

## Chemical Crystallography – CHE 580-001 (Spring 2007)

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 books cover most of the material reasonably well. The first, which I recommend you buy, is purely an introduction and should be sufficient, while the second is very much more involved, *i.e.* it is good bedtime reading for insomniacs.

“Crystal Structure Determination” by Werner Massa

English translation by Gould

Springer: ISBN 3-540-65970-6

“Fundamentals of Crystallography” by Carmelo Giacovazzo

Oxford University Press: ISBN 0-19-855578-4

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

There will be homework assignments (most weeks) as well as mid-term and final examinations. The real intent of the course though 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. To this end there will be regular sessions in the x-ray laboratory either in groups or individually to allow hands-on exposure to the apparatus and computers.

Lecture and lab. attendance is absolutely mandatory without the express consent of the instructor. This rule applies to people taking the course for credit, audit and to those who are ‘just sitting in’.

Revision 5: January 10th 2007

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### Course requirements

Assignment of grades for this course will be based upon homework problem sets, a take-home midterm exam and the successful completion and write up (as if for publication in the electronic journal Acta Crystallographica section E) of a crystal structure determination. The latter will constitute 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.

Homework assignments and the mid-term exam. will contribute 25% each of the total score for the course with the remaining 50% from the "final." Grades will be assigned according to the following scheme, but consideration of the particular experience level of students is taken into account.

A:	80	< score ≤	100%
B:	60	< score ≤	80%
C:	40	< score ≤	60%
D:	20	< score ≤	40%
F:	0	< score ≤	20%

Collaboration on homework assignments is perfectly o.k. and reasonable but verbatim copying is not a good idea. It is fairly easy to tell the difference between collaborative effort and copied work. Collaboration on the mid-term exam. is not allowed, but reference to books, lecture notes, journals *etc.* is fine. The ultimate goal of the course is to get the student comfortable with crystallography, competent to determine structures and capable of describing and interpreting published work. To this end, collaboration with others is encouraged and help from the instructor is available (as a last resort and within reason!) during the "final."