

X-ray Structure Determination

Overview

X-ray crystallography is a scientific method used to determine the arrangement of atoms of a crystalline solid in three dimensional form. This is also a most favoured technique for structure elucidation of molecules of both chemical and biological interest including structures of proteins and biological macromolecules. The course aims to take a step forward to unravel the mysteries of this fascinating technology.

This course is organized in two modules that should be taken together. The topics in Module A will expose the participants to the entire process of X-ray crystallography including crystal growth and selection, data collection, solution and refinement. In Module B, special techniques and problems in crystallography like disorder, twinning will be emphasized. The topics in the modules include X-ray diffraction, reciprocal lattice, crystal systems, space groups, structure factors, Fourier synthesis, phase problem, refinement by least squares, challenges in crystallographic refinement and publishing crystal data.

Course participants will learn these topics through lectures and hands-on experiments. Also case studies and assignments will be shared to stimulate research motivation of participants.

Modules	A: X-ray structure determination : June 13 - June 19, 2016 B: Special techniques in crystallography : June 20 - June 26, 2016 Number of participants for the course will be limited to fifty.
You Should Attend If...	<ul style="list-style-type: none">▪ You are scientists, engineers and researchers from manufacturing, service and government organizations including R&D laboratories.▪ You are students or faculty from reputed academic institutions and technical institutions.▪ You are technicians interested to learn handling of X-ray diffractometer and applications of single crystal X-ray diffraction studies.
Fees	The participation fees for taking the course is as follows: Participants from abroad : US \$500 Industry/ Research Organizations: Rs. 4000 Academic Institutions: Rs. 2000 The above fees includes all instructional materials, computer use for tutorials and assignments, 24 hour free internet facility. The participants will be provided accommodation on payment basis.

The Faculty



Prof. Ray J. Butcher is a renowned crystallographer and Professor in Inorganic and Structural Chemistry at the Howard University, USA. He received B.Sc. (Hons.) degree in Chemistry in 1968 and a Ph.D. in X-ray Crystallography from the University of Canterbury, New Zealand in 1974. He spent two years (1974-1976) as Instructor at the University of Virginia and further one year as Post-doctoral Fellow (1976-77) at Georgetown University, Washington DC before he joined Howard University as Assistant Professor in 1977, Associate Professor in 1982 and Professor in 1997. In 1997, he received Sigma Xi Visitors Medal for Outstanding Research at the University of Virginia. He served in several places around the world as Visiting Professor, Visiting Scientist, NASA Fellow, Fulbright International Scholar, etc. He has been Co-Editor of Acta Crystallographica, Section E, an International Journal in the field of X-ray Crystallography and also editor of a special issue in 2007. He has been awarded a Fulbright-Nehru Fellow at IIT Bombay during 2009-10 and Visiting Professor at the same place from December 2012 to January 2013. He has rare distinction of publishing more than 1100 research papers covering all aspects of chemistry and biology.



Prof. Sushil Kumar Gupta has been involved in teaching inorganic chemistry since 1991 at Jiwaji University, Gwalior, India. His fields of research include co-ordination compounds of transition metals and organometallic compounds of bulky silyl ligands bearing donor groups. He has published more than 60 research papers in international journals, and orally presented his research findings in a number of conferences held in India and abroad. Fourteen PhD and 12 MPhil candidates have obtained their research degrees under his guidance. He has completed nine research projects with financial support from Indian agencies (DST, CSIR, UGC, DRDO, MPCST), and 3 research projects with support from the Royal Society of Chemistry, UK. He was Commonwealth Academic Staff Fellow at University of Sussex, UK (October 1996-September 1997), JWT Jones Fellow of RSC at University of Sussex, UK (January-April 2001), and Fulbright-Nehru Senior Research Fellow at Howard University, Washington DC, USA (September 2011-April 2012). He has been admitted as Fellow of The Royal Society of Chemistry in 2013. He has also made contributions to school chemistry textbooks of NCERT. He participated in the designing of postgraduate level courses dealing with instrumentation and commercial methods of analyses; environmental chemistry; and chemical sales and marketing management.

Course Coordinator

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