

Service Crystallography at Advanced Photon Sources

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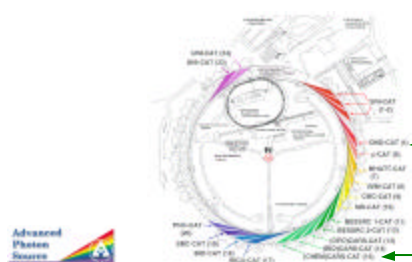
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Synopsis

Synchrotrons are not commonly used for routine small molecule service crystallography due to the additional technical expertise required and logistical problems surrounding their use. This usually means that extremely small crystals are rejected and never measured, despite any significance they might hold. SCrAPS (Service Crystallography at Advanced Photon Sources), is a collaboration directed at addressing this issue and providing academic service crystallographers with access to the specialized instrumentation and tunable / high-brilliance radiation available only at synchrotron sources located at national laboratories. The project involves a cooperative of crystallographers who take turns measuring problematic samples collected from the entire group during time at a participating beamline. The concept of making the high brilliance source at the Argonne National Laboratory (ANL) available for service crystallography was first proposed by Richard Harlow (DuPont) at the St. Paul ACA meeting during the summer of 2000. After assembling interested scientists and attending several orientation sessions, we submitted proposals, obtained beamtime, and successfully collected multiple datasets. In addition, we began work on establishing a communication network to allow for transmission, storage, and remote analysis of large scientific data sets and thus enable researchers to remotely take part in the data collection process and collaborate via the internet to process data. Ideally suited for these tasks is the project XPort described below.

Participating Crystallographers

John C. Bollinger	Indiana University
Phil Fanwick	Purdue University
James C. Fettingner	University of Maryland
Stephen Geib	University of Pittsburgh
John C. Huffman	Indiana University
Kianosh Huffman	Indiana University
Jeanette A. Krause-Bauer	University of Cincinnati
Xaing Ouyang	Texas A&M University
Maren Pink	Indiana University
Nigam Rath	University of Missouri
Ewa Skrzypczak-Jankun	University of Toledo
Charlotte Stern	Northwestern University
Dale Swenson	University of Iowa
Don Ward	Michigan State University
Victor G. Young Jr.	University of Minnesota



Why synchrotron radiation for small molecule crystallography?

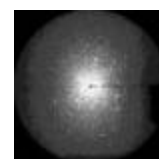
Synchrotrons deliver tunable high-intensity X-ray beams with a very low divergence. This allows for measuring micro crystals that cannot be studied at laboratory sources at all and at reasonably short exposure times. Advantages of interest are:

- High photon flux for micro-crystals (<math><1 \mu\text{m}</math>)
- Tunable energy for special experiments and to circumvent absorption problems
- Shorter exposure times reduce 'dark current' noise in detectors and for time-dependent studies

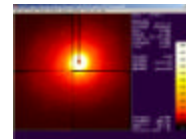
Participating Beamlines

DND-CAT, under the direction of John P. Quintana, is shared between Dow, DuPont, and Northwestern U.

In addition to their industrial and academic projects, DND-CAT provides part of the beamtime to independent investigators and has agreed to a collaboration with SCrAPS for small molecule data collection. In this way data have already been collected during three separate runs. We have also installed an XPort server on premises and are currently engaged in trials to test collaboration tools and data transfer.

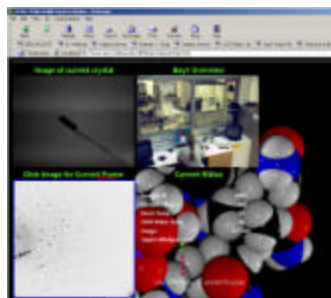


ChemMatCARS is directed by Jim Viccaro (U. of Chicago) and was established as a beamline for the study of surface and interfacial properties of liquids and solids as well as their bulk structure at atomic, molecular and mesoscopic length scales using single



(micro)crystal diffraction, surface-sensitive X-ray scattering, and small and wide-angle X-ray scattering. Viccaro has agreed to work with SCrAPS in providing beam-time for small molecule crystallographers (on a proposal basis from the user cooperative). Under the guidance of Victor G. Young and during commission time of the beamline, numerous data sets have been collected and results published.

XPort for Communication and Data Transfer



The XPort project (X-ray Portal) is a set of grid-based collaborative tools for real-time data acquisition, reduction and visualization for X-ray crystallography. XPort addresses the issue of remote instrument access, as well as Internet based collaboration tools for researchers working with crystallographic data. The project is designed to allow "same as being there" access to the remote instrument by having a variety of video and audio capabilities, as well as remote data access. Additional information on the XPort project is available at, <http://www.cs.indiana.edu/ngi/> and http://www.iumsc.indiana.edu/XPort/video_systems.htm. Xport is developed in collaboration with the IU school of informatics, the Computer Science Department, UIITS, and MCS at Argonne.

