

CHM 6225 Advanced Principles of Organic Chemistry – Syllabus

Physical Organic Chemistry
syllabus version 1.0

Spring 2023, CHM 6225, Class#23017

Tuesdays & Thursdays 11:45 am–1:40 pm, FLI 109

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Course Description. Principles of organic chemistry and their application to reaction mechanisms. A detailed introduction to the theory and principles of organic chemistry; bonding and structure in organic chemistry, stereochemistry, reactive intermediates in organic chemistry and transition state theory; kinetics and thermodynamic approaches. Exploration of these concepts via computational chemistry will also be emphasized. Prerequisites: CHM 2210, 2211 (or one year of undergraduate organic chemistry) and CHM 5224.

Syllabus. The syllabus below is subject to change. Updated versions and reading assignments will be available on Canvas (see below). The chapters refer to the principal textbook for the course, *Advanced Organic Chemistry: Part A: Structure and Mechanism, Fifth Edition*. Additional course reading from *Stereochemistry of Organic Compounds (SOC)* and *Mechanism and Theory in Organic Chemistry, Third Edition (MTOC)* will be made available.

Class #1	January 10	Class Introduction/Overview. 1.1 Molecular Structure and Valence Bond Concepts
Class #2	January 12	1.2 Molecular Orbital Theory and Methods
Class #3	January 17	T1.1, T1.2, T1.3 Bonding Topics
Class #4	January 19	2.1 Configuration
Class #5	January 24	SOC 4.1–4.6 Symmetry, Point Groups
Class #6	January 26	2.2–2.3 Conformation, Molecular Mechanics PS#1 DUE
Class #7	January 31	2.4–2.6, T2.1, T2.2, T2.3 Stereochemistry of Reactions, Stereoelectronic Effects
Class #8	February 2	3.1, MTOC 2.3 Thermodynamic Stability, Benson Group Additivities PS #2 DUE
Class #9	February 7	Midterm Exam I (Chapters 1–3.1)

Class #10	February 9	3.2 Chemical Kinetics
Class #11	February 14	3.3 Thermodynamic Stability and Reaction Rates
Class #12	February 16	3.4–3.5 Electronic Substituent Effects, Isotope Effects
Class #13	February 21	3.6 Linear Free-Energy Relationships
Class #14	February 23	3.7–3.8 Catalysis, Solvent Effects
Class #15	February 28	4.1 Mechanisms for Nucleophilic Substitution PS #3 DUE
Class #16	March 2	4.2–4.3 Structural and Solvation Effects, Neighboring-Group Effects
Class #17	March 7	4.4, T4.1 Carbocations, Carbocations in Petroleum Processing PS #4 DUE
Class #18	March 9	Midterm Examination II (Chapters 3.2–4)
	March 14	No Class – UF Spring Break
	March 16	No Class – UF Spring Break

Class #19	March 21	5.1–5.9 Addition Reactions
Class #20	March 23	5.10 Elimination Reactions
Class #21	March 28	6.1–6.5, T3.1 MTOC 3.3–3.4 Hydrocarbon Acidity, Carbanions and Carbon Nucleophiles
Class #22	March 30	7.1–7.7 Carbonyl Compounds PS #5 DUE
Class #23	April 4	8.1–8.6 Aromaticity
Class #24	April 6	9.1–9.5 Aromatic Substitution PS #6 DUE
Class #25	April 11	Midterm Examination III (Chapters 5–9)

Class #26	April 13	10.1–10.6 Concerted Pericyclic Reactions
Class #27	April 18	11.1–11.6 Generation and Characterization of Free Radicals, Mechanisms, Reactions
Class #28	April 20	12.1–12.4 Photochemistry, Photochemical Reactions
Class #29	April 25	TBD, Final Exam Review PS #7 DUE
Final Exam	May 4	Final Exam (cumulative) Thursday, May 4, 10:00 am – 12:00 pm

Required Textbook: Carey, F. A.; Sundberg, R. J. *Advanced Organic Chemistry: Part A: Structure and Mechanism, Fifth Edition*; Springer: New York, 2007 (ISBN 978-0-387-68346-1, Paperback, Amazon.com, \$50.27).

A pdf version of the required textbook is freely available through UF online via either of the following links:

<https://link.springer.com/book/10.1007/978-0-387-44899-2>

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Required Software: Spartan, Student Edition (for Macintosh or Windows). *Wavefunction*. wavefun.com (\$50) <https://www.wavefun.com/spartan-student-pricing> Or, you can use a full version on the iMac in SIS A119. There are many other suitable and free software applications that will substitute for this—especially for the PC platform. For example, NWChem <https://nwchemgit.github.io/>, ORCA <https://orcaforum.kofo.mpg.de/app.php/portal>, HyperChem <https://it.chem.ufl.edu/services/available-software/>
See: https://en.wikipedia.org/wiki/List_of_quantum_chemistry_and_solid-state_physics_software

Recommended Textbooks:

