

X-ray Crystallographic Facility Sample Submission Form

**X-ray Crystallographic Facility
Department of Chemistry, University of Rochester
B14 Hutchison Hall, 120 Trustee Road
Rochester, NY 14627
(585) 273-4715**

Chemist's Information

Name: _____ Phone: _____
Email: _____ Adviser: _____
Billing Account Number: _____
Billing Contact Address: _____

Sample Information

Sample Name: _____ Formula: _____
Crystal Growth Temperature: _____ °C Color: _____ Shape: _____
All Solvents Used: _____
Sensitivities: ☐ Oxygen ☐ Water ☐ Shock ☐ Temperature _____ °C (melts / decomposes)
Special Handling: _____

Proposed Structure (with labeled atoms if you have a preference):

Possible Impurities (starting materials, etc.):

Upon completion of the structural analysis, the submitter receives a CIF (crystallographic information file) for journal and database submission and a full report file with diagrams.

Samples will not be returned unless requested so at the time of submission.

Experimental Data

[FOR INTERNAL USE ONLY]

Submission Information

XCF Code: _____
Received: _____ Collected: _____ Completed: _____ Billed: _____

Initial Data

Color: _____ Cell ($\text{\AA}$, $^\circ$): a : _____ α : _____ Volume ($\text{\AA}^3$): _____
Shape: _____ b : _____ β : _____ Reflections: _____
Size (mm): _____ x _____ x _____ c : _____ γ : _____ Centering: _____

Collection Parameters

Detector Distance (cm): _____ Frame Time (s): _____ Total Time (hr): _____
Temperature ($^\circ\text{C}$): _____ Scan Scenario: _____
Frame Width ($^\circ$): _____

Data Manipulation, Solution, Refinement, and Results

Integration Resolution ($\text{\AA}$): _____ Solution Program: _____ ☐ Patterson
Transmission Maximum: _____ Space Group: _____ (Number: _____)
Transmission Minimum: _____
Final Cell ($\text{\AA}$, $^\circ$): a : _____ α : _____ Volume ($\text{\AA}^3$): _____
 b : _____ β : _____ Reflections: _____
 c : _____ γ : _____
Refinement Final Resolution ($\text{\AA}$): _____ Bond Precision, C—C ($\text{\AA}$): _____
Reflections (Total): _____ (Unique): _____ (Observed): _____ [Flack: _____]
Parameters: _____ Restraints: _____ Data-to-Parameter Ratio: _____ [Friedel pairs: _____]
 R (internal): _____ $R1$ (observed): _____ $R1$ (all data): _____
GooF: _____ $wR2$ (observed): _____ $wR2$ (all data): _____
[Twin Law: _____ Twin Description: _____]
[Reflections (Component 1): _____ (Component 2): _____ (Both): _____]
[Twin Mass Ratio: _____]