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

Course Code: CHI-503 **Title of the course:** Concepts in Molecular Symmetry and Spectroscopy

Number of Credits: 04

Effective from AY: 2022-23

Prerequisites for the course:	Students should have studied Inorganic chemistry courses at M.Sc. Chemistry in semester I	
Course Objective:	1. To train the students to understand the concepts of molecular symmetry and their applications in chemistry 2. To train the students to understand different spectroscopic techniques viz. magnetic resonance, vibrational & Mössbauer spectroscopy with emphasis on spectral interpretation.	
Content	**1. Molecular symmetry** a. Symmetry elements and symmetry operations, symmetry planes and symmetry reflections, inversion center, proper axes and proper rotations, improper axis and improper rotations. b. Products of symmetry operations, equivalent symmetry elements and equivalent atoms, relations among symmetry elements and operations, symmetry elements and optical isomerism, symmetry point groups, symmetries with multiple high order axes, classes of symmetry operations, procedure for symmetry classification of molecules. c. Group and it's defining properties, order of the group, examples of group, group multiplication table, cyclic group, acyclic group, abelian group, non-abelian group. Sub groups, classes, properties of conjugate elements. *d.* Some properties of matrices and vectors, the great orthogonality theorem, reducible and irreducible representations, irreducible representations and their characters, character tables. Bases for irreducible representations, direct product. Symmetry Adapted Linear Combinations and its applications. Cage and cluster compounds, metal sandwich compounds. *e.* Crystal symmetry, space groups.	No of hours 30
	2. Spectroscopy a. Magnetic Resonance Spectroscopy; interaction between electron spin and magnetic field, interaction between nuclear spin and magnetic field, Resonance condition, instrumental requirements, b. Presentation of ESR (electron spin resonance) and NMR (nuclear magnetic resonance) spectra, line widths of ESR and NMR spectra, hyperfine coupling in isotropic systems (e.g. H atom, methyl radical etc.), anisotropic system, number of expected ESR signals for one electron paramagnetic species, zero field splitting and Kramer's degeneracy, Spin energy levels of octahedral Mn(II) complexes, nuclear quadrupole interaction, spin Hamiltonian, ESR spectra of	30

	some transition metal compounds, Electron delocalization, NMR spectral interpretation of a few nuclei like ^{19}F, ^{29}Si, ^{31}P. c. Mössbauer spectroscopy; Mössbauer effect, Mössbauer principle, Recoilless emission and absorption spectral line widths, Doppler shift, experimental arrangement of Mössbauer spectroscopy, chemical shift (isomer shift), quadrupole splitting, magnetic hyperfine interaction, discussion of selected Mössbauer nuclei like ^{57}Fe, ^{129}I. d. Vibrational spectroscopy: Infrared spectroscopy and Raman spectroscopy, principle, their use in determination of molecular structure.	
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. F. A. Cotton, Chemical Applications of Group theory, 3rd Ed.; John Wiley,1990 2. J. E. Huheey, E. A. Keiter, R.L. Keiter, Inorganic Chemistry: Principles of structure and reactivity, 4thEd.; Pearson, 1993. 3. G. R. Desiraju, J. J. Vittal, A. Ramanan, Crystal Engineering, IISC Press, world Scientific, 2011. 4. R. L. Dutta, A. Syamal, Elements of Magnetochemistry, 2nd Ed.; Affiliated East-West Press, New Delhi, 1993. 5. C. N. Banwell, E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th Ed.; Tata McGraw Hill, New Delhi, 1994. 6. G. Aruldhas, Molecular structure and spectroscopy, Prentice Hall of India, 2001 7. P. Atkins, J. De Paula, J. Keeler, Atkins' Physical Chemistry, International Ed.; Oxford University Press, 2018. 8. M. Weller, T. Overton, J. Rourke, F. Armstrong, Inorganic Chemistry, International Ed.;Oxford University Press, 2018. 9. E. A. V. Ebsworth, D. W. H. Rankin, S. Cradock, Structural Methods in Inorganic Chemistry, ELBS, 1988. 10. K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, Part A: Theory and Applications in Inorganic Chemistry, 6thEd.; Wiley, 2009. 11. K. Nakamoto, Infrared and Raman Spectra of Inorganic and Coordination Compounds, Part B: Applications in Coordination, Organometallic and Bioinorganic Chemistry, 6thEd.; Wiley, 2009. 12. R. S. Drago, Physical Methods in Inorganic Chemistry, Affiliated East West Press Pvt. Ltd., 2017 13. G. C. Miessler, D. A. Tarr, Inorganic Chemistry, 3rd Ed.; Pearson, 2004	
Course outcomes:	1. Students will be able to explain symmetry aspects of simple molecules and their applications in chemistry. 2. Students will be able to explain IR, Raman, ESR, NMR, Mössbauer spectra of simple molecules to determine molecular geometry. 3. Students will understand fundamental difference between various spectroscopic techniques. 4. Students will be able to explain the space groups.	