Syllabus
M.Sc. (Chemistry) Programme
(SEMESTER – I)

Physical Chemistry – I
Programme Code- (MSCCH -21)
Course Code – (MSCCH -503)
Block I Thermodynamics

Unit 1: Classical Thermodynamics

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropy. Partial molar quantities and their physical significance. Concepts of activity and fugacity.

Unit 2: Statistical Thermodynamics

Role and importance of Statistical Mechanics in Chemistry, Fundamentals of Statistical Mechanics, Concept of distribution, Thermodynamic probability and most probable distribution. Types of statistics: Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac Statistics. Idea of microstates and macrostates. Thermodynamic probability (W) for the three types of statistics. Derivation of Distribution laws (most probable distribution) for the three types of statistics. Lagrange's undetermined multipliers. Stirling's approximation, Molecular partition function and its importance.

Unit 3 Applications of Statistical Mechanics

The molecular partition function and its factorization. Evaluation of translational, rotational and vibrational partition functions for monoatomic, diatomic and ploy atomic gases. The electronic and nuclear partition functions. Calculation of thermodynamic properties of ideal gases in terms of partition function. Statistical definition of entropy. Calculation of equilibrium constants of gaseous solutions in terms of partition function, perfect gas mixtures. Specific Heat of solids- Einstein and Debye Theory of heat capacities of monatomic solids. Third Law of Thermodynamics, Residual Entropy.

Block II Chemical Kinetics and Catalysis

Unit 4 Theories of Reaction Rates

Collision theory. Potential energy surfaces (basic idea). Transition state theory (both thermodynamic and statistical mechanics formulations). Theory of unimolecular reactions, Lindemann mechanism, Hinshelwood treatment, RRKM model (qualitative treatment).

Unit 5 Solution Kinetics

Factors affecting reaction rates in solution. Effect of solvent (dielectric constant) and ionic strength (primary salt effect) on the rate constant. Secondary salt effects.

Unit 6 The Fast Reaction Kinetics

Relaxation methods, flow and flash photolysis. Preliminary ideas of molecular reaction dynamics. Kinetics of Chain reaction involving Hydrogen- Chlorine, Hydrogen- Bromine reaction and pyrolysis of acetaldehyde. Kinetics of enzyme reactions.

Unit 7 Catalysis

Gibbs adsorption isotherm, estimation of surface area (BET equation without derivation), catalytic activity at surfaces.

Block III Electrochemistry

Unit 8 Electrochemistry-I

Debye-Huckel theory theory for electrolytic solution, recall of activity, activity coefficients and their determination including ionic strength, electrochemistry of solution, Debye-Huckel treatment of dilute solutions.

Unit 9 Electrochemistry-II

Determination of activity coefficient, Debye-Huckel theory of strong electrolytes with derivation, ionic atmosphere and thickness of ionic atmosphere, Debye-Huckel-Onsagar theory, theory of conduction, Onsagar equation including mathematical deduction, overvoltage and decomposition potential.