

# CHM 6225 Advanced Principles of Organic Chemistry – Syllabus

(Physical Organic Chemistry – syllabus version 2.0)

Spring 2014, CHM 6225-3550

Tuesday 11:45 am–1:40 pm, MAT 005; Thursday 11:45 am–1:40 pm, LIT 237 (locations subject to change)

Professor Stephen A. Miller, miller@chem.ufl.edu, Office Leigh Hall 318A

**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 e-Learning (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.

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Class #1	January 7	Class Introduction/Overview. 1.1 Molecular Structure and Valence Bond Concepts
Class #2	January 9	1.2 Molecular Orbital Theory and Methods
Class #3	January 14	T1.1, T1.2, T1.3, Bonding Topics
Class #4	January 16	2.1 Configuration
Class #5	January 21	SOC 4.1–4.6 Symmetry, Point Groups
Class #6	January 23	2.2-2.3 Conformation, Molecular Mechanics <a href="#">PS#1 DUE</a>
Class #7	January 28	No Class. Travel
Class #8	January 30	2.4–2.6, T2.1, T2.2, T2.3 Stereochemistry of Reactions, Stereoelectronic Effects
Class #9	February 4	3.1, MTOC 2.3 Thermodynamic Stability, Benson Group Additivities <a href="#">PS #2 DUE</a>
Class #10	February 6	<a href="#">Midterm Exam I</a> (Chapters 1–3.1)

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Class #11	February 11	3.2 Chemical Kinetics
Class #12	February 13	3.3 Thermodynamic Stability and Reaction Rates
Class #13	February 18	3.4–3.5 Electronic Substituent Effects, Isotope Effects
Class #14	February 20	3.6 Linear Free-Energy Relationships
Class #15	February 25	3.7–3.8 Catalysis, Solvent Effects
Class #16	February 27	4.1 Mechanisms for Nucleophilic Substitution <a href="#">PS #3 DUE</a>
	March 4	No Class. Spring Break
	March 6	No Class. Spring Break
Class #17	March 11	4.2–4.3 Structural and Solvation Effects, Neighboring-Group Effects
Class #18	March 13	4.4, T4.1 Carbocations, Carbocations in Petroleum Processing <a href="#">PS #4 DUE</a>
Class #19	March 18	<a href="#">Midterm Examination II</a> (Chapters 3.2–4)

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Class #20	March 20	5.1–5.9 Addition Reactions
Class #21	March 25	5.10 Elimination Reactions
Class #22	March 27	6.1–6.5, T3.1 MTOC 3.3–3.4 Hydrocarbon Acidity, Carbanions and Carbon Nucleophiles
Class #23	April 1	7.1–7.7 Carbonyl Compounds <a href="#">PS #5 DUE</a>
Class #24	April 3	8.1–8.6 Aromaticity
Class #25	April 8	9.1–9.5 Aromatic Substitution <a href="#">PS #6 DUE</a>
Class #26	April 10	<a href="#">Midterm Examination III</a> (Chapters 5–9)

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Class #27	April 15	10.1–10.6 Concerted Pericyclic Reactions
Class #28	April 17	11.1-11.6 Generation and Characterization of Free Radicals, Mechanisms, Reactions
Class #29	April 22	12.1–12.4 Photochemistry, Photochemical Reactions <a href="#">PS #7 DUE</a>
Final Exam	May 2	<a href="#">Final Exam</a> (Chapters 1–12) Friday, May 2nd, 12:30 pm – 2:30 pm, TBD

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**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, \$51.38).

**Required Software:** Spartan, Student Edition (for Macintosh or Windows). Wavefunction. wavefun.com (\$50)

[http://wavefun.com/products/macintosh/Student/mac\\_student.html](http://wavefun.com/products/macintosh/Student/mac_student.html)

[http://wavefun.com/products/windows/Student/win\\_student.html](http://wavefun.com/products/windows/Student/win_student.html)

(There are many other suitable and free software applications that will substitute for this—especially for the PC platform.)

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**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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**e-Learning Website.** All students will have access to the e-Learning website: <https://lss.at.ufl.edu/>

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.

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**Class Requirements.**

- 1) Seven problem sets (35 points each; 210 points max; the lowest score will be dropped)
  - 2) Ten in-class quizzes (10 points each = 100 points total)
  - 3) Three midterm examinations (150 points each = 450 total)
  - 4) Final examination (240 points)
- = 1000 points total**

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**Problem Sets.** Problem sets will be **due at 4:00 pm** on the designated due dates. They can be turned in after class or into the plastic in/out box outside of Leigh 318A (on the file cabinet). Answer keys will be posted at this time. Please print out the posted problem sets and write your answers in the space provided. The problem sets *may* be spot-graded; this means that only some or parts of the problems may be scored and contribute to the 35 points. The lowest of the seven scores must 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.

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**In-Class Quizzes.** You are expected to read the assigned chapter sections before each class. The ten 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 fairly easy for those who have read the assigned material. Quizzes can only be taken during the class period in which they are administered. They cannot be made up without an official, written University excuse. Each quiz will be worth 10 points.

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**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.

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**Final Examination.** The final examination will be cumulative. The best way to study for it will be 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.

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**Extra Credit.** Opportunities *may* arise for extra credit (e.g., extensive class participation, attending a lecture outside of class, 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 a maximum of one letter grade increment (e.g., from a B+ to an A-).

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**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.

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**Teaching Assistant.** Amr Feteha ([feteha@ufl.edu](mailto:feteha@ufl.edu)) is scheduled to be the teaching assistant/grader for this course. He can usually be found in Sisler 113 or 119 or can be reached via email.

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**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.

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**Online Notes Templates** will be available at e-Learning (see above) in pdf format. They are organized by book chapter. The templates are made and posted to help you follow the lecture; hopefully this will allow you to spend less time writing and more time thinking. Students are encouraged to print the note templates and bring them to class to facilitate notetaking.

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**Office Hours.** Office hours are scheduled for 3:00 pm – 3:50 pm on Thursdays. They will likely be held in Leigh Hall 328 (the Polymer Conference Room). Additional/individual office hours should be possible and should be scheduled by email.

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**Conflict Examinations.** *Conflict examinations* will be given only for University-excused absences provided the appropriate documentation is supplied **one week in advance of the examination period**. Conflict exams are administered before the regularly scheduled examination; no makeup examinations will be given after the regularly scheduled examination.

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

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**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.

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**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.

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**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.**

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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. A reduction of the final course grade is also likely. 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:

<http://www.dso.ufl.edu/sccr/honorcodes/honorcode.php>

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**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, review sheets, problem sets, or other materials. Tutors and tutoring services are expressly forbidden from copying any or all of these materials. Only students currently enrolled in the class may make a single copy of this material for their personal use.

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