

X-ray Crystallographic Laboratory Sample Submission Form
192 Kolthoff Hall, Chemistry Department, The University of Minnesota

Please complete **all** requested information in shaded boxes and provide a labeled molecular drawing!

Adviser: _____	Telephone: _____	Email: _____
Student: _____	Telephone: _____	Email: _____
Address if not UM Chemistry: _____		
UM CUFS/EFS number/PO number: _____		
Service: <input type="checkbox"/> Single crystal, \$250 (\$364 External Univ., \$1200 Non-Univ);		
<input type="checkbox"/> Twin surcharge, \$100; <input type="checkbox"/> Unit Cell, \$50; <input type="checkbox"/> CSD check, \$25.00 (revised 02/17/2016)		

Sample name: _____
Empirical formula: _____ Sample Location: <input type="checkbox"/> Call <input type="checkbox"/> Refrigerator
Temperature (°C): <input type="checkbox"/> 25, <input type="checkbox"/> 0, <input type="checkbox"/> -50, <input type="checkbox"/> -100 (usual), <input type="checkbox"/> _____ Container: <input type="checkbox"/> Tube <input type="checkbox"/> Vial <input type="checkbox"/> Flask
List all solvents used in crystal preparation: _____
Sample stability: <input type="checkbox"/> Stable in open container at 25 °C <input type="checkbox"/> Loses solvent* <input type="checkbox"/> Air sensitive <input type="checkbox"/> Water sensitive
Special instructions or precautions: _____
*Please supply crystals in the mother liquor

Crystal Data

Cell	Initial	Final	Lattice	Centering	Other information
a, (Å)	= _____	_____	<input type="checkbox"/> Triclinic	<input type="checkbox"/> P	Color = _____
b, (Å)	= _____	_____	<input type="checkbox"/> Monoclinic	<input type="checkbox"/> A	Shape = _____
c, (Å)	= _____	_____	<input type="checkbox"/> Orthorhombic	<input type="checkbox"/> B	Size (max, mm) = _____
α, (°)	= _____	_____	<input type="checkbox"/> Tetragonal	<input type="checkbox"/> C	Size (mid, mm) = _____
β, (°)	= _____	_____	<input type="checkbox"/> Trigonal	<input type="checkbox"/> F	Size (min, mm) = _____
γ, (°)	= _____	_____	<input type="checkbox"/> Hexagonal	<input type="checkbox"/> R	Quality (1 - 5) = _____
V, (Å ³)	= _____	_____	<input type="checkbox"/> Cubic	<input type="checkbox"/> I	Temperature (°C) = _____
Refls.	= _____	_____	<input type="checkbox"/> Supercell	<input type="checkbox"/> Notes: _____	
Faces:	_____				

Data Collection

Instrument: <input type="checkbox"/> APEX-II(Mo) <input type="checkbox"/> PHOTON-II(Cu) Operator: _____ XCL Code: 16
Detector (cm) _____ Frame time (sec.) _____ Reciprocal space collection: <input type="checkbox"/> Random <input type="checkbox"/> Astro set
X center (pixels) _____ Frame width (°) _____ <input type="checkbox"/> Quadrant <input type="checkbox"/> Hemisphere <input type="checkbox"/> Sphere <input type="checkbox"/> Repeat set
Y center (pixels) _____ Collection (hrs.) _____ Notes: _____

