CHEM 2310
Advanced Organic Chemistry I
Fall 2017, W/F 8 to 9:15 AM
228 Eberly Hall

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Office hours: Θ 10 - 12, F 9:30 - 11 (subject to revision)

Course description: A discussion of the tools, both modern and classical, that are the basis of mechanistic interpretations of relations between structure and reactivity. Special emphasis is placed on the detailed molecular level analysis of organic molecules, including the transient reactive intermediates: carbanions, carbocations, carbenes, and radicals, to develop a predictive sense for reactivity. The factors that influence equilibria, product distribution, and reaction mechanisms are also explored. *This is graduate-level physical organic chemistry course; if you are an undergraduate, please come talk to me at the end of the first class meeting.*

Learning objectives: By the end of this course, you should be able to: 1) predict or rationalize the outcome of a reaction on the basis of molecular structure and chemical principles; 2) propose a reasonable mechanism for a reaction using known reactivity patterns and experimental data; 3) select and apply appropriate experimental tools to elucidate a reaction mechanism.

Grading Policy: Course grades will be based on the total number of points earned on quizzes, problem sets, and exams, assigned according to the following scheme. Final letter grades will reflect how well learning objectives are met; they will neither be assigned using an absolute scale, nor fitted to a predetermined distribution ("on a curve"). Thus, you are not competing with your classmates.

- In class quizzes (unannounced): five × 10 pts. = 50 pts. (5%)
- Problem sets: two × 100 pts. = 200 pts. (20%)
- Midterm exams: three × 150 pts. = 450 pts. (45%)*
- Final exam: 300 pts. (30%)*

  ∑ = 1000 pts. (100%)

* Before you hand in your final exam, you may elect to scale your final exam score by 3/2, converting its point value of the final to 450 pts.; your lowest midterm score will be dropped. Your choice, as indicated on the cover page of your final exam, is binding once you turn in your exam.

Textbook: *(Required)* Anslyn, E. V.; Dougherty, D. A. *Modern Physical Organic Chemistry*; University Science Books: Mill Valley, Calif., 2006 (ISBN: 1891389319). *(Optional solutions manual)* Sponsler, M. B.; Anslyn E. V.; Dougherty, D. A. *Student Solutions Manual to Accompany Modern Physical Organic Chemistry*; University Science Books: Mill Valley, Calif., 2006 (ISBN: 189138936X). *(Also available at the University Store, optional)* Grossman, R. B. *The Art of Writing Reasonable Organic Reaction Mechanisms*, 2nd ed.; Springer: New York, 2003 (ISBN 0387954686).

Useful references and further reading (optional): [1]Carey, F. A.; Sundberg, R. J. *Advanced Organic Chemistry Part A: Structure and Mechanism*, 5th ed.; Springer: New York, 2008 (ISBN 0387683461). [2]Lowry, T. H.; Richardson, K. S. *Mechanism and Theory in Organic Chemistry*, 3rd ed.; HarperCollins: New York, 1987 (ISBN 0060440848). [3]Fleming, I. *Molecular Orbitals and Organic Chemical Reactions, Student Edition*; Wiley: Chichester, U. K., 2009 (ISBN: 0470746599). [4]Albright, T. A.; Burdett, J. K.; Whangbo, M. H. *Orbital Interactions in Chemistry*, 1st ed.; Wiley: New York, 1985 (ISBN 0471873934). [5]Eliel, E. L.; Wilen, S. H. *Stereochemistry of Organic*

Compounds; Wiley: New York, 1994 (ISBN 0471016705). [6]Crabtree, R. H. *The Organometallic Chemistry of the Transition Metals*, 6th ed.; Wiley: Hoboken, N. J., 2014 (ISBN 1118138074).

An excellent review of undergraduate organic chemistry: Clayden J.; Greeves, N.; Warren, S. *Organic Chemistry*, 2nd ed.; Oxford University Press: Oxford, U. K., 2012 (ISBN 0199270295).

A graduate organic chemistry workbook: Burgess, K. *Organic Chemistry by Inquisition 1. General Reactions*; Inquisition Press, 2009 (ISBN 0615290744). Can be ordered from www.byinquisition.org.

Assigned reading: At the end of each Friday class meeting, portions of *Modern Physical Organic Chemistry* (on average 40-50 pages per week) will be assigned as required reading for the following week. It is important to come to class prepared by doing the assigned reading before class. (However, it is okay if you do not understand everything that you read.)

Quizzes: Unannounced quizzes (5 min., 10 pts.) based on the assigned reading will take place five times during the semester, at the beginning of class (beginning no later than 8:05 am). These quizzes cannot be made up if you miss class. If you miss one or more quizzes, and your absences are excused, your other *n* quiz scores will be scaled by a factor of 5/*n* to calculate your total quiz score.

