University of Wisconsin-Madison: Chemistry 843 (3 credits)

Advanced Organic Chemistry: Proposing and Evaluating Reaction Mechanisms

Face-to-face instruction: 9:30–10:50am, MW, Room 2373 Chemistry

Instructor: Prof. Zachary Wickens
email: wickens@wisc.edu / office: 6365

Office hours: either immediately after class for up to an hour or *any other time* (by appointment)

Course description: CHEM843 is a graduate level course focused on mechanisms in organic chemistry. The ability to think mechanistically about organic reactions will allow you to explain why a reaction you tried in lab gave you an unexpected product and will help you hone in on the right set of experiments to improve reactions of interest. However, fundamentally, this class is about acquiring the skills you will need to *generate* knowledge. This class will facilitate your transition into graduate school by equipping you to interrogate problems where the answer is not known by any other human on the planet.

Primary course goal: To prepare you to construct viable mechanistic models to explain brand new chemical reactions. *Yes, this is really, really hard. Don't worry, you'll get there by learning how to:*

1. Propose plausible mechanisms to explain chemical reactions
2. Analyze papers from the primary scientific literature.
3. Recognize and predict how different mechanisms would result in different observable outcomes.
4. Evaluate several competing mechanistic hypotheses.
5. Exclude mechanisms unambiguously from further consideration using data.

Secondary course goals: The course will be structured such that in addition to the primary learning goal, we will also:

1. Build your comfort discussing chemistry and your ideas with your peers.
2. Familiarize you with synthetically important reactions in organic chemistry.
3. Expose you to the types of experiments commonly used to study mechanisms.

Course structure: This course will be highly fluid and interactive. Ultimately, I want to transfer an intellectual skillset to each and every one of you. I believe the most efficient way to do this is to work on problems together. A typical course period will be heavily focused on group work and students presenting their work at the board but will sometimes also contain brief lectures. Every student will be expected to propose potential solutions to the class at the board. Everyone will go once, then twice, etc. Sometimes the problems discussed at the board will be posed in class and sometimes they will be from problem sets.

Friday class session: The Friday session is *completely optional* and no additional tested content will be provided. The Friday class period will typically be used as an opportunity to clarify or delve deeper into content you encounter as part of this course. Occasionally it will be leveraged as an opportunity to workshop your final project with your colleagues, assisted by me. If no one arrives by 9am, I will return to my office but remain available until 9:40. I will *never* help you with a "completion-based" problem set before it is due.

Required text: "*The Art of Writing Reasonable Organic Reaction Mechanisms"* Grossman (ebook available)

Strongly recommended text: "*Modern Physical Organic Chemistry"* Anslyn and Dougherty

Useful reference books:

1. *"Advanced Organic Chemistry Part B"* Carey and Sundberg (ebook available)
2. *"Frontier Orbitals and Organic Chemical Reactions"* Fleming (ebook available)

Overview of topics: Overall, the course will initially emphasize the *generation* of mechanistic hypotheses and later the *evaluation* of mechanistic hypotheses.

Phase 1: Proposing reasonable reaction mechanisms

1. Factors governing reactivity
2. Polar reactions
3. Radical reactions

Phase 2: Distinguishing between several plausible mechanisms

1. Determination of transition state molecularity (kinetics)
2. Linear free energy relationships
3. Kinetic isotope effects

Phase 3: Uniting hypothesis generation and evaluation.

