

Approval: 5th Senate Meeting

Course Name : Chemical Crystallography
Course Number : CY-547
Credit : 2-0-2-3
Prerequisites : Consent of Teacher
Students intended for : M.Sc., Ph.D.
Elective or Compulsory : Elective
Semester : Odd or Even

Objectives: This course aim to cover both theoretical and practical aspects of Single Crystal X-ray diffraction technique.

Course Outline:

Unit 1: Crystallography overview, X-ray generation, properties of X-rays, crystal lattices, the unit cell and crystal systems, Bravais lattices, lattice planes and hkl indices, Bragg's law, reciprocal lattice, structure factors and phase problem. [3hrs]

Unit 2: Crystal symmetry, symmetry elements, space groups, asymmetric unit, Laue groups, systematic absences. [4hrs]

Unit 3: Experimental methods, crystal growth, crystal mounting, four circle diffractometer, area detectors, data reduction, absorption correction. [4hrs]

Unit 4: Structure solution and refinement, Patterson methods and Direct methods, least squares refinement, crystallographic R-values, refinement techniques. [6 hrs]

Unit 5: Anomalous dispersion and Absolute Structure, chiral and polar space groups, disorders, twinning, space group errors. [5hrs]

Unit 6: Interpretation and presentation of results, crystallographic information file, checkcif, bond lengths and angles, torsion angles, Ortep plots, crystallographic literature and data bases. [6hrs]

Topics to be covered in practical sessions: [28 hrs]

Using appropriate sample crystals, practical training will be given on the following topics: crystal selection and mounting, unit cell determination and setting up data collection strategy, data reduction and absorption correction using the software package provided, structure solution and refinement using SHELX/ provided package, preparation of cif file, checkcif and preparation of ortep diagram and other publication data of the structure. Brief training will be given in structure refinement of special cases like those with twinning, disorders etc. using standard structural data available on internet resources. Data base search.

Text Book:

Crystal Structure Determination, Werner Massa, 4th Edn. Springer, 2010.

References:

1. Crystal Structure Analysis for Chemists and Biologist, J. P. Glusker, M. Lewis M. Rossi, VCH New York, 1994.
2. An Introduction to X-ray Crystallography, M. M. Woolfson, 2ndEdn., Cambridge University Press, 1997.
3. Structure Determination by X-ray Crystallography: Analysis by X-rays and Neutrons, M. F. C. Ladd, R. A. Palmer, 5thEdn., Springer, 2012.
4. The SHELX-97 Software Manual.