

CHEM*3750 ORGANIC CHEMISTRY II (0.5 credits)

Spring Semester, 2019

Dept. of Chemistry, CEPS, University of Guelph

GENERAL INFORMATION AND COURSE OUTLINE

Instructor: Adrian L. Schwan, MacN 336 X58781

Office Hours: TBA

- and most any other time you find me in my office
- I will try to visit lab sections on a regular cycle
- schwan@uoguelph.ca (not for scientific discourse)

Required Materials

- (a) CHEM*3750 Organic Chemistry II Class Notes, Spring 2019 *edition* by A. L. Schwan provided on CourseLink
- (b) Text:
Organic Chemistry, 12th Edition and accompanying Study Guide
Graham Solomons and Craig Fryhle (henceforth shortened **SF12**)
or
Organic Chemistry, 11th Edition and accompanying Study Guide
Graham Solomons and Craig Fryhle (henceforth shortened **SF11**)
or
Organic Chemistry, 10th Edition and accompanying Study Guide
Graham Solomons and Craig Fryhle (henceforth shortened **SF10**)
- (c) Laboratory Manual:
CHEM*3750 Organic Chemistry II Laboratory Manual (lab manuals will be available in SCI 2106 starting May 13).

Additional Materials

- (d) A molecular model set is often useful in “seeing” organic chemistry principles. The Bookstore sells one or maybe two types.
- (e) Wiley-Plus additional study materials

Method of Presentation There are two meetings each week (Tues., Thurs. 11:30-12:50 MacN 118). The Tuesday slots will be solely lecture material sometimes roughly following the Schwan notes and the sections indicated in **SF10/11/12**. The Thurs. period will be 30-40 min of new material as per a Tues. lecture and the remainder will be review and examples, e.g., tutorial. This proposed allotment may occasionally be changed to accommodate scheduling or in-class tests.

Tutorial time will be used to:

- a) discussion of lecture material and how to write or understand mechanisms
- b) developing expertise, recognition skills and solving problems related to compound elucidation and synthetic chemistry
- c) discussion of (homework) problems
- d) material of your request and/or
- e) the laboratory.

As stated, the option is available to dedicate some tutorial time to new lecture material, depending on the pace of the throughout the term.

In CHEM*3750 we continue the organic chemistry education from CHEM*1040 and CHEM*2700. A knowledge of the reactions, mechanisms, terminology and concepts covered in those courses will be assumed and may be required as part of a satisfactory answer to examination questions. You should look over past course material and review any reactions as necessary as soon as possible.

Laboratory The CHEM*3750 laboratory consists of one three-hour period per week. There are laboratory sections on Tues. and Thurs. afternoons in Summerlee Science Complex 3108 (Enter via east doors close to library). See the last few pages on this document for a few details about the lab. Labs begin in the week of May 13, 2019.

Problem Assignments Problems different from those available in Solomons or Wiley-Plus and are placed at strategic locations in the Schwan notes. Solutions to those problems are placed nearby in the notes. As well there will be a listing of problems from **SF** for which you are responsible. We should also have the opportunity to discuss some of them in the tutorial period, particularly upon your request. For the spectroscopy unit, a number of problems from a problem set will be submitted for grading and that grade will contribute significantly to your final mark.

Course Grade The final grade will be calculated as follows:

| Item | Value | Comments |
|-------------------|-------|---|
| Problem Questions | 14% | Available May 9/19; due June 11/19 <i>at/by the beginning of class.</i> (hardcopy or CourseLink dropbox feature) |
| Mini Class test | 6% | In class on Thurs. June 20/19 (covers part of Chapter 2) |
| Full Class test | 20% | In class on Thurs. July 11/19 (covers Chapters 2 and some of Chapter 3) |
| Final examination | 30% | Cumulative; (Aug. 15 2019) |
| Laboratory | 30% | Breakdown for lab grades will be provided elsewhere. |

YOU WILL NOT PASS THE COURSE UNLESS YOU HAVE RECEIVED A PASSING GRADE ON AT LEAST ONE OF: [THE PROBLEM QUESTIONS (14%)]; [THE SUM OF THE CLASS TESTS (26%)]; OR [THE FINAL EXAM (30%)] A GRADE OF 48% WILL BE ASSIGNED REGARDLESS OF THE OUTCOME OF A CALCULATION.

NOR WILL YOU PASS THE COURSE IF YOU DO NOT RECEIVE A PASSING GRADE IN THE LABORATORY.

**** 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, 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.**

Academic misconduct

Students in CHEM*3750 are expected to be familiar with University of Guelph Academic Misconduct expectations and regulations found at:
<http://www.uoguelph.ca/registrar/calendars/undergraduate/current/c08/c08-amisconduct.shtml>

Types of offenses are described at:

<http://www.uoguelph.ca/registrar/calendars/undergraduate/current/c08/c08-amisconductoffen.shtml>

from which I particularly note copying

Copying is similar to plagiarism in that it involves the appropriation of others' work as one's own. It includes copying in whole or in part another's test or examination answer(s), laboratory report, essay, or other assignment.

