18 June 2018

PXRD Usage Policy and Fee System

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).

Director: Dmitriy Soldatov, MACN-338 or 122, x53548
Manager: Grzegorz Szymanski, MACN-120, x53495
Advisor: Kathryn Preuss, MACN-335, x56711
Advisor: Emily Chiang, THRN-3507, x58217

Access to the Facility

The powder diffractometer will become a fee-based multiuser facility for a trial period starting from May 2018. Researchers can be granted access to the Facility rooms and permitted to use the instrumentation after taking the University X-ray Safety training course (provided by EHS), on-site instruction session (arranged by the Manager), and the instrument operation training (provided by a qualified person assigned).

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 (G Szymanski, 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 Director. Measurements for outside users cannot be conducted without consulting first with the Director and obtaining his permission (different fees will apply in this case).

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, the Manager, or the Director. Non-registered users can visit the Facility only as observers accompanied by a registered user, with an approval from the Manager or the Director.

Access to the instrument and to the Facility rooms may be withdrawn any time from individual users on the Director or Manager's discretion, and the user's supervisor may become responsible in case of damage to the equipment or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

For the trial period, low fees will be set to allow new users to get familiar with the powder diffractometer and to determine the number of potential users. Current fees can be obtained from the Manager or the Director. In the future, 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 a booking system accessible from the Departmental webpage:

http://www.chemistry.uoguelph.ca/cgi-bin/uschedule.exe?ac=v_login

or from the X-Ray Facility webpage:

http://www.chemistry.uoguelph.ca/soldatov/lab_x-lab.html

Instrument time can be booked in half hour increments from 9 am to 6 pm, as well as for overnight periods for long-term program-controlled experiments.

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.

During the periods of instrument service or break-downs, the scheduling system will be made inaccessible. Users can enquire with the Manager or the Director on the status and availability of the instrument in the near future.

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. The Facility Personnel or other people assisted in an experiment may be acknowledged in case extensive help was received during the data acquisition and/or processing.

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 CuK_α radiation source and PIXcel^{1D} linear detector. The diffractograms were recorder in the 5 – 40^o 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.