Semester	**2**
Programme	**CHEMISTRY**
Course	**MAJOR (PHYSICAL CHEMISTRY 1)**
Paper Code	**C1CH230221T**
Credits	**4 THEORY**
Hours/week	**4 (THEORY: 4)**
Category: Core/MDC/SEC/VEC	**CORE**
Theory/Practical/Composite	**THEORY**
Number of Modules	**4 (THEORY: 4)**
Syllabus	**Theory:** **Module 1: Chemical Thermodynamics 1 (12 Lectures)** 1. Why to study and what to study. 2. Basic concepts and definitions – Applicability of thermodynamics, thermodynamic systems and their classification, Universe, system, surroundings and different types of boundaries. 3. Zeroth law and temperature. 4. Processes, reversible and irreversible process, thermodynamic equilibrium and steady state. 5. Work and heat involved in a thermodynamic process. 6. Calculation of work in different type of processes 7. Thermometry and calculation of heat exchanged 8. First law and Concept of internal energy 9. Change in Internal energy and its calculation. 10. State and path functions, exact and inexact differentials. 11. Joule's experiment and consequences: ideal and van der Waals gases. 12. Enthalpy 13. Specific heat at constant volume and pressure, relationship between them and their differences for ideal and van der Waals gases 14. Joule-Thomson experiment 15. Thermo-chemistry and Standard states. 16. Kirchoff equation. 17. Definition of entropy change of the system 18. Entropy as a state function and calculation of entropy change in different type of processes 19. Entropy change of the surrounding; impact of vastness of the surrounding and its consequence in calculating entropy change of the surrounding **Module 2: Chemical Kinetics and Homogeneous Catalysis (12 Lectures)** 1. Rate of a reaction, rate law 2. Crude approximation: all binary collision leads to product. 3. Calculation of binary collision frequency and collision number in gaseous state. 4. Refinement: concept of activation energy and Boltzmann distribution to introduce the effect of activation energy in the rate law 5. Rate constant and its variation with temperature: Arrhenius

equation

6. Order of a reaction
7. Integrated rate laws and characteristic plots
8. Half-life and its significance
9. Determination of order of a reaction
10. Rate expression for complex reactions
11. Unimolecular reaction and reaction mechanism
12. Multi step reactions
13. Rate determining step
14. Zero and fractional order reactions
15. Steady state approximation and Equilibrium approximation
16. Arrhenius and van't Hoff complexes
17. Further refinement: steric requirements (Basic qualitative overview)
18. Catalysis: pseudo-order reaction
19. Homogeneous catalysis, criteria
20. Generalized acid- base catalysis

Module 3: Intermolecular Forces and Non-Ideal Gases (12 Lectures)

1. Ideal gases: absence of intermolecular force
2. Nature of Intermolecular forces: Charge-charge interaction, charge-dipole and dipole-dipole, dipole-induced dipole interaction
3. Lennard-Jones potential
4. Temperature dependence of intermolecular forces
5. Deviation from ideal behaviour: Andrew’s and Amagat’s experiment, Joule (qualitative idea) and Joule-Thompson experiment (qualitative idea)
6. Compressibility factor
7. van der Waals equation of state
8. A van der Waals gas at Critical state
9. Boyle temperature, inversion temperature and their form for a van der Waals gas.
10. Virial equation of state, first and second virial coefficient, their relation to other constants and their significance.
11. Reduced equation of state and the Law of corresponding states
12. Continuity of states

Module 4: Quantum Chemistry I (12 Lectures)

1. Black body radiation, Classical Theory of Rayleigh-Jean, Ultraviolet catastrophe and Planck’s theory, Thermodynamic viewpoint
2. Photoelectric effect, Einstein’s Quanta,
3. Compton effect
4. Dual nature of electromagnetic radiation
5. de Broglie’s hypothesis
6. Wave particle duality
7. Matter wave
8. Concept of wave packets