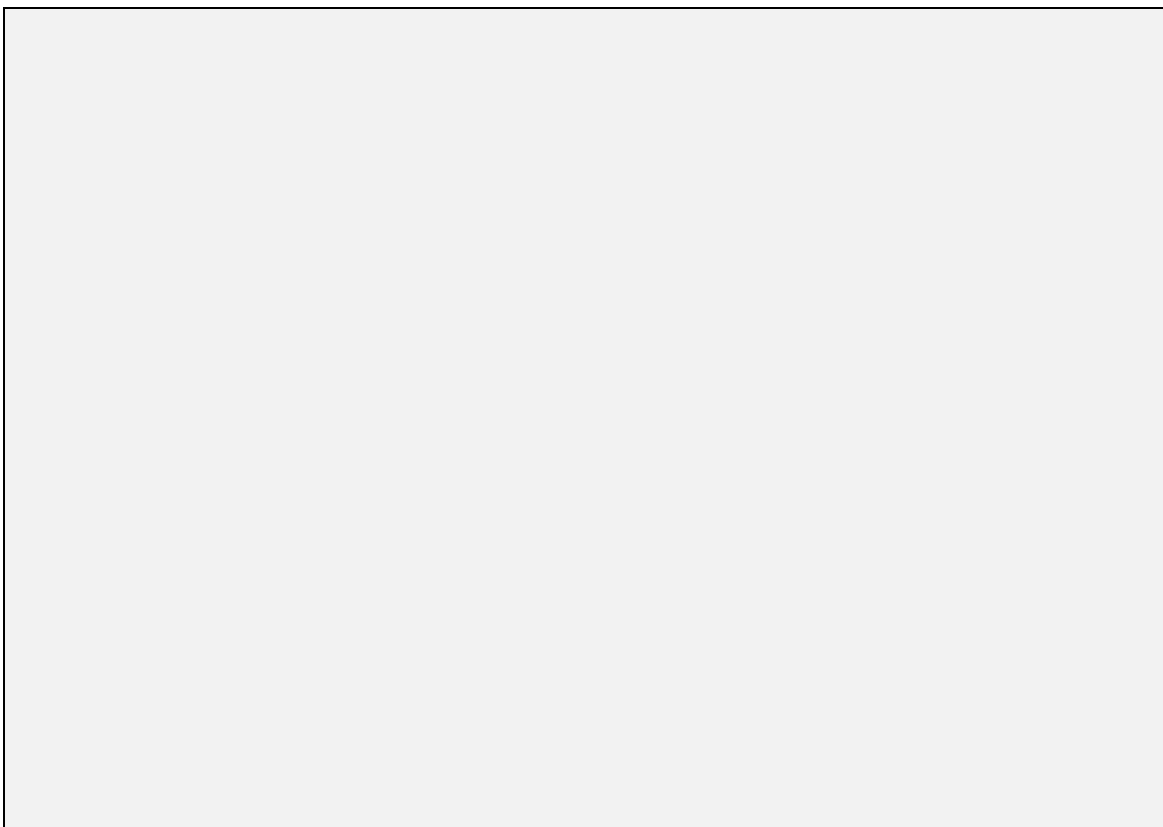
Results

Decay (%) _____	R(int) _____	Absorption correction: <input type="checkbox"/> Empirical <input type="checkbox"/> Face-indexed
Total refls. _____	Refls. F > 4σ(F) _____	Trans. min. _____ Trans. max. _____
Data resolution (Å): _____	<input type="checkbox"/> 0.84 <input type="checkbox"/> 0.77 <input type="checkbox"/> Other _____	Space group _____ (no. _____)
RI _____	wR ² _____	Goof _____ Flack parameter _____
Parameters _____	Restraints _____	Notes: _____

Sample History Record

Sample submitted on	(/ / 2016)	Applicable codes: _____
Sample initiated on	(/ / 2016)	Abandoned, Completed, Data only, Known, Publishable,
Report completed on	(/ / 2016)	Questionable, Supercell, Twinned, Unpublishable
Work billed on	(/ / 2016)	Notes: _____

The following panel is provided for a **labeled** molecular drawing. Please label all atoms with a four character maximum length. If no labeling scheme is specified the crystallographer will assign one. Requests to change the labeling scheme after the report is complete will cost an additional \$50.



Notes:

Policies:

1) Clients of our facility are encouraged to arrange that CIF (crystallographic information file) and SFT (structure factor table) files be transferred to their local computers for future publications. Most journals **require** CIF files currently and all will likely require them in the near future. CIF files are compact and can be transferred by email easily. If email is not convenient, the CIF file can be written on a 3.5" DOS formatted disk, but the requester must supply a new, formatted disk with his sample.

2) The generation of chemical waste from off-site submissions is a serious problem for the XCL. Samples with up to 5 ml of solvent are acceptable. Should a sample exceed this volume, the XCL must be contacted first and the requester may be required to arrange return shipment of these materials in advance. All leftover materials will be returned via mail.