Macromolecular X-ray Crystallography

SC/CHEM 4092 / 5092

Fall 2018

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.

Prerequisites: SC/CHEM 2011 & SC/CHEM 3051

Lectures: Tues. / Thurs. 10:00 – 11:30 – 13:00 in SC 224
Office Hours: Wed. 12:30 – 13:30, LSB 213

Course Director: Gerald Audette
Office: LSB 327C / E-mail: audette@yorku.ca

Important Dates:

September 5	First Day of Classes
October 2	Last Day to Enrol in Course with Permission of CD
Oct. 6 – 12	Fall Reading Week
November 6	Last Day to Drop Course without Receiving a Grade
December 4	Last Day of Classes
December 6-21	Final Examination Period for F18 Courses

Registrar's Calendar: http://registrar.yorku.ca/enrol/dates/fw18

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 (or my.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.

Remarking Policy:

- If, after graded exams are returned, there is a question concerning the grading of the exam, the entire exam should be returned for remarking.
- All requests for remarking must be made in writing and must be submitted to the CD no later than the end of lecture 1 week after the exam is returned in class. The request should include your name, student number, date of request, identify the question of concern and briefly explain the scientific reason why your answer merits further consideration.
- Note that the *entire* exam will be remarked and that any exams, or portions of exams written in pencil will not be re-graded.

Academic Integrity:

York students are expected to maintain high standards of academic integrity and to abide by rules set forth by York University. Any cases of academic misconduct will be treated accordingly. Ignorance of the Policies is not an acceptable excuse and students are strongly encouraged to become familiar with such Policies. The link to the Academic Integrity for Students web-site (www.yorku.ca/academicintegrity/students/index.htm) is provided for convenience. Students MUST also complete the Academic Integrity Tutorial (www.yorku.ca/tutorial/academic_integrity/) if they haven't already done so.

Counselling and Disabilities:

- According to York University policy, arrangements for students with disabilities should be made before the start of the academic term. Failure to notify the CD to your needs in a timely manner may jeopardize the opportunity to arrange for academic accommodation. (www.yorku.ca/web/futurestudents/requirements/disabilities.html)
- Attending university and coping with all the expectations, over and above other responsibilities you may have outside school, can be very challenging. A number of options are available to you, on and off campus, to help you deal and cope with difficult situations. For example, York University offers personal counselling services (www.yorku.ca/cds/pcs). They are located in Room N110 of the Bennett Centre for Student Services and can be reached at ext. 55297). Alternatively, postsecondary students in Ontario can call 1-866-925-5454 to reach the Good2Talk helpline (www.good2talk.ca).

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 and Processing
9. Solution of the Phase Problem
    a. Multiple Isomorphous Replacement
    b. Multiple Wavelength Anomalous Dispersion
    c. Molecular Replacement
10. Model Building, Refinement and Structure Validation

Textbook, Library Material and Course Readings:

The "official" textbooks for Chem 4092/5092 are:

a. Principles of Protein X-ray Crystallography (3rd ed.), by Jan Drenth

b. Biomolecular Crystallography, by Bernhard Rupp

Both texts are held on reserve in the Steacie Library (1 day loans). There is also an e-version of the Drenth text that is available through the Library.

Below is a list of some useful reference materials. Most of these are available in Steacie Library, and the library code is provided if they are.

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)