

Syllabus and General Information
CHEM 575. Diffraction and Crystal Structure

Spring 2023 T-TR 2.10-3.30 pm. GILMAN 1312

Lecture--3 hours. Prerequisite: analogues of course 301 or 324 or consent of instructor.
Introduction to X-ray structure determination; crystals, symmetry, diffraction geometry, sample preparation and handling, diffraction apparatus and data collection, methods of structure solution and refinement, presentation of results, crystallographic databases. Brief description of neutron and electron diffractions will be given.

Website: Canvas

Dr. Kirill Kovnir

kovnir@iastate.edu

Office Hours: by appointment

Recommended books: Texts 1 and 2 are directly related to the content of this class. Texts 3 and 4 are additional information for advanced users related to the methods beyond single crystal diffraction.

1. Werner Massa.
Crystal Structure Determination.
Springer, ISBN 978-3-662-06431-3.
2. Gregory Girolami.
X-ray Crystallography.
University Science Book, ISBN: 978-1891389771.
3. Vitalij Pecharsky, Peter Zavalij,
Fundamentals of Powder Diffraction and Structural Characterization of Materials. 2nd Edition.
Springer, ISBN: 978-0-387-09579-0.
4. Simon Billinge, Takeshi Egami.
Underneath the Bragg Peaks: Structural Analysis of Complex Materials. 2nd Edition.
Elsevier. ISBN: 9780080971339

Homeworks – will be assigned during class based on lecture materials.

Midterm 1: TBD.

Midterm 2: TBD.

Final: crystallographic report on assigned structure(s)

All exams will be open book & open notes.

Homeworks: 10%
Midterm1: 20%
Midterm2: 20%
Final: 50%

The final grade will be determined per the following ranges, no curve:

A⁺-A⁻ >90%

B⁺-B⁻ 80-90%

C⁺-C⁻ 70-79%

D⁺-D⁻ 60-69%

F <60%

Course Outline:

General topics: unit cells, lattices, Miller indices, generation of X-rays, diffraction, Bragg's Law, reciprocal lattice, structure factors, space groups, data collection, Fourier synthesis, methods for structure solution, use of the SHELX package for solution and refinement, data validation, plotting crystal structure, crystallographic databases.

The experimental part of the course will be devoted to practical aspects of structure solution and refinement using the SHELX package. Actual data sets will be passed out with different crystallographic challenges. There will be an opportunity to collect experimental data pending diffractometer availability. Final will be a short structure report on crystal structures determined from single crystal diffraction dataset (more details on the format and requirements will be provided). Final is due the last day of class.

Course outcomes:

After having successfully completed the course student is expected to be able to

- understand the translational symmetry and space groups,
- determine main symmetry elements from the symbol of the space group,
- figure out relations between the diffraction pattern and unit cell dimensions and symmetry,
- determine possible space groups from the analysis of the diffraction data and extinctions,
- determine crystal structure from the single crystal diffraction data,
- analyze crystal structure and prepare crystallographic files and images for publication,
- use crystallographic databases.

Cheating/Plagiarism:

Cheating or plagiarism will result in a referral to Student Judicial Affairs (SJA), automatic failure of the respective assignment, and may result in dismissal/suspension from the class. *Students are encouraged to work together*, however students are not allowed to copy data or calculations from any other person. All suspected violations will be referred to SJA.

At half of lectures for practical exercises you will need **to bring your laptop** with following free programs installed:

1. **SHELX** <https://shelx.uni-goettingen.de/>
2. **WinGX** <http://www.chem.gla.ac.uk/~louis/software/wingx/>
3. **X-Seed** - <http://academic.sun.ac.za/barbour/Software.html>
Install v. 4.1, go to "Program Settings" and link all SHELX executable

Attendance: It is an understanding that you may miss classes when ill, you are strongly encouraged to stay at home. Additional absences may occur due to your self-isolation in the cases of positive COVID testing of you or person you have been in contact. All those cases are legit absences and will be accommodated with possibilities for making up homework and exams. Those will be dealt with on a case-by-case basis.

Academic Integrity

Academic Integrity, based on the values of honesty, trust, fairness, respect, and responsibility, is a fundamental principle of scholarship in higher education. Iowa State's Academic and Research Misconduct Policy prohibits: plagiarism (using another person's writing or copying any work without proper citation); falsification; unauthorized collaboration during a test or on an assignment or substitution for another student to take an exam, course or test; and other forms of academic dishonesty. If you are to benefit from this class and be properly evaluated for your contributions, it is important for you to be familiar with and follow Iowa [State's Academic Dishonesty and Research Misconduct policies](#). Students are also encouraged to review these [Student Resources](#). Work that violates this policy will not be tolerated. Students who are found responsible for a violation of the Academic Misconduct Policy will have both a university process sanction and an academic outcome that could include a failing grade on the assignment or exam, or a failing grade for the course.

Accessibility

Iowa State University is committed to assuring that all educational activities are free from discrimination and harassment based on disability status. Students requesting accommodations for a documented disability are required to work directly with staff in Student Accessibility Services (SAS) to establish eligibility and learn about related processes before accommodations will be identified. After eligibility is established, SAS staff will create and issue a Notification Letter for each course listing approved reasonable accommodations. This document will be made available to the student and instructor either electronically or in hard-copy every semester. Students and instructors are encouraged to review contents of the Notification Letters as early in the semester as possible to identify a specific, timely plan to deliver/receive the indicated accommodations. Reasonable accommodations are not retroactive in nature and are not intended to be an unfair advantage. Additional information or assistance is available online at www.sas.dso.iastate.edu, by contacting SAS staff by email at accessibility@iastate.edu, or by calling 515-294- 7220. Student Accessibility Services is a unit in the Dean of Students Office located at 1076 Student Services Building.

Discrimination and Harassment

Iowa State University does not discriminate on the basis of race, color, age, ethnicity, religion, national origin, pregnancy, sexual orientation, gender identity, genetic information, sex, marital status, disability, or status as a U.S. Veteran. Inquiries regarding non-discrimination policies may be directed to Office of Equal Opportunity, 3410 Beardshear Hall, 515 Morrill Road, Ames, Iowa 50011, Tel. 515-294-7612, Hotline 515-294-1222, email eooffice@iastate.edu.

Free Expression

Iowa State University supports and upholds the First Amendment protection of [freedom of speech](#) and the principle of [academic freedom](#) in order to foster a learning environment where open inquiry and the vigorous debate of a diversity of ideas are encouraged. Students will not be penalized for the content or viewpoints of their speech as long as student expression in a class context is germane to the subject matter of the class and conveyed in an appropriate manner.

Prep Week

This class follows the Iowa State University Prep Week policy, as noted in the ISU Policy Library and section 10.6.4 of the Faculty Handbook. Visit the [ISU Policy Library website](#) for policy wording.

Religious Accommodations

Iowa State University welcomes diversity of religious beliefs and practices, recognizing the contributions differing experiences and viewpoints can bring to the community. There may be times when an academic requirement conflicts with religious observances and practices. If that happens, students may request reasonable accommodation for religious practices. In all cases, you must put your request in writing. The instructor will review the situation in an effort to provide a reasonable accommodation when possible to do so without fundamentally altering a course. For students, you should first discuss the conflict and your requested accommodation with your professor at the earliest possible time. You or your instructor may also seek assistance from the [Dean of Students Office](#) at 515-294-1020 or [the Office of Equal Opportunity](#) at 515-294-7612.

Contact Information for Academic Issues: If you are experiencing, or have experienced, a problem with any of the above issues, email academicissues@iastate.edu