Name of the Programme: M.Sc. Part-I (Chemistry)

Course Code: CHP-500 **Title of the course:** General Physical Chemistry

Number of Credits: 04

Effective from AY: 2022-23

Prerequisites for the course:	Students should have studied chemistry courses at graduate level or must have cleared change of discipline entrance test conducted by Goa University.	
Course Objective:	1. Introduction of various concepts on thermodynamics. 2. Introduction of electro chemistry and kinetics. 3. Learning quantum chemistry.	
Content	**1. Mathematical Preparations** a. Introduction to various functions and function plotting (exponential, logarithmic, trigonometric etc.), functions of many variables. Complex numbers and complex functions. b. Linear equations, vectors, matrices and determinants. c. Basic rules of differentiation and integration, Partial differentiation, location and characterization of critical points of a function, Regression methods, curve fitting. d. Introduction to series, convergence and divergence, power series, Fourier series e. Probability (permutations and combinations).	No of hours 12
	2. Quantum Chemistry a. Operators, Functions, Eigen value equations, Postulates. b. Schrodinger equation, application to simple system viz. free particle, particle in one dimensional, two dimensional and three-dimensional box (quantization, separation of variables, degenerate wave functions). c. Hydrogen like atoms, Schrodinger equation and its solutions, atomic orbital wave functions and interpretation. d. Hückel MO theory, Secular equations, Secular determinant, delocalization energy, charge density, π-bond order, free valence, applications to C_2H_4, C_3H_5 (radical), C_4H_6, C_4H_4, C_6H_6, C_6H_8.	20
	3. Thermodynamics a. Thermodynamic properties: Gas laws, Real gasses, Boyle temperature, Critical temperature, State and path properties. Intensive and extensive properties. Exact and inexact differentials. Internal energy, enthalpy, entropy, free energy and their relations and significances. Maxwell relations. Thermodynamic equations of state b. Joule-Thomson effect. Joule-Thomson coefficient for van der Waals' gas. Joule-Thomson effect and production of low	12

	temperature, adiabatic demagnetization, Joule-Thompson coefficient, inversion temperature. c. The third law of thermodynamics. Need for the third law. Apparent exceptions to third law. Application of third law. Use of thermodynamic functions in predicting direction of chemical change. Entropy and third law of thermodynamics. d. Phase equilibria: Phase rule, Discussion of two component systems forming solid solutions with and without maximum or minimum in freezing point curve. Systems with partially miscible solid phases. e. Three component systems: Graphical representation. Three component liquid systems with one pair of partially miscible liquids. Influence of temperature. Systems with two pairs and three pairs of partially miscible liquids. The role of added salts.	
	4. Electrochemistry a. EMF series, The cell potential: The Nernst equation, Cells at equilibrium. Determination of thermodynamic functions. b. Decomposition potential and overvoltage, electronegativity, basic principles, completeness of deposition, Separation with controlled potentials, constant current electrolysis, composition of electrolyte, potential buffers, physical characteristics of metal deposits. c. Electroplating and electroless plating, electrosynthesis. d. Concepts of acid-base aqueous and non-aqueous solvents, hard and soft acid-base concept and applications.	8
	5. Chemical Kinetics a. General introduction to various types of order of reaction including fractional order, Molecularity of the reaction. b. Introduction to reversible and irreversible reactions and reactions leading to equilibrium. Van't Hoffs equation and analysis of Gibbs free energy of equilibrium reactions. c. Collision Theory and Maxwell Boltzmann distribution of energies of colliding molecules (derivation not required). The concept of collisional cross section and reactive cross section and its significance. d. Comparative study of transition state and collision state theory (derivation not required). e. Reaction Mechanisms: elementary reactions, Consecutive elementary reactions, steady state approximation, the rate determining step and pre-equilibria f. Free radical reactions, Complex reactions such as acetaldehyde decomposition and reaction between H_2 and Br_2, Homogeneous reactions and acid-base catalysis. g. Elementary enzyme reactions. Lineweaver-Burk plot and its analysis	8

Pedagogy	Mainly lectures and tutorials. Seminars / term papers /assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.
References / Readings	1. P. W. Atkins and J. D. Paula, Physical Chemistry, 8th Ed., Oxford University Press, New Delhi. 2007 2. G. M. Barrow, Physical Chemistry, 5th Ed., Tata McGraw Hill, New Delhi. 2016 3. J. E. House, Principles of Chemical Kinetics, 2nd Ed., Academic Press, Elsevier Burlington, USA, 2007 4. I. N. Levine, Quantum Chemistry, 7th Ed., Prentice-Hall, New Delhi. 1999
Course outcomes:	1. Students should be in a position to understand and explain various concepts in physical chemistry. 2. Students should be in a position to apply these concepts during the lab course in physical chemistry. 3. Students will understand concepts of electrochemistry. 4. Students will be able to apply fundamentals of chemical kinetics for understanding reaction mechanisms.