Programme: M. Sc. Part-II (Chemistry)
Title of the Course: Group Theory and Spectroscopy
Course Code: PCC-504
Number of Credits:03 **Effective from AY:** 2019-20

Prerequisites for the course:	Should have studied the courses PCC-401, PCC-402 and PCO-401. Should have basic knowledge of Physical Chemistry.	No. of lectures
Course Objectives:	To introduce concepts in Group Theory and it applications to chemistry. To introduce some advance topics in spectroscopy.	
Course Outcomes:	Students should be in a position to understand various concepts of in Group Theory. Should be able to apply character table to solve various problems. Students should be in a position to apply the knowledge of spectroscopy for their dissertation and research work.	
Content:	4. **Elements of Group Theory** 1.1 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). 1.2 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. 1.3 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. **2. Microwave, IR and Raman Spectroscopy** 2.1 Theoretical treatment of Rotational and Vibrational spectroscopy. 2.2 Principle of Fourier Transform (FT) spectroscopy, FTIR spectroscopy Theory, instrumentation and applications. 2.3 Quantum theory of Raman effect, Raman shift, Instrumentation, Resonance Raman spectroscopy, Complimentary nature of IR and Raman spectroscopy in structure determination, Applications. **3. NMR Spectroscopy** 3.1 Basic principles of NMR. 3.2 Theory of pulse NMR and Fourier analysis, FT-NMR. 3.3 Solid state NMR, magic angle spinning (MAS), dipolar decoupling and cross polarization, applications of solid state NMR. 3.4 Double resonance, NOE, Spin tickling, Solvent and shift reagents, Structure determination by NMR. **4. ESR Spectroscopy**	18 hours 6 hours 8 hours 4 hours

	4.1 Theory and experimental techniques, Identification of odd-electron species (methyl and ethyl free radicals) and radicals containing hetero atoms. 4.2 Spin trapping and isotopic substitution, Spin densities and McConell relationship, Double resonance techniques.	
Pedagogy:	Mainly lectures/ tutorials /assignments/ presentations/ self-study or a combination of these could also be used. Sessions shall be interactive in nature to enable peer group learning.	
Text Books/ Reference Books	8. P.W. Atkins & J. De. Paulo, *Atkins' Physical Chemistry,* Oxford Univ. Press, 2007, 8th Ed. 9. F.A. Cotton, *Chemical Applications of Group Theory,* John Wiley & Sons-Asia, New Delhi, 1999, 3rd Ed. 10. K. V. Raman, *Group Theory and its applications to chemistry*, Tata McGraw-Hill, New Delhi. 11. C. N. Banwell & E.M. McCash, *Fundamentals of Molecular Spectroscopy,* Tata McGraw-Hill, New Delhi, 1994. 12. W. Kemp, *NMR in Chemistry a multinuclear introduction*, Macmillan, 1986. 13. R.S. Drago, *Physical Methods in Chemistry,* W.B. Saunders Company, 1977.	