

Semester	8
Programme	CHEMISTRY
Course	MAJOR (INORGANIC CHEMISTRY 8)
Paper Code	
Credits	4 (THEORY: 3 PRACTICAL: 1)
Hours/week	6 (THEORY: 6 PRACTICAL: 3)
Category: Core/MDC/SEC/VEC	CORE
Theory/Practical/Composite	COMPOSITE
Number of Modules	3
Syllabus	Module 1 (12 Lectures) Advanced Bioinorganic Chemistry: Metal ion transport across membranes, Hydrolytic enzymes : Carbonic anhydrase, Carboxypeptidase, Urease, Photosystem, Biological Nitrogen fixation and Nitrogenase, Cytochrome C-oxidase, Multicopper oxidase, Superoxide dismutase, Biomimetic modelling, Chelation therapy and Anticancer drugs (preliminary ideas) Module 2 (12 Lectures) Chemical Applications of Group theory: Application of group theory and symmetry in the context of chemical bonding: Construction of symmetry adapted linear combinations of orbitals and applications in Valence bond theory, LCAO approach for qualitative construction of Molecular orbital diagrams for representative symmetries and applications in coordination chemistry, Application of group theory to electronic spectroscopy: Selection rules and Splitting of d-orbitals in different symmetries, Tanabe-Sugano diagrams and correlation diagrams, Method of descending symmetries and its applications to electronic spectroscopy. Module 3 (12 Lectures) Frontiers of Inorganic Chemistry: Mechanism of electron transfer reactions and preliminary ideas of Marcus Theory, Mixed Valence, Proton-coupled electron transfer reactions and its applications, Redox non-innocence and applications of redox-innocent systems, Preliminary ideas on small molecule activation (O₂, N₂, CO₂, H₂) and their applications, C-H activation, Energy conversion and storage.

	Practical Group A • Multi tryptophan proteins and drug binding – studies at low temperatures (77K). • Fluorescence spectra in caged environments – an analysis with highly efficient fluorophores. • Drugs purity assessment by atomic absorption spectroscopy. Group B • Investigating the suitability of transition metal complexes of redox non-innocent azo ligands to act as homogeneous catalyst to ethanol dehydrogenation under solvent free condition. • Exploring the ability of transition metal complexes of conjugated imino-quinone type of ligands to act as electro-catalyst for NRR. • Exploring the potential of complexes with ligands having pyridyl/ benzothiazole functions as anti-microbials. Group C • Synthesis of di/ tri peptides incorporating sugar unit. • Different cyclisation/ cycloaddition reactions involving appropriate precursors. • Optimization of reaction conditions for click and RCM reactions with respect to catalyst, solvent, temperature, and time. Group D • Study of phase diagram in microemulsion. • Determination of droplet size distribution in microemulsion. • Particle size and band gap determination of nanoparticles from spectral study. Group E • Execution of the hybrid optimization suite to find the Global Minimum of a specific target system. • Implementation of clustering algorithms. • Visualization, final code documentation, and release of the complete package on GitHub. Group F • Synthesis of FRET based chemosensors - i) Isolation and Purification. • Synthesis of FRET based chemosensors - ii) Characterisation. • Synthesis of FRET based chemosensors - iii) Photo physical studies.
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	Group G • Study of catalytic efficiency in coupling reactions and related transformations leading to value-added products. • Synthesis and characterization of drug-conjugated organic molecules designed for gelation and metallogelation. • Assessment of plausible applications of drug-conjugated gels, including catalytic performance, stability, and functional utility. Group H • Investigation of Water oxidation catalysis by mixed metal oxides. • Investigation of Water oxidation catalysis by surface confined molecular heterogeneous catalysts. • Investigation of electro catalytic pathways pertinent to electrosynthesis
Course Overview	Theory: 1. Biological Metal Homeostasis & Transport: Explores the mechanisms of essential and toxic metal ion transport across biological membranes, including ion channels, pumps, and siderophore-mediated iron acquisition. 2. Metalloenzyme Structure-Function Relationships: Provides an in-depth analysis of hydrolytic Zn-enzymes (Carbonic anhydrase, Carboxypeptidase), Ni-enzyme (Urease), and their catalytic mechanisms involving metal centers as Lewis acids. 3. Energy Conversion in Nature: Examines the inorganic chemistry behind Photosystem II (Mn_4CaO_5 cluster for water oxidation), Nitrogenase (FeMo-cofactor for N_2 fixation), and respiratory enzymes (Cytochrome C-oxidase for O_2 reduction). 4. Molecular Symmetry in Chemical Bonding: Applies group theory to construct Symmetry Adapted Linear Combinations (SALCs) and qualitatively build Molecular Orbital diagrams for coordination complexes with representative symmetries. 5. Spectroscopic Interpretation via Symmetry: Utilizes character tables and group theory to understand electronic selection rules, d-orbital splitting patterns in various ligand fields, and the interpretation of UV-Vis spectra using Tanabe-Sugano diagrams. 6. Electron Transfer Dynamics: Covers the fundamentals of inner-sphere and outer-sphere electron transfer mechanisms, the Marcus Theory (including the inverted region), and Proton-Coupled Electron Transfer (PCET) processes in chemical and biological systems. 7. Ligand Participation in Catalysis: Introduces the concept of redox non-innocent ligands and demonstrates how they enable transition metal complexes to perform small molecule activation

