CHEM 430/530: Physical Organic Chemistry

M/W/F 1:30 – 2:20 pm, ZOOM

Th (<u>Optional</u> Tutorial) 1:30 – 2:20, ZOOM

COURSE OBJECTIVES:

This course is designed for first year graduate students or advanced undergraduates with a desire to use fundamental principles of organic chemistry to predict structure and reactivity. A broad overview of organic reactions with an emphasis on mechanism will be covered. This course assumes a firm understanding of organic chemistry at the sophomore level and builds on that foundation. By the end of this course, students should be able to propose reaction pathways using arrow-pushing mechanisms and be able to justify these pathways using fundamental physical organic principles such as frontier molecular orbital theory, resonance, sterics, electrostatics, and thermodynamics. CHEM 430/530 is a prerequisite for CHEM 431/531.

INSTRUCTOR:

Professor Matthew Golder (goldermr@uw.edu)
Office hours: During & After Thursday Tutorial

Teaching Assistant: Meredith Pomfret (mpomfr@uw.edu)
Office hours: TBA

COURSE WEBSITE, COMMUNICATION, & TECHNOLOGY:

The course will be run synchronously (M/W/F and Th optional tutorial). All sessions will be recorded to the best of my ability and posted on Canvas (this is especially important if you are in a different time zone!).

Canvas: https://canvas.uw.edu/courses/1396363
Questions regarding content on problem sets and exams should be directed to the Canvas discussion board. Chances are high that if you have a question, someone else likely has a question as well. I will answer questions on Canvas for the whole class to see.

For all email correspondences, please include CHEM 430 or CHEM 530 in the subject line. Please only email from your @uw.edu account; emails from personal accounts may be inadvertently missed.

You should have all received communication earlier in the summer about having a tablet (such as a Surface or iPad) for this course. If you don't have one and haven't already requested one for free through the UW Student Technology Loan program (https://stlp.uw.edu/). If you have other technology issues, please contact me directly ASAP so we can figure out a solution.

We will be using Ziteboard for online collaborations and problem solving. Please signup for a free account with your @uw.edu email address: https://ziteboard.com/. I will create workspaces for our Tutorial sessions; you can create your own limited number of Ziteboards to work on problems with each other yourselves.

TEXTBOOKS:

E. V. Anslyn & D. A. Dougherty. *Modern Physical Organic Chemistry*. University Science Books: Sausalito, CA, 2006.
(Note: Anslyn & Dougherty is a "classic" reference book. You'll likely use it to look up information for the duration of your graduate career and beyond. However, we will do our best to post PDFs of the relevant sections on Canvas; the material should only be used for the purposes of this course).

I. Fleming. *Molecular Orbitals and Organic Chemical Reactions*. John Wiley & Sons: New York, 2010.
(Note: This book is available online through UW Libraries as a PDF from any UW-campus/VPN connection -- https://onlinelibrary.wiley.com/doi/book/10.1002/9780470689493)

Also recommended for graduate students:
F. A. Carey and R. A. Sundberg. *Advanced Organic Chemistry. Part A. Structure and Mechanism, 5th Ed.* Kluwer Academic/Plenum Publishers, New York, 2007.

A.J. Kirby, *Stereoelectronic Effects*. Oxford Scientific Publishers, 1996.
(Note: Readings from Kirby will be posted on Canvas for use in this course only).

Additional articles and handouts will be assigned periodically for reading. Content from these materials may or may not show up on Take Home Challenges.

PROBLEM SETS:

Problem sets will be assigned throughout the course (approximately seven in total). Problem sets will be spot checked and will be graded on a "check-plus", "check", "check-minus" scale. Submission of problem sets will be done through Gradescope (see Canvas for links). Due dates/times will be listed on each problem set and Canvas. Solutions will also be posted on Canvas prior to the Thursday Tutorials.

TUTORIALS:

We will go over problem sets and THCs during optional tutorials (Thursdays, 1:30-2:20p on Zoom). We'll review problems as a group on virtual whiteboards (Ziteboard)

TAKE HOME CHALLENGES (THC):

THC #1: Through Lecture #7, Assigned F 10/23, Due W 10/28
THC #2: Through Lecture #19, Assigned F 11/20, Due W 11/25
Final THC: Cumulative, M 12/14 (Format TBD)

Assessment of your newfound knowledge will consist of problems in the form of Take Home Challenges (THCs). These will be assigned twice during the course of the quarter on Friday at the end of class and will be due the following Wednesday at the beginning of class (on Gradescope). You are welcome to work in groups online (you will have access to the virtual whiteboards), but I ask that you only write down answers you are comfortable defending. Ultimately, this is an upper level course and your goal should be to learn and understand as much material as possible as opposed to simply "getting a good grade". You may use your notes and books for the THCs, but please do not use Scifinder, Reaxys, Google Scholar, etc to look up the original references. Please communicate to me ahead of time if you have an issue with any of the dates. Except for religious reasons (see below), all other unavoidable conflicts will need to be approved by Dr. Eric Camp (BAG 303D, ericcamp@uw.edu).

