

*The University of Western Ontario*  
Chemistry 9541B, Winter 2022  
X-ray Crystallography I

**Instructor:**

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**Enrollment:**

No limit

**Description:**

1) To give registrants 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.

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.

**Topics:**

What is a crystal and how do you grow them?

Crystals, Symmetry and Space Groups

Generation of X-rays

Diffraction of X-rays by Crystals

Single Crystal Diffractometry

Data Reduction

Fourier Syntheses in X-ray Crystallography

The Phase Problem

Solving the Phase Problem I: Traditional Methods

Solving the Phase Problem II: Modern Methods

Completing the Structure Determination

Calculation of Molecular Parameters

Sources of Error in X-ray Structure Determinations

**Resources:**

No text book required. Notes taken during lectures and problem sets given out in class.

### ***Crystallographic Textbooks 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" 2<sup>nd</sup> ed., 2009  
Massa, W. "Crystal Structure Determination", 2<sup>nd</sup> ed. 2004  
Giacovazzo, *et al.* "Fundamentals of Crystallography", 1992

### **Lectures / seminars:**

Day/s: Fridays

Time/s: 1:30 – 4:00 pm

Mode of instruction: In person

### **Evaluation**

Five problem sets (45%) , class participation (5%), and a final exam (50%)

### **Course attendance and missed/late assignments**

If you are unable to meet a course requirement due to illness or other serious circumstances, you must provide valid medical or other supporting documentation to your instructor immediately. 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.

### **Notes on Academic Honesty**

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:

[www.uwo.ca/univsec/pdf/academic\\_policies/appeals/scholastic\\_discipline\\_grad.pdf](http://www.uwo.ca/univsec/pdf/academic_policies/appeals/scholastic_discipline_grad.pdf)

All required papers may be subject to submission for textual similarity review to the commercial plagiarism detection software under license to the University for detection of plagiarism. All papers submitted for such checking will be included as source documents in the reference database for the purpose of detecting plagiarism of papers subsequently submitted to the system. Use of the service is subject to the licensing agreement, currently between The University of Western Ontario and Turnitin.com (<http://www.turnitin.com>).

### **Health and Wellness**

As part of a successful graduate student experience at Western, we encourage students to make their health and wellness a priority. Western provides several on campus health-related services to help you achieve optimum health and engage in healthy living while pursuing your graduate degree. For example, to support physical

activity, all students, as part of their registration, receive membership in Western's Campus Recreation Centre.

Numerous cultural events are offered throughout the year. For example, please check out the Faculty of Music web page <http://www.music.uwo.ca/>, and our own McIntosh Gallery <http://www.mcintoshgallery.ca/>. Information regarding health- and wellness-related services available to students may be found at <http://www.health.uwo.ca/>. Students seeking help regarding mental health concerns are advised to speak to someone they feel comfortable confiding in, such as their faculty supervisor, their program director (graduate chair), or other relevant administrators in their unit. Campus mental health resources may be found at [http://www.health.uwo.ca/mental\\_health/resources.html](http://www.health.uwo.ca/mental_health/resources.html).