CHEMISTRY 652

Chemical Kinetics and Reaction Dynamics

Fall 2020, Bilger Hall 335

Prof. Ralf I. Kaiser
Bilger Hall 301
Fr 1:30 – 5:30 pm (SKYPE)

Office Hours: SKYPE
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1. **Kinetics**

   1.1. Basic concepts: reaction order, molecularity, rate laws
   1.2. Reaction mechanisms: time dependence of reactants, intermediates, and products
   1.3. Rate constants: Arrhenius rate law and deviation; activation energy versus entrance barriers
   1.4. Experimental determination of rate constants and solutions to coupled differential equations
   1.5. Modern photoionization techniques

2. **Macroscopic and microscopic processes**

   2.1. Cross section and impact parameter
   2.2. Relationship between rate constants and cross sections
   2.3. Attractive interaction potentials in bimolecular reactions
   2.4. Experimental determination of doubly differential cross sections
   2.5. Modern molecular beam techniques

3. **Potential energy surfaces**

   3.1. Two dimensional representation
   3.2. Features on potential energy surfaces
   3.3. Experimental probing of potential energy surfaces and reaction mechanisms
   3.4. Dynamics calculations in the gas phase and condensed phase

4. **Transition state theory**

   4.1. Partition functions and chemical equilibrium
   4.2. Transition state theory
   4.3. Application of transition state theory to unimolecular decomposition
   4.4. RRKM theory

Required Textbooks (HARDCOPY ONLY; NO ELECTRONIC VERSION)

1. Molecular Reaction Dynamics, Levine, Cambridge.
2. Chemical Kinetics and Dynamics, Steinfeld, Francisco, Prentice Hall.

This is a 3-credit class arranged in eight blocks Fridays, 1:30 pm – 5:30 pm. Dates to be finalized August 28, 2020. This class will deliver lectures and discussion through skype; please add me asap as rikaiser@hotmail.com or rikaiser2010 to your skype account.