Advanced Organic Chemistry Chemistry 511 Fall 2024

Thursdays 6:00-9:00 PM, Smith 240

Instructor: Prof. Stacey Brenner-Moyer (http://www.brennermoyer.com/)

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Office Hours: Thursdays 4:30-5:30 PM in Room 201E Life Sciences Building 1.

Course Description: This physical organic chemistry course builds upon the basic organic reaction mechanisms taught in undergraduate and introductory graduate coursework. We will learn about the experimental tools employed to derive the fundamental organic reaction mechanisms that have come to be accepted as fact, and we will evolve our understanding of organic reaction mechanisms beyond the simplified versions presented in undergraduate textbooks. Specifically, the physical chemistry experimental tools to be emphasized include molecular orbital theory, kinetic data, linear free-energy relationships, and isotope effects. We will learn how these data are integrated to provide comprehensive, self-consistent, and sophisticated models for the reactivity of organic molecules.

Learning Goals:

Upon completion of the course, students should be able to:

- Predict relative thermodynamic, kinetic, and stereochemical outcomes of selected reactions.
- Interpret thermodynamic, kinetic, and stereochemical data to draw reasonable conclusions with respect to reaction mechanisms.
- Illustrate the mechanism of selected reactions.

Required Texts and Materials:

1. Carey, Francis A.; Sundberg, Richard J. *Advanced Organic Chemistry, Part A: Structure and Mechanism.* 5th ed. Springer, 2007.

NOTE: This entire book can be downloaded for FREE from campus or login via Rutgers account: <u>https://link-springer-com.proxy.libraries.rutgers.edu/book/10.1007/978-0-387-44899-2</u>

Recommended Materials:

1. Molecular Model Set for Organic Chemistry, Prentice Hall

Course Evaluation:

Your grade for the course will be determined as follows: Take Home Exam 1: 30% Take Home Exam 2: 30% Final Presentation: 40%

Take home exam 1: The practice problems for Chapter 3 (below) will comprise take home exam 1. These will be due prior to the beginning of class on October 10. Prof. Brenner-Moyer will randomly select a maximum of 6 out of the 12 practice problems to grade.

Take home exam 2: Questions for take home exam 2 will be derived from the lectures covering, and practice problems for, Chapters 4-12. This take home exam will be distributed by Nov. 26, and will be due prior to the beginning of class on Dec. 5.

Final presentation: Each student will select a paper from the recent (i.e., since 2020) literature that discusses the reaction mechanism of a reaction class covered in Chapters 4-14, and utilizes some of the principles introduced in Chapter 3 (i.e., Hammett correlations, kinetic isotope effects, solvent [isotope] effects, specific/general acid catalysis). Students must OK their choice of paper with Prof. Brenner-Moyer. Students will then prepare and present a 15 minute power point lecture on their paper selection. Thoroughness of material covered, accuracy of information conveyed, and quality of oral presentation will factor heavily into the grading of the presentation. As an example of a suitable paper choice, see: Bulger, A. S.; Turner, D. W.; Zhou, Q.; Houk, K. N.; Garg, N. K. "Evaluation of Retro-Aldol vs Retro-Carbonyl-Ene Mechanistic Pathways in a Complexity-Generating C-C Bond Fragmentation." *Org. Lett.* **2024**, *26*, 3602-3606. In this paper, the authors describe an experiment designed to differentiate between possible aldol (Ch. 7) and concerted ene (Ch. 10) reaction pathways, by using the stereochemical outcome of the reaction in conjunction with isotopic labelling.

Policy for Late Submission of Take Home Exams: In the event of late submission of a take home exam, 1.5 points will be deducted for each late day. Take home exams will not be accepted beyond 7 late days, and a grade of "0" will be recorded.

Policy for Absence from Final Presentation: In the event of an excused absence from the final presentation, contact Professor Brenner-Moyer as soon as possible. In the event of an absence that is not deemed by Professor Brenner-Moyer to be excused, a grade of "0" will be recorded for the final presentation.

Issues of Courtesy: Lecture will start as scheduled, at 6:00 PM. Please try to arrive <u>on time</u>, with your <u>electronic devices turned off</u>. If you must arrive late to lecture, please enter quietly, so as not to disrupt those who were on time and are listening intently.

Please note: There will be a 15 minute break during every lecture.