	(O₂, N₂, CO₂, H₂) and C-H functionalization. 8. Sustainable Inorganic Chemistry: Surveys modern applications of inorganic compounds in energy conversion and storage technologies, including solar energy harvesting, fuel cells, and electrocatalytic pathways for sustainable chemical synthesis Practical: 1. Multidisciplinary Research-Oriented Projects: Engages students in hands-on research spanning diverse areas including fluorescence spectroscopy (protein-drug interactions), atomic absorption spectroscopy (drug purity), advanced organic synthesis (Click chemistry, RCM), nanomaterial characterization, and computational chemistry with coding and GitHub documentation. 2. Catalysis & Electrocatalysis: Provides practical training in synthesizing transition metal complexes with redox-active ligands and evaluating their performance as homogeneous catalysts (e.g., alcohol dehydrogenation) and electrocatalysts (e.g., Nitrogen Reduction Reaction, Water Oxidation), along with the synthesis and characterization of functional materials like FRET-based chemosensors and drug-conjugated metallogels.
Course Outcomes (COs)	CO1: Explain the mechanisms of metal ion transport across biological membranes, including ion channels, pumps, and siderophore-mediated acquisition, and describe the role of metal ions in biological homeostasis. CO2: Analyze the structure-function relationships and catalytic mechanisms of key metalloenzymes (carbonic anhydrase, carboxypeptidase, urease, photosystem II, nitrogenase, cytochrome c oxidase, and superoxide dismutase) in terms of metal center reactivity. CO3: Apply group theory principles to construct Symmetry Adapted Linear Combinations (SALCs) and qualitatively build molecular orbital diagrams for coordination compounds of representative symmetries. CO4: Utilize character tables and group theory to interpret electronic spectra of transition metal complexes, including predicting d-orbital splitting patterns, selection rules, and using Tanabe-Sugano and correlation diagrams. CO5: Differentiate between inner-sphere and outer-sphere electron transfer mechanisms, explain the Marcus Theory (including the inverted region), and describe Proton-Coupled Electron Transfer (PCET) processes. CO6: Evaluate the role of redox non-innocent ligands in transition metal complexes and explain their application in small molecule activation (O₂, N₂, CO₂, H₂) and C-H functionalization. CO7: Discuss the principles and applications of biomimetic modelling, chelation therapy, and anticancer drugs, highlighting the interdisciplinary connection between inorganic chemistry and

