

INTRODUCTION TO CHEMICAL THERMODYNAMICS AND KINETICS

PROF.ARIJIT KUMAR DE Department of Chemical Sciences IISER Mohali

INTENDED AUDIENCE : BSc/BS/BE/BTech/Int-MSc/Int-MTech 1st or 2nd year students

COURSE OUTLINE :

This course will cover classical thermodynamics and kinetics developed to explain a variety of macroscopic physico-chemical phenomena with applications in Chemistry. This course is designed as an introductory level course to the broad area of thermodynamics and kinetics and the lectures will be pitched at the level of undergraduates (both freshman and sophomore level).

ABOUT INSTRUCTOR :

Prof. Arijit Kumar De completed his BSc (2003) with Chemistry major from University of Calcutta (WB, India) and MSc (2005) in Chemistry from IIT Kanpur (UP, India). He pursued his PhD with Debabrata Goswami at IIT Kanpur (2005-2010). He was a postdoctoral fellow at Lawrence Berkeley National Lab and University of California Berkeley (CA, USA) with Graham R. Fleming (2010-2014). In 2014, he joined IISER Mohali (PB, India) as an Assistant Professor in the Department of Chemical Sciences.

COURSE PLAN :

Week 1: Review of states of matter, Equations of state for ideal and real gases, Heat capacities at constant volume and pressure. Introduction to Thermodynamics, Laws of thermodynamics, Zeroth law. **Week 2**: First law, Concept of work and heat, Work done in reversible and irreversible processes.

Week 3: Concept of enthalpy, Joule's experiment and Joule-Thompson experiment, Thermochemistry.

Week 4: Second law, Concept of entropy, Carnot cycle, Clausius inequality, Concept of maximum work.

Week 5: Gibbs and Helmholtz free energies, Maxwell's relations, Chemical potential, Gibbs-Helmholtz equation, Gibbs-Duhem equation.

Week 6: Phase equilibrium, Clapeyron equation and Clausius-Clapeyron equation, Phase rule, Phase diagrams of one and two-component systems.

Week 7: Thermodynamics of mixtures, Partial Molar Properties, Ideal, Ideal-dilute and Real Solutions, Colligative properties.

Week 8: Chemical equilibrium, Equilibrium constant, van't Hoff equation, Le Chatelier's principle.

Week 9: Equilibrium electrochemistry, Types of electrochemical cells, Standard electrode potential, Nernst equation, Liquid junction potential.

Week 10: Introduction to chemical kinetics, rate laws for elementary reactions of different orders, competing reactions.

Week 11: Mechanisms of composite reactions, steady state and rate determining step approximations, homogeneous (acid-base catalysis and enzyme catalysis) and heterogeneous catalysis (Langmuir adsorption isotherm).

Week 12: Temperature dependence of rate constant, Introduction to gas-phase chemical reaction dynamics, Maxwell-Boltzman distribution of molecular speeds and its application in collision theory, Unimolecular reactions.