

4:235 Chemical Kinetics Spring 2007

Instructor: Christopher M. Cheatum

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Lecture: 10:55-12:10 Tuesday/Thursday in N103 LC

Office Hours: 1:30-3:00 Tuesday/Thursday or by appointment

Text: *Molecular Reaction Dynamics*, Raphael D. Levine, ©2005 Cambridge University Press

Course Objectives:

To develop both a conceptual and a quantitative understanding of the rates of chemical reactions and what those rates can reveal about the underlying nature of reactive processes. We will explore the quantitative description of reaction rates and mechanisms. We will also study fundamental chemical processes to understand how reactions happen at a molecular level and what aspects of the chemistry are most important in controlling the rate and outcome of a chemical reaction.

Topics:

Elementary Kinetics

- Rate Laws and Mechanisms

- Numerical Methods

- Experimental Methods

- Examples: Free Radical Chain Reactions and Enzyme Catalysis

- Factors That Influence Rates: Pressure and Temperature

Reactions at Surfaces

- Gas Surface Collisions

- The Adsorption Isotherm

- Surface Diffusion

Theories of Reaction Rates

- Collision Models

 - Hard Sphere and Line-of-Centers Cross Sections

 - Microscopic Reversibility and Detailed Balance

 - State-to-State Rates and Thermal Averages

 - Potential Energy Surfaces

- Statistical Models

 - Transition State Theory

 - Isotope Effects, Tunneling

 - Unimolecular Processes

 - Nonstatistical Behavior and Energy Transfer

Reactions in Solution

- Diffusion

- Solvation and Solvent Effects on Solutes

- Diffusion Controlled Reactions

- Kramers' Theory

- Marcus Theory

Grading:

Exam 1	February 27 (Tentative)	25%
Exam 2	April 19 (Tentative)	25%
Problem Sets	Approximately 6	25%
Final Paper/Oral Presentation	April 26-May 5	25%

Final grades will use +/- designations.

General Information:

The prerequisite for this course is 4:132 (Physical Chemistry II). Although I will make every effort to develop concepts from first principles, basic elements of quantum mechanics and statistical mechanics will be necessary background material.

This is a 3 credit hour course, so under University policy you should expect to spend six hours per week outside of class on activities related to this course.

I would like to hear from anyone who has a disability which may require some modification of seating, testing, or other class requirements so that appropriate arrangements may be made. Please contact me during my office hours.

If a student has a complaint concerning a course instructor including inappropriate faculty conduct, inequities in assignments, scheduling of exams at inappropriate or unauthorized times, failure to provide disability accommodations, or grading grievances, the University has established a process by which those concerns can be handled. The appropriate procedure is to contact me first if you have any questions, concerns, or complaints, and I will do my very best to address any issues you raise. If the matter cannot be resolved you can go to the Chemistry Department office, 305 Chemistry Building, and speak with the Department Executive Officer, David Wiemer. Finally if the matter remains unresolved, the student may submit a written complaint to the Office of the Graduate College. The complete procedure for student complaints can be found in the Schedule of Courses or in the Student Academic Handbook.

Plagiarism and cheating may result in grade reduction and/or other serious penalties. The University has an established policy on academic misconduct that outlines a series of steps for faculty who discover a case of academic misconduct. The first step involves confronting the student with the misconduct. The ultimate consequences of academic misconduct are varied but can include grade reduction to an F for the course, suspension, or expulsion. The complete policy on student academic misconduct can be found in the Student Academic Handbook.

If you are ill or a personal emergency makes it impossible to be present for a scheduled exam, please contact me as soon as possible. If there is a conflict with an exam time that you are aware of in advance, it may be possible to take the exam early depending on the nature of the conflict. Permission to take a make-up exam will require an Explanatory Statement of Absence which is available at the Registration Center, 30 Calvin Hall. Problem sets turned in late will not be accepted for a grade.

I want to emphasize again that if you have any questions or concerns, please communicate those to me so that I can help you. I am available and I will be happy to talk with you.