Course: Discipline Specific Core 2

Semester	**1**
Paper Number	**HCHCR1022T (60 MARKS) & HCHCR1022P (40 MARKS)**
Paper Title	**CORE COURSE 2: PHYSICAL CHEMISTRY**
No. of Credits	**Theory-04, Practicals-02**
Theory/Composite	Composite
No. of periods assigned	Th: 4 Pr: 3
Name of Faculty member(s)	Dr. Asish K. Nag Dr. Rina Ghosh Dr. Indranil Chakraborty
Course description/objective	***Theory:*** 1. To enable students to develop a distinction between the macroscopic and microscopic viewpoints of matter. 2. In this context, students will be introduced to the microscopic world of the gaseous state and understand the statistical nature of distribution of molecular velocities, speeds and energies. 3. They will also develop the concepts of classical thermodynamics at the macroscopic level and learn through problem solving at different levels of complexity. 4. Students will be introduced to the various mechanistic aspects of chemical kinetics and will learn to formulate rate expressions based on various kinetic models. ***Practical:*** 1. To develop skills and to understand the underlying principles in acid-base titrimetric analysis. ***2.*** Using titrimetric analysis to perform kinetic experiments like decomposition of peroxide and acid catalysed hydrolysis of ester. ***3.*** To prepare buffers of a given pH. ***4.*** To fabricate simple instruments like a calorimeter to measure heat of solution of certain compounds.
Syllabus	Annexure Core Course: 3
Texts	
Reading/Reference Lists	**Theory:** 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 Press 4. Engel, T. & Reid, P. *Physical Chemistry*, Pearson 5. Levine, I. N. *Physical Chemistry*, Tata McGraw-Hill 6. Ball, D. W. *Physical Chemistry*, Thomson Press 7. Mortimer, R. G. *Physical Chemistry*, Elsevier 8. Laidler, K. J. *Chemical Kinetics*, Pearson 9. Glasstone, S. & Lewis, G.N. *Elements of Physical Chemistry* 10. Rakshit, P.C., *Physical Chemistry* Sarat Book House 11. Zemansky, M. W. & Dittman, R.H. *Heat and Thermodynamics*, Tata-McGraw-Hill

<table>
<tr><td></td><td>12. Rastogi, R. P. & Misra, R.R. An Introduction to Chemical Thermodynamics, Vikas
13. Koltz & Rosenberg, Chemical Thermodynamics

Practical:
1. Viswanathan, B., Raghavan, P.S. Practical Physical Chemistry Viva Books (2009)
2. Mendham, J., A. I. Vogel’s Quantitative Chemical Analysis 6th Ed., Pearson
3. Harris, D. C. Quantitative Chemical Analysis. 6th Ed., Freeman (2007)
4. Palit, S.R., De, S. K. Practical Physical Chemistry Science Book Agency
5. University Hand Book of Undergraduate Chemistry Experiments, edited by Mukherjee, G. N., University of Calcutta
6. Levitt, B. P. edited Findlay’s Practical Physical Chemistry Longman Group Ltd.
7. Gurtu, J. N., Kapoor, R., Advanced Experimental Chemistry S. Chand & Co. Ltd.</td></tr>
<tr><td>Evaluation</td><td><table>
<tr><td>Theory: 60 marks</td><td>Practical: 40 marks
(Continuous Assessment)</td></tr>
<tr><td>CIA: 10
End-Sem: 50</td><td>Internal Assessment Exams: 30
Viva (End Sem): 8
Attendance: 2</td></tr>
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<tr><td>Paper Structure for the End Sem Theory Exam (50 marks)</td><td>6 (SIX) Questions (each of 10 marks) will be set and the students will have to answer any 5 (FIVE).
Each of the Questions (10 marks) will consist of 2 or 3 parts (of 2/ 3/ 4/ 5)</td></tr>
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Annexure Core Course (CC): 2

(Credits: Theory-04, Practicals-02)

