Chemistry 537: Physical Organic Chemistry I

Yan Zhao Fall 2022 3101D Hach Hall M & W

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This course covers important classes of organic reactions. Reactive intermediates including cations, anions, and radicals will be introduced along the way. We will discuss in detail how these intermediates are generated, how molecular structures affect reactions involving these intermediates, and how to apply these learnings in organic reactions and mechanisms.

Text:

F. A. Carey and R. J. Sundberg, Advanced Organic Chemistry, Part A, 5th Ed.

Supplementary Text:

R. B. Grossman, The Art of Writing Reasonable Organic Reaction Mechanisms, 2nd Ed.

E. V. Anslyn and D. A. Dougherty, *Modern Physical Organic Chemistry*.

Virtual Office Hour by Appointments:

Meeting URL: https://iastate.webex.com/meet/zhaoy

Grading:

The grade will be based on a total of 500 points: two midterms (150 points each), and a comprehensive final (200 points).

Bonus: Find two examples of INNOVATIVE applications of physical organic chemistry in chemical journals and patents, respectively. They should be published within the last three years (2020–2022). In a four-page summary (2 pages for each example), <u>illustrate how</u> physical organic chemistry is used to solve the research and industrial problems, and <u>explain why</u> the solution is innovative (i.e., the <u>creative approach</u> instead of the significance/importance of the research should be discussed). Maximum bonus: 40 points (20 for research and 20 for industrial application). <u>I need to approve the paper/patent before you start working on the summary</u>. The summary (submitted via email attachment in MS Word, with the pdf files) is due by 5:00 p.m. on Monday November 21. **Important:** Name the files as "Your Last Name_paper.docx" and "Your Lame Name_patent.docx" and send me the pdf files of the papers named as "Your Last Name_paper.pdf" and "Your Last Name_patent.pdf", respectively. Every violation causes 5 points.

Practice Homework Problems:

Chap 4: 1, 2, 3, 12, 13, 16

Chap 6: 1, 2, 4, 9; Chap 5: 1, 2, 9, 13

Chap 7: 5, 8, 21, 27

Chap 9: 2, 7, 20, 21

Chap 11: 1, 4, 5, 6, 16, 19

Chap 10: 2, 5, 7, 12, 14, 19

Chap 12: 4

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Tentative Lecture Schedule:

Week	Monday	Wednesday
Aug 22	Nu. Substitution: S _N 2 & S _N 1	Nu. Substitution: S _N 1 & Borderline
Aug 29	Problems (S _N)	Neighboring Group Participation
Sept 5	Labor Day (no class)	Carbocations & Electron-Deficient Nitrogen and Oxygen
Sept 12	Problems (Carbocations)	Carbanions
Sept 19	Problems (carbanions)	Addition/Elimination
Sept 26	Addition/Elimination	Carbonyl Chemistry
Oct 03	Carbonyl Chemistry	Problems (Add/Elim)
Oct 10	Exam Review	Problems (Carbonyl)
Oct 17	Aromatic Substitution	Aromatic Substitution/Problems
Oct 24	Radical Chemistry	Radical Chemistry
Oct 31	Radical Chemistry	Radical Chemistry
Nov 07	Problems (Radical)	Pericyclic Reactions
Nov 14	Exam Review	Pericyclic Reactions
Nov 21	Thanksgiving (no class)	Thanksgiving (no class)
Nov 28	Problems (Pericyclic Rxn)	Photochemistry
Dec 05	Photochemistry	Problems (Photochemistry)

Reading Assignments:

Nucleophilic Substitution Chapter 4, Chapter 6.1, 6.2, & 6.5 Chapter 11.9 (Anslyn and Dougherty) Electron-Deficient Nitrogen and Oxygen

Addition and Elimination Chapter 5

Carbonyl Chemistry Chapter 7, Chapter 6.3 & 6.4

Aromatic Substitution Chapter 8, Chapter 9

Radicals Chapter 11 Pericyclic Reactions Chapter 10

Photochemistry Chapter 12

Tentative Exam Dates:

