

CHM 432H: Organometallic Chemistry and Catalysis

Course Syllabus: Fall 2023

I TEACHING TEAM

**INSTRUCTOR**

Name: Datong Song
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Student hours: by appointment

**CO-INSTRUCTOR – Computational project**

Name: Mima Staikova
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II COURSE OVERVIEW

COURSE DESCRIPTION:

This course will cover a series of topics on organometallic chemistry and catalysis, including key reactions in organometallic chemistry such as transmetalation, oxidative addition, reductive elimination, insertion, elimination, and metathesis, as well as their applications in catalytic transformations. Typical bonding modes, structures, and reactivity patterns of various types of organometallic compounds will be discussed, including compounds with σ -bound ligands, compounds with π -bound ligands, and carbene complexes.

STUDENT LEARNING OUTCOMES:

By the end of the course, successful students are expected to demonstrate:

- knowledge and understanding of important concepts in catalysis
- knowledge and understanding of the mechanistic details of key organometallic reactions
- knowledge and understanding of the synthesis and structural features of important organometallic compounds
- general knowledge and understanding of physical methods used to study organometallic compounds and reactions
- knowledge and understanding of important catalytic reactions and topical areas in the fields of organometallic chemistry and catalysis
- ability to carry out DFT calculations to explore catalytic reaction mechanism and to interpret the computation data

PREREQUISITE COURSE(S):

CHM 338H (Intermediate Inorganic Chemistry)

READINGS:

Required: The Organometallic Chemistry of the Transition Metals, 6th ed., Robert H. Crabtree, John Wiley & Sons, Inc. 2014. The electronic version is available to University of Toronto students free of charge at <http://onlinelibrary.wiley.com.myaccess.library.utoronto.ca/book/10.1002/9781118788301>

III COURSE ORGANIZATION

Two classes each week (T and R at 11:10 am Toronto time) starting on Thursday September 7 in BL 114.

COURSE SCHEDULE & RELEVANT SESSIONAL DATES:

DATES	WEEK	TOPICS
Sept. 7	0	Introduction to CHM 432H
Sept. 11 – Sept. 22	1,2	Electron Counting and Concepts in Catalysis Key Reactions in Organometallic Chemistry
Sept. 25 – Oct. 6	3,4	Complexes of σ -Bound Ligands
Oct. 10 – Oct.13	5	Two Guest Lectures by Mima Staikova Introduction to DFT and overview of computation project Problem Set 1 Due on Oct. 12 at 11:59 pm
Oct. 16 – Oct. 20	6	Complexes of σ -Bound Ligands
Oct. 23 – Nov. 3	7,8	Complexes of π -Bound Ligands
Nov. 6 – Nov. 10	Reading Week	No Classes
Nov. 13 – Nov. 17	10	Complexes of π -Bound Ligands Computation Data Upload Due on Nov. 16 at 11:59 pm
Nov. 16	10	Guest Lecture by Mima Staikova: Summary of computation project and guidelines for writing the report Problem Set 2 Due on Nov. 16 at 11:59 pm
Nov. 20–Dec. 1	11,12	Carbene Complexes Computation Project Report Due on Dec. 1 at 11:59 pm
Dec. 5	13	Concluding remarks and preparation for final assessment
Dec. 9 – 20	Final Assessment Period	Final Assessment

IV EVALUATION/GRADING SCHEME

OVERVIEW:

Two Problem Sets worth 15% each¹

Computation Project worth 30% (10% for completing the computation jobs and upload the data; 20% for the report)²

Final Assessment (end of course) worth 40%

¹ Textbooks, journal articles, and lecture notes are the **ONLY** allowed aids. Students are expected to work independently on their own problem sets, i.e., no discussion with others by any means.

² Computational project is performed remotely, on the UG computational cluster, using special interface, WebMO. The project computationally explores reaction mechanisms of two catalytic cycles and discussion of their similarities and differences. Each student will receive specific structures from the cycles and calculate the energy and its geometry. You will have personal password protected directory to perform the calculations. The calculations do not need to be done in one sitting. You can login, send one calculation, logout, repeat, until you have done all of them. The project is collective work. The results you calculated you will upload on Quercus for everybody to use for their project paper and discussion. There will be 3 weeks interval to finish the calculations. Please, note, if you do not provide your share of the calculations, nobody will be able to write their papers. You can contact Dr. Staikova if you need assistance. After all data are uploaded, you will have two weeks to finish and submit your project paper. The submission will be on Quercus.

