

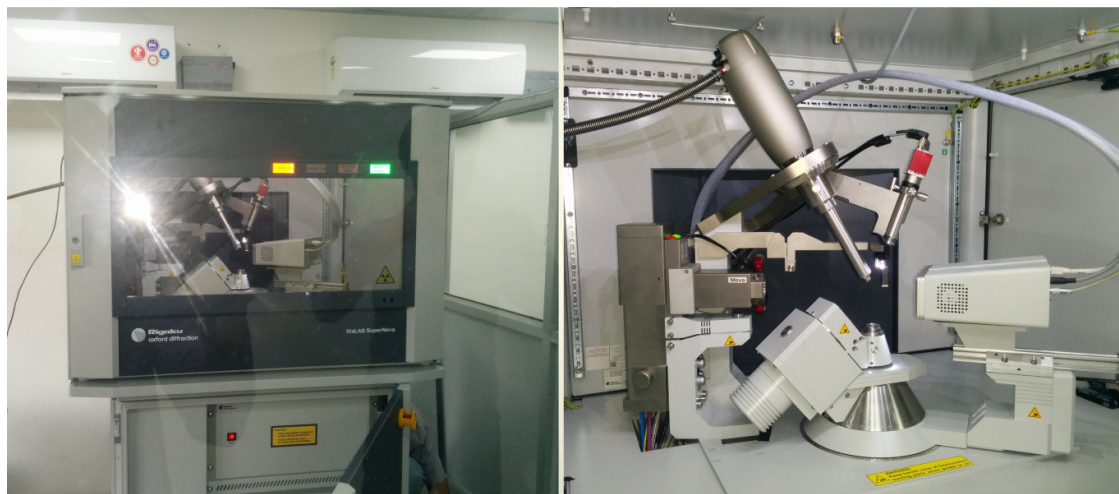
Single Crystal X-ray Facility at PU, Chandigarh

Mission of the Facility

Welcome to the Single Crystal X-ray Diffraction (SCXRD) facility at Department of Chemistry, Panjab University Chandigarh. It was funded by the Department of Science and Technology (DST) under FIST grant. The X-ray facility is primarily available to the faculty members of Panjab University, Chandigarh. External samples from academia and industry are also accepted (see details below). Our services include single-crystal diffraction studies of solid materials of small Organic, Inorganic and Organometallic compounds. The purpose of the facility is to provide X-ray diffraction analysis of the samples and to use it for research and to educate our students in the field of Chemical Crystallography. Please feel free to contact us about your diffraction needs.

Single Crystal X-ray Diffractometer: Description of the Instrument

The SuperNova system for single crystal X-ray diffraction is manufactured by Oxford-Rigaku Analytical X-ray Systems. The system consists of a four-axis KAPPA goniometer module with a HyPix3000 detector with a micro-focus Mo source. For variable temperature data collection (100-500 K), an Oxford Cryosystem 800 series (requires liquid nitrogen) with a dry air unit setup is installed. Both hardware and software are from standard packages supplied with the instrument. The entire system is automated and controlled by a computer based on windows operating system



Services

The X-ray Facility accepts samples for structural analysis from academia as well as from industry. Our SCXRD can handle samples that suffer from small size, solvent loss or twinning. On a regular basis, a course on Chemical Crystallography, which covers theory and provides hands-on trainings on the instruments, is offered.

Sample Submission procedure

Each sample should be accompanied by a submission form (see below) providing the required information and the purpose of crystal structure determination.

Single Crystal - Samples may be submitted in person or by mail. Single crystal samples may be left in a small amount of their mother liquor or in oil.

For our industrial users: A sample testing Agreement that will cover all legal aspects of nondisclosure can be prepared by the requester, if needed. This testing agreement should go to meet top and/or exceed your requirements for non-disclosure, while maintaining Panjab University stature as a non-profit public institution and can be approved by the data recorder with mutual consent.

