CHM 6225
Advanced Principles of Organic Chemistry
Spring 2017

Instructor: Lisa McElwee-White, Sisler 429, 392-8768, lmwhite@chem.ufl.edu

Web Page: Course materials are on Canvas at https://elearning.ufl.edu/.

Text: "Modern Physical Organic Chemistry," Eric V. Anslyn and Dennis A. Dougherty.

Class Time: TR 11:45 – 1:40 p.m. in Flint 121
Approximately 10 one-hour periods will be problem sessions.

Due to my travel there will be probably be a couple of Saturday mornings where we have makeup lecture 9-11 am. I provide coffee and donuts. I will let you know the dates of these lectures when I have it all sorted out.

Office Hours: MWF 3:00 - 4:00 p.m.

Exams: February 9, March 21, April 27 (final)
In addition, there will be a short (5-6 page) original proposal due April 13.

Grading:

	Points Possible
Exam 1	125
Exam 2	125
Problems	50
Proposal	75
Final Exam	125
Total	500

Note: Problem sets are not collected for grading but participation in the problem session is graded.

Prerequisites:

It will be assumed that you are familiar with the basic mechanisms of the reactions taught in sophomore organic and CHM 5224. Also assumed is a minimal knowledge of symmetry and group theory. That is, you should be able to determine the symmetry elements and point group of a molecule. You should also be able to read a character table. If you need help in this regard, the workbook "Molecular Symmetry and Group Theory" by Alan Vincent is on reserve in Marston Science Library. Working programs 1-3 will provide you with more than enough background.

Course Topics:

I. Philosophy of Mechanistic Study

II. Direct Characterization of Products and Intermediates
   A. Product Identification
   B. Stereochemical Studies
   C. Isotopic Labeling Studies
      1. Symmetry
      2. Crossover
   D. Direct Observation of Intermediates

III. Thermodynamics and Kinetics
   A. Energetics and Equilibria
   B. Group Increments
   C. Strain
   D. Molecular Modeling
   E. Kinetics
   F. Transition State Theory
   G. Arrhenius Parameters

IV. Substituent Effects
   A. Linear Free Energy Relationships
      1. Hammett Plots
   B. Kinetic Isotope Effects
      1. Primary KIE
      2. Secondary, α, β, γ KIE
   C. Equilibrium Isotope Effects

V. Medium Effects
   A. Solvent Effects
      1. Grunwald-Winstein Plots
      2. Solvent Isotope Effects
   B. Binding Forces
      1. Ion Pairing
      2. H-bonding

C. Acid-Base Reactions
    1. Acidity Functions
    2. Acid/Base Catalysis
    3. Brønsted Plots

VI. Orbital Symmetry Control
A. Hückel Molecular Orbitals
B. Woodward-Hoffmann, Dewar-Zimmerman, and FMO analyses
C. Cycloadditions
D. Electrocyclic Processes
E. Sigmatropic Reactions

VII. Molecular Orbital Analysis of Non-Pericyclic Reactions
A. Introduction to Perturbation Theory
B. Group Orbitals
C. Molecular Orbitals from Group Orbitals
D. Stereoelectronic Effects
    1. Baldwin's Rules
    2. Donor-Acceptor Analysis
    3. Anomeric Effect
E. Hard and Soft Acids and Bases
F. Ambident Nucleophiles/Ionic Reactions