ASSESSMENT DATES & MARK BREAKDOWN:

Problem sets: $2 \times 15\% = 30\%$ of overall grade

Computation Project: $10\% + 20\% = 30\%$ of overall grade

Final Assessment: 40% of final grade

Total: 100%

IMPORTANT: if an unexpected technical issue occurs with a university system (e.g., Quercus services, network outage) that affects availability or functionality, it may be necessary to revise the timing or weighting of the quizzes/term tests.

V COURSE POLICIES

- Each member of this course is expected to maintain a:
 - (i) professional and respectful attitude during all course activities, including classes, laboratories, tutorials and online activity.
 - (ii) personal calendar/schedule/organizer to ensure that all course activities are completed, and due dates are met.
 - (iii) collection of notes recorded independently based on concepts covered in course activities (students registered with Accessibility Services requiring a class note-taker will have access to this accommodation)
 - (iv) familiarity with the university policy on Academic Integrity (overleaf)

- The University of Toronto is committed to equity, human rights and respect for diversity. All members of the learning environment in this course should strive to create an atmosphere of mutual respect where all members of our community can express themselves, engage with each other, and respect one another's differences. As a Course Instructor, I will neither condone nor tolerate behaviour that undermines the dignity or self-esteem of any individual in this course and wish to be alerted to any attempt to create an intimidating or hostile environment. It is our collective responsibility to create a space that is inclusive and welcomes discussion. Discrimination, harassment and hate speech will not be tolerated. If you have any questions, comments, or concerns, we encourage you to reach out to the staff in our Equity Offices.
- Process for signaling course absences and requesting make-up tests or other missed pieces of work.

If you are absent from your studies due to illness or other reasons and unable to complete course work (e.g., a term test or an assignment) then a piece of written documentation is required. The following four items are the recognized forms of documentation:

1. Absence Declaration via ACORN (please note the circumstances under which an absence declaration can and cannot be submitted)
2. U of T Verification of Illness or Injury Form
3. College Registrar's letter
4. Letter of Academic Accommodation from Accessibility Services

Students who complete the ACORN Absence Declaration form must additionally contact me/the course coordinator/the course administrator to discuss their situation within five business days of the missed piece of work. This is essential action for any consideration to be granted.

For extended absences and for absences due to non-medical reasons, make sure to contact your College Registrar's Office. They can help you decide between a request for an extension or other types of academic consideration.

If you suspect or know that you have a disability that is affecting your studies, learn about the services and supports available through Accessibility Services. A disability can be physical disability, sensory disability, a learning disability, mental health disorder or a short-term disability like an injury. If you are not sure whether you have a disability, you can confidentially contact Accessibility Services with your questions.

- The use of generative artificial intelligence tools and apps is strictly prohibited in all course assignments unless explicitly stated otherwise by the instructor in this course. This includes ChatGPT and other AI writing and coding assistants. Use of generative AI in this course may be considered use

of an unauthorized aid, which is a form of cheating. This course policy is designed to promote your learning and intellectual development and to help you reach course learning outcomes.

- We will respond to emails within 24 hrs. on business days.
- The late penalty for each item in the marking scheme is 10% of its full mark per day.
- Submission methods: use Quercus only.

VI TECHNOLOGY REQUIREMENTS

- Advice for students more broadly regarding online learning is available here: <https://onlinelearning.utoronto.ca/getting-ready-for-online/>
- This course requires the use of computers, and technical issues are possible. When working on a piece of academic work, students are responsible for scheduling enough time to allow for reasonable delays due to technical difficulties to be overcome, so such issues will not be acceptable grounds for deadline extension. Particularly, maintaining an up-to-date independent backup copy of your work is strongly recommended to guard against hard-drive failures, corrupted files, lost computers, etc.

