Indian Institute of Science Education and Research, Mohali
Sector 81, S. A. S. Nagar, Manauli PO, Mohali, 140306.
FIRST SEMESTER 2012-2013
Course Handout

Date: 07/08/2014

Course No : **CHM607**
Course Title : **CHEMICAL CRYSTALLOGRAPHY**
Instructor : **Angshuman Roy Choudhury**
Tutor : **Angshuman Roy Choudhury**

1. **Scope and Objective of the Course**: The course has been designed to give an overview of chemical crystallography. The course will highlight the topics such as symmetry in crystallography, crystals systems, Bravais lattices, crystal symmetry, crystallographic point groups and space groups, Miller indices, theory of X-ray diffraction, data collection, data reduction, structure factors and Fourier syntheses, Phase problem, direct methods, Patterson method, crystal structure refinement etc. The course will also highlight the application of single crystal and powder X-ray diffraction techniques and will include hand on training on crystal structure solution and refinement.

2. Text Book : X-ray structure determination: A Practical Guide (2^{nd} Ed.) by George H. Stout and Lyle H Jensen, Wiley-Interscience, New York, 1989.
3. Reference Books : (1) Fundamentals of Crystallography (2^{nd} Ed.) by C. Giacovazzo, Oxford University Press, USA, 2002; (2) X-ray analysis and The Structure of Organic Molecules (2^{nd} Ed.) Wiley-VCH, New York, 1996; (3) Chemical Applications of Group Theory (3^{rd} Ed.) by F. A. Cotton, Wiley-India Edition, India, 2009.

4. Course Plan :

Lect. No	Topics	Learning Objectives
1	Introduction	Introduction to Chemical Crystallography
2-10	Crystallographic Symmetry	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, stereographic projections, Laue symmetry; glide planes, screw axes and their notations, space groups, equivalent points, space group symmetry diagrams etc. Miller Indices, crystallographic planes and directions, close pack structures, linear density, planar density, Miller-Bravais indices for hexagonal systems, various ceramic structures (NaCl, ZnS, CaF_2, CsCl etc.)
11-16	Theory of X-ray diffraction	What is X-ray, 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, Laue Method, Oscillation, rotation and precession methods.
17-20	Data reduction	L-P corrections, structure factor, scaling, interpretation of intensity data, temperature factor, symmetry from intensity statistics, 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.

21-24	The Phase Problem	Definition, Direct Methods, structure invariants and semi invariants, probability methods, Phase determination in practice, Patterson Methods, Patterson Symmetry, completion of structure solution, ΔF synthesis.
25-27	Refinement of Crystal Structure	Refinement by Fourier synthesis, refinement by ΔF synthesis, Refinement by least squares method, weighting functions, Goodness-Of-Fit (GOF) parameter, treatment of non-hydrogen atoms, and treatment of hydrogen atoms.
28-32	Practical example	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.
33-37	Powder X-ray diffraction (PXRD)	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, structure solution from PXRD etc.), Reitveld method for structure refinement, indexing of PXRD, handling of PXRD using DASH.
38-40	Neutron and Electron Diffraction	Basics of neutron and electron diffraction and their applications.

5. Evaluation Scheme:

Component	Duration	Marks	Weightage%	Remarks
Mid Sem. I	1hr	40	20%	Closed Book
Mid Sem. II	1hr	40	20%	Closed Book
Tutorials*		20 x 4	20%	Closed Book
End Sem. Examination	3 hrs.	100	40%	Closed Book

***Tutorials** : The tutorial hours are designated for quick review of the highlights of the material covered in the lectures, clarification of doubts, and problem solving. Further, set of problems will be assigned periodically, of which the instructor will specify one to be solved by the students in the tutorial hour of the following week. The second method of evaluation in tutorial will be of a test based on the lectures covered recently. There will likely be tutorial test/quiz of 20 marks in any four tutorial classes.

6. **Office Consultation Hours** : Wednesday 3:00-4:00 p.m.

7. **Notices** : Notices, if any, concerning the course will be displayed on the Notice Board of Hostel 5 and Hostel 7 and e-mail will also be sent to all the students

Instructor
CHM 607