- 1) Carey, F. A.; Sundberg, R. J. **Advanced Organic Chemistry: Part B: Reactions and Synthesis, Fifth Edition**; Springer: New York, **2007** (ISBN 978-0-387-68354-6, Paperback).
 - 2) **SOC** = Eliel, E. L.; Wilen, S. H.; Mander, L. N. **Stereochemistry of Organic Compounds**; Wiley-Interscience, New York, **1994** (ISBN 0-471-01670-5).
 - 3) **MTOC** = Lowry, T. H.; Richardson, K. S. **Mechanism and Theory in Organic Chemistry, Third Edition**; HarperCollins Publishers: New York, **1987** (ISBN 0-06-044084-8).
 - 4) Smith, M. B.; March, J. **March's Advanced Organic Chemistry, Fifth Edition**; Wiley-Interscience: New York, **2001** (ISBN 0-471-58589-0).
 - 5) Carroll, F. A. **Perspectives on Structure and Mechanism in Organic Chemistry**; Brooks/Cole, Pacific Grove, CA, **1998** (ISBN 0-534-24948-5).
 - 6) Anslyn, E. V.; Dougherty, D. A. **Modern Physical Organic Chemistry**; University Science Books, Sausalito, CA, **2006** (ISBN 1-891389-31-9).
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Canvas/Instructure Website. All students will have access to the Canvas website: <https://ufl.instructure.com/> You will login with your Gatorlink account username and password. This is where you will find general class information, important news, office hours, problem sets, handouts, class notes, and keys. This is also where you will be able to find out your point totals and histograms.

Class Requirements.

- 1) Seven problem sets (40 points each; 240 points max; the lowest score will be dropped)
 - 2) Six in-class quizzes (10 points each = 60 points total)
 - 3) Three midterm examinations (150 points each = 450 total)
 - 4) Final examination (250 points)
- = 1000 points total**
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Problem Sets. Problem sets will be **due at 11:59 pm** on the designated due dates. Answer keys will be posted around this time. Please write your answers in the space provided on the problem set itself. The usual submission method will be for students to convert Problem Sets into a pdf and submit it on Canvas under Assignments. The problem sets may be spot-graded; this means that only some or parts of the problems may be scored and contribute to the 40 points. The lowest of the seven scores will be dropped. You may work in groups or alone. But, you may not copy answers. The problem sets are designed to prepare you for the examinations.

In-Class Quizzes. The six in-class quizzes, which will be **unannounced and randomly distributed** during the semester, will be short and are designed to encourage you to attend class and to keep up with the course. They should be very easy for those who have read the assigned material for that day.

Midterm Examinations. There will be three midterm examinations and each will focus on the chapters designated. The midterms are not designed to be cumulative; but you may expect some natural amount of material from a previous midterm to be important and necessary.

Final Examination. The final examination will be cumulative. To do well, it will be important to keep up during the semester and review all notes and assignments for the course. **Working problems—frequently and consistently—**may be the best overall approach to mastering the course material.

Extra Credit. Additional opportunities *should* arise for extra credit (e.g., extensive class participation, attending a lecture outside of class, extra credit quizzes, extra credit problems on the homework, or an extra credit question on an exam). In any event, no more than 50 extra credit points may be earned. Extra credit will be applied after the curve is assigned for the course. This may allow some students to raise their grade by one grade increment (e.g., B+ to A-).

Grading. Grades will be curved based on points earned out of 1000. The extra-credit will then be added to those who have earned it to determine if an increase in the final grade is achieved.

Assignment Regrading. If you have a question concerning the grading of an assignment, you may submit the entire assignment for complete regrading. The assignment must be submitted for regrading by the first class meeting after the date the assignment was returned to the class.

Online Lecture Notes (Templates) will be available on Canvas (see above) in pdf format. They are organized by book chapter. The Lecture Notes show important course material, but have blank space for your notes to be taken during lecture. This method is designed to require less time writing and allow more time thinking. Students are encouraged to download and/or print the Lecture Notes and bring them to class to facilitate notetaking.

Office Hours. Office hours are scheduled for Thursdays from 3:00 to 3:50 pm in room 340 Sisler Hall. If I am not present, check my office (LEI 318A). Additional office hours will likely be held during times of greater demand.

Conflict Examinations. *Conflict examinations* will be given only for University-excused absences provided the appropriate documentation is supplied. Conflict exams are ideally administered *before* the regularly scheduled examination—not after. If for some reason you take an exam late, do not download or otherwise view the posted exam or exam key, or consult any classmates about exam content. Any such downloading or consultation will result in a zero for the exam.

Attendance. Attendance for this class is not recorded. However, the six unannounced and random in-class quizzes will generally reflect your attendance pattern.

Class Numbers. To facilitate the grading and return of assignments, I request that you write your name and class number on each one. The class numbers will be assigned after a few classes.

Accommodations for students with disabilities. Students requesting classroom accommodation must first register with the Dean of Students Office. The Dean of Students Office will provide documentation to the student who must then provide this documentation to the Instructor when requesting accommodation.

