theory and its applications to chemistry, Tata McGraw-Hill, New Delhi, 1999 4. C. N. Banwell and E.M. McCash, Fundamentals of Molecular Spectroscopy, Tata McGraw-Hill, New Delhi, 1994 5. W. Kemp, NMR in Chemistry a multinuclear introduction, Macmillan, 1986. 6. R.S. Drago, Physical Methods in Chemistry, W.B. Saunders Company, 1977.	
Course outcomes:	1. Students should be in a position to explain various concepts in Group Theory. 2. Should be able to apply character table to solve various problems. 3. Students should be in a position to apply the knowledge of spectroscopy for their dissertation and research work. 4. Students will understand the fundamental difference between various spectroscopic techniques.	