Semester	**7**
Programme	**CHEMISTRY**
Course	**MAJOR (INORGANIC CHEMISTRY 7)**
Paper Code	**C4CH230722T / C4CH230722P**
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 Organometallic Chemistry: Oxidative additions, Reductive Eliminations, Migratory Insertions, β-Hydride Elimination, Phosphine ligands in catalysis (stereo-electronic effects), Fischer and Schrock Carbenes and Carbynes, Organometallic catalysis (including Wilkinson's Catalyst, Cobalt and Rhodium catalysts in hydroformylation, Ziegler-Natta Catalysis, Wacker process), Asymmetric hydrogenation reactions, Directing group catalysis **Module 2 (12 Lectures)** Advanced Coordination chemistry: d-orbital splitting in linear, triangular, trigonal bipyramidal, square pyramidal environment, Thermodynamic and Kinetic stability of coordination complexes, Kinetics of octahedral substitution, Crystal Field Activation Energy, Ligand field effects, Mechanism of substitution in octahedral complexes, Substitution reactions in square planar complexes, Trans- effect and its application in complex synthesis, theories of trans effect, Mechanism of nucleophilic substitution in square planar complexes, **Module 3 (12 Lectures)** Magnetochemistry and Chemistry of f-block elements: Orbital and spin magnetic moments, spin only moments of dn ions and their correlation with effective magnetic moments, including orbital contribution; quenching of magnetic moment: super exchange and antiferromagnetic interactions (elementary idea with examples only); L-S coupling, Single Molecular Magnets (preliminary idea). Lanthanoids and Actinoids: General Comparison on Electronic configuration, oxidation states, colour, spectral and magnetic properties. **Practical** Group A • Singlet –state dimerization processes in certain specific molecules. • Isolation and identification of essential oils from citrus fruit peels. • Determination of the fluorescence quantum yield with respect to certain standard compounds.

	Group B • Spectral analysis (NMR and IR) of redox non-innocent ligands possessing conjugated azo skeleton. • Investigation of the redox behaviour and electronic structures of certain imino-quinone type of ligands using spectroscopic, electrochemical, and theoretical methods. • NMR and Infra-red spectroscopic characterization of conjugated pyridyl/ benzothiazole ligands. Group C • O-alkylation/ arylation of Diisopropylidene D- glucose. • Synthesis of symmetrically di/ tri substiruted aryl derivatives. • Click reaction. Group D • Study of variation in cmc of surfactants on variation of temperature. • Analysis of thermodynamic parameters of micellization process. • Effect of additives on micellization of surfactants. Group E • Implementation of a pairwise potential energy function (e.g., Lennard-Jones or Morse) and calculation of analytical gradients and Hessian. • Development of a deterministic Optimization scheme like Steepest Descent or Conjugate Gradient algorithm for function minimization. • Interfacing the potential energy function with the local minimizer to relax random molecular structures to their nearest local minima. Group F • Preparation of coumarin based sensors - Isolation and purification of the product. • Preparation of coumarin based sensors - ii) Characterisation of the product. • Preparation of coumarin based sensors - iii) Photo physical (UV- VIS) and Luminescence studies. Group G • Synthesis of metal–organic frameworks under solvothermal, hydrothermal, or ambient laboratory conditions. • Synthesis of metallacycles and coordination polymers using suitable metals and organic ligands. • Structural and physicochemical characterization of metallacycles, metal–organic frameworks, and coordination polymers.

	Group H • Spectral analysis (NMR and IR) of redox non-innocent ligands possessing macrocylic amine/amide skeleton. • Investigation of the redox behaviour and electronic structures of different ligand frameworks capable of Water Oxidation catalysis using multiple spectroscopic methods. • Electrochemical investigations of mixed metal oxide compounds.
Course Overview	**Theory:** 1. **Master Fundamental Organometallic Reactions:** Students will develop a deep mechanistic understanding of the core reactions that drive catalytic cycles, including oxidative addition, reductive elimination, migratory insertion, and β-hydride elimination. 2. **Analyze Industrial Catalytic Processes:** The course provides a critical analysis of major industrial homogeneous catalytic processes, including hydroformylation, Ziegler-Natta polymerization, and the Wacker process, linking molecular-level mechanisms to large-scale applications. 3. **Evaluate Ligand Design Principles:** Students will learn to assess and predict the influence of ligand properties—specifically the stereo-electronic effects of phosphines—on the activity and selectivity of organometallic catalysts. 4. **Understand Advanced Coordination Geometries:** The curriculum extends beyond classic octahedral complexes to systematically analyze d-orbital splitting patterns and electronic structures in linear, triangular, trigonal bipyramidal, and square pyramidal environments. 5. **Differentiate Thermodynamic and Kinetic Stability:** Students will be able to distinguish between thermodynamic and kinetic stability in coordination complexes and apply concepts like Crystal Field Activation Energy (CFAE) to predict substitution rates in octahedral complexes. 6. **Apply the Trans Effect in Synthesis:** The course covers the mechanistic theories behind the trans effect and its practical application as a powerful tool for the stereospecific synthesis of square planar complexes. 7. **Interpret Magnetic Properties of Metal Complexes:** Students will learn to interpret magnetic susceptibility data, correlating spin-only moments with effective magnetic moments, and understand concepts like orbital contribution, quenching, and superexchange in transition metal and lanthanide systems. 8. **Explore f-Block Element Chemistry:** The course provides a comparative study of lanthanoids and actinoids, analyzing their unique electronic configurations, variable oxidation states, and the resulting spectral and magnetic properties that distinguish them from d-block elements.

