Topics of the oral examination 2015

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 via solving time-dependent Shrödinger equations.
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. Complete (or detailed) reaction mechanisms and their reduction. Computer modelling of reaction kinetics.
10. Photochemistry. Jablonski diagram and quantum efficiency. Photochemical reaction types. Photochemical background of various photobiological harms.
11. Radiation Chemistry. Absorbed dose and LET; their units and application. Radiation chemistry reaction types as initiated by different kinds of radiation. Radiation harms. Radiation chemistry in nuclear reactor design.
12. Femtochemistry: experimental studies of elementary reactions at femtosecond timescale. Interpretation of experimental data. Types of reactions studied. Quantum control of reactions.
13. Nonlinear chemical kinetics: oscillatory reactions, pattern formation and chaos in reaction-diffusion systems.
14. Kinetics of enzyme reactions. Interpretation of experimental results on enzyme reactions. Types of enzyme reactions. Basics of drug design.

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