CHEM 633
Advanced Organic Chemistry: Physical
Fall 2016

Instructor: Mary Watson (209 LDL, 831-1529, mpwatson@udel.edu)

Office Hours: 2:30-3:30pm, Wed

Lectures: 11–12:15, Tues/Thurs, 205 BRL

TA: Scott Shuler (grader)

Website:
http://www.udel.edu/chem/mpwatson/mpwatson/Courses.html

The website will be updated regularly. Please check it for announcements, lecture notes, problem sets, answer keys, etc.

Course Capture: Lectures will be recorded and available on UD Course Capture. Link is coming shortly.

> "The mind of man cannot conceive an effect without a cause, so that the sight of a phenomenon always awakens an idea of causation. All human knowledge is limited to working back from observed effects to their cause."
>
> Claude Bernard, *An Introduction to the Study of Experimental Medicine,* 1865

Textbooks: *All texts are On Reserve in the Chemistry Library.*

Modern Physical Organic Chemistry (**A&D**)
by Anslyn, Eric V. & Dougherty, Dennis A.
Publisher: University Science Books
ISBN: 9781891389313
Edition: 2006
Required

The Art of Writing Reasonable Organic Reaction Mechanisms (**Grossman**)
By Grossman, Robert B.
Publisher: Springer
ISBN: 9781441930163
Edition: 2010
Required

Advanced Organic Chemistry/Part A: Structure & Mechanisms (**C&S)**
by Carey, Frank A. and Sundberg, Richard J.
Publisher: Springer
ISBN: 9780387448978
Edition: June 2007
Recommended
NOTE: This book also comes in paperback and is electronically available through the UD library.

Stereoelectronics Effects (**Kirby**)
by Kirby, A.J.
Publisher: Oxford University Press
ISBN: 9780198558934
Edition: 1996
Recommended

Molecular Orbitals and Organic Chemical Reactions, Student Edition (**Fleming**)
by Fleming, Ian
Publisher: John Wiley & Sons
ISBN: 9780470746592
Edition: 2009
Recommended

Other Tools: Molecular model kit

Grades:		
	6 Problem Sets	30%
	2 Midterms (10/6, 11/17)	40%
	Final Exam (TBA)	30%

Midterms and Final: Closed note, closed book tests. You may use your molecular model kit.

Problem Sets: Concepts will be introduced in lecture, but only by practicing their application will you gain the depth of understanding necessary for your PhD (and to pass the exams). Detailed solutions will be posted on the class website. You may collaborate on the problem sets, but be sure you turn in your own work. Do not use Reaxys, SciFinder Scholar or consult the literature to find the answers, unless specifically directed to do so.

Do not plagiarize or cheat. Any student who commits academic dishonesty will be punished according to the University of Delaware's guidelines (http://www.udel.edu/stuguide/09-10/code.html#honesty).

CHEM 633 Course Learning Goals

After successful completion of this course, a student should be able to:

1. Describe various theories of chemical bonding. (1)*
2. Propose reasonable arrow-pushing mechanisms based on Frontier Molecular Orbital theory. (1)
3. Rationalize the results of chemical reactions based on steric, electronic or stereoelectronic effects. (1)
4. Predict whether a reaction is exo- or endo-thermic based on bond dissociation energies. (1)
5. Predict the lowest energy conformations of organic molecules. (1)
6. Understand the stereochemical relationships between molecules. (1)
7. Describe a qualitative energy surface for a reaction using a reaction coordinate diagram. (1)
8. Understand the difference between ground states and transition states of molecules. (1)
9. Analyze experimental results to determine the thermodynamic and kinetic profile of an organic reaction. (1)
10. Derive rate laws for single and multiple step reactions, including catalytic reactions. (1)
11. Understand other tools used for studying reaction mechanisms. (1)
12. Understand the theory of catalysis. (1)
13. Understand the theory of asymmetric catalysis and stereochemical communication between molecules. (1)
14. Computationally predict ground and transition states using Density Functional Theory (DFT) methods. (5)
15. Describe the various classes of pericyclic reactions and analyze them based on an understanding of the molecular orbitals involved. (1)
16. Describe the types of noncovalent interactions and examples of these interactions in organic chemistry. (1)
17. Search and understand primary literature. (5)
18. Communicate ideas clearly and effectively in written and oral formats. (10)

*(*Numbers in parentheses indicate the departmental learning goals with which each course goal is aligned. Please see: http://www.udel.edu/chem/goals.html.)*

Proposed Course Outline and Readings

Week (Dates)	Topic	Recommended Reading	Notes
1 (8/30, 9/1)	Bonding Theories	A&D, Ch 1 C&S, Ch 1 Kirby, Ch 2 Fleming, Ch 1–2	
2 (9/6, 9/8)	Bonding Theories Arrow-pushing mechanisms (based on FMO)	Kirby, Ch 4 A&D, Appendix 5	**9/8: Problem Set 1 Due**
3 (9/13, 9/15)	Steric, electronic and stereoelectronic effects	Kirby, Ch 5 Fleming, Ch 3	
4 (9/20, 9/22)	Baldwin's rules HSAB Theory Thermodynamics	A&D, Ch 2 C&S, Ch 3 A&D, Ch 6, C&S, Ch 3	**9/22: Problem Set 2 Due**
5 (9/27, 9/29)	Conformational Analysis	A&D, Ch 7 C&S, Ch 3	9/29: Meet in 221 BRL (Computer Lab)
6 (10/4, 10/6)	Conformational Analysis		**10/6: Midterm 1**
7 (10/11, 10/13)	Transition State Theory Kinetics: Rate Equations		
8 (10/18, 10/20)	Kinetics: Multi-Step Reactions		**10/20: Problem Set 3 Due**
9 (10/25, 10/27)	Catalysis		
10 (11/1, 11/3)	Catalysis Asymmetric Catalysis	C&S, Ch 2	**11/3: Problem Set 4 Due**
(11/8)	No Class (Election Day)		
11 (11/10)	Other Mechanistic Tools		**11/10: Problem Set 5 Due**
12 (11/15, 11/17)	Pericyclic Reactions	A&D, Ch 15 C&S, Ch 8 & 10 Fleming, Ch 6	**11/17: Midterm 2**
(11/22, 11/24)	No Class (Fall Break)		
12 (11/29, 12/1)	Pericyclic Reactions		
13 (12/6, 12/8)	Noncovalent Interactions	A&D, Ch 3 & 4	**12/8: Problem Set 6 Due**