	Practical: 1. **Apply Advanced Analytical and Synthetic Techniques:** In the laboratory, students will gain hands-on proficiency in a range of modern techniques, including multi-nuclear NMR and IR spectroscopy for characterizing redox-active ligands, fluorescence spectroscopy for quantum yield determination, and electrochemical methods for investigating catalytic processes. 2. **Develop Interdisciplinary Research Skills**: The practical component is designed to bridge chemistry sub-disciplines, requiring students to synthesize complex molecules (e.g., coumarin-based sensors, MOFs), perform computational chemistry (e.g., potential energy function optimization), and investigate real-world problems like water oxidation catalysis and micellization thermodynamics.

Course Outcomes (COs)	**CO1 :**Recall and explain the mechanisms of fundamental organometallic reactions, including oxidative addition, reductive elimination, migratory insertion, and β-hydride elimination. **CO2:** Analyze the role of stereo-electronic properties of phosphine ligands in influencing the activity and selectivity of homogeneous catalysts. **CO3:** Distinguish between Fischer and Schrock carbenes/carbynes and predict their reactivity based on electronic structure. **CO4:** Evaluate the mechanisms and applications of industrially significant catalytic processes, such as hydroformylation, Ziegler-Natta catalysis, and the Wacker process. **CO5:** Analyze the d-orbital splitting patterns and predict the electronic spectra and magnetic properties of complexes in linear, triangular, trigonal bipyramidal, and square pyramidal geometries. **CO6:** Differentiate between thermodynamic and kinetic stability in coordination compounds and apply concepts like Crystal Field Activation Energy (CFAE) to predict substitution rates in octahedral complexes. **CO7:** Apply the mechanistic theories of the trans effect to design synthetic routes for specific square planar complexes. **CO8:** Interpret magnetic susceptibility data to correlate spin-only moments with effective magnetic moments, and explain concepts like orbital contribution, quenching, and superexchange in transition metal and f-block systems. **CO9:** Synthesize and purify complex organic-inorganic hybrid molecules (e.g., coumarin-based sensors, MOFs, metallacycles) using appropriate laboratory techniques. **CO10:** Analyze and interpret spectroscopic (NMR, IR, UV-Vis) and electrochemical data to characterize the structure and redox behavior of coordination compounds and catalysts. **CO11:** Implement a computational algorithm (e.g., Steepest Descent) and utilize a potential energy function to optimize

	molecular structures and calculate analytical gradients. **CO12:** Investigate the thermodynamic parameters of a physicochemical process (e.g., micellization) and correlate the effects of additives and temperature on the system.
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	**Core Reaction Mechanisms**	**K2 (Understand)**	**PO1**
CO2	**Ligand Stereo-electronic Effects**	**K4 (Analyze)**	**PO1**
CO3	**Carbene/Carbyne Distinction**	**K4 (Analyze)**	**PO1, PO3**
CO4	**Industrial Catalysis Evaluation**	**K5 (Evaluate)**	**PO1, PO3**
CO5	**Advanced d-Orbital Splitting**	**K4 (Analyze)**	**PO1**

CO6	**Stability & Substitution Rates**	**K3 (Apply)**	**PO1**
CO7	**Trans Effect in Synthesis**	**K3 (Apply)**	**PO1, PO3**
CO8	**Magnetic Property Interpretation**	**K4 (Analyze)**	**PO1, PO3**
CO9	**Advanced Synthesis Skills**	**K3 (Apply)**	**PO2,PO3, PO4,PO7**
CO10	**Spectroscopic & Electrochemical Analysis**	**K4 (Analyze)**	**PO2, PO3, PO4,PO7**
CO11	**Computational Chemistry Application**	**K3 (Apply)**	**PO2, PO3, PO4,PO7**
CO12	**Physicochemical Investigation**	**K4 (Analyze)**	**PO2, PO3, PO4,PO7**

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.	