Assigned Problems:

Ch. 1: 1a, 2a,d, 4, 5, 8, 9, 11, 12c, 15, 16, 17, 19 Ch. 2: 1, 5, 6, 7, 8, 10, 12, 14, 16, 23a, 26c,d,f,h,l, 30 Ch. 3: 2, 5, 6, 8, 9, 10, 11, 12, 13, 19, 20, 21 Ch. 4: 2b,d,f, 3, 8, 9, 11, 13a,e, 14, 16, 20, 21, 23, 26 Ch. 5: 1, 4, 6, 8, 12, 13, 14, 15, 17, 19 Ch. 6: 2, 3, 7, 8, 9, 10, 13, 15, 16, 18b, 24 Ch. 7: 1, 2b,c, 9, 10c,e, 11, 15, 17, 20, 21, 24, 25, 26 Ch. 8: 2, 4, 7, 8, 10, 11, 13, 14, 15, 18 Ch. 9: 1, 2, 3, 4, 6, 8, 11, 14, 15, 17, 19a, c Ch. 10: 1, 2a,b,c, 4, 6, 7c,d,f,g, 10, 12, 13, 14b,d,e, 15, 17, 18, 21 Ch. 11: 3, 4, 5, 8, 9, 13, 17, 18, 19, 20 Ch. 12: 2b,3b,4a-e,8,13,17,19,21

Tentative Schedule of Course Topics, Exams and Reading Assignments:

<u>Week</u>	<u>Date</u>	Topic	<u>Reading</u>
1	Th. Sept. 5	Chemical Bonding and Molecular Structure	1.1 – 1.2
2	Th. Sept. 12	Stereochemistry, Conformation,	2.1
3	Th. Sept. 19	Stereochemistry, Conformation,	2.2-2.3
4	Th. Sept. 26	Structural Effects on Stability	Chapter 3
5	Th. Oct. 3	No lecture	
6	Th. Oct. 10	Nucleophilic Substitution	Chapter 4
7	Th. Oct. 17	Polar Addition and Elimination	5.1 – 5.3, 5.6, 5.9- 5 10
8	Th. Oct. 24	Carbanions and Other Carbon	6.1, 6.3-6.5
9	Th. Oct. 31	No lecture	
10	Th. Nov. 7	Addition, Condensation and Substitution	7.1 – 7.2
11	Th. Nov. 14	Aromaticity and Aromatic Substitution	8.1 – 8.3, 9.1 – 9.5
12	Th. Nov. 21	Concerted Pericyclic Reactions	10.1 – 10.6
13	Tues. Nov. 26	Free Radical Reactions	11.1 – 11.6
14	Th. Dec. 5	Photochemistry ~take home exam 2 due~	Chapter 12
	Th. Dec. 19	student presentations during final exam period (6:20-9:20pm)	

Academic Integrity: As an academic community dedicated to the creation, dissemination, and application of knowledge, Rutgers University is committed to fostering an intellectual and ethical environment based on the principles of academic integrity. Academic integrity is essential to the success of the University's educational and research missions, and violations of academic integrity constitute serious offenses against the entire academic community. The entire Academic Integrity Policy can be found here: <u>http://academicintegrity.rutgers.edu/academic-integrity-policy/Links to an external site.</u>

Accommodations and Support: Rutgers University Newark (RU-N) is committed to the creation of an inclusive and safe learning environment for all students. RU-N has identified the following resources to further the mission of access and support:

- Students with Disabilities: Rutgers University welcomes students with disabilities into all of the University's educational programs. The Office of Disability Services (ODS) is responsible for the determination of appropriate accommodations for students who encounter barriers due to disability. In order to receive consideration for reasonable accommodations, a student with a disability must contact ODS, register, have an initial appointment, and provide documentation. Once a student has completed the ODS process (registration, initial appointment, and documentation submitted) and reasonable accommodations are determined to be necessary and appropriate, a Letter of Accommodation (LOA) will be provided to the student. The student must give the LOA to each course instructor, followed by a discussion with the instructor. This should be completed as early in the semester as possible as accommodations are not retroactive. More information can be found at <u>rutgers.eduLinks to an external site.</u>. Contact ODS: (973) 353-5375 or ods@newark.rutgers.edu.
- Religious Holiday Policy and Accommodations: Students are advised to provide timely notification to instructors about necessary absences for religious observances and are responsible for making up the work or exams according to an agreed-upon schedule. The Division of Student Affairs is available to verify absences for religious observance, as needed: (973) 353-5063 or DeanofStudents@newark.rutgers.edu.
- Counseling Services: Counseling Center Room 101, Blumenthal Hall, (973) 353-5805 or <u>http://counseling.newark.rutgers.edu/Links to an external site.</u>
- Students with Temporary Conditions/Injuries: Students experiencing a temporary condition or injury that is adversely affecting their ability to fully participate in their courses should submit a request for assistance at: https://temporaryconditions.rutgers.eduLinks to an external site.
- Students Who are Pregnant: The Office of Title IX and ADA Compliance is available to assist students with any concerns or potential accommodations related to pregnancy: (973) 353-1906 or <u>TitleIX@newark.rutgers.edu</u>.
- Gender or Sex-Based Discrimination or Harassment: Students experiencing any form of gender or sex-based discrimination or harassment, including sexual assault, sexual harassment, relationship violence, or stalking, should know that help and support are available. To report an incident, contact the Office of Title IX and ADA Compliance: (973) 353-1906 or <u>TitleIX@newark.rutgers.edu</u>. To submit an incident report: com/RUNReportingForm. To speak with a staff member who is confidential and does NOT have a reporting responsibility, contact the Office for Violence Prevention and Victim Assistance: (973) 353-1918 or run.vpva@rutgers.edu.