

CHEM 763 – Instructor: Dr. Michael Gau, 14 classes

Practical X-ray Crystallography course, Graduate level course

Class Structure for Spring 2023

- Course is aimed to instruct students how to solve, refine and complete their own crystal structures. This includes navigating the software, identifying problems and how to solve them, and being well-versed in crystallography.
- Lecture style course with follow-along worksheets/labs for instruction.
- This course can be adapted to online or in-person lectures. We will tackle a different crystallographic problem each week with tutorials on how to solve them. Then the students will complete a weekly problem/crystal structure and be graded on the completed product.
- M/W: Introduce the crystallographic problem the first class, then proceed with a tutorial of how to solve. May take two classes to complete. Assign a crystal structure to the class to complete and turn in the following week.

Tentative Schedule:

Class 1 and 2 – Introduce software and revisit important concepts of X-ray crystallography. Outline course and the crystallographic problems we will be tackling. Begin with a simple structure with no issues and teach how to solve structure, assign atoms, refine, edit/examine the results, and generate a cif/report.

Class 3 and 4 – Tutorial on most common crystallographic problem, positional disorder, and using restraints/constraints on badly behaving atoms.

Class 5 and 6 – Disorder on symmetry operation (inversion center or mirror plane) and using FRAG/FEND. Compositional disorder.

Class 7 and 8 – Whole molecule disorder and absolute configuration.

Class 9 and 10 – Using SQUEEZE and when to use it.

Class 11 and 12 – Unknown structures, multiple molecules in asymmetric unit. Intro to twinning.

Class 13 and 14 – Pseudomerothedral twinning, non-merohedral twinning. Schedule may shift and some topics may not be covered based on timing.

Outline of Assignments & Assessments

- Weekly worksheets/labs
- 10 points per weekly worksheet
- Midterm and Final exam will be worth 100 points

Essential Course Policies

- Laptops required/necessary for course