

Preliminary syllabus for Chemistry 111

Chemical Kinetics

Class meets: Mon, Wed, Fri **11:00 – 11:50 AM**

Arts 1426

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Office Hours: Wed and Thu (12:30-1:30 PM) or by appointment
Course website: <http://www.chem.ucsb.edu/~kalju/chem111>

Lecture Textbooks:

Required: "Reaction Kinetics" by M. J. Pilling and P. W. Seakins, Oxford UP, 2nd ed
Recommended: "Chemical Kinetics and Reaction Dynamics" by Paul Houston (\$ 111)

The Course:

The main goal of Chem 111 is to teach principles of reaction kinetics and catalysis. Topics covered include the laws and theories governing rates of chemical reactions and reaction mechanisms in the gas phase, in solution, and at the solid-liquid interface. Emphasis is placed on modern experimental approaches to study kinetics in complex chemical and biochemical systems. Analysis of experimental data is introduced. Computational approaches to estimate rates of chemical reactions and study the mechanism of catalysis are discussed

Expectations of Students:

- 1) Attendance and taking good lecture notes is expected. Supplementing the lecture notes with study notes based on the textbook is a good way to improve your chances to be successful in this course.
- 2) The practice problems in the book are quantitative and require a good understanding of the math. I am typically suggesting which ones are good to solve but you are free to tackle more difficult problems on your own.
- 3) Two mid-terms (each 100 points) and a final exam (200 points) will be given. The two mid-terms test your *knowledge* of topics covered prior to exam. The final will cover all the topics that were taught in this course and also tests your ability to *understand* the material.
- 4) Honesty and academic integrity must be always preserved. While working with others is encouraged outside the classroom, you must answer the exam questions individually. No supplemental material should be used during an exam.
- 5) There are no excuses for class absence, especially on the exam days. There are no make-up exams. If you must miss a test, contact the lecturer in advance and provide a verifiable doctors excuse.
- 6) The grade is based on the number of points out of 400 points total.

Study tips:

- Read the relevant textbook material before the class meets. I like to interact with students during our meetings and you enjoy the lectures more if you can think along
- Review (or rewrite) your class notes the same day and supplement them with material from the textbook and other resources (books, Internet). Ask for help if something remains unclear.
- Do not even hope that you can be successful by trying to memorize all the material few days before the exam. The final exam expects that you understand, not only remember the material.

Proposed Topics for Fall 2004

Note: I am open to suggestions from students, so if you have some special interests, please let me know.

1) Experimental techniques to study reaction kinetics

- Principles of signal detection
- Quantitative UV, fluorescence, CD, MS, HPLC, NMR, autoradiography
- Basics of data analysis
- Sealed ampoule approach for very slow reactions
- Rapid mixing techniques
- Pressure and temperature jump methods
- Flash photolysis
- Pulse radiolysis
- Discharge flow
- Monitoring of protein folding and unfolding

2) Theories of chemical reactions

- Potential energy surfaces
- Collision theory
- Activated complex model

3) Determination of potential energy surfaces

- Finding transition states and following reaction paths with quantum chemistry
- Probing the features of PES with experiments

4) Transition state theory

- Fundamental assumptions
- Thermodynamic formulation: Rate constants and activation barriers
- Quantum effects, tunneling
- Practical applications
- Femtosecond experiments to look at transition states

5) Kinetic Isotope Effects

- The origin and general interpretation
- Calculation for gas phase reactions

6) Reaction dynamics in the gas phase

- Photodissociation
- Atmospheric chemistry

7) Reactions in solution

- Description of solvent effects
- Diffusion in solution

9) Surface reactions and surface catalysis

10) Modeling of chemical reactions with Mathematica®

11) Complex reactions:

- Parallel
- Opposing
- Consecutive

12) Enzyme catalysis

- Methods to measure enzyme kinetics
- Steady state measurements without inhibitors
- Sequential and ping-pong mechanisms
- Introduction to pre-steady state kinetics
- Kinetic isotope effects in enzyme kinetics

13) Oscillatory behavior, chain reactions, chaos

14) Molecular simulations of complex reactions

- Enzyme catalysis
- Protein folding

Good luck! — Kalju