X-ray Practicals

Instructor: Joseph Reibenspies Ph.D.

Synopsis. This course is intended to teach students how to use the X-ray instrumentation available in the department. The course will not discuss the theory of X-ray diffraction only its practice.

See www.chem.tamu.edu/xray/practicals.htm for details, class notes and data.

The SHELXTL and XSEED tutorials are part of a LAPTOP university course. Students are encouraged to download the programs to their laptops and bring the laptops to class.

The XSEED program can be downloaded from http://x-seed.net/ and will run without registration for the first 30 sessions. Be sure to download POVRAY (http://www.povray.org/download/).

The SHELXTL program is restricted to laptops owned by Texas A & M University. Please do not ask the X-ray Diffraction managers to load these programs on personal computers.

The data for both sessions is at www.chem.tamu.edu/xray/practicals.htm. Please follow the Examples link.

All programs should be fully functional at the time of the class. The instructor cannot spend class time setting up computers.

Dates : January 7,8,9 and 10 Time : 12:30 Room 2122.
Instructor : Joseph Reibenspies

Syllabus:

January 7: Data Collection and Data Reduction
Beginners: 12:30-1:30
Advanced Techniques: 1:30-2:30

January 8: Absorption Correction and Initial Preparation (space group etc..)
Beginners: 12:30-1:30
Advanced Techniques: 1:30-2:30

January 9: Structure Solution and Refinement
SHELXTL tutorial 12:30-1:30
Bring your laptop with SHELXTL pre-installed
XSEED tutorial 1:30-2:30
Bring your laptop with XSEED pre-installed

January 10: Advanced Refinement and Structure Verification
Advanced Refinement techniques (disorder, absolute configuration etc..)
12:30-1:30
Structure Verification and Publication
1:30-2:30