**Department of Chemistry Syllabus**

This syllabi is advisory only. For details on a particular instructor's syllabus (including books), consult the instructor's course page. For a list of what courses are being taught each quarter, refer to the Courses page. *Every instructor has prerogative to teach the course as they see fit and ultimately the instructor's syllabus supersedes all others.*

***CHE 233: Physical Organic Chemistry***

Approved:

 2016-08-23, Dean Tantillo

Suggested Textbook: (actual textbook varies by instructor; check your instructor)

Anslyn, E. V.; Dougherty, D. A. *Modern Physical Organic Chemistry*.

University Science Books, 2006 (a student solutions manual also exists)

*a running list of corrections to the first printing can be found here:*

 http://www.uscibooks.com/anserr.htm

Suggested Schedule:

**I. Point Group Symmetry** (~11/2 week)

 • symmetry elements, operations, and point groups

 • chirality and topicity

• symmetry as a mechanistic tool

• symmetry and efficiency

**II. Intro to Arrow-Pushing** (~1 week)

 • conventions, drawing

 • arrow-pushing strategies

 • typical reactivity patterns for various reactive intermediates

**III. Kinetics and Thermodynamics** (~3 weeks)

 • types of energy

• potential energy surfaces

 • intro to chemical kinetics

 • rate theory

 • isotope effects

 • solvent effects

• Hammond postulate and Curtin-Hammett principle

• linear free energy relationships

• kinetic vs. thermodynamic control

 • dynamics and tunneling

**IV. Molecular Orbital Theory** (~41/2 weeks)

 • what does the Schrödinger equation mean?

• simple Hückel theory 🡪 doing quantum mechanics by hand!

*\* frontier orbital concepts (FMO) and geometric effects*

• computational chemistry

 *\* aromaticity*

 *\* pericyclic reactions*

Additional Notes:

 **Additional Useful References, Not Required:**

• Fleming, I. *Molecular Orbitals and Organic Chemical Reactions*. Wiley, 2010

(both a reference edition and student edition are available)

• Grossman, R. B. *The Art of Writing Reasonable Organic Reaction Mechanisms*,

Springer, 2002 (hardback) and 2010 (paperback).

• Sundberg, R. J.; Carey, F. A. *Advanced Organic Chemistry, Part A: Structure*

*and Mechanism, 4th Edition*. Kluwer/Plenum Press, 2000.

• Gómez-Gallego, M.; Sierra, M. A. *Organic Reaction Mechanisms–40 Solved*

*Cases*. Springer, 2004.

• Isaacs, N. *Physical Organic Chemistry, 2nd Edition*, Addison-Wesley-Longman,

1995

• Fleming, I. *Frontier Orbitals and Organic Chemical Reactions*. Wiley, 1996.

• Carpenter, B. K. *Determination of Organic Reaction Mechanisms*. Wiley, 1994.

• Smith, M. B.; March, J. *March’s Advanced Organic Chemistry: Reactions,*

*Mechanisms, and Structure, 6th Edition*. Wiley, 2007.

 • Lowry, T. H.; Richardson, K. S. *Mechanism and Theory in Organic Chemistry,*

 *3rd Edition*. Harper Collins, 1987.

• Quinkert, G.; Egert, E.; Griesinger, C. *Aspects of Organic Chemistry: Structure*.

 VCH, 1996.

• Moss, R. A.; Platz, M. S.; Jones, M. *Reactive Intermediate Chemistry*. Wiley,

2004.

• Eliel, E. L.; Wilen, S. H. *Stereochemistry of Organic Compounds*. Wiley, 1994.

• Young, D. *Computational Chemistry: A Practical Guide for Applying*

*Techniques to Real World Problems*. Wiley, 2001.

 **A Great Source of Practice Arrow-Pushing Problems:**

http://evans.harvard.edu/problems/

others are listed on SmartSite

 **The IUPAC Glossary of Terms Used in Physical Organic Chemistry:**

http://www.chem.qmw.ac.uk/iupac/gtpoc/

Learning Goals:

• *This class is not about memorization. It is about developing analytical thinking*

*and problem solving skills*.

• By the end of the course, when given an experimental observation on a particular reaction, you should

be able to:

(1) write down a reasonable arrow-pushing mechanism for the reaction

(2) decide whether existing theories can explain the observed reactivity

(3) design experiments to test your proposed mechanism/explanation

(4) evaluate the validity/plausibility of others’ explanations