Birla Institute of Technology & Science, Pilani
Hyderabad Campus

FRIST SEMESTER 2023-2024

Course Handout Part II

Date: 11-08-2023

In addition to part-I (General Handout for all courses appended to the time table) this portion gives further specific details regarding the course.

Course No. : *CHEM F416*
Course Title : ***Applied Crystallography***
Instructor-in-Charge : Arijit Mukherjee

Scope and Objective of the Course:

The course intends to cover the fundamentals of crystallography as well as to explore its broader applications in contemporary research areas (such as crystal engineering), especially in chemistry. By the end of the course, students should be able to appreciate the role that crystal structure analysis and crystallography play in material design, evaluate crystal structures and symmetry elements, and communicate about crystal structures using technical, verbal, and visual means. The course also includes a hands-on experience in crystal structure analysis. The course may help the students in decision-making about pursuing crystallography as a tool in a research career.

Textbooks (TB):

1. W. Massa, Crystal Structure Determination, Springer Verlag, Berlin, 2000.
2. G. R. Desiraju, J. J. Vittal, A. Ramanan, Crystal Engineering. A Textbook, World Scientific, Singapore, 2011.

Reference books (RB):

1. Jenny P. Glusker, K. N. TrueBlood Crystal Structure Analysis A Primer, Oxford University Press, New York, Third Edition, 2010,
2. W. Clegg, Crystal Structure Analysis: Principles and Practice, Oxford University Press, 2001.

1. Course Plan:

Lecture No.	Learning objectives	Topics to be covered	Chapter in the Text Book	Learning Outcome
1	**Introduction to crystallography**	Symmetry, crystallization, and crystallography	T1-Ch 1, Lecture notes	Learning the broad definition of the subject
2-6	**Symmetry operations**	Review of symmetry operations, symmetry in the real world, symmetry operations in two dimensions, review of point groups, review of crystal systems and Bravais lattice types, crystal lattice, unit cell concepts	T1 Ch2, Ch 6.1-6.3, Lecture notes	Theoretical knowledge about multiple symmetry operations in two and three dimensions.

7-12	**Space groups**	Space groups, symmetry diagrams and equivalent point diagrams, general and special positions, crystallographic directions, and planes. Explanation with crystal structures.	T1 Ch 6, Lecture notes	Representation of symmetry elements and space groups
13-18	**Fundamentals of X-ray diffraction-I**	X Rays: Origin, production, absorption, filtering, detectors, selection of radiation, interference of waves, X-ray scattering, Laue's conditions, Bragg's law,	T1 Ch 3, Lecture notes	Theoretical knowledge about X-ray generation, X-ray interaction with matter, X-ray diffraction,
19-25	**Fundamentals of X-ray diffraction-II**	Ewald construct, reciprocal lattice, diffraction in reciprocal space, limits of resolution, structure factors, systematic absences, Fridel's law, intensity calculation, phase problem	T1 Ch 4, 5, 6, Lecture notes	Theoretical knowledge about reciprocal space and its importance, structure factors, systematic absences, Friedel's law, intensity calculation, phase problem
26-28	**Basics of Crystallization**	Crystal nucleation and growth, techniques to grow single crystals, morphology of crystals	T2, Ch 4, Lecture notes	1. How does a crystal nucleate and grow? 2. Relation with morphology
29-32	**Structure determination by X-ray crystallography**	Choosing a crystal, crystal mounting, optical alignment, data collection, data reduction, solving a crystal structure, refinement of crystal structures, completing the structure, and crystallographic information files.	T1 Ch 7,8,9, Lecture notes	Understanding and correlating the structure-property relationship
33*	**Analysis of SCXRD Data (Hands-on)**	Demonstration of some components of Single Crystal X-ray Diffraction (SCXRD) and analysis of crystal structures of some organic molecules.	Lecture Notes	Students will get some experience in the analysis of single crystal structures of some organic molecules.
34-41	**Applications of crystallography**	Some milestones related to Chemistry (Selected crystal structures), introduction to crystal engineering, cocrystals and polymorphism, coordination polymers, crystallographic databases, application of X-ray diffraction in pharmaceuticals	T2 Ch 1, 2, 3, 5, 6, 7, T1 Ch 13, Lecture notes	Appreciating the application of crystallography to real-life/industry-relevant problems
42*	**Analysis of PXRD Data (Hands-on)**	Demonstration of some components of Powder X-ray Diffraction (PXRD) related to data collection and analysis of organic molecular solids.	Lecture notes	Students will get some experience in the analysis of PXRD.

*Hands-on experience in crystal structure analysis.

5. Evaluation Scheme:

Component	Duration (minutes)	Weightage (%)	Date & Time	Nature of Component
Midsemester Test	90	30	11/10 - 4.00 - 5.30PM	Closed book (10% Open book)
Assignment + Presentation	-	30	-	Open book
Comprehensive Examination	180	40	13/12 AN	Closed book

6. Chamber Consultation Hour: Will be announced in class.
7. Notices: Will be updated in CMS
8. Make-up Policy: Make up would be considered only for **genuine reasons**.
9. Academic Honesty and Integrity Policy: Academic honesty and integrity are to be maintained by all the students throughout the semester and no type of academic dishonesty is acceptable.

INSTRUCTOR-IN-CHARGE