Course Evaluations. “Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available at <https://gatorevals.aa.ufl.edu/students/>. Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their Canvas course menu under GatorEvals, or via <https://ufl.bluera.com/ufl/>. Summaries of course evaluation results are available to students at <https://gatorevals.aa.ufl.edu/public-results/>.”

UF Honor Code: We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity.

On all work submitted for credit by students at the university, the following pledge is either required or implied: **“On my honor, I have neither given nor received unauthorized aid in doing this assignment.”** “The university requires all members of its community to be honest in all endeavors. A fundamental principle is that the whole process of learning and pursuit of knowledge is diminished by cheating, plagiarism and other acts of academic dishonesty. In addition, every dishonest act in the academic environment affects other students adversely, from the skewing of the grading curve to giving unfair advantage for honors or for professional or graduate school admission. Therefore, the university will take severe action against dishonest students. Similarly, measures will be taken against faculty, staff and administrators who practice dishonest or demeaning behavior.”

Cheating and Plagiarism. Cheating and/or plagiarism will not be tolerated. The minimum penalty will be an automatic zero on the assignment in question. Suspension from the University may also result. Do not risk it. It is not worth it. Plagiarism consists of passing off as one’s own the ideas, words, writings, etc. that belong to someone else. You are committing plagiarism if you copy the work of another person and turn it in as your own, even if you have that person’s permission. See: <https://sccr.dso.ufl.edu/policies/student-honor-code-student-conduct-code/>

Copyright Notice. All handouts used in this course are copyrighted and may not be copied without my expressly granted permission. “Handouts” include all materials generated for this class, which include but are not limited to syllabi, quizzes, exams, problems, in-class materials, lecture note templates, lecture notes, review sheets, problem sets, or other materials. Tutors and tutoring services are expressly forbidden from copying any or all of these materials, unless you pay me two million U.S. dollars. Only students currently enrolled in the class may make a single copy of this material for their personal use.

COVID-19 Statements:

Privacy. Our class sessions may be audio-visually recorded for students in the class to refer and for enrolled students who are unable to attend live. Students who participate with their camera engaged or utilize a profile image are agreeing to have their video or image recorded. If you are unwilling to consent to have your profile or video image recorded, be sure to keep your camera off and do not use a profile image. Likewise, students who un-mute during class and participate verbally are agreeing to have their voices recorded.

If you are not willing to consent to have your voice recorded during class, you will need to keep your mute button activated and communicate exclusively using the "chat" feature, which allows students to type questions and comments live. The chat will not be recorded or shared.

As in all courses, unauthorized recording and unauthorized sharing of recorded materials is prohibited.

Safety Practices. We will have face-to-face instructional sessions to accomplish the student learning objectives of this course. In response to COVID-19, the following practices are in place to maintain your learning environment, to enhance the safety of our in-classroom interactions, and to further the health and safety of ourselves, our neighbors, and our loved ones.

- If you are not vaccinated, get vaccinated. Vaccines are readily available at no cost and have been demonstrated to be safe and effective against the COVID-19 virus. Visit this link for details on where to get your shot, including options that do not require an appointment: <https://coronavirus.uflhealth.org/vaccinations/vaccine-availability/>. Students who receive the first dose of the vaccine somewhere off-campus and/or outside of Gainesville can still receive their second dose on campus.
- You are expected to wear approved face coverings at all times during class and within buildings even if you are vaccinated. Please continue to follow healthy habits, including best practices like frequent hand washing. Following these practices is our responsibility as Gators.
 - Sanitizing supplies are available in the classroom if you wish to wipe down your desks prior to sitting down and at the end of the class.
 - Hand sanitizing stations will be located in every classroom.
- If you sick, stay home and self-quarantine. Please visit the UF Health Screen, Test & Protect website about next steps, retake the questionnaire and schedule your test for no sooner than 24 hours after your symptoms began. Please call your primary care provider if you are ill and need immediate care or the UF Student Health Care Center at 352-392-1161 (or email covid@shcc.ufl.edu) to be evaluated for testing and to receive further instructions about returning to campus. UF Health Screen, Test & Protect offers guidance when you are sick, have been exposed to someone who has tested positive or have tested positive yourself. Visit the [UF Health Screen, Test & Protect website](#) for more information.
 - Course materials will be provided to you with an excused absence, and you will be given a reasonable amount of time to make up work.
 - If you are withheld from campus by the Department of Health through Screen, Test & Protect you are not permitted to use any on campus facilities. Students attempting to attend campus activities when withheld from campus will be referred to the Dean of Students Office.
- Continue to regularly visit coronavirus.UFHealth.org and coronavirus.ufl.edu for up-to-date information about COVID-19 and vaccination.
- Course materials will be provided to you with an excused absence, and you will be given a reasonable amount of time to make up work. To find more information on the university attendance policies, click here <https://catalog.ufl.edu/UGRD/academic-regulations/attendance-policies/>.

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