Problem sets: Two problem sets will be assigned for homework. They will be handed out on the Sep 6 and Oct 25, 2017. Completed problem sets will be due Oct 11 and Dec 6, 2017, respectively. *Please start these problem sets early!* Problem sets solutions will be posted one week following the due date. Unexcused late problem sets submitted after the due date but before solutions are posted will receive 80% credit. Problem sets will not be accepted after solutions are posted. Working with your classmates is permitted and encouraged. *However, the solutions you submit need to reflect your own understanding, and plagiarism will not be tolerated. If you obtain a key insight for solving a problem from a classmate, please include an acknowledgement for his/her contribution.* For each problem set, five of the twelve problems will be selected for grading (five × 20 pts. = 100 pts.). Please staple the pages of your submitted work. Sheets of unlined 8.5" × 11" are preferred over lined loose-leaf paper. You are strongly encouraged to provide your responses in block letters (rather than cursive), using ink (rather than pencil). Illegible responses may incur a loss of credit.

Exams: Midterm exams (75 min., 150 pts.) will take place in class on the Fridays of Weeks 4, 8, and 12. Midterm exams will focus on the topics covered after the previous exam. However, fundamental concepts from earlier in the semester may appear in later midterms. Each midterm exam will consist of a true/false section (30 pts.), a short answer section (30 pts.), and three free response questions (three × 30 pts. = 90 pts.). The final exam (180 min., 300 pts.) will consist of twelve free response questions, from which you will choose ten to answer (ten × 30 pts. = 300 pts.). During each exam, you may bring one handwritten 8.5" × 11" sheet of notes, as well as a molecular model set of your choosing. No other exam aids are permitted. You will be provided with scrap paper to work out your answers, but only the responses contained in your exam packet will be graded. Again, answers are expected to be legible, and points may be deducted if they are not.

Student Opinion of Teaching Surveys: Students in this class will be asked to complete a *Student Opinion of Teaching Survey*. Surveys will be sent via Pitt email and appear on your *CourseWeb* landing page during the last three weeks of class meeting days. Your responses are anonymous. Please take time to provide comments, suggestions, and criticisms for any aspect of the course, including format, content, policies, and overall effectiveness. Your feedback is very valuable, and the things I learn from you will be taken into account when I teach this or another course in the future.

University Policies on Academic Integrity: Students in this course will be expected to comply with the University of Pittsburgh's Policy on Academic Integrity. Any student suspected of violating this obligation will be required to participate in the procedural process, initiated at the instructor level, as

outlined in the University's *Guidelines on Academic Integrity* (provost.pitt.edu/sites/default/files/academic_integrity_guidelines.pdf). In particular, please take note of the following University statement on academic integrity:

> *Cheating/plagiarism will not be tolerated. Students suspected of violating the University of Pittsburgh Policy on Academic Integrity, from the February 1974 Senate Committee on Tenure and Academic Freedom reported to the Senate Council, will be required to participate in the outlined procedural process as initiated by the instructor. A minimum sanction of a zero score for the quiz or exam will be imposed.* — Academic Integrity Statement for Syllabi

University Policies on Disability Services: If you have a disability for which you are or may be requesting an accommodation, you are encouraged to contact both your instructor and Disability Resources and Services (DRS, www.studentaffairs.pitt.edu/drs/), 140 William Pitt Union, (412) 648-7890, drsrecep@pitt.edu, (412) 228-5347 for P3 ASL users, as early as possible in the term. Disability Resources and Services will verify your disability and determine reasonable accommodations for this course.

Absences: Attendance will not be taken (however, there will be unannounced quizzes, *see above*). If you have a planned absence for a family obligation, medical appointment, or religious observance, please let me know as soon as possible, in order to make reasonable accommodations. If you were absent due to an illness or an emergency, and you missed a quiz or turned in a problem set late as a result, please provide documentation to have your absence excused.

Course Schedule & Outline:

Week 1-4 (Aug 30 to Sep 20, 7 class meeting days): Nomenclature, Lewis structures and valence bond theory, weaker-than-covalent interactions and intermolecular forces, thermochemistry, conformational analysis and strain, acid-base theories, hybridization, orbital interactions, hyperconjugation. (*Problem set #1 handed out Sep 6, 2017*)

Midterm #1 Sep 22, 2017: 8 – 9:15 am, 228 Eberly

Week 5-8 (Sep 27 to Oct 18, 7 class meeting days): Transition state theory, reaction mechanism and kinetic analysis, catalysis, linear free energy relationships, kinetic isotope effects.
Problem set #1 due Oct 11, 2017 at 9:15 am

Midterm #2 Oct 20, 2017: 8 – 9:15 am, 228 Eberly

Week 9-12 (Oct 25 to Nov 15, 7 class meeting days): Reactive intermediates (carbanions, carbocations, carbenes, radicals), stereochemistry, mechanisms for additions, eliminations, substitutions & rearrangements, introduction to organometallic chemistry of transition metals. (*Problem set #2 handed out Oct 25, 2017*)

Midterm #3 Nov 17, 2017: 8 – 9:15 am, 228 Eberly

Thanksgiving (University holiday) Nov 22 – 26

Week 13-15 (Nov 29 to Dec 13, 5 class meeting days): Aromaticity, Hückel theory, orbital correlation diagrams, pericyclic reactions, Woodward-Hoffmann rules.
Problem set #2 due Dec 6, 2017 at 9:15 am

Final exam Dec 15, 2017: time and location to be announced