Copying also includes submitting the same work, research or assignment for credit on more than one occasion in two or more courses, or in the same course, without the prior written permission of the instructor(s) in all courses involved (including courses taken at other post-secondary institutions).

Please note: Whether or not a student intended to commit academic misconduct is not relevant for a finding of guilt. Hurried or careless submission of assignments does not excuse students from

responsibility for verifying the academic integrity of their work before submitting it. Students who are in any doubt as to whether an action on their part could be construed as an academic offence should consult with a faculty member or faculty advisor.

Recording of Materials

Presentations which are made in relation to course work—including lectures—cannot be recorded or copied without the permission of the presenter, whether the instructor, a classmate or guest lecturer. Material recorded with permission is restricted to use for that course unless further permission is granted.

Resources

The Academic Calendars are the source of information about the University of Guelph's procedures, policies and regulations which apply to undergraduate, graduate and diploma programs.

E-mail Communication

As per university regulations, all students are required to check their <mail.uoguelph.ca> e-mail account regularly: e-mail is the official route of communication between the University and its students.

When You Cannot Meet a Course Requirement

When you find yourself unable to meet an in-course requirement because of illness or compassionate reasons, please advise the course instructor (or designated person, such as a teaching assistant) in writing, with your name, id#, and e-mail contact. See the undergraduate calendar for information on regulations and procedures for Academic Consideration.

Drop Date

The last date to drop one-semester courses, without academic penalty, is July, 2019. For regulations and procedures for Dropping Courses, see the Undergraduate Calendar.

Copies of out-of-class assignments

Keep paper and/or other reliable back-up copies of all out-of-class assignments: you may be asked to resubmit work at any time.

Accessibility

The University of Guelph is committed to creating a barrier-free environment. Providing services for students is a shared responsibility among students, faculty and administrators. This relationship is based on respect of individual rights, the dignity of the individual and the University community's shared commitment to an open and supportive learning environment. Students requiring service or accommodation, whether due to an identified, ongoing disability or a short-term disability should contact the Student Accessibility Services as soon as possible.

For more information, contact Student Accessibility Services at 519-824-4120 ext. 56208 or email accessibility@uoguelph.ca or see the website: <https://wellness.uoguelph.ca/accessibility/>

Course Content

1 - INTRODUCTION TO ORGANIC SPECTROSCOPY

1. ^1H NMR Spectroscopy
2. ^{13}C NMR Spectroscopy
3. Infrared (IR) Spectroscopy
4. Other Spectroscopic Methods

2 - ALDEHYDES AND KETONES

1. Synthetic Routes to Aldehydes and Ketones
2. Acidity and Enolization of Aldehydes and Ketones
3. Halogenation of Ketones and Aldehydes
 - haloform reaction
4. Alkylation Reactions and Enamines
5. The Aldol Condensation
6. Other Related Condensation Reactions
 - Claisen, Dieckmann, Reformatsky condensations
7. Synthetic Applications of Condensation Reactions
 - acetoacetate synthesis
 - malonate synthesis
 - Robinson annelation
8. The Wittig Olefination of Aldehydes and Ketones
9. Reductive Conversion of $\text{C}=\text{O}$ to CH_2

3 - CONJUGATION

1. Terminology and Nomenclature
2. Allyl
3. Conjugated Dienes
4. The Diels Alder Reaction
5. Molecular Orbital Description of Conjugation

4 - BENZENE: AROMATICITY, CONJUGATION AND ASSOCIATED REACTIVITY

1. Aromaticity
 - ($4n + 2$) rule, resonance energy
2. NMR Spectra of Benzene Derivatives
3. Side Chain Chemistry of Benzene Derivatives
 - radical bromination
4. Birch Reduction (The destruction of aromaticity)

5 - REACTIVITY OF SOME SUBSTITUTED AROMATIC COMPOUNDS

1. Aromatic Amines
2. Diazonium Salts

-Sandmeyer reaction

3. CHEM*2700 and aromatic synthetic strategies.

4. Aryl Halides

-nucleophilic aromatic substitution

-benzyne

5. Phenols and Phenyl Ethers

6 - SYNTHESIS

As part of lecture or tutorial sessions, occasional synthetic strategies will be presented that comprise an effort to tie together the various chapters of this course and of CHEM*2700.

Course Learning Objectives

Chapter 1: To be able to:

- elucidate simple organic structures based on available characterization data
- draw conclusions about structural features based on characterization data
- predict spectral data of simple structures based on available data and analogies
- develop a trust and confidence in the value of tabulated spectral data

Chapter 2: To be able to:

- write reactions equations for the preparation of aldehydes and ketones
- cite several pK_a values and have a sense of the origin of their magnitude
- apply pK_a values to understand the direction of equilibrium in acid or basic environments
- understand significance of racemization as well as exchange and deuteration reactions of aldehydes and ketones
- understand the basis of and draw reaction equations for reactions of aldehydes, ketones and esters
- assemble simple synthetic sequences for the construction of organic molecules using reactivity characteristics of aldehydes, ketones and esters
- understand and apply the various features of reactivity pertaining to of aldehydes, ketones and esters
- develop a sense of the driving force for particular mechanistic steps for chemical conversions of aldehydes, ketones and esters

