Course: Discipline Specific Core 5

Semester	**3**
Paper Number	**HCHCR3052T (60 MARKS) & HCHCR3052P (40 MARKS)**
Paper Title	**CORE COURSE 5: 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:*** **Applications of Thermodynamics** Concept of chemical potential is developed showing that it is a particular case of properties called partial molar quantities. Then it explores how to use the chemical potential of a substance to describe the physical properties of mixtures. The concept of chemical potential is used to account for the equilibrium composition of chemical reactions. The former corresponds to a minimum in the Gibbs energy plotted against the extent of reaction. The thermodynamic formulation of equilibrium enables one to establish the quantitative effects of changes in the conditions like temperature and pressures. **Foundation of Quantum Mechanics** This part reviews 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. The Schrodinger equation will be introduced with the ground work of operators. Some examples with zero and non-zero potentials will be discussed. Solution of the corresponding Schrodinger equation, leading to the eigenstates and corresponding eigenvalues will be analysed. Finally, students will be taught how determination of the average quantities lead to the uncertainty Principle, one of the most profound departures from classical mechanics. **Transport properties** The focus here is on molecular motion. The concept of flux and the relation between flux and force will be introduced. Expressions will be derived that govern the migration of properties through matter. One of the most useful consequences of this general approach is the formulation of the diffusion equation. ***Practical:*** 1. Experimental method of determining the viscosity of solutions and studying the concentration dependence. Realisation of the conditions governing the validity of Poiseullie’s equation. 2. Study of precipitation titrations and construction and explanation of the curves. 3. Obtaining the conductance variation of a mixture containing both strong and weak acids and indication of the neutralisation points. Explaining the variations from the point of view of ionic mobilities. 4. Using the conductometric method to study time dependences of the concentration of reactant/product of a chemical reaction. Obtaining the correct plot for determination of the rate constant of the reaction. 5. Performing conductance measurements in weakly conducting solutions and verifying the dilution law. Learning to calculate the pK_a of weak acids.
Syllabus	Annexure Core Course: 5
Texts	

<table>
<tr>
<td>Reading/Reference Lists</td>
<td>
Theory:

1. Atkins, P. W. & Paula, J. de Atkins’, Physical Chemistry, Oxford University Press
Castellan, G. W. Physical Chemistry, Narosa
McQuarrie, D. A. & Simons, J. D. Physical Chemistry: A Molecular Approach, Viva Press
Levine, I. N. Physical Chemistry, Tata McGraw-Hill
Rakshit, P.C., Physical Chemistry, Sarat Book House
Moore, W. J. Physical Chemistry, Orient Longman
Mortimer, R. G. Physical Chemistry, Elsevier
Denbigh, K. The Principles of Chemical Equilibrium Cambridge University Press
Engel, T. & Reid, P. Physical Chemistry, Pearson
Levine, I. N. Quantum Chemistry, PHI
Atkins, P. W. and Friedman, Molecular Quantum Mechanics, Oxford
Zemansky, M. W. & Dittman, R.H. Heat and Thermodynamics, Tata-McGraw-Hill
Rastogi, R. P. & Misra, R.R. An Introduction to Chemical Thermodynamics, Vikas
Klotz, I.M., Rosenberg, R. M. Chemical Thermodynamics:Basic Concepts and Methods Wiley
Glasstone, S. An Introduction to Electrochemistry, East-West Press

Practical:

1. Viswanathan, B., Raghavan, P.S. Practical Physical Chemistry Viva Books (2009)
Mendham, J., A. I. Vogel’s Quantitative Chemical Analysis 6th Ed., Pearson
Harris, D. C. Quantitative Chemical Analysis. 6th Ed., Freeman (2007)
Palit, S.R., De, S. K. Practical Physical Chemistry Science Book Agency
University Hand Book of Undergraduate Chemistry Experiments, edited by Mukherjee, G. N., University of Calcutta
Levitt, B. P. edited Findlay’s Practical Physical Chemistry Longman Group Ltd.
Gurtu, J. N., Kapoor, R., Advanced Experimental Chemistry S. Chand & Co. Ltd.

