Course Title: Chemical Crystallography

Course Code: CH-808

Credit Hours: 3-0

Prerequisite: Nil

Course Objectives

The course is designed to introduce X-ray diffraction methods as a tool for materials characterization. The specific course objectives are:

- Introduction of crystallographic point groups, transitional symmetry elements and space groups in crystals
- Diffraction of X-rays and Bragg's Law, Reciprocal space and construction of Ewald's sphere and sphere of reflections
- Data collection strategies for single crystals and powdered crystalline materials and interpretation of data
- Phase problem and methods of determination of phases
- Structure solution and refinement of single crystal data using SHELXT and SHELXL through crystallographic packages such as Olex2.
- Refinement of powder XRD data, indexing of PXRD patterns, determination of accurate lattice parameters and identification of new/unknown phases

Course Outcomes

At the end of the course the students are expected to have learned the following:

• A basic understanding of symmetry elements and the theory of X-ray crystallography in crystalline materials.

• Usage of X- ray crystallography in both single crystals and powder crystalline materials for research applications.

Course Contents

Crystal systems and Bravais lattice, introduction to symmetry elements in crystals, crystallographic point groups, glide planes, screw axes, space groups, Miller Indices, crystallographic planes and directions.

What are X-rays, generation and classification of X-ray, diffraction of X-rays, Bragg's law. The reciprocal lattice, Bragg's law in reciprocal space, Ewald's sphere and sphere of reflection.

Data collection strategies for single crystals, interpretation of intensity data, temperature factor, Structure factor, Friedel's law, determination of systematic absences for various symmetry, Anomalous scattering and absolute configuration.

Phase problem, Phase determination in practice, Patterson Methods, Patterson Symmetry.

Refinement by least squares method, weighting functions, Goodness-of-Fit (GOF) parameter, treatment of non-hydrogen atoms, and treatment of hydrogen atoms, treatment of disordered structures.

Methods of crystal growth and selection of crystals, data collection, data reduction, space group determination, structure solution and refinement using SHELXT and SHELXL through crystallographic packages (OLEX2)

PXRD: determination of accurate lattice parameters, identification of new/unknown phases, indexing of PXRD

Recommended Books

1. Fundamentals of Crystallography (3rd Ed.) by C. Giacovazzo, Oxford University Press, USA, 2011. (DOI: 10.1093/acprof:oso/9780199573653.001.000)

2. Crystal Structure Determination (2nd Ed.) Massa Werner, Translated into English by R. O. Gould. New York, NY: Springer, 2004. ISBN: 3540206442.

3. Crystal Structure Refinement: A Crystallographer's Guide to SHELXL, Peter Müller, Oxford Scholarship Online (OSO), 2010. (DOI:10.1093/acprof:oso/9780198570769.001.0001)