Grading: Your course grade will be determined from four components

1. **Participation (20%):** Class attendance for MW sessions is mandatory but only a part of this grade. I expect that if I ask you to work a problem or read something prior to class and you will come to class prepared and ready to engage. Regular reflection worksheets will be included in the participation grade. *If you are losing a significant amount of credit in this category I will warn you by email unless your points are being lost due to skipping class.*

2. **Completion of problem sets (20%):** On the deadline for a problem set, upload a photographed/scanned copy of your work to Canvas or furnish a hard copy to me in person (slide it under my door in 6365 if I'm not there). You should always your work to class the next day for your reference. The deadline will be 1 or 2 days before class because I will base the in-class discussion on the answers I receive. *Full credit will be awarded for all good faith answers received prior to the deadline. Bringing a finished problem set to class the day after the deadline merits half credit.*

3. **Midterm exam (30%):** Two *take home* exams will be given. The first will be *due no earlier than* October 11th and the second will be *due no earlier than* November 26th. You will be given the opportunity to turn in revised answers to questions on the exam one week after it is returned to you for up to half of the credit back. The exams are intended to be a learning experience. *Collaboration is strictly forbidden on exams but is permitted and recommended for the revision*.

4. **Final project (30%):** Each student will select a unique recently reported reaction and will critically evaluate the *current* level of mechanistic understanding we have of the reaction and discuss opportunities to further develop our mechanistic model for the reaction.

   Tentative deadlines for this project (subject to change):
   a. October 5th: Initial paper reviews
   b. October 17th: Second round of paper reviews
   c. October 29th: Selection of reaction mechanism from reviewed papers for further evaluation
   d. November 22nd: Preliminary mechanistic analysis of selected reaction
   e. December 5th: Submission for peer review
   f. December 9th: Peer reviews due
   g. December 16th: Final project deadline

Course expectations: Looking up solutions in online (or getting answers from folks who took it last year!) to any questions posed in exams or problem sets *defeats the purpose of those exercises and is completely off limits*. Collaboration with your colleagues is encouraged (except on exams) but you must always still turn in your own original work.

A personal note on diversity and inclusion: In my classroom and in the department as a whole, we support and celebrate diversity of all kinds, including racial, cultural, sexual orientation, mental health, nation of origin, gender identity, marital status, political, age and experience. I am committed to making my class an open and safe learning environment for *everyone* involved and I will do everything in my power to foster and maintain that environment. Please be mindful and respectful of your colleagues in this interactive class.

McBurney Resource Center: The University of Wisconsin-Madison supports the right of all enrolled students to a full and equal educational opportunity. The Americans with Disabilities Act (ADA), Wisconsin State Statute (36.12), and UW-Madison policy (Faculty Document 1071) require that students with disabilities be reasonably accommodated in instruction and campus life. Reasonable accommodations for students with disabilities is a shared faculty and student responsibility. Students are expected to inform faculty [me] of their need for instructional accommodations by the end of the third week of the semester, or as soon as possible after a disability has been incurred or recognized. Faculty [I], will work either directly with the student [you] or in coordination with the McBurney Center to identify and provide reasonable instructional accommodations. Disability information, including instructional accommodations as part of a student's educational record, is confidential and protected under FERPA.

Justification regarding 3 credit hours awarded: Three hours of classroom or direct faculty/instructor instruction and a minimum of six hours of out of class student work each week over the course of the ~3 month semester makes this a 3 credit hour course.

Academic Integrity: By enrolling in this course, each student assumes the responsibilities of an active participant in UW-Madison's community of scholars in which everyone's academic work and behavior are held to the highest academic integrity standards. Academic misconduct compromises the integrity of the university. Cheating, fabrication, plagiarism, unauthorized collaboration, and helping others commit these acts are examples of academic misconduct, which can result in disciplinary action. This includes but is not limited to failure on the assignment/course, disciplinary probation, or suspension. Substantial or repeated cases of misconduct will be forwarded to the Office of Student Conduct & Community Standards for additional review. For more information, refer to studentconduct.wiscweb.wisc.edu/academic-integrity/.

Institutional statement on diversity: "Diversity is a source of strength, creativity, and innovation for UW-Madison. We value the contributions of each person and respect the profound ways their identity, culture, background, experience, status, abilities, and opinion enrich the university community. We commit ourselves to the pursuit of excellence in teaching, research, outreach, and diversity as inextricably linked goals."