**X-ray Diffraction (XRD) Facility**

**Access and training:**

1. Training will be provided for all PXRD instruments. Requests for SCXRD training will be evaluated on a case-by-case basis.
2. The trainee must submit the registration form, see below, signed by the research supervisor.
3. Training is provided by the facility manager only.
4. Training is scheduled with the facility manager and trainees can provide training samples for this purpose.
5. It is the trainees’ responsibility to acquire basic knowledge of XRD before the training.
6. Once the training requirements have been fulfilled, the user will be granted access to the online booking system (<https://faces.ccrc.uga.edu>) and will be able to carry the experiments independently.
7. Trained users are NOT allowed to train other users. Violation of this rule will result in loss of access to the facility.
8. For external users, the facility working hours are from 8:00 am to 6:00 pm, Monday to Friday.
9. The facility manager must be informed of any cancellations for a scheduled session.

**Safety rules:**

1. All users are expected to wear personal protective equipment (lab coat, gloves, and goggles) and follow Departmental and University regulations (mcgill.ca/ehs). WHMIS training certification is required before any work in the XRD facility.
2. Never bypass any safety interlock on the XRD machines. Violation of this rule will result in loss of access and usage of the facility and charges will be made for any damage.
3. Users must maintain a clean and tidy lab environment during and after usage of the facility.
4. Please report any hazardous situation (such as a water leak) to the facility manager or McGill security immediately.
5. The XRD facility is NOT liable for any injury acquired in the XRD facility. All users should obtain appropriate safety training prior to using the facility.

**Facility rules**

1. Users must record the number of samples and the starting and ending times of their experiments in the logbook.
2. The user and supervisor/PI will be held responsible for repairing damage resulting from improper operation of the instruments.
3. It is every user’s responsibility to report directly to the facility manager any abnormal status of the XRD instruments. Users are not allowed under any circumstances to attempt to adjust or repair the instruments.

**Agreement:** I have read, understood and agree to comply with the terms and conditions

Date: Users name: Signature:

Date: Supervisor/PI name: Signature:

**Training Form/non-routine measurements**

**for Powder X-ray Diffraction (PXRD)**

Date: FOAPAL:

**Supervisor/PI’s information:**

Name: Phone:

Email: Signature:

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**Personal Information of the user**:

Name: E-mail:

Room Number & Building: Department:

Group: Signature:

Tel.:

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**Compound Details for non-routine measurements (for submission samples only)**:

Sample name/Empirical Molecular formula:

Type of measurement: hot-stage/capillary:

Name of the sample(s):

comments:

Contact the crystallographer(s)/manager for more information about the general experiment for this technique, user fees, or general discussion.

**Sample Submission Form for SCXRD**

Date: FOAPAL:

**Supervisor/PI’s information:**

Name: Phone:

Email: Signature:

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**Personal submitting the sample**:

Name: E-mail:

Room Number & Building: Department:

Tel.: Signature:

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**Compound Details**:

Sample Empirical Molecular formula:

Color and shape of the crystal:

Air-stable /air-sensitive; Moisture sensitive: Yes/No; Sensitive to solvent loss: Yes/No

Other characterization methods used: NMR; MS; IR; TGA

Solvents used in the reaction or during crystallization:

Preferred Temperature of Analysis

**Sketch of anticipated structure and any preferred atom labeling scheme:**

Contact the crystallographer(s)/manager for more information about the general experiment for this technique, user fees, or general discussion.

**SCXRD rates:\***

|  |  |  |  |
| --- | --- | --- | --- |
|  | Department of Chemistry | Other Academic Researchers | Industry |
| Determination of unit cell | $20 | $30 | $80 |
| Data collection | $120 | $200 | $500 |
| Full structural determination\*\* | $200 | $300 | $800 |
| Non-routine structural determination | $350 | $400 | Contact facility manager |
| Service (data interpretation, report writing, etc.) | $30/hr | $40/hr | $100/hr |

\* Data collection and structure determination charges on SCXRD will be applied regardless of the sample composition (e.g. starting material etc).

\*\* Additional charges are possible for non-routine structural determination (difficult cases of structure determination and refinement require considerable extra time and effort to analyze the sample. Weakly diffracting materials, twinning, air-sensitive crystals, or crystals with highly disordered fragments and high-solvent content often belong to this category). The users will be contacted by the facility manager.

**PXRD rates:**

|  |  |  |  |
| --- | --- | --- | --- |
|  | Department of Chemistry\* | Other Academic Researchers | Industry |
| Training | $50 | $50 | N/A |
| Data collection by user | $15/hr | $25/hr | N/A |
| Data collection by facility manager | $30/hr | $45/hr | $80/hr |
| Setup for data collection by facility manager | N/A | N/A | $20 |
| Variable Temperature PXRD | $20/hr +  $30 service fee | $30/hr +  $50 service fee | $120/hr +  $100 service fee |
| Service (eg. data collection by facility manager) | $30/hr | $45/hr | $100/hr |

\* long acquisition can be applied for Department of Chemistry only at rate of $100 / 12 hr