Terms & conditions for ownership of the Samples and analysis:

- Samples submitted to the X-ray Facility are the proprietary of the investigator and she/he should ensure the quality of crystal for data collection. It may not be possible to return the sample.
- The data obtained by the X-ray Facility that are directly relevant to the sample(s) will be given to the requester upon completion of analysis as indicated in the sample submission form. The results of the data collection will be copied in CD/DVD and will be mailed.
- A compulsory acknowledgement of this DST-FIST facility is needed in all research publication resulting out of using the SCXRD facility of chemistry department of Panjab University.
- The sample analysis charges will be received in favour of **The Chairman, Department of Chemistry** either in form of DD or can be directly deposited to the account **(AC No: 10444977226, IFSC: SBIN0000742)** via online transfer and proof-copy must be attached.

- The sample analysis charges, once received, are non-refundable.
- The data obtained from the data collection, need not always be publishable due to various reasons (poor diffraction, complex twinning, multiple natures of crystals, small satellite crystal sitting on the main crystal, diffuse scattering etc. The data requester cannot assume to get a publishable data in every data collection. No legal or financial matter can be linked with the quality of the data. This condition is assumed to be valid from the requestor once the sample is submitted.
- Preservation of collected data in any form for more than a month, from the date of data collection is not possible at the department. It is the duty of the requestor to preserve the data safely once the data is received from our end.

Charges:

Measurement type	Academic Users		Industry Users	
	Room temp	Low temp	Room temp	Low temp
Optical observation and photography	Rs. 500	----	Rs 1000	
Cell determination	Rs. 1000	Rs. 1500	Rs. 2500	Rs. 3000
Full data collection	Rs. 4000	Rs. 5000	Rs. 8000	Rs. 10,000

For Industry Users

A sample testing agreement that will cover all legal aspect of nondisclosure can be prepared by the requestor. This testing agreement should go to meet top and or exceed your requirements for non-disclosure, while maintaining Panjab University Stature as a non-profit public Institution.

Address for sending samples

The Chairman,

Department of Chemistry, Panjab University Chandigarh

Sector 14, Chandighr-160014

Tel: +91-1722541435, 2534414

Email: chemdept@pu.ac.in

For more information related data analysis, please contact:

Dr Subash Chandra Sahoo

Department of Chemistry, Panjab University

Chandigarh

Ph: 8968718364

Email: subash.chem@gmail.com, scsahoo@pu.ac.in

Request form





Department of Chemistry, Panjab University Chandigarh.
Sector 14, Chandigarh-160014.

Single Crystal Sample Request Form

Name:	Supervisor:
Address:	
Telephone:	Account # :
E-mail:	Date:
Sample Label:	
Chemical Formula:	
Are the crystals air, moisture, light, heat sensitive?	
Color and Shape of the crystals:	
Solvents used in reaction, crystallization:	
Is the sample chiral and a single enantiomer?	
Data collection temperature: RT_____, 100 K_____, other_____	
Indicate your requirement: Unit cell only_____ Full data set_____ Complete solution_____	
What other analytical data (CHN analysis, FTIR, UV-Vis, Mass Spec, etc.) do you have for the sample to support the proposed structure below?	
Is there any specific information needed (non-bonded distances, dihedral angles, stereochemistry, etc.)?	
Proposed Structure with a reaction Scheme (<i>on the reverse side</i>):	
Special hazards and precautions for sample (toxicity, explosion risk, etc.):	
Sample disposition: Save and Return_____ Dispose of after analysis_____	
Signature of Supervisor:	

Notes:

(1) After finding your sample suitable for SCXRD study the requested work will be completed within two weeks from the date of submission if the instrument does not have an issue or additional crystallographic challenges are present. Also, if more than two samples are submitted from a supervisor on the same date it will take longer than two weeks for considering your sample.

(2) Please acknowledge the work done by this facility in your publication for **DST-FIST**.

Note: if the sample is not picked up within two weeks from the date of providing

results, it will be discarded automatically.

Please provide proposed structure with a reaction scheme/used conditions etc:

A large, empty rectangular box with a dark blue border, intended for the user to draw a chemical structure, reaction scheme, or reaction conditions.