CHEMISTRY 832
GOALS AND OBJECTIVES

Chemistry 832, Undergraduate Bulletin Course Description: *Solid-State Structural Methods*. Structure determination for single-crystal and multi-phase organic and inorganic solids by techniques such as single-crystal and powder X-ray and neutron diffraction, electron microscopy, and X-ray microanalysis. Integration of theoretical and practical perspectives through laboratory exercises. Two hours lecture and three hours laboratory-discussion. Prereq: CHEM. 721 and CHEM. 741 or 802. 3 q.h.

Goal 1. By the end of this course, the students will understand how molecules and extended solids pack in the solid state in terms of *unit cell structures*.

Objective 1. The students will learn what a unit cell is and how to identify unit cells in both two and three dimensional solids by a combination of lecture content, lecture exercises, analysis of two dimensional solids (including Escher prints and wall paper samples), and computer aided solids visualization.

Objective 2. The students will learn the principle types of solid state symmetry, including: point group symmetry elements (e.g. rotation axes, inversion center, mirror planes, and their combinations), symmetry in extended solids (e.g. glide planes, and screw axes), and how this relates to the crystallographic space groups.

Objective 3. The students will learn the basic principles of how intermolecular forces and entropy interact with experimental variables to influence the contents and imperfections of unit cells.

Goal 2. By the end of this course, the students will understand how the *macroscopic morphologies* of single crystalline, powder, and multi-phase samples are characterized and relate to their microscopic structures.

Objective 1. Through a combination of lecture content and lab exercises, the students will learn how unit cells are organized to give macroscopic samples having single crystalline, powder, and multi-phase morphologies.

Objective 2. Through a combination of lecture content and lab exercises, the students will learn the basic principles of how solid state defects effect single crystalline, powder, and multi-phase morphologies.

Objective 3. The students will learn the basic principles of how intermolecular forces and entropy interact with experimental variables to influence the packing of unit cells into macroscopic objects.

Goal 3. By the end of this course, the students will understand how crystals grow from solutions, melts, etc., and be able to plan and carry out a systematic approach to growing single crystals suitable for diffraction experiments.

Objective 1. Through a combination of lecture content and laboratory exercises the students will understand how to plan and carry out a systematic survey of crystallization conditions.

Objective 2. Through a combination of lecture content and laboratory exercises the students will understand how to plan and carry out a systematic approach to growing single crystals based on their survey of crystallization conditions.

Objective 3. Through laboratory exercises the students will learn how to select and mount crystals suitable for single-crystal diffraction analyses.

Goal 4. By the end of this course, the students will understand the principles of atomic scale diffraction by x-rays, neutrons, and electrons and how it relates to practical aspects of crystallography.

Objective 1. Through a combination of lectures, assignments, and computer based laboratory exercises the students will understand how the scale of molecular sizes and molecular assemblies interact with the wavelengths of the x-rays, neutrons, and electrons to set limits on possible information from the experiment.

Objective 2. Through a combination of lectures, assignments, and computer based laboratory exercises the students will understand how the motions and disorder of molecules and molecular assemblies interact with the x-rays, neutrons, and electrons to set limits on possible information from the experiment.

Objective 3. Through a combination of lectures, assignments, and computer based laboratory exercises the students will understand how the absorption of x-rays, neutrons, and electrons by molecules sets effects the information from the experiment.

Objective 4. Through a combination of lectures, assignments, and computer based laboratory exercises the students will understand how contents of unit cells and the unit cell sizes and geometry interact with the x-rays, neutrons, and electrons to give the positions, intensities, and phases of reflections in diffraction patterns.

Goal 5. By the end of this course, the students will understand how an x-ray diffractometer operates and is used to collect diffraction data and how this relates to the analogous neutron and electron diffraction instruments.

Objective 1. Through a combination of lecture content, assignments, and laboratory exercises the students will gain a firm understanding of the rationale behind, and appreciation for, the safety procedures in a diffraction laboratory.

Objective 2. Through a combination of lecture content and laboratory exercises the students will understand how x-rays are generated and converted into collimated monochromatic beams.

Objective 3. Through a combination of lecture content and laboratory exercises the students will understand how a crystal is centered and oriented in an x-ray beam under both manual and computer control.

Objective 4. Through a combination of lecture content and laboratory exercises the students will understand how the quality of crystals are evaluated, particularly via: optical microscopy, x-ray rotation photographs, and peak profiles.

Objective 5. Through a combination of lecture content and laboratory exercises the students will understand how the intensities and positions of diffracted x-ray beams are measured by serial and area detectors.

Objective 6. Through a combination of lecture content and laboratory exercises the students will understand how one uses diffractometer software to plan and carry out a diffraction experiment.

Objective 7. Through a combination of lecture content and laboratory discussion students will develop a basic appreciation of how the procedures used for neutron and electron diffraction experiments are related to those for the x-ray experiment.

Goal 6. By the end of this course, the students will understand the principles and practice of how diffraction data is processed and analyzed to give atomic scale structural information.

Objective 1. Through a combination of lecture content and assignments and laboratory and computer based exercises, the students will gain a basic understanding of how raw diffraction data is processed to correct for experimental factors and give corrected data appropriate for use in structural analyses.

Objective 2. Through a combination of lecture content and assignments and laboratory and computer based exercises, the students will gain a basic understanding of how the correct space group for a particular crystal is deduced.

Objective 3. Through a combination of lecture content and assignments and laboratory and computer based exercises, the students will gain a basic understanding of how the processed diffraction data is analyzed to guess trial structures and how this relates to general solutions to the phase problem.

Objective 4. Through a combination of lecture content and assignments and laboratory and computer based exercises, the students will gain an understanding of how the trial structure is checked for validity and used to assign initial atomic positions.

Objective 5. Through a combination of lecture content and assignments and laboratory and computer based exercises, the students will gain an understanding of how the initial atomic positions are refined by least squares methods in an iterative cycle to give the final three dimensional structure.

Objective 5. Through a combination of lecture content and assignments and laboratory and computer based exercises, the students will gain an understanding of how the final three dimensional structure is converted to molecular and crystal plots and tables of data suitable for publication.

Goal 7. By the end of this course, the students will understand the strengths and limitations of the atomic scale structural information provided by diffraction experiments.

Objective 1. Through a combination of lecture content and assignments and laboratory and computer based exercises, the students will learn to evaluate the reliability of a structure determination (i.e. does one have the correct structure).

Objective 2. Through a combination of lecture content and assignments and laboratory and computer based exercises, the students will learn to evaluate the reliability of structural data (what is the chemical significance of specific structural features such as a particular bond length or angle).

Objective 3. Through a combination of lecture content and assignments, the students will learn to evaluate the reliability of structural information in the literature for small molecules, polymers, biological macromolecules, minerals, metals, etc.