PRESENTATIONS (CHEM 530 ONLY):

Graduate students will be responsible for preparing a short flash talk (~ 3-5 minutes, one slide) on a young (pre-tenure) organic chemistry faculty member. Undergraduates in CHEM 430 will not prepare presentations but are expected to attend the sessions. These presentations will happen after Thanksgiving. I will provide a list of assigned "topics" later in the quarter. One major goal of this assignment is to expose everyone to the broad/diverse nature of organic chemistry (both personnel and topics).

GRADING:

430: Final THC (35%), higher THC (30%), lower THC (20%), problem sets (15%).
530: Final THC (35%), higher THC (30%), lower THC (20%), problem sets (10%), presentation (5%).

The final THC can replace your lower THC score. Problem sets will be graded with a "check", "check-plus", or "check-minus". If you do not hand in a problem set, then you'll receive a 0 on that assignment.

RELIGIOUS ACCOMODATIONS:

Washington state law requires that UW develop a policy for accommodation of student absences or significant hardship due to reasons of faith or conscience, or for organized religious activities. The UW's policy, including more information about how to request an accommodation, is available at Religious Accommodations Policy (https://registrar.washington.edu/staffandfaculty/religious-accommodations-policy/). Accommodations must be requested within the first two weeks of this course using the Religious Accommodations Request form:
https://registrar.washington.edu/students/religious-accommodations-request/.

TENTATIVE SCHEDULE (SUBJECT TO CHANGE):

Lecture #	Date	Week #	Topics
1	W 9/30	1	Introduction, Bonding/Molecular Orbitals, Hybridization I
2	F 10/2	1	Hybridization II, Arrow Pushing
3	M 10/5	2	Molecular Orbital Trends, Energy Diagrams
4	W 10/7	2	"4 Types of Energy", Kinetics and Selectivity
5	F 10/9	2	TS Theory (Hammond Postulate/Curtin-Hammett), Carbocations (Empty p-orbital) I- SN1 Rxns, Stability
6	M 10/12	3	Carbocations (Empty p-orbital) II- Lone Pair v. Pi v. Sigma Donation, norbornyl cations, cyclopropyl cations
7	W 10/14	3	Carbocations (Empty p-orbital) III- More Sigma Donation (beta metal carbocations, neighboring group effects, solvent effects)
8	F 10/16	3	Addition to π^* I- Additions to C=O (Cram model, Felkin-Anh)
9	M 10/19	4	Addition to π^* II- Additions to C=O (Lewis Acid, Relative trends)
10	W 10/21	4	Addition to π^* III- Additions to C=O + C=N (Organocatalysis/LUMO-lowering reactions, Reductive amination, Conjugate addition)
11	F 10/23	4	Addition to σ^* I- Proton transfer, SN2 + Addition to σ^* II- Steric effects, SN1 v. SN2 v. SN2'
12	M 10/26	5	Addition to σ^* III- Migratory rearrangements (Pinacol, Tiffeneau-Demjanov, Wolff, Hofmann, Beckman, Baeyer-Villiger)
13	W 10/28	5	Finish σ^* III (Hofmann, Beckmann, B-V, Migratory Apptitutde, Orbitals)
14	F 10/30	5	Elimination Reactions I- E1 v. E2 v. E1cb
15	M 11/2	6	Elimination Reactions II- Beta metals, Peterson Olefination, Grob, Thermal
16	W 11/4	6	Nucleophlic filled n orbitals I- Acid/Base, pKa Nucleophilic filled n orbitals II- Anions, Organometallics (-Li, -Mg, -Cu)

17	F 11/6	6	Nucleophilic π orbitals I- Heteroatom electrophiles (H-X addition, epoxidation, hydroboration/oxidation/migration)
18	M 11/9	7	Nucleophilic π orbitals II- Carbon-carbon bond formation (Prins, allylation/crotylation, enols/enamines/enolates: regioselectivity… thermodynamic v. kinetic)
VETERAN'S DAY (No Class)	W 11/11	7	No Class
19	F 11/13	7	Nucleophilic π orbitals III- Carbon-carbon bond formation (Finish enols/enamines/enolates: C-alkylation v. O-acylation, Ireland TS, Z-T TS, stereoselectivity)
20	M 11/16	8	Nucleophilic σ orbitals- Hydrides
21	W 11/18	8	, Other Stereoelectronic Effects I- Definition, Anomeric Effect, Cyclic Structures and Other Stereoelectronic Effects II- Alkanes, Alkenes, Conformational analysis & A values, Baldwin's Rules
22	F 11/20	8	Pericyclic Reactions I- Introduction + Electrocyclization
23	M 11/23	9	Pericyclic Reactions II- Finish Electrocyclizations + Cycloaddition
THANKSGIVING BREAK (No Class)	W 11/25	9	No Class
THANKSGIVING BREAK (No Class)	F 11/27	9	No Class
24	M 11/30	10	Pericyclic Reactions III- Finish Cycloaddition, Sigmatropic
25	W 12/2	10	Pericyclic Reactions IV- Chelotropic + Group Transfer
26	F 12/4	10	CHEM 530 Student Presentations (~5/day)
27	M 12/7	11	CHEM 530 Student Presentations (~5/day)
28	W 12/9	11	CHEM 530 Student Presentations (~5/day)
29	F 12/11	11	CHEM 530 Student Presentations (~5/day)
Final Exam	M 12/14		Cumulative Final Exam