	9. Uncertainty principle: its various mathematical forms and its justifications
Course Overview	Theory: 1. This is a core theoretical course designed for Semester 2 students to provide a deep understanding of macroscopic and microscopic chemical behavior. 2. To enable students to develop a distinction between the macroscopic and microscopic viewpoints of matter. 3. The curriculum is divided into two primary domains: **Chemical Thermodynamics** and **Chemical Kinetics & Quantum Chemistry**. 4. Students will explore the laws of thermodynamics, entropy, and equilibrium, alongside the kinetic theories of gases and the mathematical foundations of quantum mechanics. 5. The course emphasizes the transition from classical observations to wave mechanical models, preparing students for advanced chemical analysis. 6. They will develop the concepts of classical thermodynamics at the macroscopic level and learn through problem solving at different levels of complexity, up to the first law of thermodynamics. 7. Students will be introduced to the various mechanistic aspects of chemical kinetics and will learn to formulate rate expressions based on various kinetic models. 8. Students will review the experimental results that over threw the concepts of classical physics. The conclusion derived from the experiments was that classical concepts of 'particle' and 'wave' blend together giving rise to a new set of rules that lead to the formulation of quantum mechanics.
Course Outcomes	Upon successful completion of this course, students will be able to: **CO1:** Define and differentiate thermodynamic systems, boundaries, and state vs. path functions. **CO2:** Apply the First Law of Thermodynamics to calculate work, heat, and internal energy changes for ideal and van der Waals gases under isothermal, adiabatic, and free-expansion conditions. **CO3:** Derive and apply thermodynamic relations (Joule-Thomson coefficient, Kirchhoff's equation) to analyze the enthalpy and heat-capacity behaviour of gases. **CO4:** Calculate entropy changes of the system and surroundings for different thermodynamic processes and apply entropy criteria to evaluate the spontaneity of a process. **CO5:** Construct rate laws and analyze reaction mechanisms, including multi-step and unimolecular reactions, using integrated rate equations and the steady-state and equilibrium approximations. **CO6:** Interpret the temperature dependence of reaction rates using the Arrhenius equation and Collision Theory. **CO7:** Evaluate the kinetics of homogeneous catalysis, including pseudo-order behaviour and generalized acid-base catalysis, to explain catalytic rate enhancement. **CO8:** Analyze the origin and temperature dependence of intermolecular forces (charge-charge, charge-dipole, dipole-dipole, and dipole-induced dipole interactions) using the Lennard-Jones potential. **CO9:** Evaluate the deviation of real gases from ideal behaviour using the compressibility factor, the van der Waals and virial equations of state, and the Law of Corresponding States. **CO10:** Explain the failure of classical mechanics (black-body radiation, photoelectric effect, Compton effect) and the necessity of wave-particle duality for electromagnetic radiation and sub-atomic

	particles. **CO11:** Apply de Broglie's hypothesis and the concept of wave packets to derive and interpret Heisenberg's Uncertainty Principle in its various mathematical forms.
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 Statement**	**Bloom's Taxonomy**	**Mapped POs**
CO1	**Define and differentiate thermodynamic systems, boundaries, and state vs. path functions.**	**K1 (Remember)**	**PO1**
CO2	**Apply the First Law of Thermodynamics to calculate work, heat, and internal energy changes for ideal and van der Waals gases under isothermal, adiabatic, and free-expansion conditions.**	**K3 (Apply)**	**PO1, PO3**
CO3	**Derive and apply thermodynamic relations (Joule-Thomson coefficient, Kirchhoff's equation) to analyze the enthalpy and heat-capacity behaviour of gases.**	**K4 (Analyze)**	**PO1, PO3**
CO4	**Calculate entropy changes of the system and surroundings for different thermodynamic processes and apply entropy criteria to evaluate the spontaneity of a process.**	**K4 (Analyze)**	**PO1, PO3**
CO5	**Construct rate laws and analyze reaction mechanisms, including multi-step and unimolecular reactions, using integrated rate equations and the steady-state and equilibrium approximations.**	**K4 (Analyze)**	**PO1, PO3**
CO6	**Interpret the temperature dependence of reaction rates using the Arrhenius equation**	**K3 (Apply)**	**PO1, PO3**

