Chemical Crystallography – CHE 640 (Fall 2023)

Instructor - Dr. Sean Parkin

Course overview

This course is an *introduction* to structure determination by X-ray diffraction. It is intended to be suitable for graduate students whose primary area of interest is either synthetic organic, inorganic, or organometallic chemistry.

The course does not revolve around any particular textbook, but the following cover most of the material reasonably well. There are of course other books, and they all contain much the same sort of information.

"**Crystal Structure Determination**" by Werner Massa
English translation by Gould
Springer: ISBN 3-540-65970-6

"**X-Ray Crystallography**" by Gregory S. Girolami
University Science Books: ISBN-13: 978-1-891389-77-1

The progression of the course loosely follows the steps involved in a typical routine structure determination, but will occasionally stray off target to introduce some concept necessary for a deeper understanding of the subject. The nature of the material requires that some mathematical derivations are presented, but these will be kept to a minimum. The general level of mathematics required for a typical bachelor's degree in chemistry should be sufficient (algebra, trigonometry, calculus, probability, statistics, matrices and tensors, and some group theory).

There will be homework assignments (some weeks) as well as mid-term (take home) and final examinations (more of a semi-independent project). The intent of the course is to provide sufficient background information that students can collect X-ray diffraction data, solve, and refine a relatively well-behaved small-molecule crystal structure and correctly interpret the results. To this end there will be regular sessions in the X-ray laboratory, mostly in groups, but perhaps also individually, to allow hands-on exposure to the microscopes, diffractometers, and computers.

Lecture and laboratory attendance is mandatory unless you have the consent of the instructor. If you think you might be late, please let me know *via* e-mail as early as possible! This rule applies to everyone - you will not learn anything unless you do the work.

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Course requirements

Assignment of grades for this course is based upon homework problem sets, a take-home midterm exam and the successful completion and write up (as if for publication in the journal *Acta Crystallographica section E*) of a crystal structure determination. The latter constitutes the final exam and can be begun after the mid-term exam, *i.e.* as soon as a student feels ready to tackle semi-independent practical work. Crystals for this "final exam" may be from the students own research project (preferred), or could be selected from random crystals found in the X-ray lab.

Homework assignments and the mid-term exam will each contribute 25% of the total score for the course with the remaining 50% from the final. Grades will be assigned according to the following scheme.

A:	85	< score ≤	100%
B:	70	< score ≤	85%
C:	55	< score ≤	70%
D:	40	< score ≤	55%
F:	0	< score ≤	40%

Working together on homework assignments is ok with me, but *verbatim copying* is **not ok**. It is fairly easy to tell the difference between collaborative effort and copied work.

<u>If your handwriting is lousy then it is your job to ensure that it is readable.</u>

Collaboration on the mid-term exam is not allowed, but reference to books, lecture notes, journals *etc*. is ok. If you are completely stuck the instructor *might* help, provided you ask *sensible* questions *well before* the end of the exam week. The ultimate goal of the course is to get students comfortable with elementary crystallography, competent to determine routine structures, and capable of describing and interpreting published work. To this end, collaboration with others is encouraged and help from the instructor is available throughout the course.

Note: The instructor is British and therefore has no concept of either 'grading curves' or 'extra credit'. Don't ask.

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