Semester	**7**
Programme	**CHEMISTRY**
Course	**MAJOR (PHYSICAL CHEMISTRY 6)**
Paper Code	**C4CH230732T / C4CH230732P**
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 and Reaction Rate Theories 1 (12 Lectures)** 1. Energy states and levels 2. Micro and macro states 3. Thermodynamic probability 4. Entropy and probability 5. Nernst Heat Theorem and 3rd law of thermodynamics 6. Maxwell-Boltzmann statistics 7. Distribution of molecular states: Boltzmann distribution 8. Application to Maxwell's velocity distribution and barometric distribution 9. Partition function and its significance 10. Translational, rotational and vibrational partition function and their significance 11. Thermodynamic properties (internal energy, enthalpy, Helmholtz free energy, Gibb's free energy, chemical potential, entropy and value of beta) 12. Reaction coordinate and PES 13. Transition state theory and activated complex 14. Expression of rate constant in terms of partition function, the Eyring equation **Spectroscopy II (12 Lectures)** 1. Vibration of a diatomic molecule and simple harmonic oscillator 2. Review of Solution of quantum harmonic oscillator (general expression) 3. Selection rule for harmonic oscillator 4. Spectrum 5. Anharmonicity and its effect on energy levels 6. Selection rule for anharmonic oscillator 7. Vibrational spectrum 8. Rotational – vibrational coupling in the limit of Born-Oppenheimer approximation 9. Raman spectroscopy (Qualitative) 10. Rayleigh and Raman scattering 11. Polarizability ellipsoids 12. Features and condition for Raman activity (for linear and non-linear AB2 molecule) 13. Rotational and vibrational Raman spectra and its characteristics

	Intermolecular Forces (12 lectures) 1. van der Waal's forces, its importance in colloid chemistry. 2. Colloid Stability, van der Waals attraction, and potential energy curves. 3. Molecular interactions and power laws. 4. Molecular origins of van der Waals attraction. 5. Macroscopic implications. 6. van der Waals forces between large particles and over large distances. 7. Electromagnetic radiation of the London force. 8. Calculation of van der Waals forces between macroscopic bodies. 9. DLP theory 10. Theory of coagulation in dilute dispersion: rapid and slow coagulation 11. Hamaker constant for several systems and introduction to DLVO theory. **Practical:** Group A • To identify different plastic recyclable classes using infrared spectra. • Study of the binding efficiency of certain antibiotics with globular proteins – theoretical correlation. • FTIR analysis of benzoic acids samples. Group B • Investigating the suitability of redox non-innocent ligands possessing conjugated azo skeleton to act as an electrocatalyst to bring about CO2RR. • Assessing conjugated imino-quinone type of ligands as homogeneous catalyst for alcohol dehydrogenation and cascade synthesis of N-heterocycles. • Exploring the potential of conjugated pyridyl/ benzothiazole ligands as anti-microbials. Group C • Synthesis of di/ tri peptides incorporating sugar unit. • Different cyclisation/ cycloaddition reactions involving appropriate precursors. • Different types of allylation/ propargylation reactions of sugar derivatives. Group D

	• Determination of cmc in mixture of surfactants in aqueous medium. • Thermodynamic analysis of mixed surfactant solution in aqueous solution. • Analysis of interaction between surfactants in mixture. Group E • Interfacing the potential energy function with the local minimizer to relax random molecular structures to their nearest local minima. • Implementation of a Simulated Annealing algorithm with adjustable cooling schedules. • Application of Simulated Annealing algorithm for Lennard-Jones cluster optimization. Group F • Synthesis of Rhodamine based fluorophores - i) Isolation and purification of the product. • Synthesis of Rhodamine based fluorophores - ii) Characterisation of the product. • Synthesis of Rhodamine based fluorophores - iii) Photo physical (UV- VIS and Luminescence studies). Group G • Evaluation of heterogeneous catalytic activity of the synthesized materials in selected chemical transformations. • Assessment of interaction with metals and water purification properties of the synthesized coordination materials. • Study of biocatalytic applications and recyclability of metallacycles, metal–organic frameworks, and coordination polymers. Group H • Investigation of different electrode surfaces (Carbon, garpehene, ITO, FTO, Pt) for electrocatalysis. • Benchmarking different electrode surfaces for efficient electron kinetics. • Digital Simulation of different electron transfer kinetic phenomena and reaction mechanisms pertinent to catalysis.
Course Overview	**Theory:** A composite course bridging the microscopic quantum world with macroscopic thermodynamic observables, alongside high-level instrumental and computational laboratory training.

