

# Chemistry 9513S/T: Elucidation of Organic and Bioorganic Mechanisms

## 2020–21 Course Outline (draft)

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Instructor: Kim Baines

Office: Chemistry Building 310A

Office Hours: By appointment (in person or by Zoom); e-mail for an appointment. Students must use their Western (@uwo.ca) email addresses when contacting Prof. Baines.

E-mail: [kbaines2@uwo.ca](mailto:kbaines2@uwo.ca)

### *Lectures and Tutorials*

Section	Day	Time	Room
001	Tu	9:30 – 11:20 am	NS 7
	Th	9:30 – 10:20 am	NS7

\*Note: I am trying to get the time changed to MWF 8:30 am to 9:20 am

In-person lectures will be posted online following the class.

### *Prerequisites*

Unless you have either the prerequisites for this course or written special permission from your Dean to enroll in it, you will be removed from this course and it will be deleted from your record. This decision may not be appealed. You will receive no adjustment to your fees in the event that you are dropped from a course for failing to have the necessary prerequisites.

Prerequisites: Chemistry 3373F (or equivalent)

### *Course Description*

Calendar description: Techniques for diagnosing and testing mechanisms of chemical reactions, with an emphasis on organic and bioorganic examples: kinetics, activation parameters, Bronsted catalysis law, Hammett and Taft relations, Marcus Theory, kinetic isotope effects, solvent effects. An introduction to pericyclic reactions with a discussion of aromaticity and orbital symmetry.

## *Course Topics (draft)*

### **Review of Chemical Kinetics and Thermodynamics:**

- deriving rate laws; 1st, pseudo-first, parallel reactions, 2nd order reactions
- steady-state and equilibrium approximations
- experimental determination of rate and equilibrium constants
- Eyring and Arrhenius Equations, temperature effects on rate constants
- qualitative look at the location of the transition-state; Hammond Postulate
- reaction coordinate diagrams, microscopic reversibility, selectivity

### **Kinetic Methods in the Elucidation of Reaction Mechanisms:**

- the rate law and stoichiometry of the transition state
- kinetic isotope effects
- structure-reactivity relationships, linear free energy relationships
- solvent/medium effects
- acids/bases/nucleophiles/electrophiles/homogeneous catalysis
- mechanistic probes

## *Course Materials*

There is NO text book required. Notes and course materials will be provided through OWL.

For the enthusiasts in the crowd there are a few further reference texts:

*Advanced Organic Chemistry* (4th Edition) by J. March, Wiley, 1991. Physical organic chemistry is not one of the strengths of the book, but it has an excellent bibliography of organic reactions and mechanisms.

*Mechanism and Theory in Organic Chemistry* (3rd Edition) by T. H. Lowry and K. S. Richardson, Harper and Row, 1987.

*Physical Organic Chemistry* (2nd Edition) by Niel Isaacs, Longman Scientific, 1995.

*Advanced Organic Chemistry* (3rd Edition) by F.A. Carey and R.A. Sundberg, Plenum, 1990, especially Part A.

*Modern Physical Organic Chemistry* by E. V. Anslyn and D. A. Dougherty, University Science, 2006.

## *Course Evaluation (draft)*

The overall course grade will be calculated as listed below:

<b>Component</b>	<b>Value</b>
Problem Sets	20
Midterm	30
Presentation	50

## *Accommodation and Accessibility*

### **Accommodation Policies**

Students with disabilities work with Accessible Education (formerly SSD) which provides recommendations for accommodation based on medical documentation or psychological and cognitive testing. The Academic Accommodation for Students with Disabilities policy can be found at:

[https://www.uwo.ca/univsec/pdf/academic\\_policies/appeals/Academic Accommodation\\_disabilities.pdf](https://www.uwo.ca/univsec/pdf/academic_policies/appeals/Academic_Accommodation_disabilities.pdf)

### **Academic Consideration for Student Absence**

Students will have up to two (2) opportunities during the regular academic year to use an on-line portal to self-report an absence during the semester, provided the following conditions are met: the absence is no more than 48 hours in duration, and the assessment for which consideration is being sought is worth 30% or less of the student's final grade. Students are expected to contact their instructors within 24 hours of the end of the period of the self-reported absence, unless noted on the syllabus. Students are not able to use the self-reporting option in the following circumstances:

- for exams scheduled by the Office of the Registrar (e.g., December and April exams)
- absence of a duration greater than 48 hours,
- assessments worth more than 30% of the student's final grade,
- if a student has already used the self-reporting portal twice during the academic year

If the conditions for a Self-Reported Absence are *not* met, students will need to provide a Student Medical Certificate if the absence is medical, or provide appropriate documentation if there are compassionate grounds for the absence in question. Students are encouraged to contact their Faculty academic counselling office to obtain more information about the relevant documentation.

