

Course Title: Chemical Crystallography

Semester: VII

Course Code: CH-451

Credit Hours: 3-0

Pre-requisite: Nil

Course Objectives

1. Students will acquire knowledge about techniques involving X-rays, their production, detection, geometry of crystals, symmetry, diffraction of X-rays, structure refinement.

Text Books

2. B.D. Culity and S.R. Stock, *Elements of X-ray Diffraction*, 3rd ed., Prentice Hall(2003).

Recommended Books

3. L. Smart and M. Gagan, *The Molecular World: The Third Dimensions*, RSC, UK(2002).

3. J.P. Glusker, *Crystal Structure Analysis for Chemists and Biologists*, Wiley-VCH(1994).

Detailed Contents

4. Introduction: Techniques involving X-rays, historical background, the eye and microscope analogy, interatomic and intermolecular forces, solid-crystalline, amorphous. X-rays: Production, X-ray tubes, absorption and filtering, selection of radiation, detection of X-rays. Geometry of the crystal: Introduction, unit cells, lattices, crystal systems, crystal classes, space groups. Symmetry: Macroscopic and microscopic symmetry elements, crystal symmetry and properties. Diffraction of X-rays: Bragg's equation and Bragg's law, reciprocal lattice, Bragg's law in reciprocal lattice. Diffractometer: Powder methods camera and diffractometer, single crystal methods camera (Rotation, Oscillation, Weissenberg and Precession) and diffractometer. Intensities of the diffracted beam; measurement, data reduction. Solution of the structure, refinement and interpretation of the result.

Course Outcomes

5. At the end of the course, students will be able to understand the X-ray crystallography, unit cells, lattices, crystal systems, crystal classes, space groups, crystal symmetry and diffractometer methods.