Topics in Organic Chemistry - 4473 - CHEM 3703 - 1
Syllabus—Spring 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:

- As discussed in class.

Grading. Your grade will be determined by:
Homework (15%)
Presentation on an experimental method (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 experimental methods. In the final weeks of the course, groups of students will present on experimental methods used to measure the kinetics and thermodynamics of binding and, in some cases, provide structural information. The expectations for these presentations will be discussed during the course.

Midterm Exam. This exam will take place in early May and will cover the material in parts 1 and 2.

Final Exam. 10:00–11:50 am, June 3 in Olin 103. The exam will be cumulative.

Background Reading and Review

This is a graduate level course that assumes familiarity with principles of organic chemistry (primarily structure and energetics) and physical organic chemistry. Students should be comfortable with the conformational analysis of organic molecules, acidity and basicity, basic ideas of coordination chemistry, principles of kinetics and thermodynamics, and have a general understanding of the structures of biological molecules including nucleic acids and proteins. If you have concerns regarding your preparation, then please make an appointment to meet with the instructor.

Part 1. Solutions and Non-Covalent Binding Forces

Solvent and solution properties, the problems with vacuums, solvent scales, solubility, solute mobility, the thermodynamics of solutions, binding forces, ion pairing, electrostatics interactions of dipoles, hydrogen bonding, π effects, induced-dipole interactions, halogen bonds, pinctogen bonds, the hydrophobic effect.

Assigned reading: Textbook chapter 3

Part 2. Analysis of the Thermodynamics and Kinetics of Intermolecular Interactions

a) Thermodynamic analysis of binding phenomena, the relevance of the standard state, heat capacity, cooperativity and allostery, enthalpy–entropy compensation, binding isotherms.

b) Energetic contributions to binding, enthalpic vs. entropic driving forces, maximizing attractions and minimizing repulsions, chemical and biochemical double mutant cycles, measurements of interaction energies.

c) Equilibrium kinetics, kinetic vs. thermodynamic stability of complexes.

Assigned reading: Textbook Section 4.1 & other

Part 3. Examples from Supramolecular Chemistry and Biological Chemistry

Molecular recognition, binding motifs, concave and cavity-containing molecules, molecular recognition of surfaces, complex and emergent architectures. Drug-receptor interactions, DNA duplex formation and stability, polar interactions in non-polar environments. Hydrogen bonds, heat capacity, and protein thermal stability.

Assigned reading: provided in class

Part 4. Experimental Methods

A general discussion on experimental approaches and group presentations on modern methods, including NMR, isothermal titration calorimetry, surface-based methods, UV/vis and fluorescence, and other approaches.

Assigned reading: provided in class.