VII INSTITUTIONAL POLICIES & SUPPORT

ACADEMIC INTEGRITY

Academic integrity is essential to the pursuit of learning and scholarship in a university, and to ensuring that a degree from the University of Toronto is a strong signal of each student's individual academic achievement. As a result, the University treats cases of cheating and plagiarism very seriously. The University of Toronto's Code of Behaviour on Academic Matters

(governingcouncil.utoronto.ca/secretariat/policies/code-behaviour-academic-matters-july-1-2019) outlines the behaviours that constitute academic dishonesty and the processes for addressing academic offences. Potential offences include, but are not limited to:

In computational project reports:

1. Using someone else's ideas or words without appropriate acknowledgement.
2. Submitting your own work in more than one course without the permission of the instructor.
3. Making up sources or facts.
4. Obtaining or providing unauthorized assistance on any report. **Please note that the use of websites (such as Chegg.com or the course discussion board) to post virtual laboratory report material/questions or to post/access answers to questions is an academic offence under the**

University of Toronto's Code of Behaviour on Academic Matters. Alleged instances of this nature are forwarded to the Faculty of Arts & Science Student Academic Integrity office.

On problem sets and tests/exams:

1. Using or possessing unauthorized aids. **Please note that the use of websites (such as Chegg.com or the course discussion board) to post quiz/term test questions or to post/access answers to questions is an academic offence under the University of Toronto's Code of Behaviour on Academic Matters. Alleged instances of this nature are forwarded to the Faculty of Arts & Science Student Academic Integrity office.**
2. Looking at someone else's answers or collaborating/discussing answers.
3. Misrepresenting your identity.

In general academic work:

1. Falsifying institutional documents or grades.
2. Falsifying or altering any documentation required by the University.

All suspected cases of academic dishonesty will be investigated following procedures outlined in the Code of Behaviour on Academic Matters. If you have questions or concerns about what constitutes appropriate academic behaviour or appropriate research and citation methods, you are expected to seek out additional information on academic integrity from your instructor or from other institutional resources (see www.academicintegrity.utoronto.ca/).

The University's plagiarism detection tool

Normally, students will be required to submit their course essays to the University's plagiarism detection tool for a review of textual similarity and detection of possible plagiarism. In doing so, students will allow their essays to be included as source documents in the tool's reference database, where they will be used solely for the purpose of detecting plagiarism. The terms that apply to the University's use of this tool are described on the Centre for Teaching Support & Innovation web site (<https://uoft.me/pdt-faq>).

COPYRIGHT

If a student wishes to copy or reproduce class presentations, course notes or other similar materials provided by instructors, he or she must obtain the instructor's written consent beforehand. Otherwise, all such reproduction is an infringement of copyright and is absolutely prohibited. More information regarding this is available here: <https://teaching.utoronto.ca/ed-tech/audio-video/copyright-considerations/>

ACCESSIBILITY NEEDS

Students with diverse learning styles and needs are welcome in this course. The University of Toronto is committed to accessibility: if you require accommodations for a disability, or have any other accessibility concerns about the course, please contact [Accessibility Services](#) as soon as possible.

ACCOMMODATIONS FOR RELIGIOUS OBSERVANCES

Following the University's policies, reasonable accommodations will be made for students who observe religious holy days that coincide with the due date/time of an assignment, tutorial, class or laboratory session. Students must inform the instructor **before** the session/assignment date to arrange accommodations.

ADDITIONAL SERVICES & SUPPORT

The following are some important links to help you with academic and/or technical service and support:

- General student services and resources at [Student Life](#)
- Full library service through [University of Toronto Libraries](#)
- Resources on conducting online research through [University Libraries Research](#)
- Resources on academic support from the [Academic Success Centre](#)
- Learner support at the [Writing Centre](#)
- Information for [Technical Support/Quercus Support](#)

ACKNOWLEDGEMENT OF TRADITIONAL LANDS

We wish to acknowledge this land on which the University of Toronto operates. For thousands of years, it has been the traditional land of the Huron-Wendat, the Seneca and, most recently, the Mississaugas of the Credit River. Today, this meeting place is still the home to many Indigenous people from across Turtle Island and we are grateful to have the opportunity to work on this land.