Instructor: Jeffrey L. Petersen, Professor
Office: 257 CRL
Lecture Periods: Monday, Wednesday, and Friday, 8:30 a.m., Room 300, Clark Hall
E-mail address: jpeterse@wvu.edu

Course Overview: This course provides students with a practical understanding of the application of single-crystal X-ray diffraction methods for the determination of molecular structure. The first half of the course focuses on the concepts of space group symmetry and diffraction theory. The second half of the course covers the various steps associated with a single-crystal X-ray structural analysis, including crystal growing methods, data collection, space group determination, structure solution and refinement, computer graphics, and the use of the SHELXTL crystallographic software for molecular structure determination.

Text:

Crystal Structure Determination, W. Massa, 2nd ed.

Problem Assignments: Problem assignments will be assigned on a weekly basis and must be completed and handed in on time. A homework assignment that is turned in late will be penalized 50% of the maximum credit assigned to that particular assignment. The completed homework assignments should reflect each student’s individual effort and not the work of others.

Reserve Materials:

The answer keys to all of the assigned problems and the hour examinations will be placed on reserve in the Wise Library. The reserve desk is located on the left side of the main floor as you enter the new addition of the Wise Library. The reserve materials can also be retrieved electronically by going to the University Library website located at http://www.libraries.wvu.edu. These materials are saved in pdf format, which will require the use of Adobe Acrobat Reader to retrieve them. If you do not have Adobe Acrobat Reader on your computer, the latest version can be downloaded at no charge from the University Library website.
**Exams and Grading:** Two hour examinations and a comprehensive final examination will be administered during the semester.

- Exam 1  week 7
- Exam 2  week 14
- Final Exam  Friday, December 14, 2012 at 11 am

The overall course grade will be determined as follows:

- Homework Assignments  20%
- Hour Examinations  40%
- Final Examination  40%

**Social Justice Statement**

West Virginia University is committed to social justice. I concur with that commitment and will maintain a positive learning environment based upon open communication, mutual respect, and non-discrimination. Our University does not discriminate on the basis of race, sex, age, disability, veteran status, religion, sexual orientation, color or national origin. All suggestions as to how to further a positive learning environment in Chemistry 547 are welcomed.

*Cell phones and portable listening devices, such as a MP3 player, iPod, or radio, are to be turned off and stowed during periods and examinations.*

**Reserved Reference Materials in Wise Library:**

1. Stout and Jensen, "X-Ray Structure Determination - A Practical Guide"
2. Drago, "Physical Methods in Chemistry", see chapter devoted to crystallography
3. Ladd and Palmer, "Structure Determination by X-Ray Crystallography"
Other references covering crystallographic methods of structural analysis:

1. Glusker and Trueblood, "Crystal Structure Analysis"
2. Rhodes, “Crystallography Made Crystal Clear”
5. Woolfson, “X-Ray Crystallography”
7. Donohue and Bunn, “Chemical Crystallography”
11. McKie and McKie, “Crystalline Solids”
General Course Outline
CHEMISTRY 547

I. General Principles of Molecular Structure
   A. Basic Molecular Geometries
   B. Fundamental Chemical Bonding Principles
   C. Deviations from Idealized Geometries

II. Concepts of Diffraction Theory
   A. Origin of X-Ray Radiation
   B. Unit Cell
   C. Lattice Planes and Miller Indices
   D. Bragg's Law
   E. Reciprocal Lattice

III. General Aspects of Molecular and Crystallographic Symmetry
   A. Rotation and Reflection Symmetry
   B. Stereographic Projections and Point Group Symmetry
   C. Symmetry of Crystal Systems
   D. Translational Symmetry
   E. Bravais and Primitive Lattices
   F. Glide Planes and Screw Axes

IV. The Structure Factor
   A. Friedel's Law
   B. Amplitude and Phase
   C. Systematic Absences

V. Space Group Symmetry
   A. Triclinic, Monoclinic, and Orthorhombic Lattices
   B. Equivalent and Special Positions
   C. Symmetry Properties of Reciprocal Space

VI. Crystal Structure Analysis
   A. Crystal Growing
   B. X-ray Diffraction Instrumentation
   C. Preliminary Crystallographic Information
   D. X-ray Data Collection and Reduction
   E. Phase Problem
   G. Patterson and Direct Methods for Structural Analysis
   H. Refinement of the Structural Model
   I. Computation of Structural Parameters
   J. Computer Graphics and 3D Molecular Structure Display