Title of the course: Reaction Kinetics

Credits: 3
Coordinator: Keszei, Ernő

Department: Physical Chemistry

Prerequisits: B.Sc. courses physical chemistry 1 and 2

Topics of the course:

Molecular theories of chemical reactions. The Collision Theory. Potential energy surfaces. Quasi-equilibrium and dynamic derivation of the Transition State Theory rate constant. Variational Transition State Theory. Classical and quantum-mechanical simulations to calculate rate constants. Analytical and numerical solutions of large reaction mechanisms. Reduction of the number of species and reactions. Quasi-steady-state approximation and its error. Reactions in liquid solutions. Ionic and polar transition states in polar solvents. Kinetic salt effects. Diffusion controlled and kinetically controlled reactions. Reaction-diffusion systems. Isotope effects. Linear free energy relationships and other semi-quantitative relations. Photochemistry. Radiation chemistry. Kinetics of enzyme-catalyzed reactions. Drug design. Acido-base catalysis. Experimental methods in chemical kinetics. Molecular dynamics and laser photolysis experiments. Ultrafast lasers and femtochemistry. Exact quantum mechanical calculations of rate constants for reactions containing 3-4 atoms. Exotic dynamic systems; oscillations, pattern formation a chaos.

Textbooks to use

Mandatory: M.J. Pilling, P.W. Seakins: Reaction Kinetics, Oxford University Press, 1995
Recommended: P. W. Atkins: Physical Chemistry, Oxford University Press, 2005

Other material for study

Several auxiliary materials and projected presentations available at the website of the course: http://keszei.chem.elte.hu/rkinetika/