PXRD Usage Policy and Fee System

Date modified: Oct 28, 2021

General Information

The Chemistry Department X-Ray Facility is located in MACN-351 (instrumental room) and MACN-341 (computer room). Established in Spring 2011, it currently includes a single crystal diffractometer (SuperNova), a powder diffractometer (PANalytical Empyrean, "Panda"), and an X-ray fluorescent spectrometer (PANalytical Zetium, “Zeus”).

Manager: Dr. Katherine (Kate) Marczenko, SSC-2503, x53721
Director: Prof. Dmitriy Soldatov, MACN-338, x53548
Advisor: Prof. Kathryn Preuss, MACN-335, x56711
Advisor: Prof. Emily Chiang, THRN-3507, x58217

The X-Lab Facility has a website accessible at https://uogxlab.uoguelph.ca/.

Access to the Facility

The powder diffractometer is part of a fee-based multiuser facility. Researchers can gain access to the Facility rooms and be permitted to use the instrumentation after taking the University X-ray Safety training course (provided by EHS), on-site instruction session to the X-Lab Facility (arranged by the Manager), and the instrument operation training (includes one-on-one training session with the Manager and a score of 75% or higher on an instrument-specific quiz).

Researchers with access to the instrument and/or other equipment are referred to as Users. They should obey the rules existing within the Facility and introduced to them during training, including those for switching the instrument between working and stand-by regimes, changing sample stages, using and cleaning workspace, and storing samples.

Users must register with the Manager (K. Marczenko, see contacts above). Non-faculty registered users may only use the powder diffractometer for experiments approved by their faculty supervisor. Any non-standard experiments should be discussed with, and approved by, the Manager.

Users are only allowed to operate the equipment within the rooms to which they were given permission to operate. Undergraduate students should typically be supervised by a designated senior user, research supervisor, or the Manager. Non-registered users can visit the Facility only as observers accompanied by a registered user, with an approval from the Manager.

Access to the instrument and to the Facility rooms may be withdrawn any time from individual users on the Director or Manager's discretion, and the user's supervisor may become responsible in case of damage to the equipment or to the data security.

Fee and Scheduling System

Current fees are shown below; more details can be obtained from the Manager. The fee system and fee amounts may be adjusted periodically to account for changing needs, the number of users, and availability of the instrument. The collected fees will be used to cover the cost of everyday needs of the Facility (tools, consumables, minor repairs).

Registered users will book time on the instrument through the Skedda X-lab booking system (https://uogxlab.skedda.com/booking). You will only be able to book time after you have been designated as a trained user.

Instrument time can be booked in half hour increments, 24 hours a day. It is the responsibility of the user to book time in advance, and to unbook it in advance if they no longer need the time. Past slots cannot be unbooked. Booked time will be subjected to fees, regardless of actual usage. Regardless of booking, the users must make a record in the logbook each time they used the instrument.

The fee schedule for Panalytical Empyrean is included below.

	Department of Chemistry	Other Academic	Industry
Training	$40/person	$50/person	NA
Data Collection by user	$10/hr	$15/hr	NA
Data Collection by Facility Manager	$15/hr	$20/hr	$40
Variable Temperature	$20/hr + $30 service fee	$30/hr + $30 service fee	$100/hr + $30 service fee
Service (data interpretation, report writing, etc.)	$30/hr	$40/hr	$100/hr

Notes: Minimum charge of $10 will apply even if data collection time was less than 1 hour. 12-hour PXRD data collection for Department of Chemistry users: $100. All fees are subject to change.

Acknowledgements

The usage of the Chemistry Department X-Ray Facility must be acknowledged in any publication (and optionally in conference presentations) whenever data obtained on the diffractometer are reported or used to support other results. For more details, please refer to the X-Lab Authorship Policy.

Examples of statements in a publication:

"**Experimental:** Powder X-ray diffraction data were collected on a PANalytical Empyrean diffractometer in a reflection geometry with Ni-filtered Cu*K*α radiation source and PIXcel1D linear detector. The diffractograms were recorder in the 5 – 40° 2θ range for a ground sample in a spinning holder. The data were collected and processed using the Data Collector[1] and HighScore Plus (version 4.1)[2] software."

"**Acknowledgements:** Powder XRD data were collected at the Chemistry Department X-Ray Diffraction Facility, University of Guelph."

[1] *X'pert Data Collector Software*, version 5.3; PANalytical B.V.: Almelo, The Netherlands, 2014.
[2] Degen, T.; Sadki, M.; Bron, E.; König, U.; Nénert, G. *Powder Diffr.* **2014**, *29*, S13-S18