

CHEM-3760 ORGANIC CHEMISTRY III

WINTER SEMESTER 2020

Information Sheet and Course Outline

An in-depth treatment of various aspects of organic chemistry. This will include such topics as chemistry of heterocycles, synthetic strategies, polar rearrangements, organic photochemistry and a detailed discussion of organic spectroscopy. **Prerequisite: CHEM*3750 (CHEM*2070)**

- **Instructor:** Professor Adrian L. Schwan (schwan@uoguelph.ca)

Office: MacN 336, Phone: 824-4120 (Ext. 58781)

Office hours: tba early in the term

The email is provided for logistic communication. Professor Schwan does not discuss science by email. Person-to-person communication is infinitely more effective. Professor Schwan will try to visit the lab regularly and may be able to meet with you should you simply find me in my office.

- **Textbooks:**

- (a) "Introduction to Spectroscopy", 5th Ed., by Pavia, Lampman, Kriz and Vyvyan, Brooks/Cole, 2015. (**PLK5**) OR "Introduction to Spectroscopy", 4th Ed., by Pavia, Lampman, Kriz and Vyvyan, Brooks/Cole, 2009. (**PLK4**)
- (b) "Organic Chemistry" and "Study Guide and Solutions Manual to Organic Chemistry", 10th Ed., by Solomons and Fryhle, John Wiley & Sons, Inc., 2011. (**SF**)

Also of value:

- (c) "Advanced Organic Chemistry: Reactions and Mechanisms", 2nd Ed. by B. Miller, Prentice-Hall, Inc., 2004.
- (d) It is highly recommended that you become comfortable with SciFinder Scholar

- **Lectures:** There will be three lectures each week: M, W, F 1:30-2:20 pm in ALEX, Room 117. The lecture notes for Organic Chemistry III, CHEM*3760, will be available as pdf files on CourseLink. Prof. Schwan will also supply partially-filled templates that form the basis of the lecture material. The lab manual can be purchased in SCIE 2106 (cash only). It is assumed that you are familiar with the material covered in CHEM*2700 and CHEM*3750 and you may wish to call on your notes for those courses to review topics.

- **Laboratory:** The lab manual "Organic Chemistry III, CHEM*3760, Laboratory Outline", revised Winter 2020, will be available for sale by the Department as indicated. Students must

provide their own safety goggles. A student without eye protection will not be permitted to work in the laboratory. Contact lenses are extremely hazardous in a laboratory environment and they are not recommended in the lab. SAFETY GOGGLES MUST BE WORN AT ALL TIMES IN THE CHEM*3760 LABORATORY.

*****Students must pass the lab and lecture components of the course independently to receive a passing grade for the course.*****

- **Grading:** The final grade will be obtained as follows:
Two take home Problem Sets
 - 6% Mass Spectrometry and IR Spectroscopy (due Jan. 27, 2020)
 - 14% Mass Spectrometry, IR Spectroscopy and mostly NMR Spectroscopy and structure elucidation (due Feb. 12, 2020)*Term Test* 20% (in the week Mar. 16, covering Chapters 2-3 and part of 4 (2 hrs))**
Laboratory 30% Expectations and deadlines will be defined in the lab.
Final Exam 30% Scheduled by Registrar's Office: Apr. 13, 2020, 2:30 pm

*** (The exact date of the Term Test will be decided in the first lecture)*

- **Course Outline and Reading Assignments:**

On the following pages is an outline of the course. The reading assignments in SF and PLK will provide a different and more detailed perspective of many of the topics being discussed. The lectures allocated for each topic are approximate. Practice problems are distributed through the course notes and will include questions from the texts.

- **Winter Break:** February 17-21, no classes during this week.

- **Course Statements:**

Communications The primary communication between the students and the lecturer concerning issues with the course is through discussions during the lectures. Announcements and information related to the course, will also be available on online.

Students are expected to attend EVERY lecture. Copies of course notes have diminishing value if not obtained in the current context of Prof. Schwan's lecturing. Expectation for students' understanding of chemistry will be based on the verbal content of lectures and tutorials.

Important information for students registered with Student Accessibility Services (SAS)

- (1) If you plan to write any examination at SAS, please arrange with SAS ASAP.
- (2) Please send me an e-mail ASAP to inform me that you will be writing exams at SAS.