Students should also note that individual instructors are not permitted to receive documentation directly from a student, whether in support of an application for consideration on medical grounds, or for other reasons. **All documentation required for absences that are not covered by the Self-Reported Absence Policy must be submitted to the Academic Counselling office of a student's Home Faculty.**

For policy on Academic Consideration for Student Absences - Undergraduate Students in First Entry Programs, see:

[https://www.uwo.ca/univsec/pdf/academic\\_policies/appeals/Academic Consideration for absences.pdf](https://www.uwo.ca/univsec/pdf/academic_policies/appeals/Academic_Consideration_for_absences.pdf)

and for the Student Medical Certificate (SMC), see:

[http://www.uwo.ca/univsec/pdf/academic\\_policies/appeals/medicalform.pdf](http://www.uwo.ca/univsec/pdf/academic_policies/appeals/medicalform.pdf)

### **Religious Accommodation**

Students should consult the University's list of recognized religious holidays, and should give reasonable notice in writing, prior to the holiday, to the Instructor and an Academic Counsellor if their course

requirements will be affected by a religious observance. Additional information is given in the Western Multicultural Calendar:

<https://multiculturalcalendar.com/ecal/index.php?s=c-univwo>

You may also be eligible to write the Special Exam if you are in a “Multiple Exam Situation” (see [http://www.registrar.uwo.ca/examinations/exam\\_schedule.html](http://www.registrar.uwo.ca/examinations/exam_schedule.html)).

If a student fails to write a scheduled Special Examination, the date of the next Special Examination (if granted) normally will be the scheduled date for the final exam the next time this course is offered. The maximum course load for that term will be reduced by the credit of the course(s) for which the final examination has been deferred. See Academic Calendar for details (under [Special Examinations](#)).

## *Academic Policies*

The website for Registrarial Services is <http://www.registrar.uwo.ca>.

In accordance with policy, <http://www.uwo.ca/its/identity/activatenonstudent.html>, the centrally administered e-mail account provided to students will be considered the individual’s official university e-mail address. It is the responsibility of the account holder to ensure that e-mail received from the University at his/her official university address is attended to in a timely manner.

### **Contingency plan for pivoting to 100% online learning**

In the event of a COVID-19 resurgence during the course that necessitates the course delivery moving away from face-to-face interaction, all remaining course content will be delivered entirely online, either synchronously (i.e., at the times indicated in the timetable) or asynchronously (e.g., posted on OWL for students to view at their convenience). The grading scheme will **not** change. Any remaining assessments will also be conducted online as determined by the course instructor.

**All lectures for this course will be recorded.** The data captured during these recordings may include your voice recordings. The recordings will be used for educational purposes related to this course. The recordings may be disclosed to other individuals participating in the course for their private or group study purposes. Please contact the instructor if you have any concerns related to lecture recordings.

Participants in this course are not permitted to record the sessions, except where recording is an approved accommodation, or the participant has the prior written permission of the instructor.

No electronic devices (phones, iPods, etc.) may be in your possession during tests and exams, even for timekeeping purposes. A simple calculator (without internet access) and a ruler is permitted during the exam.

It is university policy that a regularly scheduled class (lecture, lab, or tutorial) takes precedence over tests and exams. Therefore, if another course schedules a test or exam that takes place during your class, lab or tutorial, the instructor for that course must accommodate you.

**Scholastic offences** are taken seriously and students are directed to read the appropriate policy, specifically, the definition of what constitutes a Scholastic Offence, at the following Web site:

[http://www.uwo.ca/univsec/pdf/academic\\_policies/appeals/scholastic\\_discipline\\_undergrad.pdf](http://www.uwo.ca/univsec/pdf/academic_policies/appeals/scholastic_discipline_undergrad.pdf).

## *Support Services*

Please visit the Science & Basic Medical Sciences Academic Counselling webpage for information on add/drop courses, academic considerations for absences, appeals, exam conflicts, and many other academic related matters: <https://www.uwo.ca/sci/counselling/>

Please contact the course instructor if you require lecture or printed material in an alternate format or if any other arrangements can make this course more accessible to you. You may also wish to contact Student Accessibility Services (SAS) at (519) 661-2147 if you have any questions regarding accommodations.

Western University is committed to a thriving campus as we deliver our courses in the mixed model of both virtual and face-to-face formats. We encourage you to check out the Digital Student Experience website to manage your academics and well-being: <https://www.uwo.ca/se/digital/>.

Learning-skills counsellors at the Student Development Centre (<http://www.sdc.uwo.ca>) are ready to help you improve your learning skills. They offer presentations on strategies for improving time management, multiple-choice exam preparation/writing, textbook reading, and more. Individual support is offered throughout the Fall/Winter terms in the drop-in Learning Help Centre, and year-round through individual counselling.

Students who are in emotional/mental distress should refer to Mental Health@Western ([http://www.health.uwo.ca/mental\\_health](http://www.health.uwo.ca/mental_health)) for a complete list of options about how to obtain help.

Additional student-run support services are offered by the USC, <http://westernusc.ca/services>.

## *Social Media*

Twitter - Follow us @westernuchem

@kimbchemistry

Facebook - [www.facebook.com/ChemistryatWestern](http://www.facebook.com/ChemistryatWestern)