

**CHEM\*7120/712 X-RAY CRYSTALLOGRAPHY**

Fall 2017 – Course Outline

Introduction into chemical crystallography and X-ray diffraction (XRD) analysis. The course provides theoretical background for understanding the crystal structure analysis and data reported in the literature as well as hands-on training on the XRD equipment available. Part I: brief introduction into crystallography. Parts II & III: theory and practice of XRD analysis. Part IV: an individual project. Credits: 0.5.

- WEBSITE** <http://www.chemistry.uoguelph.ca/soldatov/C7120>
- SCHEDULE** Sep 12th (first class) – Nov 30th; Tuesdays, 7:00 pm – 9:30 pm  
(official class dates: Sep 12, 19, 26; Oct 3, 17, 24, 31; Nov 7, 14, 21, 28, 30)  
MiniLink Room (Guelph: MACN-203; Waterloo: C2-278)
- INSTRUCTOR** Professor Dmitriy Soldatov  
Office: U of Guelph, MACN-122 or MACN-338  
Contacts: 519-824-4120 x 53548; 519-546-6027 (cell); soldatov@uoguelph.ca
- EVALUATION** Two written assignments (20% each), in-class midterm exam (30%), project work and technical report (15%) and an in-class presentation with questions (15%). Late submission of assignments or reports will be subject to 10% grade reduction per day. Auditing students must complete the assignments and the midterm exam with min 50% grade.
- LAB / PROJECT** This course has a lab component (project) that is taken in Guelph. Waterloo students can arrange for their project to be done in Waterloo, subject to approval by the instructor.

**CONTENTS****Part I Crystallography: Introduction.**

Crystals. Crystal symmetry: translational, point and space symmetry; crystal lattice, unit cell and Miller indices. From crystal systems to space groups. System of notations in crystallography.

Major crystallographic resources. Bonding in crystals. Examples of crystal structures.

**Part II Crystal structure analysis: X-Rays and diffraction.**

X-Rays and X-ray sources. Scattering and diffraction of X-rays. The Bragg law. Equivalent reflections. Systematic absences.

Reciprocal lattice. Diffraction limits. Sphere of reflection. Structure factor. Diffraction intensities.

**Part III Crystal structure analysis: Practical.**

X-Ray diffraction techniques: powder and single-crystal methods; other XRD techniques. Diffractometer and its components. Data collection and processing.

Crystal growth; preparation of samples; general requirements. Setting up an XRD experiment.

Crystal structure solution, refinement, visualization and presentation; overview of available software; publication requirements.

**Part IV Crystal structure analysis: Individual project.**

Individual projects including experimental part (e.g. preparation of a crystal, data collection, structure solution and refinement), writing a technical report and an in-class presentation.

The presentation is scheduled during the exam period; it includes questions on the course material and replaces the final exam.

## RESOURCES

Lecture Notes will be provided in advance of the classes.

Other resources and links will be posted on the course website (see above).

A number of general texts and web resources may be used; some texts are listed below.

## OPTIONAL TEXTS

AR West, Solid State Chemistry and Its Applications, Wiley, 1984 (1st ed) or 2014 (2nd ed)

DE Sands, Introduction to Crystallography, Dover Publications, 1993 (Dover ed)

C Hammond, The Basics of Crystallography and Diffraction, IUCr and Oxford Univ. Press, 2009 (3rd ed)

GH Stout and LH Jensen, X-Ray Structure Determination: A Practical Guide, Macmillan Co, 1968 (1st ed) or Wiley, 1989 (2nd ed)

JP Glusker and KN Trueblood, Crystal Structure Analysis. A Primer, IUCr and Oxford Univ. Press, 2010 (3rd ed)

W Massa, Crystal Structure Determination, Springer, 2004 (2nd ed)

W Borchardt-Ott, Crystallography, Springer, 1995 (2nd ed)

C Giacovazzo et al, Fundamentals of Crystallography, IUCr and Oxford University Press, 2011 (3rd ed)

P Müller (ed.), Crystal Structure Refinement. A Crystallographer's Guide to SHELXL, IUCr and Oxford Univ. Press, 2006

## GENERAL POLICIES AND REGULATIONS

E-mail Communication: As per university regulations, all students are required to check their university e-mail account regularly: e-mail is the official route of communication between the university and its students.

When You Cannot Meet a Course Requirement: When you find yourself unable to meet an in-course requirement because of illness or compassionate reasons, please advise the course instructor in writing, with your name, id#, and e-mail contact. See the graduate calendar for information on regulations and procedures for Academic Consideration:

<http://www.uoguelph.ca/registrar/calendars/graduate/2017-2018/genreg/>

[http://www.registrar.uwaterloo.ca/students/accom\\_illness.html](http://www.registrar.uwaterloo.ca/students/accom_illness.html)

Drop Date: The last date to drop the course, without academic penalty, is Thursday, **3 November 2017**.

Copies of out-of-class assignments: Keep paper and/or other reliable back-up copies of all out-of-class assignments: you may be asked to resubmit work at any time.

Accessibility: Providing services for students is a shared responsibility among students, faculty and administrators. This relationship is based on respect of individual rights, the dignity of the individual and the university community's shared commitment to an open and supportive learning environment. Students requiring service or accommodation, whether due to an identified, ongoing disability or a short-term disability should contact the Student Accessibility Services as soon as possible. For more information see the following websites:

<http://www.uoguelph.ca/csd/>

<http://uwaterloo.ca/disability-services/>

Academic Misconduct: The students have the responsibility of abiding by the university's policy on academic misconduct regardless of their location of study; faculty, staff and students have the responsibility of supporting an environment that discourages misconduct. Please note: Whether or not a student intended to commit academic misconduct is not relevant for a finding of guilt. Hurried or careless submission of assignments does not excuse students from responsibility for verifying the academic integrity of their work before submitting it. Students who are in any doubt as to whether an action on their part could be construed as an academic offence should consult with a faculty member or faculty advisor.

The investigation of cases of academic misconduct cases and the cases that are heard at the Admissions and Progress Committee indicate that many graduate students, especially those new to Canada, are not aware of University regulations reflected in the attached statements. In particular, issues related to academic consideration, dropping courses, and lack of awareness of behavior that constitutes academic misconduct may all lead to disruption or delay of a student's academic studies and require considerable time and effort from faculty and administrative staff to resolve resulting problems.

In the case of the graduate academic misconduct policy, the Graduate Calendar states: "It should not be possible for a student to claim that he/she was not warned about the University's academic misconduct regulations, what constitutes academic misconduct and the potential consequences of transgressing." For further details see:

<http://www.uoguelph.ca/registrar/calendars/graduate/2017-2018/genreg/>  
<http://www.adm.uwaterloo.ca/infosec/Policies/policy71.htm>

Recording of Materials: Presentations which are made in relation to course work—including lectures—cannot be recorded or copied without the permission of the presenter, whether the instructor, a classmate or guest lecturer. Material recorded with permission is restricted to use for that course unless further permission is granted.

Resources: The Academic Calendars are the source of information about the university procedures, policies and regulations which apply to undergraduate, graduate and diploma programs:

<http://www.uoguelph.ca/registrar/calendars/index.cfm?graduate>  
<http://gradcalendar.uwaterloo.ca/group/Gen-Info-Regs>