Course Content Outline

Chapter 1: **Organic Spectroscopy** (~10 lectures and 1-3 review periods)

- (a) Mass Spectrometry
- (b) Infrared Spectroscopy
- (c) ^1H NMR Spectroscopy
- (d) ^{13}C NMR Spectroscopy
- (e) 2D NMR Experiments

Chapter 2: **Synthetic Planning and Retrosynthesis** (~3-4 lectures)

-including a review of fundamental concepts and recognition of (organic) chemistry

Chapter 3: **Heterocyclic Chemistry** (9 lectures)

- (a) Nomenclature of Heterocyclic Compounds
- (b) Properties: Aromaticity, Dipole Moment, Basicity
- (c) Synthesis of Non-Aromatic Heterocycles: Intramolecular Cyclization; Cycloaddition (Epoxidation, Paterno-Buchi Reaction, Aziridination); Hydrogenation
- (d) Reaction of Non-Aromatic Heterocycles: Ring-opening Reactions of 3-membered Ring Heterocycles; Nucleophilic addition of Aziridines; Rearrangement of Aziridines; Ring-opening of Higher-member Heterocycles
- (e) Synthesis and Reactions of Indoles: Fischer Indole Synthesis, Bischler Indole Synthesis; Aromatic Electrophilic Substitution Reactions of Indoles
- (f) Synthesis and Reactions of Quinoline: Electrophilic Aromatic Substitution;
- (g) Other Important Heterocycles: Crown Ethers, Dihydropyran & Tetrahydropyran, Dioxanes, 1,3-Dithiane; Thiirane

Chapter 4: **Polar Rearrangements** (6 lectures)

- (a) Rearrangements of Carbocations: Wagner-Meerwein Shifts, Pinacol Rearrangement, Dienone-Phenol Rearrangement, Fries Rearrangement
- (b) Rearrangement of Carbanions & Carbenoids: Favorskii Rearrangement, Semibenzillic Rearrangement, Benzillic Rearrangement, Ramberg-Backlund Rearrangement, Wolff Rearrangement
- (c) 1,2-Nucleophilic Rearrangement to Electron Deficient Nitrogen & Oxygen: Beckmann Rearrangement, Hofmann Rearrangement, Curtius Rearrangement, Schmidt Rearrangement, Baeyer-Villiger oxidation, Hydroperoxide Rearrangement

Chapter 5: **Photochemistry** (4 lectures)

- (a) Molecular Orbital View of Excitation
- (b) Jablonski diagram
- (c) Photochemical Reactions—*isomerization*, *photoreduction*, *Norrish Type I & Type II cleavage*, *photoenolization*, *cycloadditions*, *Barton reaction*

Course Objectives

Chapter 1: To be able to:

- elucidate organic structures based on available characterization data
- draw conclusions about structural features based on characterization data
- predict spectral data of structures based on viewing structural drawings, finding available data and recognizing analogies

Chapter 2: To be able to:

- analyze simple reaction sequences in a retrosynthetic manner: propose logical starting organic compounds when presented with larger substrates
- realize that seemingly unfamiliar content can be understood using fundamental (organic) chemistry principles.

Chapter 3: To be able to:

- understand the importance and structures of selected heterocyclic compounds
- recognize important heterocyclic structures and draw their mechanism of formation, based on starting material structures
- identify and draw starting materials based for selected heterocyclic compounds
- recognize the role of selected reagents in the formation of specific heterocyclic compounds
- draw the mechanism for common heterocycle-forming reactions

Chapter 4: To be able to:

- to predict and draw the structures of rearranged compounds when provided with starting materials and reagents
- draw the mechanisms using curly arrows for rearrangement reactions
- recognize and distinguish between similar rearrangement reactions

Chapter 5: To be able to:

- understand fundamentals of photophysics
- understand fundamentals of photochemical transformations of organic compounds
- draw mechanisms to account for light induced chemical transformations

Overall: To be able to:

- relate chemical structures to anticipated spectral characteristics
- to be able to recognize reaction equations and assign applicable, general classification terms
- predict reactivity aspects of molecules based on their structure
- work through reaction mechanisms, based on fundamental principles of reactivity
- work in an independent manner in the organic lab environment

Useful References

<https://onlinelibrary.wiley.com/doi/epdf/10.1002/ejoc.200700966>

Books on reserve

For lectures

- Introduction to Spectroscopy, D.L. Pavia, G.M. Lampman, G.S. Kriz QD272.S6 P38 2001 3rd Ed.
- Organic spectroscopy 3rd ed. W. Kemp QD 272.S6 K45 1991
- Spectrometric identification of organic compounds 5th ed. R. M. Silverstein, G.C. Bassler, T.C. Morrill QD272.S6S55 1991
- Aromatic Heterocyclic Chemistry, D.T. Davies, QD400 .D38 1993
- Advanced Organic Chemistry Reactions and Mechanisms by B. Miller, QD251.2 .M534 2004 *2nd Ed.*
- Polar Rearrangements, L.M. Harwood, QD 281.R35 H37 1995.
- Intermediate Organic Chemistry, 2nd. Ed., J.C. Stowell, QD251.2.S75
- Synthesis of Fused Heterocycles, G.P. Ellis, QD 400.E45
- Principals of Organic Synthesis, R.O.C. Norman and J.M. Coxon, QD 262.N6 1993
- Handbook of Heterocyclic Chemistry, A.R. Katritzky, QD 400.K29 2000
- Essentials of organic chemistry: for students of pharmacy, medicinal chemistry and biological chemistry P.M. Dewick. QD251.3.D49 2006 Chapter 11 is a good heterocyclic chapter
- Organic synthesis : the disconnection approach 2nd ed. S.G. Warren, P. Wyatt. QD262 .W284 2008
- March's advanced organic chemistry : reactions, mechanisms, and structure. 6th ed. M. B. Smith, J. March QD251.2 .M37 2007

