Semester	**8**
Programme	**CHEMISTRY**
Course	**MAJOR (PHYSICAL CHEMISTRY 7)**
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	**Theory:** **Statistical Mechanics 2 (12 lectures)** 1. Thermodynamic parameters and function for different ensembles: 2. Fluctuation in thermodynamic quantities 3. Heat capacity of solids – Einstein and Debye treatment. 4. Preliminary idea of Quantum Statistics 5. Indistinguishable and distinguishable particles 6. Derivation of Fermi-Dirac and Bose-Einstein Statistics 7. Classical limits of Fermi-Dirac and Bose-Einstein distribution 8. Application of the quantum statistics for deriving thermodynamic properties of ideal Bose-Einstein and Fermi-Dirac systems 9. Conduction electron 10. Black-body radiation 11. Bose Einstein condensation 12. Density matrix (introduction only) 13. Liouville theorem 14. Quantum Liouville theorem and its consequences **Group Theory 2 (12 lecture)** 1. The basis functions, projection and transfer operators (Bloch) 2. Reduction of a representation 3. The standard reduction formula 4. The direct product representation and its decomposition 5. Use of the projection operator to form symmetry adapted linear combination (SALC) of a simple system. 6. Spectroscopic Selection Rule 7. Normal Modes and vibrational spectroscopy 8. MO construction in pi and sigma bonded systems 9. Woodward-Hoffman Rules **Polymer chemistry & Adsorption (12 Lectures)** 1. Polymer and degree of polymerization 2. Thermoplastic and thermoset 3. Linear and branched chain polymer 4. Branching in a polymer: copolymerization and backbiting 5. Chain growth and step growth polymerization 6. Tacticity of polymers and its consequence on the physical properties

	7. Physical categories of polymers: glass transition temperature 8. Kinetics of free-radical polymerization 9. End-to-end distance of a straight chain homopolymer: unrestricted and restricted bond angle 10. Radius of gyration of a straight chain homopolymer 11. Thermodynamics of polymer solution: lattice model 12. Molecular weight of polymer 13. Number and weight average molecular weight, experimental determination 14. Adsorption of gases on solid surfaces 15. Physisorption and chemisoption: potential energy surface 16. Adsoption isotherm and their interpretation 17. Capillary condensation: explanation 18. Derivation of Langmuir adsorption isotherm 19. BET adsorption isotherm 20. Bio-polymers **Practical:** Group A • Drug delivery systems in aqueous medium at Physiological pH in 'natural supramolecular systems' • A novel insight into the interactions of different tea extracts with multi-tryptophan proteins and their related antimicrobial status. • Protein conformation in nanocavities - a theoretical study Group B • Synthesis of suitable coordination polymer of 3d transition elements • Exploration of Coordination polymers as heterogeneous catalyst in C-C bond formation. • Exploring the role of Coordination polymers as electro-catalyst in CO2RR. Group C • Synthesis of macrocycles involving RCM reactions. • Synthesis of macrocycles involving Click reactions. • Synthesis of polypeptides. Group D • Study of behaviour of surfactant in aqueous polymeric solution using tensiometry. • Study of behaviour of surfactant in aqueous polymeric solution using viscometry. • Study of behaviour of surfactant in aqueous polymeric solution using spectrophotometry. 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 trivalent Chemosensors: i) Isolation and. Purification, ii) Characterisation, iii) Photo physical studies • Synthesis of DFPC based fluorescent probes: i)Isolation and. Purification, ii) Characterisation, iii) Photo physical studies

