

# CHEM\*4720      ORGANIC REACTIVITY

## Winter Semester 2010

Introduction to physical organic chemistry, including a discussion of reactive intermediates, substituent effects, medium effects, ring strain, pericyclic reactions and a theoretical description of the bonding in organic molecules.

Prerequisite: CHEM\*3760 (may be taken concurrently). Recommended prerequisite: CHEM\*2820 or CHEM\*2880

Instructor: Professor Adrian L. Schwan, Office SCIE 2515. X53061

Office hours: **T.B.A.**

I can be available outside of office hours; you are encouraged to make an appointment to meet with me through my secretary Elizabeth Copland (SCIE 2516).

Text: Two should be available in the bookstore:

Advanced Organic Chemistry, Part A, 4th ed., by Carey and Sundberg. (may be 5<sup>th</sup> ed. available)  
Advanced Organic Chemistry Reactions and Mechanisms, 2<sup>nd</sup> ed by Bernard Miller

Either one of these texts is "recommended"; they are useful references for some of the topics to be covered in the lectures. The Miller book is particularly useful if you are currently enrolled in CHEM\*3760. Further references will be given where appropriate. Supplemental information in the form of class notes ARE REQUIRED. They will be distributed by way of CourseLink prior to lectures.

Method of Presentation: Two lectures per week (T, Th) all in MacK 238 at 8:30-9:50 AM. There will be no lecture on Tues. March 9, 2010.

Method of Evaluation: The course grade will be based on one mid-term examination, a final examination and approximately 5-8 small problem assignments. The mid-term examination will be given either on Feb. 26/10 or during the week of March 1-5/10 at a mutually convenient time. The final examination will be given during the final examination period. The problem assignments and their subsequent solutions will be posted on Courselink.

The final grade will be calculated as follows:	problem assignments	30%
	mid-term examination	30%
	final examination	40%

All midterm and examination questions are an exercise in problem recognition and solving. They are to be attempted and solved individually.

### COURSE OUTLINE

1. Substituent Effects on Organic Rates and Equilibria
  - a) Qualitative description of substituent effects
  - b) Linear free energy relationship: the Hammett equation
2. Solvent Effects on Organic Rates and Equilibria
  - a) Basic relationships; solvents and solvation
  - b) Scales for ion solvating ability

c) phase transfer catalysis

3. Angle Strain and Stereoelectronic Effects

Strained molecules and some reactivity

Radical clock reactions

Stereoelectronic requirements for reactions

4. The Huckel Molecular Orbital Method (partially a self-study section)

a) Description of the method

b) Regularities in Huckel molecular orbitals

c) Aromaticity and NMR

5. Frontier Orbital Theory and Pericyclic Reactions

a) Families of pericyclic reactions and rules governing them

b) Rates of pericyclic reactions

c) Introduction to 1,3-dipoles

**\*\* If you miss the final exam or a major mid-term assignment for medical or compassionate reasons, you are expected to provide verification of those reasons before you receive a passing grade, credit standing or a deferred privilege.**

**\*\* As part of the faculty evaluation process in the Department of Chemistry, students are reminded that written comments on the teaching performance of the lecturer may be sent to the Chair (or the Dean of CPES), Department of Chemistry, at any time. Such letters must be signed; a copy, will be made available to the instructor after submission of final grades.**

Library Reserve List The following books have been placed on reserve in the library.

Two Hour Reserve

1. I Fleming. Frontier Molecular Orbitals and Organic Chemical Reactions. QD 461.F53
2. T.L. Gilchrist and R.C. Storr. Organic Reactions and Orbital Symmetry. QD 476.G54 1979
3. B. Miller, Advanced Organic Chemistry Reactions and Mechanisms QD251.2.M534 (maybe under Chem\*3760)
4. F.A. Carroll Perspectives on Structure and Mechanism in Organic Chemistry QD476.C375 B.
5. E.V. Anslyn and D.A. Dougherty Modern Physical Organic Chemistry QD476 .A57 2006

Three Day Reserve

1. T.H. Lowry and K.S. Richardson. Mechanism and Theory in Organic Chemistry, 3rd ed. QD 476.L68
2. N.S. Isaacs. Physical Organic Chemistry. QD 475.I846
3. F.A. Carey and R.J. Sundberg. Advanced Organic Chemistry Part A. QD 251.2.C36 1983
4. E.V. Anslyn and D.A. Dougherty. Modern Physical Organic Chemistry QD476.A57 2006
5. B. Halton, ed. Advances in Strain in Organic Chemistry QD 461.a33 1991
6. A. de Meijere and S. Blechert Strain and Its Implications in Organic Chemistry QD 461.S875
7. A. Greenburg. Strained Organic Molecules. QD 476.G66
8. K. Yates. Huckel Molecular Orbital Theory. QD 461.Y37
9. A. Streitweiser Jr. Molecular Orbital Theory for Organic Chemists. QD 255.S88
10. J.D. Roberts. Notes on Molecular Orbital Calculations. QD 476.R58
11. P.J. Garratt. Aromaticity. QD 331.G28 1986
12. R.B. Woodward and R. Hoffman. The Conservation of Orbital Symmetry. QD 461.W75
13. T.L. Gilchrist and C.W. Rees. Carbenes, Nitrenes and Arynes. QD 305.H7 G5
14. C.D. Johnson. The Hammett Equation. QD 502.J63
15. F.A. Carey and R.J. Sundberg. Advanced Organic Chemistry Part B. QD 251.2.C36 1983
16. A. Pross. Theoretical and Physical Principles of Organic Reactivity. QD476.P755 1995