For laboratory

- Introduction to Organic Laboratory Techniques : a Contemporary Approach. D. L. Pavia, G.M. Lampman, G.S. Kriz. QD 261.P38 1988
- Microscale Organic Laboratory : with Multistep and Multiscale Syntheses, D.W. Mayo, R.M. Pike, P. K. Trumper, QD 261.M38 1994
- Operational Organic Chemistry : a Laboratory Course, J. W. Lehman, QD 261.L39

- **University Statements:**

1. **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. The grounds for Academic Consideration are detailed in the Undergraduate and Graduate Calendars.

Undergraduate Calendar - Academic Consideration and Appeals

<https://www.uoguelph.ca/registrar/calendars/undergraduate/current/c08/c08-ac.shtml>

Graduate Calendar - Grounds for Academic Consideration

<https://www.uoguelph.ca/registrar/calendars/graduate/current/genreg/index.shtml>

Associate Diploma Calendar - Academic Consideration, Appeals and Petitions

<https://www.uoguelph.ca/registrar/calendars/diploma/current/index.shtml>

2. **Email Communication** As per university regulations, all students are required to check their e-mail account regularly: e-mail is the official route of communication between the University and its students.
3. **Drop Date** Students will have until the last day of classes to drop courses without academic penalty. The deadline to drop two-semester courses will be the last day of classes in the second semester. This applies to all students (undergraduate, graduate and diploma) except for Doctor of Veterinary Medicine and Associate Diploma in Veterinary Technology (conventional and alternative delivery) students. The regulations and procedures for course registration are available in their respective Academic Calendars.

Undergraduate Calendar - Dropping Courses

<https://www.uoguelph.ca/registrar/calendars/undergraduate/current/c08/c08-drop.shtml>

Graduate Calendar - Registration Changes

<https://www.uoguelph.ca/registrar/calendars/graduate/current/genreg/genreg-regregchg.shtml>

Associate Diploma Calendar - Dropping Course

<https://www.uoguelph.ca/registrar/calendars/diploma/current/c08/c08-drop.shtml>

4. **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.
5. **Academic Integrity** The University of Guelph is committed to upholding the highest standards of academic integrity, and it is the responsibility of all members of the University community-faculty, staff, and students-to be aware of what constitutes academic misconduct and to do as much as possible to prevent academic offences from occurring. University of Guelph students have the responsibility of abiding by the University's policy on academic misconduct regardless of their location of study; faculty, staff, and students have the responsibility of supporting an environment that encourages academic integrity. Students need to remain aware that instructors have access to and the right to use electronic and other means of detection.

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.

Undergraduate Calendar - Academic Misconduct

<https://www.uoguelph.ca/registrar/calendars/undergraduate/current/c08/c08amisconduct.shtml>

Graduate Calendar - Academic Misconduct

<https://www.uoguelph.ca/registrar/calendars/graduate/current/genreg/index.shtml>

6. **Accessibility** The University promotes the full participation of students who experience disabilities in their academic programs. To that end, the provision of academic accommodation is a shared responsibility between the University and the student.

When accommodations are needed, the student is required to first register with Student Accessibility Services (SAS). Documentation to substantiate the existence of a disability is required; however, interim accommodations may be possible while that process is underway.

Accommodations are available for both permanent and temporary disabilities. It should be noted that common illnesses such as a cold or the flu do not constitute a disability.

Use of the SAS Exam Centre requires students to book their exams at least 7 days in advance and not later than the 40th Class Day.

For Guelph students, information can be found on the SAS website <https://www.uoguelph.ca/sas>

7. **Recording of Materials** Presentations that are made in relation to course work - including lectures - cannot be recorded or copied without the permission of the presenter, whether the instructor, a student, or guest lecturer. Material recorded with permission is restricted to use for that course unless further permission is granted.
8. **Resources** The Academic Calendars are the source of information about the University of Guelph's procedures, policies, and regulations that apply to undergraduate, graduate, and diploma programs.

Academic Calendars <https://www.uoguelph.ca/academics/calendars>