	• Synthesis of excimer based chemosensors: i)Isolation and. Purification, ii) Characterisation, iii) Photo physical studies Group G • Design and synthesis of azo-phenol based organic ligands and exploring their redox properties. • Preparation of lanthanide based Metal-Organic Frameworks and coordination polymers. • Designing metal-organic materials for purification of impurities from industrial wastewater. Group H • Synthesis and characterization of dianionic tridentate and tetradentate ligand frameworks • Synthesis and characterization of of Metal complexes of containing dianionic tridentate and tetradentate ligand frameworks • Investigation of Oxygen reduction, Nitrate reduction and similar multielectron catalytic processes and pathways using electrochemistry and chemical techniques.
Course Overview	**Theory:** Specialized course designed for final-year students, focusing on the rigorous application of statistical mechanics and group theory to quantum and macroscopic systems. Statistical Mechanics 2 (Module I): Extends the foundational Boltzmann statistics to complex ensembles. It explores thermodynamic fluctuations, heat capacity models for solids (Einstein and Debye), and provides a deep dive into quantum statistics (Fermi-Dirac and Bose-Einstein). It covers critical phenomena like Bose-Einstein condensation and introduces the Density Matrix and Liouville's Theorem. Group Theory 2 (Module II): Advances the application of group theory in quantum chemistry. It covers basis functions, projection/transfer operators (Bloch), the reduction of representations, and the use of the Great Orthogonality Theorem to form Symmetry Adapted Linear Combinations (SALCs). Applications in Spectroscopy & Bonding (Module III): Bridges theoretical group theory with practical spectral interpretation, focusing on Spectroscopic Selection Rules, Normal Mode analysis for vibrations, and MO construction for pi and sigma bonded systems.
Course Outcomes	**CO1 [Ensembles, Fluctuations & Heat Capacity]:** Derive thermodynamic parameters and functions for different statistical ensembles, analyze fluctuations in thermodynamic quantities, and apply the Einstein and Debye treatments to compute the heat capacity of solids. **CO2 [Quantum Statistics]:** Derive the Fermi-Dirac and Bose-Einstein distribution laws for indistinguishable particles, evaluate their classical limits, and apply quantum statistics to derive the thermodynamic properties of conduction electrons, black-body radiation, and Bose-Einstein condensation.

	CO3 [Density Matrix & Liouville Theorem]: Introduce the density matrix formalism and apply the (quantum) Liouville theorem to describe the time evolution of statistical ensembles. **CO4 [Representation Reduction & SALCs]:** Apply basis functions, projection/transfer (Bloch) operators, and the standard reduction formula to decompose representations and direct products, and construct Symmetry Adapted Linear Combinations (SALCs) for simple molecular systems. **CO5 [Spectroscopic & Bonding Applications of Group Theory]:** Apply group-theoretical selection rules to predict vibrational spectroscopic (normal mode) activity, construct molecular orbitals in pi- and sigma-bonded systems, and explain pericyclic reaction outcomes using the Woodward-Hoffmann rules. **CO6 [Polymer Classification, Synthesis & Kinetics]:** Classify polymers by structure, synthesis mechanism (chain-growth and step-growth polymerization), and tacticity, and analyze the kinetics of free-radical polymerization and the physical consequences of the glass transition temperature. **CO7 [Polymer Solution Statistics & Molecular Weight]:** Calculate the end-to-end distance and radius of gyration of a homopolymer chain, apply the lattice model to describe the thermodynamics of polymer solutions, and determine the number- and weight-average molecular weight of a polymer. **CO8 [Adsorption Isotherms]:** Distinguish between physisorption and chemisorption using potential energy surfaces, derive the Langmuir and BET adsorption isotherms, and explain the phenomenon of capillary condensation. **CO9 [Coordination Polymer & Macrocyclic Synthesis for Catalysis]:** Synthesize coordination polymers and macrocyclic/polypeptide compounds (via RCM and click chemistry) and evaluate their efficacy as heterogeneous and electrocatalysts (e.g., for C-C bond formation and CO_2RR). **CO10 [Surfactant-Polymer & Biomolecular Interactions]:** Investigate the physicochemical behaviour of surfactants in aqueous polymeric solutions using tensiometric, viscometric, and spectrophotometric methods, and study supramolecular drug-delivery systems and protein-ligand binding interactions. **CO11 [Chemosensor Synthesis & Photophysical Characterization]:** Synthesize and photophysically characterize chemosensor and fluorescent probe molecules, including trivalent, DFPC-based, and excimer-based systems. **CO12 [Functional Coordination Materials for Catalysis & Remediation]:** Design and synthesize functional coordination materials (azo-phenol ligands, lanthanide MOFs, and dianionic

