



CHEMICAL CRYSTALLOGRAPHY

PROF. ANGSHUMAN ROY CHOUDHURY

Department of Chemistry
IISER Mohali

- INTENDED AUDIENCE** : PhD students and 2nd year M.Sc students
PREREQUISITES : Basic knowledge about molecular symmetry
INDUSTRY SUPPORT : Pharmaceutical industry

COURSE OUTLINE :

This course would highlight the concepts and applications of widely used experimental technique of X-ray crystallography. The course would take the students through the lane of crystallographic symmetry to the structure determination and refinement of crystal structures using x-ray diffraction. Any experimental organic or inorganic chemist would be benefited from this course.

ABOUT INSTRUCTOR :

Prof. Angshuman Roy Choudhury. The instructor has obtained his Ph. D. in 2005 from Indian Institute of Science, Bangalore working in the area of small molecule X-ray crystallography. Following that he has worked in the University of Liverpool as a post-doctoral fellow from October, 2004 to September, 2007. Then he moved to BITS, Pilani as Assistant Professor in Chemistry. From there, he moved to IISER Mohali in December, 2009 as Assistant Professor in chemistry. He has more than 100 publications in various international journals, guided two PhD students and a few masters students at IISER Mohali. He offers the same course at IISER Mohali in the August Semester.

COURSE PLAN :

- Week 01** : Introduction, 1D symmetry, Concept of 2D symmetry and lattices, notations of symmetry elements, space groups in 2D, 3D lattices, 32 point groups and their notations, crystal systems and Bravais lattices.
- Week 02** : Stereographic projections, Laue symmetry; glide planes, screw axes and their notations, space groups, equivalent points, space group symmetry diagrams etc.
- Week 03** : Miller Indices, crystallographic planes and directions, close pack structures, linear density, planar density, Miller-Bravais indices for hexagonal systems, various ceramic structures (NaCl, ZnS, CaF₂, CsCl etc.), octahedral and tetrahedral sites etc.
- Week 04** : What are X-rays, generation and classification of X-ray, X-ray sources, diffraction of X-rays, Bragg's law. The reciprocal lattice, reciprocal relationship, Bragg's law in reciprocal space, Ewald's sphere and sphere of reflection
- Week 05** : Methods of crystal growth, identification of phases and morphologies, in-situ cryo crystallization, crystal growth under external stimuli etc.
- Week 06** : Data collection strategies, Laue Method, Oscillation, rotation and precession methods. L-P corrections, structure factor, scaling, interpretation of intensity data, temperature factor, symmetry from intensity statistics
- Week 07** : Structure factor and Fourier synthesis, Friedel's law; exponential, vector and general forms of structure factor, determination of systematic absences for various symmetry or lattice centering, FFT, Anomalous scattering and absolute configuration.
- Week 08** : Phase problem, Direct Methods, structure invariants and semi invariants, probability methods, Phase determination in practice, Patterson Methods, Patterson Symmetry, completion of structure solution, Del-F synthesis.
- Week 09** : Refinement by Fourier synthesis, refinement by Del-F synthesis, 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.
- Week 10** : Crystal selection, indexing of crystals, data collection, data reduction, space group determination, structure solution and refinement using SHELXS97 and SHELXL97, introduction to crystallographic packages (APEX II suite, OLEX2, WinGx, PLATON) and IUCr validation of the data
- Week 11** : Methodology, geometrical basis of powder X-ray diffraction, applications of PXRD: determination of accurate lattice parameters, identification of new/unknown phases, applications in pharmaceutical industry.
- Week 12** : Applications of powder X-ray diffraction: Structure determination from PXRD and Reitveld method for structure refinement, indexing of PXRD, handling of PXRD using DASH.