CHEMICAL SYSTEMS I (Chem 3110–1)
Syllabus—Winter 2013
MWF 10:00–10:50, F.W. Olin Hall 103

Instructor
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Text. Modern Physical Organic Chemistry. Ansyln & Dougherty. University Science Books, First edition

Additional Resources:

- Advanced Organic Chemistry parts A and B. Carey & Sundberg, Fifth edition
- Advanced Organic Chemistry. Smith & March, Sixth edition
- The Art of Writing Reasonable Organic Reaction Mechanisms. Grossman, Second edition

Grading. Your grade will be determined by:
Homework (15%)
Presentations on Named Reactions (20%, graded by your classmates)
Midterm Exam (25%)
Final Exam (40%, cumulative)

Homework. Problems will be assigned on a regular basis throughout the course.

Presentations on Named Reactions. Each class will start with a 5–7 minute mini-presentation with students taking turns to cover one named reaction from the attached list. You are also expected to provide a one-page handout summarizing the reaction. On the day of the presentation, plan to come 5 min early and write the essential mechanisms on the board before the class begins. Grading sheets will be provided to the class and your grade will be the average of the class's evaluations.

Midterm Exam. This exam will take place in mid-February and will cover the material in parts 1–3.

Final Exam. 10:00–11:50 am, March 15 in Olin 103. The exam will be cumulative.

Background Reading and Review

Basic bonding concepts. Textbook sections 1.1–1.2.2.

Part 1. Conformational, Steric and Stereoelectronic Effects.

Thermochemistry of stable molecules, potential functions, strain energy, conformational analysis of acyclic and carbocyclic compounds, electronic and stereoelectronic effects, highly strained molecules, atropisomerism, molecular mechanics.

Assigned reading: Textbook sections 2.1–2.1.2, 2.1.4, 2.1.7, 2.3–2.6 (not 2.6.1–)

Part 2. Stereochemistry

Stereogenicity and stereoisomerism, symmetry arguments, topicity relationships, stereospecific vs. stereoselective reactions, symmetry and timescale.

Assigned reading: Textbook sections 6.1–6.5

Part 3. Kinetic Analysis of Reaction Mechanisms

Energy surfaces and reaction coordinate diagrams, limitations of thermodynamic data, transition state theory, the Hammond postulate, reactivity vs. selectivity, the Curtin-Hammett principle, microscopic reversibility, kinetic vs. thermodynamic control, kinetic experiments, isotope effects, substituent effects and Hammett plots, principles of catalysis, acid-base catalysis, the Brønsted relationship.

Assigned reading: Textbook sections 7.1–7.4, 8.1–8.1.4, 8.2, 8.3, 8.5, 9.1, 9.3, Carey & Sundberg supplement (to be provided by the instructor).

Part 4. Organic Reactions Mechanisms Part A: Polar Additions and Eliminations

Predicting organic reactivity, regio- and stereochemistry of additions, Ad_E2 mechanisms, E1, E2, and E1cB β-elimination reactions, variable nature of E2 transition states, More O'Ferrall–Jencks plots.

Assigned reading: Textbook sections 10.1, 10.3-10.7, 10.13.

Part 5. Organic Reactions Mechanisms Part B: Nucleophilic Substitutions

The S_N1 and S_N2 mechanisms, borderline mechanisms, carbocations, ion pairs, effects of solvent, leaving groups, and neighboring groups. Non-classical carbocations.

Assigned reading: Textbook section 11.5