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<td>Evaluation</td>
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<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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<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>
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Annexure Core Course (CC): 5

(Credits: Theory-04, Practicals-02)

CHEMISTRY -C V: PHYSICAL CHEMISTRY-II

(Credits: Theory-04, Practicals-02)

Theory: 60 Lectures

a) Transport processes **(15 Lectures)**

Fick's law: Flux, force, phenomenological coefficients & their inter-relationship (general form), different examples of transport properties

Viscosity: General features of fluid flow (streamline flow and turbulent flow); Newton's equation, viscosity coefficient; Poiseuille's equation; principle of determination of viscosity coefficient of liquids by falling sphere method; Temperature variation of viscosity of liquids and comparison with that of gases

Conductance and transport number: Ion conductance; Conductance and measurement of conductance, cell constant, specific conductance and molar conductance; Variation of specific and equivalent conductance with dilution for strong and weak electrolytes; Kohlrausch's law of independent migration of ions; Equivalent and molar conductance at infinite dilution and their determination for strong and weak electrolytes; Debye –Huckel theory of Ion atmosphere (qualitative)-asymmetric effect, relaxation effect and electrophoretic effect; Ostwald's dilution law; Ionic mobility; Application of conductance measurement (determination of solubility product and ionic product of water); Conductometric titrations

Transport number, Principles of Hittorf's and Moving-boundary method; Wien effect, Debye-Falkenhagen effect, Walden's rule

b) Applications of Thermodynamics – I **(25 Lectures)**

Partial properties and Chemical potential: Chemical potential and activity, partial molar quantities, relation between Chemical potential and Gibb's free energy and other thermodynamic state functions; variation of Chemical potential (μ) with temperature and pressure; Gibbs-Duhem equation; fugacity and fugacity coefficient; Variation of thermodynamic functions for systems with variable composition; Equations of states for these systems, Change in G, S H and V during mixing for binary solutions

Chemical Equilibrium: Thermodynamic conditions for equilibrium, degree of advancement; van't Hoff's reaction isotherm (deduction from chemical potential); Variation of free energy with degree of advancement; Equilibrium constant and standard Gibbs free energy change; Definitions of K_P, K_C and K_X; van't Hoff's reaction isobar and isochore from different standard states; Shifting of equilibrium due to change in external parameters e.g. temperature and pressure; variation of equilibrium constant with addition to inert gas; Le Chatelier's principle and its derivation

Nernst's distribution law; Application- (finding out K_{eq} using Nernst dist law for $KI+I_2 = KI_3$ and dimerization of benzene

Chemical potential and other properties of ideal substances- pure and mixtures: a) Pure ideal gas-its Chemical potential and other thermodynamic functions and their changes during a change of; Thermodynamic parameters of mixing; Chemical potential of an ideal gas in an ideal gas mixture; Concept of standard states and choice of standard states of ideal gases

b) Condensed Phase – Chemical potential of pure solid and pure liquids, Ideal solution – Definition, Raoult's law; Mixing properties of ideal solutions, chemical potential of a component in an ideal solution; Choice of standard states of solids and liquids

c) Foundation of Quantum Mechanics (20 Lectures)

Beginning of Quantum Mechanics: Wave-particle duality, light as particles: photoelectric and Compton effects; electrons as waves and the de Broglie hypothesis; Uncertainty relations (without proof)

Wave function: Schrodinger time-independent equation; nature of the equation, acceptability conditions imposed on the wave functions and probability interpretations of wave function

Concept of Operators: Elementary concepts of operators, eigenfunctions and eigenvalues; Linear operators; Commutation of operators, commutator and uncertainty relation; Expectation value; Hermitian operator; Postulates of Quantum Mechanics

Particle in a box: Setting up of Schrodinger equation for one-dimensional box and its solution; Comparison with free particle eigenfunctions and eigenvalues. Properties of PB wave functions (normalisation, orthogonality, probability distribution); Expectation values of x, x^2, p_x and p_x^2 and their significance in relation to the uncertainty principle; Extension of the problem to two and three dimensions and the concept of degenerate energy levels

Simple Harmonic Oscillator: setting up of the Schrodinger stationary equation, energy expression (without derivation), expression of wave function for n = 0 and n = 1 (without derivation) and their characteristic features

CHEMISTRY LAB-C V LAB

(60 Lectures)

Experiment 1: Study of viscosity of unknown liquid (glycerol, sugar) with respect to water and the variation of ⍰⍰with concentration.

Experiment 2: Conductometric titration to determine the solubility product of sparingly soluble salts like AgCl.

Experiment 3: Determination of molecular weight of polymers by viscosity measurements.

Experiment 4: Conductometric titration of an acid (strong, weak/ monobasic, dibasic) against strong base

Experiment 5: Study of saponification reaction conductometrically

Experiment 6: Verification of Ostwald’s dilution law and determination of K_a of weak acid