

CHEM 850-010: Special Topics Inorganic Chemistry
X-ray Crystallography
M 12:20 – 2:50 PM, 3 credits

The course will cover basic theory and practice of single crystal X-ray diffraction and space group symmetry with emphasis the practical aspects of diffraction data collection and structure solution as performed at the X-ray Crystallography Laboratory. Students will conduct solvent-based crystallization experiments and learn the SHELXTL program suite. Students are also required to show proof of attendance for X-ray Safety Training conducted by the Radiation Safety Officer.

Prerequisites: CHEM-457 or CHEM-654 or consent of instructor

Textbook: Crystal Structure Determination by William Clegg, Oxford Chemistry Primers, ISBN 0-19-855901-1

Topics covered (each roughly covering a week):

Fundamentals of the Crystalline State
Diffraction of X-rays by Molecules and Crystals
Geometry and Symmetry of X-ray Diffraction
Forward and Reverse Fourier Transform in 3D
Generation of X-rays, Absorption and Monochromation
Crystal Growing Techniques
Preparation and Selection of Samples
X-ray Diffractometers
Measurement of Intensities
The Phase Problem & Solving the Structure
Completing and Refining the Structure
Presenting and Interpreting the Results: the checkCIF program