



Macromolecular X-ray Crystallography

SC/CHEM 4092 / 5092

Fall 2010

Course Description

This course covers the theory and practice behind macromolecular structure determination using X-ray crystallographic methods, including crystallization, X-ray diffraction, data reduction, addressing the phase problem, structure refinement and validation, and recent advances in the field.

Lectures: Tues./Thurs. 10:00 – 11:30 in FRQ 312

Office Hours: Wed. 1:00 – 2:00

Course Director: Gerald Audette
E-mail: audette@yorku.ca
Office: CB 456

Important Dates:

September 14	First Day of Classes
September 26	Last Day to Enrol in Course w/o Permission of Instructor
October 8	Last Day to Enrol in Course with Permission of Instructor
October 9-15	Fall Reading Week
November 12	Last Day to Drop Course without Receiving a Grade
December 9	Last Day of Classes
December 12-23	Final Exam Timeframe (exact date TBD)

Notes:

1. Registrar's Calendar: <http://www.registrar.yorku.ca/importantdates/fw10.htm>
2. Students are expected to be available at all times during the Fall examination period and therefore should not make travel plans within that period.

Evaluation:	In-Class Mid-Term	30%
	Term Paper & Presentation	30%
	Final Exam	40%
	Total	100%

Grading Scheme:

The grading scheme for the course conforms to the point system used in other programs at York ($A^+=9$, $A=8$, $B^+=7$, $B=6$, $C^+=5$, $C=4$, $D^+=3$, $D=2$, $E=1$, $F=0$). A letter grade for the course will be assigned based on the final percentage grade ($A^+=90-100$, $A=80-89$, $B^+=75-79$, $B=70-74$, $C^+=65-69$, $C=60-64$, $D^+=55-59$, $D=50-54$, $E=40-49$, $F=0-39$). The final grade for the course will be calculated using the weightings listed above under **Evaluation**.

Email Policy:

Course related e-mail communications should be sent from your yorku.ca account, and should include "Chem 4092" or "Chem 5092" in the subject line.

Missed Exams:

- A medical certificate and Attending Physician's Statement must be submitted for any missed midterm/quiz. This documentation must be submitted within 3 working days of the missed exam. If no documentation is submitted, the mark assigned to that midterm/quiz will be zero.
- Four (4) working days after a midterm/quiz, a deferred exam will be scheduled, to be held not more than ten (10) working days after the originally scheduled midterm/quiz. Failure to write the deferred midterm/quiz will result in the mark associated with that exam as zero.

Re-grade Policy:

If, after graded exams are returned, there is a question concerning the grading of the exam, the entire exam should be returned. The *entire* exam will be re-graded. All requests for re-grading must be made in writing and must be submitted to the Course Director no later than the end of lecture 1 week after the exam is returned in class. The request should identify the question of concern and briefly explain the scientific reason why your answer merits further consideration.

Disabilities:

Students with disabilities, including physical, medical, systemic, learning and psychiatric disabilities may need accommodation in exam requirements. Students are encouraged to notify the Course Director and seek advice from the Counseling and Development Centre. According to York University policy (www.yorku.ca/web/futurestudents/requirements/disabilities.html), arrangements for students with disabilities should be made before the start of the academic term. Failure to notify the Course Director to your needs in a timely manner may jeopardize the opportunity to arrange for academic accommodation.

Academic Integrity:

York students are expected to maintain high standards of academic integrity and to abide by rules set forth by York University, as outlined in the following web-site:

www.yorku.ca/academicintegrity/students/index.htm

Course Outline

1. History
2. Preparation of Samples
3. Crystallization
4. Diffraction Theory
5. Symmetry, systematic absences
6. Structure Factors, Fourier Transforms, Convolutions, Patterson Synthesis
7. X-ray Sources, Detectors
8. Data Collection
9. Data Reduction
10. Solution of the Phase Problem
 - a. Multiple Isomorphous Replacement
 - b. Multiple Wavelength Anomalous Dispersion
 - c. Molecular Replacement
11. Model Building, Refinement and Structure Validation

Textbook, Library Material and Course Readings:

The “official” textbook for Chem 4092/5092 is Principles of Protein X-ray Crystallography (3rd ed.), by Jan Drenth, and several copies are available from Dr. Audette’s lab for reference purposes (there is also a copy in the Steacie Library). Below is a list of some useful reference materials:

1. Introduction to Macromolecular Crystallography – A. McPherson (QD 381.9 S87 M36 2009)
2. Macromolecular Crystallography Protocols (Volumes 1 & 2) – S. Doublie (ed.) (*QP551.M332)
3. International Tables for Crystallography (in particular Volumes A & F) – IUCr (*Reserve)
4. Crystallization of Biological Macromolecules – McPherson, A. (1999) (*QD381.M43)
5. Practical Protein Crystallography – McRee, D. (1999) (*QP551.M366)
6. Crystal Structure Refinement – Muller, P. (ed.) (*QD921.C772)
7. X-ray Structure Determination: A Practical Guide – Stout, G. & Jensen, L. (*QD945S)
8. Protein Crystallography – Blundell, T.L. & Jhonson, L.N. (*QD945.B57)
9. X-ray Diffraction by Macromolecules – Kasai, N. & Kakudo, M. (*QD945.K27)
10. The Development of X-ray Analysis – Bragg, W.L. (*QD945.B688)

*In Steacie Library