

CSIR-NCL Integrative Skill Initiative

Skill development Course in

X-Ray Crystallography



About the course: X-ray crystallography is the most powerful method for determining accurate crystal structures of small as well as macromolecules. The properties of any crystalline material are very much functions of its crystal structure and internal arrangement of atoms. X-ray diffraction is a sophisticated method to determine crystal structure and related parameters. This course provides a glimpse of how X-ray diffraction can be used to solve various crystallographic problems of both single and poly crystalline materials, starting from an elementary level. In the course, both single crystal and powder X-ray diffraction methods will be covered. After completing the course the candidate will be able to analysis and interpret the diffraction data and will acquire sufficient expertise to solve and refine the crystal structure independently.

Course Content: Introduction to X-ray crystallography, Coordinate systems in crystallography, Crystal symmetry, Point groups, Laue group, Plane groups, space groups, Miller indices, Crystal lattices, X-ray diffraction and Bragg's law, Reciprocal lattice, Scattering factor, Ewald sphere, Friedel's law, Space group determination from diffraction data, Fourier transformation, Electron density equation and map, Structure factor, Thermal parameters, Background theory for data collection, Data reduction, Interpretation of intensity data, The phase problem, Crystal structure solution and refinement, Determination of absolute and relative configuration of chiral crystals, Crystal structure analysis, CIF preparation, validation and deposition to CSD, Data collection using three and four-circle diffractometers, Area detectors, Different methods of crystallization, Crystal selection to structure refinement (hands on training), Introduction to powder diffraction, Indexing powder pattern, Particle size determination, etc.

Course Instructors: Dr. Rajesh G. Gonnade, Dr. Kiran A. Kulkarni and team

Course Code: SDP-NCL09

Duration: 2nd to 20th July, 2018, 3 Weeks

Number of Participants: 20-30

Eligibility: M. Sc., M. Pharm., B. E.,
B. Tech., M. E., M. Tech.

Course Fees:

- **Students:** Rs.15,000/-
 - **Faculties:** Rs. 25,000/-
 - **Industry Participants:** Rs. 50,000/-
- (Fee includes breakfast, tea and lunch)

Accommodation (Three weeks + 2 days):

- **Students:** Rs. 500/-
- **Faculty/Professionals:** Rs. 1000/-

Participants can make payment either by DD or Online Transfer. For details see SDP website

How to Apply

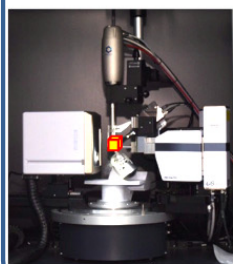
Application form is available at
<http://www.ncl-india.org/files/SDP/Default.aspx>

Mailing Address

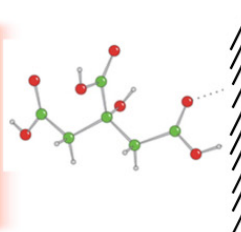
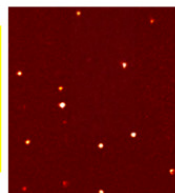
Coordinator,
CSIR-NCL Skill Development Program,
CMC Division, CSIR- National
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Bhabha Road, Pune-411008, India.

Email: ncl.sdte@ncl.res.in
(Application will also be accepted by email)

Single Crystal X-Ray Diffraction Method



Bragg's Law
 $n\lambda = 2d \sin \theta$
X-Ray
single crystal



Powder X-Ray Diffraction Method



Bragg's Law
 $n\lambda = 2d \sin \theta$
X-Ray
polycrystalline material

