

**JCL 310 (Jan) (3-1-0)**  
**Structure & Chemical Crystallography**  
**Instructor: Sebastian C. Peter**

**Introduction:** History of crystallography. introduction of crystallography, allotropy and polymorphism.

**Structure of solids:** amorphous, polycrystalline, single crystalline, metallic crystal, unit cell and lattice structure determination, atomic and density packing factor, crystallographic points, directions and planes, structural relations in known compounds, crystal morphology.

**Crystalline solids:** Pauling rules, ionic model of solids, electronegativity and bonding in solids, Van Arkel triangle and Heyes Ketelaar triangle, ionic radii, polyhedral representation of solids.

**Symmetry of solid structure:** symmetry element and operation, point group determination and representation.

**Group theory of solids:** Great orthogonality theorem, character table representations, symmetry of orbitals and functions, hybridization and molecular vibration determination by group theory, mutual-exclusion principle.

**X-ray diffraction:** Diffraction principles, reciprocal space, Ewald construction, powder X-ray diffraction, XRD line broadening, Rietveld refinement in powder diffraction, single crystal X-ray diffraction methods, different methods to grow good crystals, data collection and processing strategies, image plate and CCD detectors, intensity statistics, structure factor, phase problem in crystallography, Patterson and direct methods, electron density maps, structure refinement, structure databases, synchrotron radiation, basics of neutron diffraction, basics of electron diffraction.

**Space group:** Hermann-mauguin symbols, classification of space group, definition of crystallographic terms, identification of the crystal system by HM symbols, graphical symbols.

*Special classes on software learning ('Fullprof' and 'WinGX') for Single crystal refinement and Powder XRD refinement and data interpretation.*

**Reference books:**

1. A.R. West, Solid State Chemistry and its Applications
2. L. Smart and E. Moore, Solid State Chemistry: An Introduction
3. M F C Ladd, R A Palmer, Structure Determination by X- Ray
4. W. Massa, Crystal Structure Determination
5. C. Hammond, The Basics of Crystallography and Diffraction
6. G. H. Stout and L. H. Jensen, X-Ray Structure Determination: A Practical Guide
7. B. E. Warren, X-Ray Diffraction

8. C. Hammond, The Basics of Crystallography and Diffraction
9. T. Hahn, International Tables for Crystallography
10. P. Müller, R. Herbst-Irmer, A. Thomas Schneider, M. Sawaya, Crystal Structure Refinement: A Crystallographer's Guide to SHELXL