Approval: 8th Senate Meeting

Course Name: Chemical Thermodynamics and Electrochemistry

Course Number: CY514

Credits: 3-0-0-3

Prerequisites: B.Sc. (with Chemistry) or Teachers Consent

Intended for: UG/PG

Distribution: Core

Semester: Even

Course Preamble: This course has designed to keep a view that students will begin their studies with the different laws of thermodynamics and will apply them to understand different physical phenomena. In first module they will learn about thermodynamics and statistical thermodynamics. In second semester they will learn about equilibrium and non equilibrium thermodynamics. The third module will start with the application of Gibbs' energy in thermodynamics and further extension will be on the study of electrochemistry, kinetics of electrode reactions and overall understanding of the electrochemical processes.

Course Outline:

Unit-I The Laws of Thermodynamics [10 lectures]

Zeroth law of Thermodynamics, Equilibrium, State Functions, Probability and distribution, Chemical Systems and Surroundings, temperature, equations of state First Law of thermodynamics : Internal energy, heat capacity, enthalpy, Isothermal, Adiabatic and Isobaric Processes , Energy, Enthalpy and Exact Differentials, Heat Capacities, Joule Thompson Effect, Heat Engines and Heat Pumps Second Law of thermodynamics: Entropy, Carnot cycles, heat engines, spontaneous changes, enthalpy and surrounding, Gibbs energy and application of Gibbs Energy Third Law of Thermodynamics: Concept of the absolute zero temperature

Statistical Thermodynamics [8 lectures]

Kinetic theory of gases, Probability and Maxwell Boltzmann distribution, Molecular Partition Functions, Thermodynamics from partition Functions, Equilibrium Constants, canonical ensemble ;ideal monoatomic, diatomic and polyatomic gases, quantum statistics Electronic, Vibrational, Rotational Partition Functions, Translational Partition Function, Heat Capacities, Heat Capacities of Solids, Debye and Einstein Models

Unit-II Equilibrium and Nonequilibrium Thermodynamics [10 lectures]

Equilibrium: Free Energy and Equilibria, Application of Gibbs energy for Phase change, Helmoltz Free Energies, Gibbs Helmoltz Equation, Free Energies of Formation, phase rule, Clapeyron equation, phase diagram, Ideal and non-ideal solutions, gases, liquids and solutions, equation of states, Fugacities and their determination,Entropy and Free Energy of Mixing, Partial Molal Quantities and the Chemical Potential, Activities and Activity Coefficients, Debye Huckel Theory and Extensions, the Nernst equation, colligative properties, multicomponent phase diagram, Determination of Activity Coefficients **[2 lectures]**

Nonequilibrium Thermodynamics: Postulates and significance of nonequilibrium thermodynamics, Entropy Production for heat transfer, chemical reactions and diffusion, Onsager's formulation and limitations, Onsager's reciprocity relation – verification using chemical reactions, electrokinetic and thermoelectric effects-I, Onsager's reciprocity relation – verification using chemical reactions, electrokinetic and thermoelectric effects-II, Conductance of electrolytes using Onsager's approach.

Unit-III Electrochemistry and Kinetics of Electrode reactions:

[6 Lectures]

Electrochemistry: Introduction and over view of electrochemical processes:

[4 Lectures]

Electrochemical cell and reactions, Faradic and nonfaradiac processes, electrochemical Experiments and variables in electrochemical cells, Basic electrochemical thermodynamics, free energy and cell EMF, half reaction and reduction potentials, formal potentials , reference electrodes , measurements of potential differences, Electrochemical potentials, liquid junction potential.

Kinetics of Electrode reactions [8 lectures]

Essentials of electrode reactions, Butler Volmmer Model for electrode kinetics, One step, one electron process through potential energy diagram, standard rate constants and transfer coefficients, equilibrium condition and exchange current,

Text Books:

1. Molecular Thermodynamics by Donald A Mcquarrie and Simon Viva Student Edition byViva Books Private Limited (2010)

2. Modern Electrochemistry, Volume 1 and 2, J.O.M Bokris and A.K.N, Reddy Plenum Press N.Y. (1970)

3. Electrochemical Methods second edition, A.J. Bard and L.R. Faulkner, John Wiley and Son (2001).

Reference Books:

1. Chemical Thermodynamics by Glasstone **Publisher:** Lightning Source Inc(year 2007 March)

2. Physical Chemistry by Thomas Engel and Philips Reid Pearson Education; Third edition (2013)

3. Physical Chemistry books by Berry Rice and Ross published by OUP USA; 2 edition (11 May 2000)