Programme: M. Sc. Part-II (Chemistry)
Title of the Course: Thermodynamics and Reaction Kinetics
Course Code: PCC-502
Number of Credits:03 **Effective from AY:** 2019-20

Prerequisites for the course:	Should have studied the courses PCC-401, PCC-402 and PCO-401. Should have basic knowledge of Physical Chemistry.	No. of lectures
Course Objectives:	To introduce to classical & non-equilibrium thermodynamics. To introduce advances in reaction kinetics.	
Course Outcomes:	Students should be in a position to understand various concepts of thermodynamics and kinetics. Students should be in a position to apply the knowledge of thermodynamics and kinetics for their lab course in physical chemistry, dissertation and research work.	
Content:	2. **Equilibrium Thermodynamics** 1.1 Thermodynamic state functions. Exact and inexact differentials; partial derivatives. Maxwell relations. 1.2 Thermodynamic equations of state. Temperature and pressure dependence of Gibbs function. Gibbs-Helmholtz equation. Partial molar quantities. Free energy change accompanying a chemical reaction, chemical potential, Gibbs-Duhem equation. Duhem-Margules equation. 1.3 Entropy of mixing for gases and liquids. Gibbs paradox. 1.4 Thermodynamic derivation of phase rule. **2. Non-equilibrium Thermodynamics** 2.1 Concept of internal entropy and spontaneity of a process in relation to free energy. Chemical affinity and extent of a reaction. Mass and energy balance equations. Entropy production in heat flow, chemical reactions and open system. 2.2 Postulates and methodologies, linear laws, Gibbs equations, Onsager's reciprocal theory. Validity of Onsager's equation and its verification. Application to thermo-electric and electro-kinetic phenomena. **3. Reaction Kinetics** 3.1 Collision theory of reaction rates and treatment of unimolecular reactions. Theory of absolute reaction rates and its applications to reactions in solution. Thermodynamic study from reaction kinetics, comparison of results with Eyring and Arrhenius Equations. Solvent and salt effects; influence of ionic strength and solvent on the rates of reaction, primary and secondary salt effects. 3.2 Mechanism of photochemical, chain, coupled and Reversible reactions. Oscillatory reactions. Chemical Hysteresis in Belousov-Zhabotinskii reaction. 3.3 Fast reactions and study by stopped flow technique, relaxation method, pulse radiolysis, flash photolysis and magnetic resonance methods. 3.4 Homogeneous catalysis and Michaelis-Menten kinetics. Kinetic	9 hours 9 hours 18 hours

	rate law for autocatalytic reactions. Kinetics of heterogeneous reactions, heterogeneous catalysis, inhibition, product induced and non–reactive inhibition. 3.5 Potential energy surfaces and introduction to molecular reaction dynamics, theoretical calculation of energy of activation, chemical lasers.	
Pedagogy:	Mainly lectures/ tutorials /assignments/ presentations/ self-study or a combination of these could also be used. Sessions shall be interactive in nature to enable peer group learning.	
Text Books/ Reference Books	1. P.W. Atkins & J. De. Paulo, *Atkins' Physical Chemistry*, Oxford Univ. Press, 2007, 8th Ed. 2. J. Rajaram, J.C. Kuriacose, S.N. & Co., *Thermodynamics for students of Chemistry, Classical, Statistical and Irreversible*, Jalandhar, 1996. 3. E. N. Yeremin, *Fundamentals of Chemical Thermodynamics*. 4. K.J. Laidler, *Chemical Kinetics*, Tata McGraw, New Delhi, 1985. 5. D. A. McQuarrie & John D. Simon, *Physical Chemistry*, Viva Books Pvt. Ltd., New Delhi.	