Approval: 8th Senate Meeting

Course Name: Reaction Dynamics, Kinetics and Catalysis

Course Number: CY513

Credits: 3-0-0-3

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

Intended for: UG/PG

Distribution: Core

Semester: Odd/Even

Course Preamble: The main focus of this course is to provide the students with deeper understanding how the physical chemistry's riles and theories could be used to understand the dynamics of a chemical reaction.

Course Outline:

1. [12 Lecture]

Introduction Review of kinetic theory of gases, the kinetic model of gases, collisions with walls and surfaces, the rate of effusions, transport properties of a perfect gas, atomic and molecular collisions, collisional theory, diffusion controlled reactions, thermodynamics properties of diffusion, potential energy surface, generation, interpretation and correlation with reaction energetics; elementary ideas on conical intersection.

2. [12 Lecture]

The rates of a chemical reactions Rate theories Transition state theory and RRKM theory, scattering - classical and quantum. Reactive Collisions Potential energy surfaces, atom-diatom reactions, polyatomic reactions, state-selective, molecular beams, reaction rates and cross sections

3. [6 Lecture]

Catalytic Reactions, homogeneous catalysis, energetics, homogeneous active sites, activation and deactivation, auto catalysis and its mechanism

4. [10 Lecture]

Synthesis and reaction of polymers; thermodynamics and kinetics of polymerization; Chemical structure andmorphology, Kinetics and mechanism of chain growth and step growthpolymerisation. Fibre forming polymers, ring-opening polymerization; water-soluble polymers, gels and hydrogels; chemical aspects to polymer processing, polymer surface and its modification; introduction to

industrial polymers; application of polymers in medicine, nanotechnology, electronics; eco-friendly polymers: biodegradable, bio-sourced polymers, polymers from renewable resources

Text Books

1. R. D. Levine, Molecular Reaction Dynamics, Cambridge University Press 2005.2.
2. Theories of Molecular Reaction Dynamics, Henriksen & Hansen, Oxford University Press 2008.

Reference Books

1. Physical Chemistry: A Molecular Approach by Donald A. McQuarrie and John D. Simon, Viva Books, First South Asia Edn. 1998.
2. Physical Chemistry by Peter Atkins and Julio de Paula (Oxford University Press 7th Edn. 2002
3. Photodissociation Dynamics, by R. Schinke, cabbridge University Press 1993.
4. Principles of Polymerization, 4th edition, by G. Odian; John Wiley and Sons, Inc. 2004;
5. Introduction to Physical Polymer Science, 4th Edition L. H. Sperling, Wiley, 2006.