Course Type	Course Code	Name of Course		Т	Р	Credit
DE	NCYD514	Single crystal X-ray diffraction	3	0	0	3

Course Objective

- This course contains the theory and application of single crystal X-ray diffraction technique.
- With this course students will learn the concepts behind the technique and how to solve the structures of small molecules.

Learning Outcomes

At the end of the course students will be able to-

- Gain knowledge about X-ray diffraction technique
- Solve structure of small molecules from diffraction data

Unit	Topics to be Covered	Lecture	Learning Outcome				
NO.		Hours					
1	Introduction, History of single crystal X-	10L	Students will learn the basics of the crystal				
	ray diffraction. Crystal Geometry, The		system.				
	crystalline state, Unit cell, Bravais						
	lattice, Miller indices, symmetry						
	elements and space groups, Hermann-						
	Mauguin Symbolism., Point Groups.						
	Crystals growth, quality, X-rays: origin,	8L	Students will learn how to grow the				
2	properties, safety, X-ray diffraction and		crystals, properties of X-rays.				
	Bragg's Law, Ewald sphere						
3	Reciprocal lattice concept,	7L	Students will learn about space group and				
	determination of space groups, Laue		related topics.				
	pattern, Phase problem, Data reduction.						
4	Structure factor and its significance,	10L	Students will learn how to solve a structure				
	Patterson Fourier synthesis, direct		and theory of it.				
	methods, Isomorphous replacement,		This part will focus on how to refine a				
	of crystal structures R factor		structure to get better results.				
	Difference fourier maps.		_				
5	Treatment of disorder. Introduction to	7L	This topic enables how to resolve disorders.				
	crystallographic softwares.		Different softwares also introduced.				
TOTAL		42					

Text Books:

1. Introduction to X-Ray Structure Determination: A Practical Guide, George H. Stout and Lyle H. Jensen, Wiley-Interscience; 2nd edition (21 June 1989)

Reference Books:

- Crystal Structure Determination, Werner Massa, Robert O. Gould, 2nd Edition, Springer; 2004. Corr. 5th printing 2010 edition, 2010.
- 3. Introduction to macromolecular crystallography, Alexander McPhearson, Wiley-Liss, 2003.
- 4. Crystal structure analysis- A primer, 3rd edn. J. P. Glusker, K. N. Trueblood, Oxford Science Publications, 2010