Chemistry 549
Chemical Kinetics and Dynamics
Spring, 2004

Text: *Chemical Kinetics and Dynamics*, Steinfeld, Francisco, and Hase, Prentice Hall, 2nd Edition, and supplementary readings.

The grade will be based on periodic problem assignments, an hour exam, and a final. The final grade will be calculated as follows:

Problem sets:	49%
Hour exam	20%
Final	40%

The following is a broad outline of topics to be covered. Details, especially in the dynamics part of the course, are likely to change as the course evolves.

I. Kinetics
- A. Introduction
- B. Mechanisms and Rate Laws
    1. First order reactions
    2. Second order reactions
    3. Consecutive reactions
    4. Branched reactions
    5. Approximations
    6. Numerical solutions
- C. Condensed Phase Reactions
    1. Solution reactions
    2. Catalysis
    3. Oscillating reactions
    4. Surface reactions
- D. Bimolecular Reactions
    1. Collision theory
    2. Transition state theory
- E. Unimolecular Reactions
    1. Lindeman mechanism
    2. RRKM theory

II. Dynamics
- A. Newton Diagrams
- B. Elastic scattering
    1. Classical mechanics
    2. Quantum mechanics
- B. Inelastic scattering and energy transfer
- C. Reactive scattering
    1. Potential Energy surfaces
    2. Reaction dynamics
    3. Non-adiabatic processes

4. Resonances

D. Photo-induced processes
    1. Multiphoton excitation
    2. Coherent control
    3. Strong field effects

Syllabus

Topic 1. Introduction to kinetics: Detailed balancing and microscopic reversibility (2 lectures)
Read chapter 6

Topic 2. Kinetic rate equations (3 lectures).
Read chapters 1 and 2.1-2.3.

Topic 3. Reactions in condensed phases; catalysis; oscillating reactions; surface reactions
Read chapters 4, 5, and 12.

Topic 4. Bimolecular kinetics; collision theory and transition state theory.
Read chapter 8.1 and 10.

Topic 5. Unimolecular kinetics; RRKM theory.
Read chapter 11.

Topic 6. Energy transfer; Landau-Teller, resonance effect; the master equation

Topic 7. Introduction to dynamics; Newton diagrams and potential energy surfaces.
Read chapters 6 and 7.

Topic 8. Classical elastic scattering; central potentials
Read section 8.2 and supplemental reading.

Topic 9. Quantum mechanical scattering; partial wave analysis.
Read section 8.3.

Topic 10. Reactive scattering; experimental results
Read chapter 9.

Topic 11. Electronic effects; the Born-Oppenheimer principle, Landau-Zener transitions; Marcus theory; resonances

Topic 12. Interaction of light and matter; absorption cross sections; Rabi cycling; tunneling vs multiphoton transitions

Topic 13. Coherent control