

Topics of the oral examination 2022

1. Potential Energy Surfaces in reacting systems.
2. Transition State Theory; its quasi-equilibrium and dynamic formulations. Its relation to the Collision Theory.
3. Calculation of the rate constant by simulations. Calculation of the PES using the Born-Oppenheimer approximation. Simulations using quasi-classical trajectory calculations.
4. Reaction dynamics; early methods, molecular beams and laser kinetics.
5. Experimental methods in kinetic studies. Time-window of different methods, fields of their application.
6. Temperature and pressure dependence of the rate constant. Discussion of relevant quantities determining these dependences.
7. Characteristics of reactions in solution (liquid phases). Reactions involving ionic species and dipole molecules. Primary and secondary salt effects. Effect of polarity of the solvent on the reaction rate.
8. Diffusion controlled reactions. Diffusion control, kinetic control and mixed control. Time-dependent rate constants.
9. Photochemistry. Jablonski diagram and quantum efficiency. Photochemical reaction types. Photochemical background of various photobiological harms.
10. Femtochemistry: experimental studies of elementary reactions at femtosecond timescale. Interpretation of experimental data. Types of reactions studied. Quantum control of reactions.

Further details at the course website: <http://keszei.chem.elte.hu/rkinetika>