Chem 613: Chemical Crystallography, Spring 2019

Instructors: John F. Berry; 6357 Chemistry; 262-7534; berry@chem.wisc.edu
Ilia Guzei; 2124 Chemistry; 263-4694; iguzei@chem.wisc.edu

Lectures: MWF 8:50-9:55 AM; 2311 Chemistry
Lab Sessions: Some Fridays 8:00-10:00 AM; 1381 Chemistry
Credits: 3 credits
Office hours: Tuesdays and Fridays at 4:30 PM (JFB); Fridays at 10:00 AM (IG)
Prerequisites: Chem 511 (Advanced Inorganic Chemistry) or equivalent

Objectives: In this graduate level course, students will learn the fundamental and practical aspects of crystallography in sufficient detail to solve the structures of crystalline materials from X-ray diffraction data, and critically evaluate crystal structures reported in the literature.

Organization: The course consists of lectures and lab practical sessions, see the course schedule for more details

Topics:

Symmetry and the Crystalline State: Transitional symmetry and the unit cell; notation for lattice planes and directions; symmetry operations; point groups and space groups.

The Theory and Experimental Aspects of X-ray Diffraction: The geometrical conditions for diffraction; the reciprocal lattice and Ewald sphere; the form and structure factors; the selection and mounting of crystals; diffraction experiments and data analysis.

Fourier Analysis: Fourier transforms; the relationship between diffraction data and the electron density distribution within a crystal; the phase problem; Fourier maps.

Structure Solution and Refinement: Methods of structure solution, including Patterson maps, direct methods, and the charge-flipping algorithm; structure models and their refinement; validation and critique of structure refinements.

Special Topics: Depending on the time available and interest of class, additional topics could include neutron diffraction, electron diffraction, synchrotron radiation, or protein crystallography.

Grading: Grades for this course will be based on the completion of the ten problem sets to be assigned, lab practical assignments, midterm exam, and oral and written components of the final exam.

Ten problem sets	15 points each	150 points
Ten practical assignments (you can do more for extra credit!)	15 points each	150 points
Midterm exam		100 points
Oral final presentation		50 points
Written final presentation		50 points
Total		500 points

Final grades are on an absolute scale. If you earn 450 points, you are guaranteed an A. Likewise for the other point totals. You are competing against this scale, and not other students. It is therefore to your benefit to help each other.

A	450 – 500 points	(90 %)
AB	439 – 449 points	(87.7 %)
B	400 – 438 points	(80 %)
BC	389 – 399 points	(77.7 %)
C	350 – 388 points	(70 %)
D	300 – 349 points	(60 %)
F	< 300 points	(< 60 %)

This scale may be adjusted upward. It will never be adjusted downward.

Suggested textbooks:

G. S. Girolami, *X-Ray Crystallography* (University Science Books)
W. Massa, *Crystal Structure Determination* (Springer)

On-line resources useful for Chem 613 include the instructional pamphlets of the International Union of Crystallography (http://www.iucr.org/education/pamphlets), and the on-line crystallography course of G. Chapuis at EPFL (http://escher.epfl.ch/eCrystallography/).

Chem 613 Problem Sets

Problem Set 1: Crystallographic Point Groups.

Problem Set 2: Plane groups.

Problem Set 3: Space groups.

Problem Set 4: More Space Symmetry.

Problem Set 5: Crystal Data and Crystal Directions.

Problem Set 6: Powder Diffraction

Problem Set 7: Structure Factors

Problem Set 8: Space Group Determination

Problem Set 9: Structure Factor and Patterson Analysis

Problem Set 10: Direct Methods

Problem Set 11: TBA

Schedule of Topics, Reading Assignments, Suggested Problems, and Assignment Due Dates
CHEM 613 – X-Ray Crystallography – Spring 2019

Week	Day	Date	Topic	Reading Assignment	Assignments
1	W	23.1.2019	Overview of crystallography	Campana	
	F	25.1.2019	Point group symmetry	Girolami, Chapters 1 and 2	
2	M	28.1.2019	Translational symmetry	Girolami, Chapters 4 and 5	
	W	30.1.2019	Lattices	Giroalmi, Chapter 6	
	F	1.2.2019	Bravais lattices	Girolami, Chapter 7	
3	M	4.2.2019	Growing crystals		
	W	6.2.2019	Plane groups	Girolami, Chapter 8	
	F	8.2.2019	Space groups	Girolami, Chapters 10, 11, 12	
4	M	11.2.2019	Vector algebra and matrices	Girolami, Appendix A, B	Problem Set 1
	W	13.2.2019	Diffraction of X-rays, Laue equations	Girolami, Chapters 13, 16, 17, 18	
	F	15.2.2019	Lab – Structure Solution		
5	M	18.2.2019	Reciprocal lattice	Girolami, Chapters 19, 20	Problem Set 2
	W	20.2.2019	Bragg's law, scattering planes, *d* spacings	Girolami, Chapter 21	
	F	22.2.2019	Lab – Structure Solution		
6	M	25.2.2019	Ewald construction	Girolami, Appendix C	Problem Set 3
	W	27.2.2019	Structure factors	Girolami, Chapter 23	
	F	1.3.2019	Lab – Structure Solution		
7	M	4.3.2019	Phases, Friedel's law, Laue classes	Girolami, Chapter 24	Problem Set 4
	W	6.3.2019	Systematic absences	Girolami, Chapter 26, 27	
	F	8.3.2019	Midterm Exam!		
8	M	11.3.2019	Fourier transform	Girolami, Chapter 28	
	W	13.3.2019	Structure solution, the Patterson map	Girolami, Chapter 31	Problem Set 5
	F	15.3.2019	Lab – Structure Solution		
9	NO CLASS – SPRING BREAK				
10	M	25.3.2019	Direct methods	Girolami, Chapter 34, 35	
	W	27.3.2019	Charge flipping	Girolami, Chapter 30	

	F	29.3.2019	Lab – Structure solution		
11	M	1.4.2019	Modeling the electron density	Girolami, Chapter 36	Problem Set 6
	W	3.4.2019	Refinement	Girolami, Chapter 37	
	F	5.4.2019	Lab – Structure solution		
12	M	8.4.2019	Twinning	Girolami, Chapter 38	Problem Set 7
	W	10.4.2019	Powder diffraction	Girolami, Chapter 41	
	F	12.4.2019	Lab – Structure Solution		
13	M	15.4.2019	Neutron diffraction	Girolami, Chapter 42	Problem Set 8
	W	17.4.2019	Synchrotron radiation		
	F	19.4.2019	Lab – Structure Solution		
14	M	22.4.2019	Protein crystallography	Girolami, Chapter 33	Problem Set 9
	W	24.4.2019	Other Topics		
	F	26.4.2019	Other Topics		
15	M	29.4.2019	Student presentations		Problem Set 10
	W	1.5.2019	Student presentations		
	F	3.5.2019	Student presentations		
*** FINAL EXAM: Due May 10th at noon ***					