Chapter 3: To be able to:

- recognize double bond containing compounds and intermediates and appreciate their geometry
- understand and draw resonance structures of allylic and related intermediates, and understand their significance to the distribution of reaction products
- understand and draw potential energy diagrams for simple intermediates and transition states.
- draw Diels-Alder products and starting materials with stereochemical components, where applicable

Chapter 4: To be able to:

- understand fundamentals of aromaticity, antiaromaticity and applications of the $4n$ and $4n+2$ rules and their electronic structure-based origins
- recognize significance of aromaticity as a driving force
- understand and draw resonance structures of benzylic and related intermediates, and understand their significance to reaction product distributions
- draw and understand radical and anionic intermediates of benzene derivatives, and their origins
- understand the synthetic value and mechanism of the Birch reduction

Chapter 5: To be able to:

- draw and understand reaction of aromatic amines
- draw and understand reactions of diazonium salts and benzene intermediates
- understand role of substituent effects in the electrophilic aromatic substitution and nucleophilic aromatic substitution reactions
- assemble strategically chosen syntheses of aromatic compounds based on various aromatic substitution mechanisms

Overall:

- the student should be able to recognize reaction equations and assign applicable, general classification terms**
- the student should understand and appreciate that “the structure of the molecule tells you everything”!**

Helpful Websites

organic chemistry:

<http://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/intro1.htm>

<http://www.organic-chemistry.org/namedreactions/>

Also see under “Web Pages” on the left column at:

<https://www.chem.wisc.edu/areas/reich/group/index.htm>

videos:

<https://www.khanacademy.org/science/organic-chemistry>

<http://www.chemtube3d.com/Main%20Page.html>

spectroscopy related:

http://sdbs.riodb.aist.go.jp/sdbs/cgi-bin/cre_index.cgi

<http://www.chem.wisc.edu/areas/reich/handouts/nmr-h/hdata.htm>

<http://www.nmrdb.org/predictor>

Molecule Drawing Software

1. The Chemistry Department has a site license for ChemDraw - Standard.

To download ChemDraw proceed to the URL below.

<http://sitelicense.cambridgesoft.com/sitelicense.cfm?sid=1627>

You will be prompted for a qualifying email. All emails ending in @uoguelph.ca qualify.

You will be prompted to login into your Cambridge Soft account. The username is your email. If you've forgotten the password they will email it to you. If you don't have an account, you can easily register.

Once you log in, you will see two sections. The top is for Windows. The bottom is for Macs. You will also receive an email with your serial number to be used with ChemDraw.

2. <http://www.acdlabs.com/download/>

Reference Books on Reserve

- Arrow pushing in organic chemistry an easy approach to understanding reaction mechanisms
Author: Levy, D. E.
- Essentials of organic chemistry : for students of pharmacy, medicinal chemistry and biological chemistry
Author: P.M. Dewick
- Introduction to Spectroscopy 3rd ed
Author: D.L. Pavia, G.M. Lampman, G.S. Kriz
- March's advanced organic chemistry : reactions, mechanisms, and structure. 5th ed.
Author: Michael B. Smith, Jerry March.
- Organic chemistry demystified
Author: Bloch, D. R.
- Organic Chemistry 5th ed.
Author: Morrison, Robert Thornton, Boyd, Robert Neilson
- Organic chemistry 8th ed.
Author: Solomons, T. W. Graham. Fryhle, Craig B
- Organic chemistry. 7th ed.
Author: T.W. Graham Solomons, Craig B. Fryhle.
- Principals of Organic Synthesis
Author: R.O.C. Norman and J.M. Coxon
- The nuts and bolts of organic chemistry : a student's guide to success
Author: Karty, Joel.

Chem*3750 Experiment Schedule SUMMER 2019.

| WEEK | DATE | EXPERIMENT WEEK |
|------|----------|---|
| | WEEK OF: | |
| 1 | May 13 | CHECK IN/Safety Talk/Equipment review. Expt. 1 Benzoin Preparation (Start). |
| 2 | May 20 | Finish Experiment #1 Expt. 2 Benzil Preparation (Oxidation of Benzoin). |
| 3 | May 27 | Expt. 3 Preparation of Tetraphenylcyclopentadieneone. Lab book grading #1. |
| 4 | June 4 | NO LABS THIS WEEK. CSC Conference |
| 5 | June 10 | Expt. 4 Preparation of Dibenzalacetone. |
| 6 | June 17 | Test Experiments #1-#4. Expt. 5. Molecular Modeling: Gaussview program. Calculation of Keto/enol tautomers of Acetylacetone. Computer Lab in SC 1303 |
| 7 | June 24 | Expt. 6 Preparation of Dimedone. (Start) Lab book grading #2. |
| 8 | July 1 | Expt. 6 Preparation of Dimedone. (Finish) Expt. 7 Wittig. |
| 9 | July 8 | Expt. 8 Diels-Alder: Benzyne. |
| 10 | July 15 | Lab Clean-up, Check Out & Lab Final Test (all experiments). Hand in Lab Books. |
| 11 | July 22 | Check your Lab Grade. |
| 12 | July 29 | Last week of lectures. |