CHEMISTRY -C II: PHYSICAL CHEMISTRY-I

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

Kinetic Theory and Gaseous state **(20 Lectures)**

Kinetic Theory of gases: Concept of pressure and temperature; Collision of gas molecules; Collision diameter; Collision number and mean free path; Frequency of binary collisions (similar and different molecules); Wall collision and rate of effusion

Maxwell's distribution of speed and energy: Nature of distribution of velocities, Maxwell's distribution of speeds in one, two and three dimensions; Kinetic energy distribution in one, two and three dimensions, calculations of average, root mean square and most probable values in each case; Calculation of number of molecules having energy $\geq \varepsilon$, Principle of equipartition of energy and its application to calculate the classical limit of molar heat capacity of gases

Real gas and virial equation: Deviation of gases from ideal behavior; compressibility factor; Boyle temperature; Andrew's and Amagat's plots; van der Waals equation and its features; its derivation and application in explaining real gas behaviour, other equations of state (Berthelot, Dietrici); Existence of critical state, Critical constants in terms of van der Waals constants; Law of corresponding states; virial equation of state; van der Waals equation expressed in virial form and significance of second virial coefficient; Intermolecular forces (Debye, Keesom and London interactions; Lennard-Jones potential - elementary idea)

Chemical Thermodynamics **(25 Lectures)**

Zeroth and 1^{st} law of Thermodynamics: Intensive and extensive variables; state and path functions; isolated, closed and open systems; zeroth law of thermodynamics; Concept of heat, work, internal energy and statement of first law; enthalpy, H; relation between heat capacities, calculations of q, w, U and H for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions; Joule's experiment and its consequence.

Thermochemistry: Standard states; Heats of reaction; enthalpy of formation of molecules and ions and enthalpy of combustion and its applications; Laws of thermochemistry; bond energy, bond dissociation energy and resonance energy from thermochemical data, Kirchhoff's equations and effect of pressure on enthalpy of reactions; Adiabatic flame temperature; explosion temperature

Second Law: Need for a Second law; statement of the second law of thermodynamics; Concept of heat reservoirs and heat engines; Carnot cycle; Physical concept of Entropy; Carnot engine and refrigerator; Kelvin – Planck and Clausius statements and equivalence of the two statements with entropic formulation; Carnot's theorem; Values of §dQ/T and Clausius inequality; Entropy change of systems and surroundings for various processes and transformations; Entropy and unavailable work; Auxiliary state functions (G and A) and their variation with T, P and V. Criteria for spontaneity and equilibrium.

Thermodynamic relations: Maxwell's relations; Gibbs- Helmholtz equation, Joule-Thomson experiment and its consequences; inversion temperature; Joule-Thomson coefficient for a van der Waals gas; General heat capacity relations

c) Chemical kinetics **(15 Lectures)**

Rate law, order and molecularity: Introduction of rate law, Extent of reaction; rate constants, order; Forms of rates of First, second and nth order reactions; Pseudo first order reactions (example using acid catalyzed hydrolysis of methyl acetate); Determination of order of a reaction by half-life and differential method; Opposing reactions, consecutive reactions and parallel reactions (with explanation of kinetic and thermodynamic control of products; all steps first order)

Role of Temperature and theories of reaction rate: Temperature dependence of rate constant; Arrhenius equation, energy of activation; Rate-determining step and steady-state approximation – explanation with suitable examples; Collision theory; Lindemann theory of unimolecular reaction; outline of Transition State theory (classical treatment)

Homogeneous catalysis: Homogeneous catalysis with reference to acid-base catalysis; Primary kinetic salt effect; Enzyme catalysis; Michaelis-Menten equation, Lineweaver-Burk plot, turn-over number

Autocatalysis; periodic reactions

CHEMISTRY LAB-C II LAB

(60 Lectures)

Experiment 1: Construction of a simple calorimeter.

Experiment 2: Determination of the heat of solution of simple compounds by solubility measurements.

Experiment 3: Study of kinetics of acid-catalyzed hydrolysis of methyl acetate by titrimetric method.

Experiment 4: Study of kinetics of decomposition of H_2O_2 by titrimetric method.

Experiment 5: Preparation of buffers in the acidic, neutral and alkaline ranges using a pH meter.