CHEMISTRY 652

Chemical Kinetics and Reaction Dynamics

Spring 2017

Prof. Ralf I. Kaiser
Bilger Hall 301

Office Hours M, 1:00-2:00
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1. **Kinetics**

   1.1. Basic concepts: reaction order, molecularity, rate laws
   1.2. Reaction mechanisms: time dependence of reactance, 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

5. **Classical versus quantum mechanical treatment of elastic and reactive scattering**

6. **Experimental Reaction Dynamics – Gas Phase and Surface Science**

Required Textbooks

1. Molecular Reaction Dynamics and Chemical Reactivity, R.D. Levine, R.B. Bernstein (Oxford, New York).
2. Chemical Kinetics and Reaction Dynamics, Paul L. Houston (Mc Graw Hill, New York).

KNOWLEDGE OF SOLVING COUPLED DIFFERENTIAL EQUATIONS, MATRICES, AND INTEGRALS IS MANDATORY; NO CALCULUS REVISION WILL BE GIVEN.

This is a 3-credit class (150 min instructions per week). Class times will be arranged with the students on January 10, 2017, 9:30 am, Bilger 302.