Topics of the oral examination 2025

- 1. Potential Energy Surfaces in reacting systems.
- 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. Characteristics of reactions in solution (liquid phase). Reactions involving ionic species and dipole molecules. Primary and secondary salt effects. Effect of polarity of the solvent on the reaction rate.
- 7. Diffusion controlled reactions. Diffusion control, kinetic control and mixed control. Time-dependent rate constants.
- Photochemistry. Jablonski diagram and quantum efficiency. Photochemical reaction types. Photochemical background of various photobiological harms.
- 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