7:00-9:30 p.m., Friday, 10/07 Midterm 1 7:00-9:30 p.m., Friday, 11/11 Midterm 2

12:00-2:00 p.m., Wednesday, December 14th Final

Student Learning Outcomes:

There are two major learning objectives for this class. First, to help you develop a deeper understanding of organic mechanisms. The knowledge will enable you to understand "unfamiliar" reactions found in the literature based on the types of intermediates involved. It will also help you troubleshoot reactions that do not work as expected in your research, e.g., by analyzing how reaction conditions affect the kinetics and the selectivity of the reaction. Second, to help you understand how to design experiments to test scientific hypotheses. Mechanisms are actually hypothesized reaction pathways supported by experimental evidence. By understanding how chemists have verified their hypotheses in different organic mechanisms, you will better understand hypothesis-driven research in general and learn to design experiments in your own research to test your hypotheses, whether reaction-based or not.

Key intermediates: You will learn about key intermediates in organic reactions including carbocations, carbanions, and radicals. You will learn different ways to stabilize them through both substituent effects and external conditions such as solvents.

Organic reactions: You will learn about major types of organic reactions including nucleophilic substitution, addition/elimination, nucleophilic addition, electrophilic and nucleophilic aromatic substitution, radical chemistry, pericyclic reactions, and photochemistry.

Arrow-pushing mechanisms: You will apply the above learning to complex organic transformations that involve multiple steps of bond making and breaking. You are expected to propose reasonable mechanisms for these transformations based on the structure of the substrate(s) and reaction conditions.

Applications of physical organic chemistry in modern scientific research: You will see examples of physical organic principles being employed in both academic and industrial research. These examples are meant to help you understand how simple concepts in one area of chemistry can be used creatively in other areas to solve difficult research problems.

Academic Dishonesty

The class will follow Iowa State University's policy on academic dishonesty. Anyone suspected of academic dishonesty will be reported to the Dean of Students Office.

http://www.dso.iastate.edu/ja/academic/misconduct.html

Disability Accommodation

Iowa State University complies with the Americans with Disabilities Act and Sect 504 of the Rehabilitation Act. If you have a disability and anticipate needing accommodations in this course, please contact (instructor name) to set up a meeting within the first two weeks of the semester or as soon as you become aware of your need. Before meeting with (instructor name), you will need to obtain a SAAR form with recommendations for accommodations from the <u>Disability Resources Office</u>, located in Room 1076 on the main floor of the Student Services Building. Their telephone number is 515-294-7220 or email <u>disabilityresources@iastate.edu</u>. Retroactive requests for accommodations will not be honored.

Dead Week

This class follows the Iowa State University Dead Week policy as noted in section 10.6.4 of the Faculty Handbook http://www.provost.iastate.edu/resources/faculty-handbook.

Harassment and Discrimination

Iowa State University strives to maintain our campus as a place of work and study for faculty, staff, and students that is free of all forms of prohibited discrimination and harassment based upon race, ethnicity, sex (including sexual assault), pregnancy, color, religion, national origin, physical or mental disability, age, marital status, sexual orientation, gender identity, genetic information, or status as a U.S. veteran. Any student who has concerns about such behavior should contact his/her instructor, Student Assistance at 515-294-1020 or email dso-sas@iastate.edu, or the Ompliance at 515-294-7612.

Free Expression

Iowa State University supports and upholds the First Amendment protection of <u>freedom of speech</u> and the principle of <u>academic freedom</u> in order to foster a learning environment where open inquiry and the vigorous debate of a diversity of ideas are encouraged. Students will not be penalized for the content or viewpoints of their speech as long as student expression in a class context is germane to the subject matter of the class and conveyed in an appropriate manner.

Contact Information

If you are experiencing, or have experienced, a problem with any of the above issues, email academicissues@iastate.edu.