	• Statistical Mechanics & Reaction Rate Theories (Module I): Explores the probabilistic foundations of thermodynamics, transitioning from micro/macro states and Boltzmann distributions to the calculation of partition functions (translational, rotational, vibrational). It applies these concepts to chemical kinetics via the Potential Energy Surface (PES), activated complexes, and the Eyring equation in Transition State Theory. • Spectroscopy II (Module II): Investigates the quantum mechanics of molecular vibrations, moving from ideal harmonic oscillators to anharmonic limits. It introduces rotational-vibrational coupling under the Born-Oppenheimer limit and provides a detailed exploration of Raman spectroscopy, Rayleigh scattering, and polarizability ellipsoids for linear and non-linear molecules. • Intermolecular Forces & Colloids (Module III): Focuses on the origins and macroscopic implications of van der Waals forces. It provides a rigorous theoretical treatment of colloidal stability, coagulation kinetics, Hamaker constants, and the DLVO theory. **Practical:** • Practical Component (Groups A–H): Features a highly diverse, research-oriented laboratory curriculum. Students engage in advanced FTIR analysis, electrocatalysis (e.g., CO_2 reduction), synthesis of peptides and fluorophores, surfactant thermodynamics, and computational chemistry (e.g., Simulated Annealing algorithms for Lennard-Jones cluster optimization and digital simulation of electron transfer).
Course Outcomes	**CO1 [Statistical-Mechanical Foundations]:** Relate the thermodynamic probability of a microstate distribution to entropy via Boltzmann's relation, connect this to the Nernst Heat Theorem and the Third Law of Thermodynamics, and apply the Boltzmann distribution to derive Maxwell's velocity distribution and the barometric distribution law. **CO2 [Statistical Thermodynamics]:** Calculate translational, rotational, and vibrational partition functions, and derive thermodynamic properties (internal energy, enthalpy, Helmholtz and Gibbs free energies, chemical potential, and entropy) from them. **CO3 [Reaction Rate Theories]:** Analyze Potential Energy Surfaces (PES) and apply Transition State Theory to derive the Eyring equation and compute reaction rate constants. **CO4 [Vibrational Spectroscopy]:** Evaluate the effects of anharmonicity and rotational-vibrational coupling on the energy levels and selection rules of diatomic molecules. **CO5 [Raman Spectroscopy]:** Differentiate between Rayleigh and Raman scattering, apply polarizability ellipsoids to predict the

	Raman activity of linear and non-linear molecules, and interpret the characteristics of rotational and vibrational Raman spectra. **CO6 [Molecular Origins of van der Waals Forces]:** Explain the molecular origins of van der Waals (dispersion/London) forces, their power-law distance dependence, and electromagnetic retardation effects, and extend these to calculate van der Waals interactions between macroscopic bodies using Hamaker constants. **CO7 [Colloidal Stability & DLVO Theory]:** Evaluate colloidal stability and the kinetics of rapid and slow coagulation in dilute dispersions using DLVO theory. **CO8 [Spectroscopic & Analytical Characterization]:** Execute FTIR spectroscopic analysis to classify plastics and characterize organic compounds (e.g., benzoic acid), and apply physicochemical methods to determine the critical micelle concentration and thermodynamics of mixed surfactant systems. **CO9 [Catalysis & Biomolecular Screening]:** Evaluate the catalytic efficacy of synthesized homogeneous, heterogeneous, and electrocatalytic materials (including redox-active ligands for CO_2RR and coordination polymers/MOFs, with attention to water-purification applications) in target transformations, and assess ligand-protein binding and antimicrobial activity through theoretical or spectroscopic correlation. **CO10 [Organic & Coordination Synthesis]:** Synthesize, isolate, and characterize complex organic and coordination compounds, including peptides, cyclisation/cycloaddition and allylation/propargylation products, and Rhodamine-based fluorophores, together with their photophysical (UV-Vis and luminescence) characterization. **CO11 [Computational & Electrochemical Methods]:** Implement Simulated Annealing algorithms to optimize molecular geometries (e.g., Lennard-Jones clusters), and benchmark and digitally simulate electron-transfer kinetics across different electrode surfaces (carbon, graphene, ITO, FTO, Pt).
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	Statistical-Mechanical Foundations	**K2** (Understand), **K3** (Apply)	PO1, PO3
CO2	Statistical Thermodynamics & Partition Functions	**K4** (Analyze), **K5** (Evaluate)	PO1, PO3
CO3	Transition State Theory & Eyring Equation	**K4** (Analyze)	PO1, PO3
CO4	Anharmonicity & Rovibrational Spectra	**K4** (Analyze)	PO1, PO3
CO5	Raman Scattering & Polarizability	**K3** (Apply), **K4** (Analyze)	PO1, PO3
CO6	Molecular Origins of vdW Forces & Hamaker Constants	**K2** (Understand), **K3** (Apply)	PO1, PO3
CO7	Colloidal Stability & DLVO Theory	**K4** (Analyze), **K5** (Evaluate)	PO1, PO3, PO5
CO8	Spectroscopic & Analytical Characterization	**K3** (Apply), **K4** (Analyze)	PO2, PO3

CO9	Catalysis & Biomolecular Screening	**K4** (Analyze), **K5** (Evaluate)	PO2, PO5, PO7
CO10	Organic & Coordination Synthesis	**K3** (Apply), **K6** (Create)	PO2, PO4
CO11	Computational & Electrochemical Methods	**K4** (Analyze), **K6** (Create)	PO2, PO4, PO5

Reading/Reference Lists	1. Bishop, D.M., Group Theory and Chemistry (Dover Books on Chemistry), Dover 2. Cotton, F.A., Chemical Applications of Group Theory, 3ed, Wiley 3. Davidson, G., Group Theory for Chemists, Palgrave Macmillan 4. Jaffe, H.H., Orchin, M., Symmetry in Chemistry, Dover 5. Wardle, D., Principles and Applications of Photochemistry, Wiley 6. Schulman, S.G., Fluorescence and Phosphorescence Spectroscopy: Physico-chemical Principles and Practice, Pergamon Press 7. Klessinger, M., Michl, J., Excited States and Photochemistry of Organic Molecules, VCH 8. Vemulapally, G.K., Physical Chemistry, Prentice Hall 9. Carraher, C.E., Jr., Polymer Chemistry, CRC Press Flory, T.J., Principles of Polymer Chemistry, Cornell University Press Tanford, C., Physical Chemistry of Macromolecules, John Wiley and Sons	
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.	