

## Chemistry 4483B: Elucidation of Organic and Bioorganic Mechanisms

### 2021–22 Course Outline

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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	MWF	12:30 – 1:20 am	ChB 115

### *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 for Chem 4483B: Chemistry 3373F

### *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*

#### **Administration**

## Reaction Mechanisms

### Quantitative Assessment of Operational Species in Organic/Bioorganic Reactions

- thermochemistry of reactive intermediates
- acid-base chemistry
- Lewis acids/bases and electrophiles/nucleophiles
- assessment of sterics

### Kinetic Analyses

- energy surfaces and reaction coordinate diagrams
- postulates and principles related to kinetic analyses
- kinetic analyses

### Experiments for the Elucidation of Reaction Mechanisms

- isotope effects
- substituent effects and linear free energy relationships
- other useful experiments

## Tutorials

### *Course Materials*

There is no text book required. Lectures will be “on the board” and/or materials will be provided through the OWL site.

For the enthusiasts in the crowd, here are a few reference texts for further reading:

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

*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 Neil Isaacs, Longman Scientific, 1995.

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

*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.

Students should check OWL (<http://owl.uwo.ca>) on a regular basis for news and updates. This is the primary method by which information will be disseminated to all students in the class. Students are responsible for checking OWL on a regular basis. All course material will be posted to OWL: <http://owl.uwo.ca>.

If students need assistance, they can seek support on the OWL Help page. Alternatively, they can contact the Western Technology Services Helpdesk. They can be contacted by phone at 519-661-3800 or ext. 83800.

## *Learning Outcomes*

The course also has an emphasis on the development of skills such critical-thinking, analysis, and qualitative reasoning; these professional skills are essential to success in not just chemistry but also in other courses and many occupations.

<b>Course-Specific Outcomes</b>	<b>Professional Skills</b>
Be able to predict the relative reactivity of the operational species in polar reactions	Work independently.
Recognize the importance of kinetic and thermodynamic methods in underpinning our understanding of reaction mechanisms	Form productive and collaborative working relationships with other individuals.
Think critically about, explain, integrate, and apply kinetic and thermodynamic principles and theories.	Obtain, evaluate, and integrate information from various sources, and determine its relevance.
Identify advantages and shortcomings in the methods used to elucidate reaction mechanisms.	Prioritize a set of tasks and manage the use of his or her time.
	Communicate thoughts, ideas, and observations verbally and in writing.
	Recognize when to seek assistance.
	Develop respect for, and comply with, regulations and policies.
	Learn to accept responsibility for his or her decisions, actions, and non-actions.

## *Course Evaluation*

The overall course grade will be calculated as listed below:

<b>Component</b>	<b>Notes</b>	<b>Value</b>
Problem Sets	4 at 5% each (Approx. due dates: Feb 4, Feb 18, Mar 18, Apr 1, 2022)	20
Class Participation		5
Midterm	In-person, Saturday, March 5, 2022 at 2:00 pm – 5:00 pm, Location: TBD	35
Final Exam	In-person, Cumulative; 3 hours; Scheduled by the Registrar in the April Exam Period	40

Late Problem Sets: A late penalty of 5% of the total grade for a problem set/day until the problem set is returned or the problem set is worth 0%.

There is no make-up midterm. If the midterm is missed for a valid reason, the weight of the midterm will be added to the final exam.

In the event that we cannot have the midterm/exam in-person, the midterm/exam will be proctored using Zoom\*. If that is necessary, you will be required to keep your camera on for the entire session, hold up your student card for identification purposes, and share your screen with the invigilator if asked to do so at any time during the exam. The midterm/exam session will not be recorded.

More information about the use of Zoom for exam invigilation is available in the Online Proctoring Guidelines at the following link:

<https://www.uwo.ca/univsec/pdf/onlineproctorguidelines.pdf>

In the event of having an online midterm/exam, completion of this course will require you to have a reliable internet connection and a device that meets the system requirements for Zoom. Information about the system requirements are available at the following link:

<https://support.zoom.us/hc/en-us>

\* Please note that Zoom servers are located outside Canada. If you would prefer to use only your first name or a nickname to login to Zoom, please provide this information to the instructor in advance of the test or examination.

## *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.

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) 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)