Name of the Programme: M.Sc. Part-II (Analytical Chemistry)

Course Code: CHA-621 **Title of the course:** Fundamentals of Crystallography

Number of Credits: 4

Effective from AY: 2023-24

Prerequisites for the course:	Students should have studied M.Sc. Part-I.	
Course Objective:	1. To introduce basic concepts of crystallography. 2. To impart knowledge of single crystal and powder X-ray diffraction methods. 3. To analyse Materials and understand Structure. 4. To familiarize students with various applications of Crystallography	
Content	**1. Basics of Crystallography** a. The Crystalline state, symmetry elements. b. Lattices, unit cell, crystallographic directions, planes, point groups and symmetry classes. c. The Laue classes, the seven crystal systems, Bravais lattices, space groups and International Tables. d. Description of crystal structures, unit cell projections and atomic coordinates, unit cell content. e. Ionic crystals, molecules and molecular crystals, protein crystals, physical properties of crystals.	No of hours 10
	2. Diffraction of X-rays by Crystals: a. Interaction of X-rays with matter. b. Scattering of X-rays by an electron, atom, atomic scattering factor, temperature factor, scattering by molecule or unit cell. c. Diffraction by crystals, structure factor, Bragg's law, the reflection and the limiting spheres, symmetry in reciprocal space, systematic absences, diffraction intensities. d. Experimental methods in X-ray crystallography: X-ray sources, monochromatization, collimation, and focusing of X-rays.	10
	3. Single Crystal X-ray Diffraction: a. Crystals and their properties: crystallization, growing and choosing crystals, microscopic observation b. Data collection techniques for single crystals, diffractometer geometry, measurement of the integrated intensities, data collection with area detectors, c. Data reduction: Lorentz correction, polarization correction, absorption corrections, radiation damage corrections, relative scaling.	10

	d. Solution and refinement of crystal structures: Wilson plot, the heavy atom method, Direct methods, phase determination procedures, figures of merit, e. Completing and refining the structure: difference Fourier method, least-squares method, absolute configuration. f. Introduction to crystallographic softwares (e.g. APEX 4, Olex2 etc) and IUCr validation of the data (CIF)	
	4. Powder X-ray Diffraction: a. Origin of powder diffraction pattern, position, shape, and intensity of powder diffraction peaks. b. Powder diffractometry: beam conditioning, goniometer design, nonambient powder diffractometry. c. Collecting quality powder diffraction data: sample preparation, data acquisition, quality of data, data processing. d. Determination of unit cell: indexing methods. e. Introduction to the Rietveld method. d. Introduction to powder diffraction softwares for indexing, unit cell refinement (e.g. Winplotr, UnitCell).	10
	5. Applications of Crystallography: a. Chemistry and Materials science: understanding crystal structures of compounds, alloys, metals, polymers, phase transitions etc. b. Geology, mineralogy, gemology. c. Pharmaceuticals: polymorphs, excipient analysis, active pharmaceutical ingredients. d. Forensics and environmental analysis. e. Nano materials characterization. f. Biomolecules: determination of structures of proteins, nucleic acids and other biological macromolecules. g. Other diffraction techniques: neutron diffraction, thin film, microstructure properties, pair distribution function analysis, etc.	10
	6. Analysis of Materials and Structural Understanding: a. Characterisation of Solids using diffraction techniques. b. Introduction to databases: powder diffraction files, inorganic and organic crystal structure database, protein data bank etc. c. Inspection of crystals/powders with light microscope. d. Visualization of crystal structures using softwares (e.g. Diamond, VESTA). e. Beyond ideal crystals: crystal twins, modulated structures, quasicrystals.	10

Pedagogy	Mainly lectures and tutorials. Seminars / term papers /assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning.
References / Readings	1. M. Milanesio, G. Zanotti, G. Gilli, M. Catti, H. Monaco, G. Ferraris, G. Artioli, P. Gilli, D. Viterbo, C. Giacovazzo - Fundamentals of Crystallography, 3rd Ed., Oxford University Press, 2015. 2. C. Hammond - The Basics of Crystallography and Diffraction (International Union of Crystallography Texts on Crystallography) 4th Ed., Oxford University Press, 2015. 3. R. West, Solid State Chemistry and Its Applications, 2nd Ed.; Wiley, 2022. 4. F. Hoffmann, Introduction to Crystallography, 1st Ed. Springer, 2020. 5. D. Sherwood, Crystals, X-rays and Proteins: Comprehensive Protein Crystallography, 1st Ed. Oxford University Press, 2015. 6. A. Hofmann, S. Clokie, Wilson and Walkers Principles and Techniques of Biochemistry and Molecular Biology, 8th Ed.; Cambridge University Press, 2018. 7. V. Pecharsky and P. Zavalij, Fundamentals of Powder Diffraction and Structural Characterization of Materials, 2nd Ed.; Springer, 2009. 8. R. Young, The Rietveld Method, 1st Ed., Oxford University Press, 1995 9. W. David, K. Shankland, L. McCusker, C. Bärlocher, Structure Determination from Powder Diffraction Data, 1st Ed., Oxford University Press, 2006. 10. B. He, Two-dimensional X-ray Diffraction, 1st Ed., Wiley, 2009. 11. W. Massa, Crystal Structure Determination, 2nd Ed., Springer, 2010. 12. R. Dinnebier, S. Billinge, Powder Diffraction: Theory and Practice, 1st Ed., Royal Society of Chemistry, 2008.
Course Outcome:	1. Student will acquire fundamental concepts of crystallography. 2. Students will gain insights into single crystal and powder X-ray diffraction methods. 3. Students will be able to use X-ray diffraction methods for materials characterization. 4. Students will be able to correlate crystal structure and materials properties