

Course Introduction and Overview:

This course will give registrants 1) a working knowledge of crystal structure analysis so that they will be able to make an informed reading of crystal structure results they encounter in the chemical literature and 2) provide enough background for those Chemistry Ph.D. students who would like to go on and learn how to collect their own data and solve and refine crystal structures. This course is broken up into 2 components: **CHEM-9541** (Winter 2024) and **CHEM-9542** (Fall 2024), which will cover theoretical and practical aspects of X-ray crystallography, respectively.

Contact Information:

Course Instructor:

Dr. Marcus W. Drover

Phone: 519-661-2111 ext. 86334

Email: marcus.drover@uwo.ca

OWL (www.westernu.brightspace.com)

Course Webpage

By appointment only.

Student Hours:

- Please e-mail, for instance, three (3), times convenient to you and we can arrange a mutually suitable time.

Lecture/ Tutorial times & location:

Lectures: Fridays, 2:30-5:00pm

Location: Check the secure site for location

Course-Based Learning Objectives:

Upon completion of Chem 9542, students will be able to:

1. Understand the techniques necessary to collect and interpret single-crystal X-ray diffraction (SC-XRD) data for molecular structure solution and powder X-ray diffraction (PXRD) data for materials characterization;
2. Apply modern software tools to analyze X-ray diffraction data (OLEX2, SHELX, etc.);
3. Visualize and present 3D crystal structures (Mercury, Diamond, etc.);
4. Search the literature using crystal databases from the Cambridge Crystallographic Data Centre (CCDC).

Important Dates:

Sep. 6: Class 1 -

Sep. 13: Class 2 -

Sep. 20: Class 3 -

Sep. 27: Class 4 -

Oct. 4: Class 5 -

Oct. 11: Class 6 -

Student Assessment:

CHEM-9542 comprises one lecture per week.

Problem Sets (2)	40% (Due Sep. 20 th and Oct. 4 th)
Class Participation	10%
Final Assignment	50%
Total	100% (Due Oct. 18th)

**The final assignment consists of one final assignment (a complete structure solution and submitted crystallographic paper from an experimental dataset).

Required resources:

Text: No textbook is required, notes are to be taken during class and problem sets are to be given out during class.

The following serve as utile resources and are in the Taylor library:

Luger, P. "Modern X-ray Analysis in Single Crystals: a practical guide", 2014
Clegg, W. et al. "Crystal Structure Analysis: Principles and Practice" 2nd ed., 2009
Massa, W. "Crystal Structure Determination", 2nd ed. 2004
Giacovazzo, et al. "Fundamentals of Crystallography", 1992

Course content:

Topic 1	Structure Solution and Refinement via OLEX 2 Software
Topic 2	Disorder and Twinning
Topic 3	Cambridge Structural Database (CSD) and Mercury Visualization Software
Topic 4	Powder X-ray Diffraction (if time permits)

A friendly reminder: It is extremely important, as with any course, to keep up with the required reading. One can become lost very quickly, and the pace of this course, combined with the fact that many of the topics discussed rely heavily on a firm knowledge of the prior materials, will leave you feeling behind and frustrated!

All course material will be posted to OWL: <http://owl.uwo.ca>. If students need assistance with the course OWL site, 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.

Late Policy for Chem 9542: All work is subject to a late policy of 10% per day, including weekends. Work more than three days late will not receive any credit. Late policies will be waived provided students have a valid reason that is supported by the academic counsellors from their home faculty.

Student Absences: Students who are unable to meet their academic responsibilities due to medical or compassionate reasons may submit a request for academic consideration. For each missed piece of work, regardless of its weight in the total course grade, you must apply for such consideration by providing valid medical or supporting documentation to the Academic Counselling Office of your Faculty of Registration.

Accommodation for students with disabilities: Students with disabilities are encouraged to contact Accessible Education, which provides recommendations for accommodation based on medical documentation or

psychological and cognitive testing. In cases where a student misses a piece of work for reasons related to the disability on file with Accessible Education, the student should request accommodation by contacting Accessible Education instead of the Academic Counselling Office

For further information, please consult the University's medical illness policy at https://www.uwo.ca/univsec/pdf/academic_policies/appeals/accommodation_medical.pdf.

The Student Medical Certificate is available at https://www.uwo.ca/univsec/pdf/academic_policies/appeals/medicalform.pdf.

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.

Specific to Chem 9542:

Assignments – If an assignment is not handed in for a valid reason (see process for seeking academic consideration above) the weighting will be redistributed equally to the other assignments.

Final Exam – If you miss the Final Exam, please contact your faculty's Academic Counselling Office as soon as you can do so. They will assess your eligibility to write the Special Exam (the name given by the university to a makeup Final Exam). 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).

Accommodation and Accessibility:

Religious Accommodation:

When a course requirement conflicts with a religious holiday that requires an absence from the University or prohibits certain activities, students should request accommodation for their absence in writing at least two weeks prior to the holiday to the course instructor and/or the Academic Counselling office of their Faculty of Registration. Please consult University's list of recognized religious holidays (updated annually) at:

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

Accommodation Policies:

Students with disabilities are encouraged to contact Accessible Education, which provides recommendations for accommodation based on medical documentation or psychological and cognitive testing. The policy on Academic Accommodation for Students with Disabilities can be found at:

https://www.uwo.ca/univsec/pdf/academic_policies/appeals/Academic_Accommodation_disabilities.pdf

Academic Policies:

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

In accordance with policy, https://www.uwo.ca/univsec/pdf/policies_procedures/section1/mapp113.pdf, 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 their official university address is attended to in a timely manner.

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.

Support Services:

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

Students who are in emotional/mental distress should refer to Mental Health@Western (<https://uwo.ca/health/>) for a complete list of options about how to obtain help.

Western is committed to reducing incidents of gender-based and sexual violence and providing compassionate support to anyone who has gone through these traumatic events. If you have experienced sexual or gender-based violence (either recently or in the past), you will find information about support services for survivors, including emergency contacts at https://www.uwo.ca/health/student_support/survivor_support/get-help.html. To connect with a case manager or set up an appointment, please contact support@uwo.ca.

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 Accessible Education at http://academicsupport.uwo.ca/accessible_education/index.html if you have any questions regarding accommodations.

Learning-skills counsellors at the Student Development Centre (<https://learning.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.

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

Statement on Equity, Diversity, and Inclusivity:

Western University and I are committed to a community and learning environment that embraces equity, diversity, and inclusivity including gender and gender-identity, sexuality, ethnicity, religion, culture, and national origins. This commitment is underscored by Western University being a signatory to the [Dimensions Program and Charter](#). Our community and learning are enhanced and enriched when diverse perspectives and experiences are recognized and respected, and all can contribute. In this class I hold that each student has the right to be addressed "in accordance with their personal identity" (e.g., name, personal pro-nouns).¹ Please let me know how you wish to be addressed and how I can help to support you during this class, and I will do my best to do so.

¹University of Michigan, Center for Research on Teaching and Learning.

Statement on the Use of Artificial Intelligence (AI):

The use of generative artificial intelligence (AI) tools/software/apps is unacceptable in this course.