Course Code	Course Name	Credits
26CH606	INORGANIC SPECTROSCOPY	04

Course Objectives

- This course in inorganic spectroscopy intends to make the students understand the role of spectroscopic methods in inorganic chemistry.
- To apply spectroscopic methods for structural analysis of inorganic compounds and metalloproteins.

Learning Outcomes

Upon successful completion of this course it is intended that a student will be able to:

- Understand the principles and applications of IR, Raman, ORD, CD, ESR, NMR, and NQR spectroscopy.
- Apply spectroscopic methods to analyze molecular structure, bonding, stereochemistry, and coordination compounds.
- Interpret hyperfine interactions, electronic environments, and magnetic properties using ESR and Mössbauer spectroscopy.
- Evaluate advanced techniques such as photoelectron and X-ray absorption spectroscopy for structural and electronic analysis.

Unit 1 - IR, Raman, ORD & CD spectroscopy (12 Hrs.)

Classical and quantum theories of the Raman effect; pure rotational, vibrational, and vibrational–rotational Raman spectra; selection rules and mutual exclusion principle; resonance Raman spectroscopy (RRS) and coherent anti-Stokes Raman spectroscopy (CARS); infrared and Raman spectra of metal complexes; circular dichroism (CD) spectroscopy—introduction to basic theory and terminology; Cotton effect; optical isomerism in octahedral complexes; absolute configuration of complexes; stereoselectivity and conformation of chelate rings; optical rotatory dispersion (ORD) and linear dichroism.

Unit 2 – Electron Paramagnetic Resonance spectroscopy (10 Hrs.)

Introduction; theory and instrumentation; g-values and anisotropy; hyperfine and superhyperfine splitting; line widths; interpretation of ESR spectra of single-electron and multi-electron systems; EPR of metalloenzymes

Unit 3 - Inorganic NMR, NQR spectroscopy (14 Hrs.)

NMR spectroscopy—spin and applied magnetic field; nature of spinning particles; interaction of spin with magnetic field; population of energy levels; chemical shift and coupling constants; ^{31}P and ^{19}F NMR spectra of HPX_2, P_4S_3, TiF_4, BrF_5, SF_4, SF_6, $XeOF_4$, $CsIF_6^{2-}$, $B_3H_8^-$, NF_3, $P_3N_3Cl_4F_2$, ClF_5 and ClF_3; phosphorus and hypophosphorous acid systems ($HP(O)F_2$, $HOP(O)FH$); use of lanthanide compounds as shift reagents; applications to metalloproteins and paramagnetic complexes; NQR—principles and introduction; nuclear quadrupole energy levels; energy and transition frequencies; effect of magnetic field (Zeeman effect); factors affecting line width; solid-state effects; applications of NQR—bonding in boron trichloride and its adducts; calculation of percentage ionic character of a bond.

Unit 4 – Mossbauer Spectroscopy (12 Hrs.)

Introduction; principle of the Mössbauer effect and basic concepts of Mössbauer spectroscopy; Doppler shift; experimental resonance conditions; sharpness of resonance and recoil effect; cross-section for resonant absorption; hyperfine interactions and Mössbauer parameters— isomer shift and electric quadrupole splitting; Mössbauer studies of octahedral high- and low-spin Fe(II) and Fe(III) complexes; information on oxidation state, π-back bonding, structure, and nephelauxetic effect in iron compounds; studies on halides of tin(II) and tin(IV) compounds.

Unit 5 - Photoelectron spectroscopy & X-ray Absorption spectroscopy (12 Hrs.)

Photoelectron spectroscopy (UV and X-ray)—physical principles; experimental details; Koopmans' theorem; chemical shifts and their correlation with electronic charges; applications of PES; X-ray absorption spectroscopy (XAS) and extended X-ray absorption fine structure (EXAFS); applications of X-ray absorption spectroscopy—structure determination, resolution of crystallographic disorder, determination of oxidation states, prediction of molecular symmetry, identification of atoms in the first coordination sphere (edge and EXAFS analysis), and structure of metal clusters.

Reference Books:

1. K. Nakamoto, Coordination, Organometallic, and Bioinorganic Chemistry, 6th edition, 2009, Wiley.
2. S. Hüfner, Photoelectron Spectroscopy, 3rd Edn., 2003, Springer-Verlag.
3. J.F. Watts, An Introduction to Surface Analysis by XPS and AES, 2nd Edn., 2003, J. Wiley & Sons.
4. N.N. Greenwood, T.C. Gibbs, Mossbaur Spectroscopy, 1971, Chapmann Hall.
5. Goldanski, R.H. Harber, Chemical Application of Mossbaur Spectroscopy, 1968, VAcademic Press.
6. R.S. Drago ,Physical methods in Spectroscopic Techniques, 2nd Edn., 1985, ELBS.

Websites and eLearning Sources:

1. https://nptel.ac.in/courses/104101134
2. https://archive.nptel.ac.in/content/storage2/courses/104103019/module5/lec36/1.html

COs and Bloom's Taxonomy Mapping – 26CH606		
Course Outcomes	**On completing P.G. program the students will be able to**	**BTL**
CO1	Recall and explain basic principles, terms, and instrumentation of key spectroscopic methods like IR, Raman, NMR, and Mössbauer.	K1, K2
CO2	Apply theories and concepts from Raman, Cotton Effect, EPR, NMR, and Mössbauer spectroscopy to analyze and interpret molecular spectra.	K3
CO3	Analyze and interpret data from Raman, CD, EPR, NMR, and Mössbauer spectroscopy to determine molecular structures, configurations, and metal complex characteristics.	K4
CO4	Evaluate spectroscopic techniques to predict molecular activity, analyze chelate conformations, interpret EPR and NMR spectra, and assess bonding in tin compounds.	K5
CO5	Create methods to use advanced spectroscopic techniques for studying and analyzing metal complexes, determining molecular structure and oxidation states.	K6

BTL K1 and K2 – remembering and understanding, K3- Applying, K4 – Analyse, K5- Evaluate and K6-Create

Relationship Matrix – 26CH606												
Course Outcomes	**Programme Outcomes (POs)**						**Programme Specific Outcomes (PSOs)**					**Mean Score of Cos**
	PO1	**PO2**	**PO3**	**PO4**	**PO5**	**PO6**	**PSO1**	**PSO2**	**PSO3**	**PSO4**	**PSO5**	
CO1	3	2	2	1	1	1	3	2	2	1	1	1.7
CO2	2	3	2	1	1	1	2	3	2	2	1	1.8
CO3	2	2	3	2	1	1	2	3	3	2	2	2.1
CO4	2	2	3	2	2	1	2	2	3	3	2	2.2
CO5	2	2	3	2	2	3	2	2	3	3	3	2.5
											Total	2.06

Mean Score: 3- High, 2- Medium/Moderate, 1-Low