	and Collision Theory.		
CO7	**Evaluate the kinetics of homogeneous catalysis, including pseudo-order behaviour and generalized acid-base catalysis, to explain catalytic rate enhancement.**	**K5 (Evaluate)**	**PO1, PO7**
CO8	**Analyze the origin and temperature dependence of intermolecular forces (charge-charge, charge-dipole, dipole-dipole, and dipole-induced dipole interactions) using the Lennard-Jones potential.**	**K4 (Analyze)**	**PO1, PO3**
CO9	**Evaluate the deviation of real gases from ideal behaviour using the compressibility factor, the van der Waals and virial equations of state, and the Law of Corresponding States.**	**K4 (Analyze)**	**PO1, PO3**
CO10	**Explain the failure of classical mechanics (black-body radiation, photoelectric effect, Compton effect) and the necessity of wave-particle duality for electromagnetic radiation and sub-atomic particles.**	**K2 (Understand)**	**PO1, PO5**
CO11	**Apply de Broglie's hypothesis and the concept of wave packets to derive and interpret Heisenberg's Uncertainty Principle in its various mathematical forms.**	**K3 (Apply)**	**PO1, PO3**

Reading/Reference Lists	1. Atkins, P. W. & Paula, J. de Atkins', Physical Chemistry, Oxford University Press.

	2. Castellan, G. W. Physical Chemistry, Narosa. 3. McQuarrie, D. A. & Simons, J. D. Physical Chemistry: A Molecular Approach, Viva. 4. Levine, I. N. Physical Chemistry, Tata McGraw-Hill. 5. Rakshit, P.C., Physical Chemistry, Sarat Book House. 6. Moore, W. J. Physical Chemistry, Orient Longman. 7. Mortimer, R. G. Physical Chemistry, Elsevier. 8. Engel, T. & Reid, P. Physical Chemistry, Pearson. 9. Ball, D. W. Physical Chemistry, Thomson Press. 10. Vemulapalli, G. K, Physical Chemistry, Prentice Hall India. 11. Glasstone, S, Thermodynamics for Chemists, EWP. 12. Zemansky, M. W. & Dittman, R.H. Heat and Thermodynamics, Tata McGraw-Hill. 13. Denbigh, K. The Principles of Chemical Equilibrium Cambridge University Press. 14 Nag, A. K, Physical Chemistry Vol. 1, 2, Mcgraw Hill. 15. Klotz, I.M., Rosenberg, R. M. Chemical Thermodynamics: Basic Concepts and Methods Wiley. 16. Sears, F. W., Salinger, G. L., Thermodynamics, Kinetic Theory, and Statistical Thermodynamics (Addison-Wesley Principles of Physics Series), Pearson; 3rd edition. 17. Metiu, H., Physical Chemistry: Thermodynamics, Taylor and Francis. 18. Kaufman, M., Principles of Thermodynamics, Taylor and Francis. 19. Honig, J. M., Thermodynamics, Academic Press. 20. Laidler, K. J. Chemical Kinetics, Pearson. 21. Houston, P. L., Chemical Kinetics and Reaction Dynamics, Dover Publication Inc. 22. House, J.E., Principles of Chemical Kinetics, Academic Press. 23. Metiu, H., Physical Chemistry: Kinetics, Taylor and Francis. 24. Levine, I. N. Quantum Chemistry, PHI. 25. Atkins, P. W. and Friedman, Molecular Quantum Mechanics, Oxford. 26. Eisberg, R., Resnick, R, Quantum Physics of Atoms, Molecules, Solids, Nuclei and Particles, 2ed, Wiley.
Evaluation	Theory: 100 Internal: 30 (CIA:20, Other mode of Assesment:5, Attendance: 5) Semester Exam:70

Paper Structure for the End Semester Theory Examination	Answer SEVEN out of NINE questions, of 10 marks each.