Programme: M. Sc. Part-II (Inorganic Chemistry)
Course Code: ICC-503
Title of the Course: Group Theory & Spectroscopy
Number of Credits: 03 **Effective from AY:** 2019-20

Prerequisites for the course:	The students who have done ICC-401, ICC-402 and ICO-401 at MSc-I level are eligible for attend this course.	No. of lectures
Course Objectives:	1. To train students to understand the concepts of molecular symmetry and group theory and their applications. 2. To train the students to understand different spectroscopic techniques viz. magnetic resonance, vibrational & Mössbauer spectroscopy with emphasis on spectral interpretation.	
Course Outcomes:	1. Students will be able to understand symmetry aspects of simple molecules. 2. Students will get to know about applications of group theory and concepts of molecular orbital theory. 3. Students will be able interpret IR, Raman, ESR, NMR, Mossbauer spectra of simple molecules and determine molecular geometry	
Content:	**1. Group Theory:** Basic definitions and theorems of group theory, Molecular symmetry and the symmetry groups, symmetry elements and operations, symmetry planes and reflections, inversion center, proper axes and proper rotations, improper axis and improper rotations. Products of symmetry operations, equivalent symmetry elements and equivalent atoms, symmetry point groups, systematic symmetry classification of molecules, classes of symmetry operations, representations of groups, the great orthogonality theorem, some properties of matrices and vectors, reducible and irreducible representations, properties of the characters of representations, character tables, group theory and quantum mechanics, wave functions as basis for irreducible representations, direct product, Symmetry aspects of molecular orbital theory, general principles, the secular equation, the Huckel approximation, simple LCAO-MO theory of homocyclic π systems. More general cases of LCAO-MO pi-bonding, Molecular orbitals for the metal sandwich compounds. **2. Spectroscopic Methods:** Magnetic Resonance Spectroscopy, interaction between electron / nuclear spin and magnetic field, Resonance condition, instrumental requirements, presentation of NMR, ESR spectra, line widths of NMR and ESR spectra, hyperfine coupling in isotropic systems (e.g. H atom, methyl radical etc.), anisotropic system, zero field splitting and Kramer's degeneracy, Spin energy levels of octahedral Mn(II) complexes, ESR spectra of some transition metal compounds, Electron	18 hr 18 hr

	delocalization, NMR spectral interpretation of a few nuclei like ^{19}F, ^{29}Si ^{31}P, Mössbauer spectroscopy; Recoilless emission and absorption spectral line widths, Doppler shift, experimental arrangement of Mossbauer spectroscopy, chemical shift (isomer shift), quadrupole splitting, Magnetic hyperfine interaction. Discussion of selected Mossbauer nuclei (^{57}Fe, ^{129}I) Vibrational spectroscopy (IR & Raman) – recapitulation of basics, reduced mass, isotope effect, a few applications for determination of molecular geometry (See Ref. 7 and 8)	
Pedagogy	Mainly lectures / tutorials / assignments / self-study or a combination of some of these could also be used to some extent.	
Text books / Reference books	1. F. A. Cotton, *Chemical Applications of Group theory*, John Wiley, 1990, 3rd Ed. 3. R. L. Dutta & A. Syamal, *Elements of Magnetochemistry*, Affiliated East-West Press, New Delhi, 1993, 2nd Ed. 4. C. N. Banwell & E. M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw Hill, New Delhi, 1994, 4th Ed. (Chapter 7) 5. G. Aruldhas, *Molecular structure and spectroscopy*, Prentice Hall of India, 2001. 6. P Atkins, J De Paula & J Keeler, *Atkins' Physical Chemistry*, International Edition, Oxford University Press, 2018 (Focus 16) 7. M Weller, T Overton, J Rourke & F Armstrong *Inorganic Chemistry* International Edition, Oxford University Press, 2018 (Chapter 8) 8. P Atkins, T Overton, J Rourke, M Weller & F Armstrong, *Shriver & Atkins' Inorganic Chemistry* Oxford University Press, 2010, 5th Ed. (Chapter 8) 9. E.A.V. Ebsworth, D.W.H. Rankin & S. Cradock, *Structural Methods in Inorganic Chemistry,* ELBS, 1988.	