	medicine. CO8: Summarize modern applications of inorganic compounds in sustainable energy conversion and storage technologies, including solar energy harvesting, fuel cells, and electrocatalytic synthesis. CO9: Execute advanced laboratory experiments involving fluorescence spectroscopy, atomic absorption spectroscopy, and nanomaterial characterization to assess drug-protein interactions, drug purity, and particle properties. CO10: Synthesize and characterize transition metal complexes with redox-active ligands and evaluate their catalytic performance in homogeneous reactions (e.g., alcohol dehydrogenation) and electrocatalytic processes (e.g., Nitrogen Reduction Reaction, Water Oxidation). CO11: Perform multi-step organic and inorganic syntheses (including click chemistry, RCM, peptide synthesis, and FRET-based chemosensors) and characterize products using appropriate spectroscopic and analytical techniques. CO12: Apply computational chemistry tools and coding skills to perform global minimum optimization, implement clustering algorithms, and document and share code packages on GitHub for chemical problem-solving.
Program Outcomes (POs)	PO1: Fundamental Knowledge: Demonstrate a comprehensive understanding of core concepts in chemistry, including organic, inorganic, physical, analytical, and biochemistry. PO2: Laboratory Skills: Acquire hands-on experience in laboratory techniques and instrumentation, applying safety protocols and proper methodologies to conduct experiments and analyse results. PO3: Problem Solving: Develop critical thinking and problem-solving skills by applying chemical principles to real-world scenarios, including the ability to design experiments and interpret data. PO4: Research Competency: Engage in independent and collaborative research projects, employing scientific methods to formulate hypotheses, conduct experiments, and communicate findings effectively. PO5: Interdisciplinary Applications: Understand the interdisciplinary nature of chemistry, exploring its applications in fields such as medicine, environmental science, materials science, and nanotechnology. PO6: Communication Skills: Effectively communicate scientific information, both verbally and in written form, to diverse audiences, demonstrating the ability to present complex ideas clearly and concisely. PO7: Ethics and Sustainability: Recognize the ethical implications and responsibilities of scientific research and practice in chemistry, emphasizing the importance of sustainability and environmental stewardship in chemical practices.

CO #	Course Outcome Summary	Bloom's Taxonomy (K-Level)	Mapped POs	
CO1	Metal ion transport	K2 (Understand)	PO1, PO5	
CO2	Metalloenzyme catalysis mechanisms	K4 (Analyze)	PO1, PO3, PO5	
CO3	SALCs & MO diagrams	K3 (Apply)	PO1, PO3	
CO4	Group theory in spectroscopy	K4 (Analyze)	PO1, PO3, PO4	
CO5	Electron transfer mechanisms	K4 (Analyze)	PO1, PO3, PO5	
CO6	Redox non-innocent ligands	K5 (Evaluate)	PO1, PO3, PO4, PO7	
CO7	Bioinorganic medicine applications	K2 (Understand)	PO1, PO5, PO7	
CO8	Energy conversion & storage	K2 (Understand)	PO1, PO5, PO7	
CO9	Spectroscopy & nanomaterial analysis	K3 (Apply)	PO2, PO3, PO4, PO5	
CO10	Catalysis & electrocatalysis evaluation	K5 (Evaluate)	PO2, PO3, PO4, PO5, PO7	
CO11	Multi-step synthesis & characterization	K3 (Apply)	PO2, PO3, PO4, PO5	
CO12	Computational chemistry & coding	K3 (Apply)	PO2, PO3, PO4, PO6	
Reading/Reference Lists		1. Douglas, B.E. and McDaniel, D.H. Concepts & Models of Inorganic Chemistry Oxford, 1970. 2. Atkin, P. Shriver & Atkins' Inorganic Chemistry, 5th Ed., Oxford University Press (2010).		

	3. Cotton, F.A., Wilkinson, G. and Gaus, P.L., Basic Inorganic Chemistry 3rd Ed.; Wiley India. 4. Sharpe, A.G., Inorganic Chemistry, 4th Indian Reprint (Pearson Education) 2005. 4. Huheey, J. E.; Keiter, E.A. & Keiter, R.L. Inorganic Chemistry, Principles of Structure and Reactivity 4th Ed., Harper Collins 1993, Pearson, 2006. 5. Mingos, D.M.P., Essential trends in inorganic chemistry. Oxford University Press (1998). 6. Housecraft, C. E.; Sharpe, A. G., (2018), Inorganic Chemistry, 5th Edition, Pearson. 7. Wulfsberg, G (2002), Inorganic Chemistry, Viva Books Private Limited.	
Evaluation	Theory: 60 Internal: 15 (CIA: 10; Other form of Assessment: 2; Attendance: 3) Semester Exam: 45	Practical: 40 CA: 38; Attendance: 2
Paper Structure for Theory Semester Exam	Answer THREE out of FOUR questions, of 15 marks each.	