Semester	2
Paper Number	C1CH230221T
Paper Title	Core
No. of Credits	4
Theory/Composite	Theory
No. of periods assigned	4
Name of Faculty member(s)	Asish Kumar Nag Rina Ghosh Indranil Chakraborty Rahul Sharma
Course description/objective	Theory: 1. To enable students to develop a distinction between the macroscopic and microscopic viewpoints of matter. 2. 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. 3. Students will be introduced to the various mechanistic aspects of chemical kinetics and will learn to formulate rate expressions based on various kinetic models. 4. 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.
Syllabus	Annexure Core Course
Learning Outcomes	Students will gain an understanding of: 1. the application of mathematical tools to calculate thermodynamic and kinetic properties. 2. the relationship between microscopic properties of molecules with macroscopic thermodynamic observables 3. the derivation of rate equations from mechanistic data 4. the use of simple models for predictive understanding of physical phenomena associated to chemical thermodynamics and kinetics 5. the limitations of classical mechanics at molecular length scales 6. the differences between classical and quantum mechanics
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.

Annexure Major Course

Chemical Thermodynamics I *(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

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

Intermolecular Forces and Non-Ideal Gases (12 Lectures)

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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

Quantum Chemistry I (12 lectures)

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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