Crystal Structure Determination: Principle and Application

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Overview

Only a little over a century ago X-rays were discovered by Röntgen in 1895.Their first uses were medical. In 1915 Debye, and in the 1920's von Laue and the Braggs (father and son), showed that X-rays can both scatter and absorb X-rays. Amazingly, they can be used to describe the periodic arrays of atoms and molecules in crystals, and elucidate the arrangement of the atoms that gave rise to that particular pattern of scattered X-rays, as detected on photographic film. X-ray absorption is valuable for giving atom-specific analysis data since the energies of X-rays are comparable to electronic binding energies. This course will focus on the scattering phenomenon, or, in other words, X-ray diffraction. The study of this phenomenon is called X-ray crystallography. Major advances in this field have been made possible by advances in computational technology, the adoption of powerful X-ray synchrotron radiation, and replacement of photographic film by digital 2D detectors. More Noble prizes have been awarded for research in this field than in any other—at least 32 to date. The contributions to all areas of chemistry are enormous. During the last 50 years X-ray crystallography has grown to the point that it is considered the most reliable and definitive method for description of molecular structure. This course is designed for students of chemistry who wish to know some of the fundamentals of crystallography as well as the more practical aspects.

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.

2.0 Objectives

The primary objectives of the course are as follows:
i) Exposing the participants to the fundamentals of crystallography

ii) Building in confidence and capability amongst researcher using this powerful tool

iii) Providing exposure to practical problems and their solutions through case studies

iv) Enhancing the capability of the participants for practical applications

v) Updating researcher about various problem solving techniques available

vi) Improving the skills of the researchers towards presentation of the structural data correctly

Modules	**Duration: Nov 29 - Dec 9, 2017**
You Should Attend If…	• You are a chemist or materials scientist interested in recent developments and fundamentals of crystallography. • You are a PhD students/post-doc/faculty working on X-ray structural characterization of small molecules
Fees	The participation fees for taking the course is as follows: **Participants from abroad : US $500** **Industry/ Research Organizations: Rs. 10000** **Faculty: INR 3000** **Academic Institutions: Rs. 1000** The above fee include all instructional materials, tutorials and assignments, 24 hr free internet facility. The participants will be provided with accommodation on payment basis.

The Faculty

Prof. Marilyn M. Olmstead is currently a Professor in the Department of Chemistry at the University of California, Davis (USA). She has been a leading crystallographer and outstanding scientist in the world today. She is elected fellows of both ACS and ACA and has received large number of awards/honors in recognition of her work, some of them are: UCD James H. Meyer Distinguished Achievement Award; ISI Highly Cited Researchers; Academic Federation Excellence in Research Award; UCD Professional Development Award; Administrative and Professional Staff Achievement Award; UCD Faculty Summer Planning Award; UCD Innovative Projects in Teaching Grant; Woodrow Wilson Fellow. She is also elected Members of United States National Committee for Crystallography (2002-2004 and 2013-), Continuing Education Committee of ACA (2002-2005), elected Councilor of Sacramento ACS local section (2008-2010) and President of General Interest Committee, ACA (2010-2011). She has around 850 publications in the high-impact journals (with h-index of 85), and also served in the Editorial Boards of several international Journals such as *Journal of Coordination Chemistry* (2005-2010), *Acta Crystallographica., Section E*. (2001-2011), *Inorganic Chemistry* (1988-1991 and 2003-2005).

Prof. S. P. Rath received his bachelor and masters from the Calcutta University in 1992 and 1994, respectively, and obtained his PhD in 1999 from Indian Association for the Cultivation of Science (IACS), Kolkata. After postdoctoral study at the University of California, Davis, he joined the Department of Chemistry at the IIT Kanpur in December 2004 where he is a full professor since 2014. He is presently Jagdeo N. Gupta & Smt Murti Gupta Chair Professor and also a fellow of the National Academy of Sciences (FNASc). He has published more than 95 papers in the high-impact international journals and guided 10 students for their PhD. He is the recipients of P. K. Kelkar Research Fellowship for young faculty (2009-12), Alexander von Humboldt Fellowship for Experienced Researcher (2012) and Chemical Research Society of India (CRSI) Bronze medal (2014). His current research interests are bioinorganic modeling of multi-heme proteins, binding and activation of small molecules, electron and energy transfer, and probing molecular chirality using Exciton Coupled Circular Dichroism (*ECCD*).

Course Co-ordinator

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