CHEM 730: MODERN PHYSICAL ORGANIC CHEMISTRY
San Diego State University

Fall Semester, 2014, Main Campus

Instructor	Prof. Byron W. Purse
Contact	Chemical Sciences Laboratory (CSL) 213 bpurse@mail.sdsu.edu (preferred contact); (619)-594-6215 (office)
Lectures	MW 5:00pm-6:15pm in GMCS-310
Midterm Exams	Monday, Oct. 6 Monday, Nov. 10
Final Exam	Friday, Dec. 12 from 3:30pm-5:30pm
Office Hours	MW 11:00am–12:00pm in CSL-213 or by appointment
Prerequisites	BS or equivalent degree in chemistry.

Expected Learning Outcomes

Students completing the course should have these skills:

1. To be able to propose reasonable mechanisms for a chemical reaction, evaluate the relative merits of the different mechanisms, and to be able to propose logical, viable experiments to distinguish between them.
2. To understand fundamentals of chemical kinetics and thermodynamics and their applications to the understanding of reactivity and the interactions between molecules.
3. To be able to understand the details of physical organic chemistry studies in the primary literature and to assess the quality of data and the validity of the interpretation of results.
4. To be able to relate the structure of a molecule to its expected properties and reactivity.

Textbook

Modern Physical Organic Chemistry, *1st ed*, by Anslyn and Dougherty, University Science, 2005; ISBN: 978-1891389313.

Additional Learning Materials

Advanced Organic Chemistry, Part A: Structure and Mechanisms, *5th ed*, by Carey and Sundberg, *Springer*, 2008; ISBN: 978-0387683461.

Other resources and the primary literature as discussed in class.

Exams

There will be two 2 hour midterm exams during the semester, each worth 200 points. The final exam (also 2 hours) is cumulative and is worth 250 points. Make-up exams will only be offered in exceptional circumstances, typically requiring advance notice.

Homework

Homework assignments will be given periodically during the course.

NSF-Style Proposal

The major homework assignment for the class will be to prepare a shortened NSF-style proposal to determine the mechanism of a reaction from the literature for which the true mechanism is debated or unknown. The choice of reaction will be made by you and must be approved by Prof. Purse in advance of completing the assignment. The proposal is worth 250 points.

Grades

Your final grade will be based on a maximum of 1250 points, distributed as follows:

Contribution	***Points***
midterm 1	200
midterm 2	200
final exam	250
homework	250
proposal	250
participation	100
total	**1250**

Letter Grade Assignment

A = 1075–1250
B = 925–1074
C = 760–924
D = 625-759
F < 625

Cheating and Plagiarism

Academic dishonesty is not tolerated and will result in you receiving a grade of zero for the associated activity. Moreover, I will report all violations to the SDSU Center for Student Rights and Responsibilities for investigation and possible disciplinary action, which can include expulsion from SDSU.

For information on SDSU policies, please refer to this URL: http://csrr.sdsu.edu/cheating-plagiarism.html

Students with Disabilities

If you are a student with a disability and believe you will need accommodations for this class, it is your responsibility to contact Student Disability Services at (619) 594-6473. To avoid any delay in the receipt of your accommodations, you should contact Student Disability Services as soon as possible. Please note that accommodations are not retroactive, and that accommodations based upon disability cannot be provided until you have presented your instructor with an accommodation letter from Student Disability Services. Your cooperation is appreciated.

Course Content

Background Reading and Review

Basic bonding concepts. Textbook sections 1.1.

Part 1. Qualitative Molecular Orbital Theory (QMOT)

Explanations for structure, bonding, and stability that are not adequately treated by basic bonding concepts.Textbook sections 1.2–1.4.

Part 2. Strain and Stability

Thermochemistry of stable molecules, potential functions, strain energy, QMOT analysis of stability and conformation, thermochemistry of reactive intermediates. Textbook sections 2.1–2.2.

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, Charton parameters, principles of catalysis, acid-base catalysis, the Brønsted relationship. 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. Solutions and Non-Covalent Binding Forces

Solvent and solution properties, the problem of 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, $n \rightarrow \pi^*$ interactions, halogen bonds, pinctogen bonds, the hydrophobic effect. Textbook chapter 3

Part 5. 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, competition binding experiments, Job plots.

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.

Textbook Section 4.1 & other

Part 6. Experimental Methods & Applications

Examples from the primary literature and a discussion of methods for data analysis and statistically valid interpretation of results.

Reading assigned in class.