

Department of Chemistry Online Course Syllabus

CHM 1268: X-ray Crystallography

I CONTACTS

COURSE COORDINATORS

Name: Professor Douglas Stephan

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Name: Professor Datong Song

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II COURSE OVERVIEW

COURSE DESCRIPTION:

This course is intended to give the student the theoretical and practical background for the determination of molecular structures employing single crystal X-ray diffraction methods.

STUDENT LEARNING OUTCOMES:

To give the student a clear understanding of the method and a general proficiency of solving and refining crystal structures for publication.

PREREQUISITE COURSE:

The prerequisite for this course is addition to graduate school.

Supplemental:

III HOW THE COURSE IS ORGANIZED

The zoom lecture will be announced on Quercus. The lectures are on Tuesdays at 10AM-12 PM.

THEORY (4 two-hour lectures)

The following specific theory lectures will cover:

Jan 12: Crystals: growth, quality, properties; X-rays

Symmetry in the solid state, Bravais lattices, Laue groups, site, translational symmetry

Jan 19: Space groups, International tables, implications

Miller Indices, Bragg's Law, Reciprocal Space, Bragg's law in reciprocal space
Systematic absences, symmetry determination, data collection,

Jan 26: computer automation and output

data to be collected, procedure for data reduction

The phase problem

Patterson Space and solution, direct methods

Feb 2: Structure refinement

Friedel's Law and Optical activity

A consideration of errors, a publication checklist

PRACTICAL

Feb 9 – April 6 (8 two-hour lectures)

Solve and refine routine crystal structures as well as disordered structures using SHELX software, generate .cif files, checkcif reports, plots, and tables for publications and presentations.

IV EVALUATION/GRADING SCHEME

Assignment (theory)	20%
Practical	50%
final	30%

FINAL ASSESSMENT

TBA.

V COURSE POLICIES

- I will make every effort to respond to email within 24 hrs on weekdays (Douglas.stephan@utoronto.ca).
- Office hours: I will be available M-F (1-5:30 pm); barring other commitments. Please use the link below to arrange a TEAMS meeting using the booking webpage: <https://outlook.office365.com/owa/calendar/DouglasStephan@utoronto.onmicrosoft.com/bookings/>
- *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. U of T does not condone discrimination or harassment against any persons or communities."*
- Privacy language and appropriate use of course materials: <https://teaching.utoronto.ca/ed-tech/audio-video/sample-statements/>

VI TECHNOLOGY REQUIREMENTS

Specific guidance from the U of T Vice-Provost, Students regarding student technology requirements is available here:

<https://www.viceprovoststudents.utoronto.ca/covid-19/tech-requirements-online-learning/>

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 of course sometimes things can go wrong when using them. You are responsible for ensuring that you maintain regular backup copies of your files, use antivirus software (if using your own computer), and schedule enough time when completing an assignment to allow for delays due to technical difficulties. Computer-viruses, crashed hard drives, broken printers, lost or corrupted files, incompatible file formats, and similar mishaps are common issues when using technology, and are not acceptable grounds for a deadline extension.

VII INSTITUTIONAL POLICIES AND SUPPORT

ACADEMIC INTEGRITY

On 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

(<https://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 papers and assignments:

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 assignment.

On tests and exams:

1. Using or possessing unauthorized aids.
2. Looking at someone else's answers during an exam or test.
3. Misrepresenting your identity.

In 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 <https://www.academicintegrity.utoronto.ca/>).

Use of Turnitin

Note for instructor: Turnitin (<https://teaching.utoronto.ca/ed-tech/teaching-technology/turnitin/>) is a very highly recommended tool directly integrated into Quercus that will assist in detecting textual similarities between compared works. Students must be informed at the start of the course that the instructor will be using Turnitin. If you plant to use this tool, the course syllabus must include the following statement (as is):

"Normally, students will be required to submit their course essays to Turnitin.com 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 Turnitin.com reference database, where they will be used solely for the purpose of detecting plagiarism. The terms that apply to the University's use of the Turnitin.com service are described on the Turnitin.com web site".

COPYRIGHT

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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.

ADDITIONAL SERVICES and 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](#)