PHYSICAL ORGANIC CHEMISTRY 2
3 CREDITS CHEM 538 Spring 2024

Prof. Arthur Winter
Department of Chemistry
E-mail: winter@iastate.edu; Phone: 294-2813; Office: Hach Hall 2101d.

LECTURES: Tues, Thurs 12:40pm-1:55 pm, Gilman 1312.

OFFICE HOURS: Immediately following class and by appointment.

PREREQUISITE: Basic undergraduate organic chemistry and preferably a course in physical chemistry that included quantum mechanics (but not necessary). Please address any special needs or special accommodations with me at the beginning of the semester or as soon as you become aware of your needs. Those seeking accommodations based on disabilities should obtain a Student Academic Accommodation Request (SAAR) from the Disability Resources (DR) office (515-294-7220). DR is located in Room 1076 of the Student Services Building.

REQUIREMENTS: 1) Oral presentation (12 min + questions) in class of a related **recent** research paper with background information (20%). 2) One mid-term exam (40%). 3) Final exam (40%). For the mid-term exam and the final, a paper from the primary literature will be assigned ahead of time that relates to the topics covered for that exam. One or more exam questions will relate to that paper. Homework problems will not be graded or collected, but will provide the background for tests and serve to stimulate student-led discussion.

REQUIRED MATERIAL: The 1st edition of Anslyn and Dougherty's Modern Physical Organic Chemistry and the accompanying Student Solutions Manual. These books will be available at the bookstore in the Memorial Union or online. Required reading assignments are delineated in the syllabus below. In addition, the 4th edition of Carey and Sundberg's Advanced Organic Chemistry, part A, and the 6th edition of Smith and March's Advanced Organic Chemistry are useful references available in the library.

COURSE STRUCTURE: The first half of this course (up to Exam 1) will cover molecular structure; the second portion of the course will build on this static understanding of molecular structure to introduce reactivity, complex stereochemistry, self assembly, and photochemistry. Examples from synthetic organic chemistry, bioorganic chemistry, materials/polymer chemistry will be used throughout the course to illustrate the broad applicability of these fundamentals of physical organic chemistry.

LEARNING OBJECTIVES: By the end of this course, I want you to understand:

1) How bonding works (really). I want you to correct any erroneous impressions of bonding you may have gotten from undergraduate general chemistry and organic chemistry textbooks.
2) The limitations and usefulness of the Lewis model of bonding
3) How the Hamiltonian operator works, particularly the kinetic energy term.
4) How wavefunctions work and how to draw wavefunctions for a given potential and what those wavefunctions mean.
5) How to build qualitative molecular orbital diagrams to be able to predict the structure, conformations, and reactivity of molecules
6) How computational chemistry uses approximations to the Schrodinger equation to provide quantitative answers of interest to practicing wet chemists.
7) The strengths and weaknesses of different model theories including Hartree-Fock and correlated methods such as density functional theory and configuration interaction (CI).
8) The different kinds of basis sets for building up wavefunctions and the abbreviations
9) How entropy works and how interplay of entropy and enthalpy can lead to predictions of equilibria.
10) The different types of intermolecular forces and their strengths
11) How to design non-covalent host-guest complexes using the principles of complementarity and preorganization
12) How reaction mechanisms can be deduced using stereochemistry, kinetics, isotope effects, intermediate traps, and substituent effects.
13) Understand the fundamental principles of organic photochemistry and spectroscopy (time permitting)

APPROXIMATE SYLLABUS:

Jan 16	Go over syllabus, theories of bonding Chapter 1 (pp. 1-61) /Parts of Chapter 14 (pp. 807-821)
Jan 18	Chapter 1/2/14 views of bonding
Jan 23	Chapter 1/2/14 views of bonding
Jan 25	Chapter 1/2/14 views of bonding
Jan 30	Chapter 1/2/14 views of bonding
Feb 1	**Seminar at Miami – No class**
Feb 6	Chapter 1/2/14 views of bonding
Feb 8	Chapter 1/2/14 views of bonding
Feb 13	Chapter 1/2/14 views of bonding
Feb 15	Chapter 1/2/14 views of bonding
Feb 20	Chapter 1/2/14 views of bonding
Feb 22	Chapter 1/2/14 views of bonding
Feb 27	**EXAM 1**
Feb 29	Chapter 3, solutions and non-covalent binding forces
Mar 1	Chapter 3, solutions and non-covalent binding forces
Mar 5	Chapter 3, solutions and non-covalent binding forces
Mar 7	Chapter 3, solutions and non-covalent binding forces
Mar 12	**Spring Break – No Class**
Mar 21	**Spring Break – No Class**
Mar 26	Chapter 4 Molecular recognition
Mar 28	Chapter 4 Molecular recognition
Apr 2	Chapter 4 Molecular recognition
Apr 4	Chapter 7, Energy surfaces and kinetic analysis
Apr 9	Chapter 7, Energy surfaces and kinetic analysis
Apr 16	Chapter 8, Experiments related to kinetics and thermodynamics
Apr 18	Chapter 8, Experiments related to kinetics and thermodynamics
Apr 23	Chapter 8, Experiments related to kinetics and thermodynamics
Apr 25	Chapter 8, Experiments related to kinetics and thermodynamics
Apr 30	ORAL PRESENTATIONS OF RECENT LITERATURE
May 2	ORAL PRESENTATIONS OF RECENT LITERATURE
May 7	DEAD WEEK: Finish up Oral Presentations (if needed)
TBA!!!	**FINAL EXAM**