

CHEM 9541

X-ray Crystallography I: Theory

Department of Chemistry
Faculty of Science
The University of Western Ontario

1. Course Information

Course Name: X-ray Crystallography I: Theory

Lectures:

Location:

2. Instructor

Name: Marcus W. Drover

Title: Assistant Professor

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3. Course Description

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.

4. Evaluation (tentative)

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|-----------------------|-------------|
| • Problem Sets (2) | 40% |
| • Class Participation | 10% |
| • Final Exam | 50% |
| • Total | 100% |

5. Prerequisites:

There are no prerequisites.

6. Course Materials:

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 on reserve in 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

7. Learning outcomes:

Topic 1	What is a crystal and how do you grow them?
Topic 2	Diffraction, X-rays, Tubes, Optics, Detectors, Goniometers
Topic 3	Bragg's Law, Lattices, Unit Cell, Crystal Systems, Bravais Lattices
Topic 4	Reciprocal Lattice, Miller Indices, Ewald Sphere, Limiting Sphere, Resolution
Topic 5	Symmetry, Asymmetric Unit, Point Groups, Stereographic Projections, Crystal Classes
Topic 6	Translational Symmetry Elements, Space Groups, H-M Notation, International Tables
Topic 7	Systematic Absences in Reciprocal Space
Topic 8	Structure Factors, Scattering Factors, Friedel's Law (absolute configuration)
Topic 9	Fourier Transforms, Electron Density, The Phase Problem

8. Course attendance, expectations and missed tests/exams

Course attendance is highly recommended for Chem 9541, particularly considering the interdisciplinary nature of the course and points associated with in-class activities. You are responsible for all information disseminated in class. Information missed due to course absences will not be considered for the basis of a grade appeal.

Arrival on time is expected. Please turn off all cell phones upon entering class. Reading of newspapers, work on assignments for this or other classes, or other activities that are not part of the class are not allowed during lecture. Students who do not comply with these requirements or who behave disorderly or disrespectfully may be asked to leave the classroom.

If you are unable to meet a course requirement due to illness or other serious circumstances, you must contact your instructor within 48 hours after you are able to resume academic duties with valid medical or other supporting documentation.

Once your absences have been excused, an alternate date for presentation or exam will be arranged. It is the student's responsibility to make alternative arrangements with their instructor once the accommodation has been approved and the instructor has been informed.

No "make-up" evaluation will be provided for the *in-class activities* component of the course. If the absence is excused, missed *in-class activities* marks will be transferred to the exam.

9. The fine print - University guidelines on various other issues:

A. Medical/Compassionate Excuses: Students missing work for valid medical or other reasons are governed by the regulations <https://studentservices.uwo.ca/secure/index.cfm>

B. Student Accessibility Services (SAS): Western is committed to achieving barrier-free accessibility for all its members, including graduate students. As part of this commitment, Western provides a variety of services devoted to promoting, advocating, and accommodating persons with disabilities in their respective graduate program. Graduate students with disabilities (for example, chronic illnesses, mental health conditions, mobility impairments) are encouraged to register with Student Accessibility Services, a confidential service designed to support graduate and undergraduate students through their academic program. With the appropriate documentation, the student will work with both SAS and their graduate programs (normally their Graduate Chair and/or Course instructor) to ensure that appropriate academic accommodations to program requirements are arranged. These accommodations include individual counselling, alternative formatted literature, accessible campus transportation, learning strategy instruction, writing exams and assistive technology instruction. For more information, see <http://www.sdc.uwo.ca/ssd/>

C. Academic Offences: 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/handbook/appeals/scholastic_discipline_undergrad.pdf

D. Support Services: Support is available from the Registrar: <http://www.registrar.uwo.ca>, via the university students council (<http://westernusc.ca/services/>) and at Student Development Services (<http://www.sdc.uwo.ca/>). In particular, learning-skills counsellors at the Student Development Centre 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.

E. Mental or Emotional Health: Students who are in emotional/mental distress should refer to Mental Health@Western <http://www.uwo.ca/uwocom/mentalhealth/> for a complete list of options about how to obtain help.