	polydentate ligand complexes) and evaluate their efficacy in redox catalysis, multielectron electrochemical processes, and environmental remediation (e.g., industrial wastewater purification). **CO13 [Computational Optimization & Software Development]:** Develop and implement computational optimization algorithms (global minimization and clustering) for molecular systems, and document and release the resulting software package using version-control platforms (e.g., GitHub).
Program Outcomes	**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 #	Core Curriculum Domain	Bloom's Taxonomy (K-Level)	Mapped POs
CO1	Ensembles, Fluctuations & Heat Capacity	**K3** (Apply), **K4** (Analyze)	PO1, PO3
CO2	Quantum Statistics (FD/BE)	**K4** (Analyze), **K5** (Evaluate)	PO1, PO3
CO3	Density Matrix & Liouville Theorem	**K2** (Understand)	PO1, PO3
CO4	Representation Reduction & SALCs	**K3** (Apply), **K4** (Analyze)	PO1, PO3
CO5	Spectroscopic & Bonding Applications	**K3** (Apply), **K4** (Analyze)	PO1, PO3
CO6	Polymer Classification, Synthesis & Kinetics	**K3** (Apply), **K4** (Analyze)	PO1, PO3
CO7	Polymer Solution Statistics & Molecular Weight	**K3** (Apply)	PO1, PO3
CO8	Adsorption Isotherms	**K3** (Apply), **K4** (Analyze)	PO1, PO3
CO9	Coordination Polymer & Macrocyclic Synthesis	**K3** (Apply), **K5** (Evaluate)	PO2, PO4
CO10	Surfactant-Polymer & Biomolecular Interactions	**K3** (Apply), **K4** (Analyze)	PO2, PO3, PO5
CO11	Chemosensor Synthesis & Photophysical Characterization	**K3** (Apply), **K6** (Create)	PO2, PO4, PO5
CO12	Functional Coordination Materials & Remediation	**K5** (Evaluate), **K6** (Create)	PO2, PO5, PO7
CO13	Computational Optimization & Software Development	**K4** (Analyze), **K6** (Create)	PO2, PO4, PO6

<table>
<tr><td>Reading/Reference Lists</td><td colspan="2">Theory:

1. Sears, F.W., Salinger, G. L., Thermodynamics, Kinetic Theory, and Statistical Thermodynamics (Addison-Wesley Principles of Physics Series), Pearson; 3rd edition.

2. Metiu, H., Physical Chemistry: Statistical Mechanics, Taylor and Francis

3. Laud, B.B., Statistical Mechanics, New Age

4. Chandler, D., Introduction to Modern Statistical Mechanics 1st Edition, OUP

5. Mcquarrie, D.A., Statistical Mechanics, Viva

6. Pathria, R.K., Beale, P.D., statistical Mechanics, Academic Press

7. Bishop, D.M., Group Theory and Chemistry (Dover Books on Chemistry), Dover

8. Cotton, F.A., Chemical Applications of Group Theory, 3ed, Wiley

9. Davidson, G., Group Theory for Chemists, Palgrave Macmillan

10. Jaffe, H.H., Orchin, M., Symmetry in Chemistry, Dover

Practical:</td></tr>
<tr><td>Evaluation</td><td>Theory: 60
Internal: 15 (CIA: 10; Other form of Assessment: 2; Attendance: 3)
Semester Exam: 45</td><td>Practical: 40
CA: 38; Attendance:2</td></tr>
<tr><td>Paper Structure for Theory Semester Exam</td><td colspan="2">Answer THREE out of FOUR questions, of 15 marks each.</td></tr>
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