

CHEM-769 PHYSICAL ORGANIC CHEMISTRY as of Nov. 27/11

Tentative Course Outline Winter Semester 2012 (Full document will be provided closer to the first class date)

Physical organic chemistry, including a discussion of reactive intermediates, substituent effects, photochemistry, pericyclic reactions and a theoretical description of the bonding in organic molecules.

Instructor: Professor Adrian L. Schwan, Office: SCIE 2512, Guelph Campus. 824-4120 X53061; E-mail: schwan@uoguelph.ca FAX: 1-519-766-1499

Text: Modern Physical Organic Chemistry, E.V. Anslyn and D.A Dougherty....recommended

The text is a useful reference for most of the topics to be covered in the lectures. Further references will be given where appropriate. Supplemental information in the form of class notes are provided. These will be presented to you in some form in advance of lectures.

Method of Presentation: One 2 1/2 hour lecture per week, Mon. nights starting at 7:00 pm in the main link room. First lecture is Mon. Jan. 9, 2012. It is expected that there will be no lecture on March 26/12.

Method of Evaluation: The course grade will be based on a final examination, some problem assignments and an essay of one research group's recent efforts in physical organic or related chemistry. The final examination will be given in April. Regular problem sets will be comprised of a few questions. Several practice problems will be part of the course notes. The absolute final due date for the essay is due Apr. 2, 2012.

The final grade will be calculated as follows:

research essay	30%
problem assignments	35%
final examination	35%

Should you wish to drop one of your in-course efforts (once you have completed it and seen your grade) and make the final exam worth the difference, that option is available and should be requested in writing before you write the final.

Audits: Please understand that an audit is an official entry on your transcript and there are certain course requirements to achieve this. Audit does not mean "sitting-in". Professor Schwan generally does not recommend the audit or 'sitting in' process, since 1. your graduate career will be assessed primarily by the quality of your thesis and 2. a graduate degree means that you can learn things for yourself. It follows that your time should be spent on your research project.

COURSE OUTLINE

1. Kinetics and Mechanism
 - (a) Transition state theory
 - (b) Energy profiles
2. Substituent Effects on Organic Rates and Equilibria
 - (a) Qualitative description of substituent effects
 - (b) Linear free energy relationship: the Hammett equation
 - (c) Acid and Base catalysis
3. The Hückel Molecular Orbital Method -- a tool for appreciating molecular orbitals

- (a) Description of the method
 - (b) Regularities in Hückel Molecular Orbitals
 - (c) The concept of aromaticity
4. Aromaticity
- (a) NMR analysis of aromaticity
 - (b) Homoaromaticity
 - (c) Heterocyclic aromaticity
5. Orbital Symmetry Control of Concerted Reactions
- (a) FMO analysis of pericyclic reactions
 - (b) Introduction to 1,3-dipoles
 - (c) Other reactive species in pericyclic reactions
6. Radical Reactions
- (a) Concepts and BDE's
 - (b) Prevalence
 - (c) Rearrangements
7. Photochemistry
- (a) Physical Concepts
 - (b) Some Photochemical reactions
8. Evaluation of Some Research Publications
-to take place throughout the year as a class discussion

Library Reserve List

A number of general texts applicable to the areas noted above will be put on reserve.