CHEM 730: PHYSICAL ORGANIC CHEMISTRY

Spring 2018
Schedule Number: 20769

COURSE INFORMATION

Class Days: MW
Class Times: 5:00–6:15 pm
Class Location: GMCS-306

Instructor: **Prof. Byron W. Purse**
bpurse@mail.sdsu.edu (preferred contact)
(619) 594-6215 (office)
Office Location: CSL 213
Office Hours Times: by appointment
Office Hours Location: CSL 213

Midterm Exams

Wednesday, February 28, 5:00 pm – 6:15 pm.
Wednesday, April 4, 5:00 pm – 6:15 pm.

Final Exam

Friday, May 4, 2016, 3:30 pm – 5:30 pm. **The final exam is cumulative.**

Prerequisites

BS or equivalent degree in chemistry.

Course Information

Updated information is available on the course BlackBoard site through SDSU.

Course Catalog Description

Selected topics in organic chemistry. May be repeated with new content. See Class Schedule for specific content. Maximum credit six units applicable to a master's degree.

Scope and Purpose

This course covers structure, bonding, and the study of reaction mechanisms and the interactions between molecules. The content will include fundamentals of theory and practical applications with an emphasis on the primary literature. Students completing the course should have a solid understanding of how to propose reasonable reaction mechanisms and descriptive understandings of inter- and intra-molecular interactions, and be able to assess the quality and validity of experiments used to support or refute such proposals.

Students should meet these **expected learning outcomes** as a minimum requirement in order to pass the course:

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.

Course Outline and Assigned Reading from *Modern Physical Organic Chemistry*, 1st ed.

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 valence bond theory. 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→π* 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.

Adding/Dropping Procedures

January 30 is the last day to add/drop classes or change grading basis. To add a class during the schedule adjustment period, students can request an add code from the instructor. Please email the instructor regarding add codes for other circumstances.

Course Materials

Textbook

Modern Physical Organic Chemistry, *1st ed*, by Anslyn and Dougherty, University Science, 2005; ISBN: 978-1891389313. Approximately $110.

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.

Homework

Homework assignments will be given periodically during the course.

Course Structure and Conduct

The course will use a traditional lecture format with discussion. BlackBoard will be used for course management.

Course Assessment and Grading

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 research in your lab or from the literature. The true mechanism must be the debated or unknown. The choice of reaction will be made by you and must be approved by Prof. Purse at least four weeks in advance of completing the assignment. If the reaction is from your research lab, then your topic must also be approved by your PI. The proposal is worth 250 points and is due on 4/30/18.

Midterm 1	200 points
Midterm 2	200 points
Final exam	250 points
Homework	250 points
Proposal	250 points
Participation	50 points
Total	**1200 points**

Letter Grade Assignments

A = 1030–1200
B = 890–1029
C = 730–889
D = 600-729
F < 600

+/− grades will be included in these ranges and set at the instructor's discretion

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.

Academic Honesty

The University adheres to a strict policy regarding cheating and plagiarism. These activities will not be tolerated in this class. Become familiar with the policy (http://go.sdsu.edu/student_affairs/srr/conduct.aspx). Any cheating or plagiarism will result in failing this class and a disciplinary review by Student Affairs.

Examples of Plagiarism include but are not limited to:

- Using sources verbatim or paraphrasing without giving proper attribution (this can include phrases, sentences, paragraphs and/or pages of work)

- Copying and pasting work from an online or offline source directly and calling it your own
- Using information you find from an online or offline source without giving the author credit
- Replacing words or phrases from another source and inserting your own words or phrases
- Submitting a piece of work you did for one class to another class

If you have questions on what is plagiarism, please consult the policy (http://go.sdsu.edu/student_affairs/srr/conduct.aspx) and this helpful guide from the Library: (http://library.sdsu.edu/guides/tutorial.php?id=28)