

University of Windsor
Chemistry and Biochemistry
Chemistry 59-553, Winter Term 2017

Lectures: Tues. and Thurs. 9:00-10:30 pm in Essex Hall room

Professor: Dr. Charles Macdonald (office: 355 Essex Hall (Chemistry); 236 Essex Hall (Science))

Office Hours: Open door

Material:

This course is primarily intended for graduate students and a significant amount of reading and practice with software outside of class time will be required to comprehend the material. The material concerning the fundamental principles can be found in any number of text books on X-ray crystallography. I have suggested a few books that you may want to purchase - these are listed on the course web site. Furthermore, I will provide handouts during class or post notes on my web site for most topics and provide you with URLs for a number of helpful web sites that contain tutorials or other information of value.

The course web site can be found by selecting the proper link at:

<http://cmacd.myweb.cs.uwindsor.ca/teaching.htm>

Grading for 59-553:

The overall grade will be based on assignments (30%), a final exam (40%) and a project with a short paper (total 30%).

Project and paper submission: on or prior to Mar. 29, 2017

The project and paper involve the solution, refinement and report preparation of a crystal structure in the style of an *Acta Crystallographica C* paper; more details will be provided in class.

Exam Date: Friday Apr. 21, 2017 – 12:00 noon (Exam Slot 38)

Last Date for Voluntary Withdrawal from Course: March 15, 2017

Course evaluations will be conducted sometime during the final two weeks of class, as per Senate regulations.

Course Outline:

The goals of this course are two-fold.

First, I would like the student to become familiar with the fundamental principles concerning X-ray diffraction by crystalline materials and to gain an understanding of the methods that we use to determine the structures of molecules and materials using X-ray diffraction experiments.

Second, I would like the class to become familiar with a variety of different software that we use for the purposes of structure determination, solution, refinement and presentation (including SHELX, WinGX, OLEX2, Diamond, ORTEP-3, and others). Similarly, I will introduce the class to other useful software tools including: databases (CSD and ICSD); structure confirmation software (PLATON); powder XRD tools (PowderCell) and maybe even some software for putting interactive structures on web pages.

Topics that I intend to cover include (not necessarily in this order):

- crystal growth, selection and mounting
- X-ray generation, diffractometer set-up, and safety
- crystal symmetry and space groups
- lattices and reciprocal lattices
- crystallographic planes and Miller indices
- X-ray diffraction (Bragg and Laue)
- structure factors and electron density
- The "Phase Problem"
- Structure Solution (Patterson methods, Direct Methods, Dual Space Methods, and others)
- Refinement
- Interpretation of structural data
- Presentation of structural data
- twinning
- Powder XRD