X-ray Crystallographic Laboratory Sample Submission Form
S146 Kolthoff Hall, Chemistry Department, The University of Minnesota

Please fill in the shaded boxes, including a labeled molecular drawing (on reverse).

Research Advisor: _____ *Telephone:*_____ *Email:*_____
Chemist (if different): _____ *Telephone:*_____ *Email:*_____
Address if not UM Chemistry: _____
UM fund number / PO number: _____ *Billing contact person:*_____
Request: ☐*Single crystal, $261 ($364 External University, $800 Non-University);*
☐*Unit cell only, $57.50;* ☐*CSD check, $25;*
{☐*Twin surcharge, $111.75 ($265 Non-University)}* *(revised 01/04/2005)*

Sample name / code: _____
Molecular formula: _____
Collection Temperature (°C):☐*Room temperature,* ☐*-100 (usual), Other* ☐ _____
Container: ☐*Tube* ☐*Vial* ☐*Flask* ☐*Other*
*List **all** solvents used in crystal preparation:* _____
Sample stability: ☐*Stable in open container at RT* ☐*Loses solvent** ☐*Air sensitive* ☐*Water sensitive*
*Special instructions or precautions:*_____
**Please supply crystals in the mother liquor*

Crystal Data

Cell	*Initial*	*Final*	*Lattice*	*Centering*	*Other information*
a,(Å)	= _____	_____	☐ *Triclinic*	☐*P*	*Color =* _____
b,(Å)	= _____	_____	☐ *Monoclinic*	☐*A*	*Shape =* _____
c,(Å)	= _____	_____	☐ *Orthorhombic*	☐*B*	*Size (max,mm)=* _____
α,(°)	= _____	_____	☐ *Tetragonal*	☐*C*	*Size (mid,mm) =* _____
β,(°)	= _____	_____	☐ *Trigonal*	☐*F*	*Size (min,mm) =* _____
γ,(°)	= _____	_____	☐ *Hexagonal*	☐*R*	*Quality (1 - 5) =* _____
V,(Å³)	= _____	_____	☐ *Cubic*	☐*I*	*Temperature (°C) =* ____
Refls.	= _____	_____	☐ *Supercell*	☐*Notes:* _____	

Faces: _____

Data Collection

Instrument: ☐*Siemens* ☐*Bruker* *Operator:* _____ *XCL Code:* 05

Detector (cm) _____ *Frame time (sec.)* _____ *Reciprocal space collection:* ☐*Random* ☐*Other*
X center (pixels) _____ *Frame width (°)* _____ *Coverage:* ☐*Hemisphere* ☐*Sphere* ☐*Other*
Y center (pixels) _____ *Collection (hrs.)* _____ *Notes:* _____

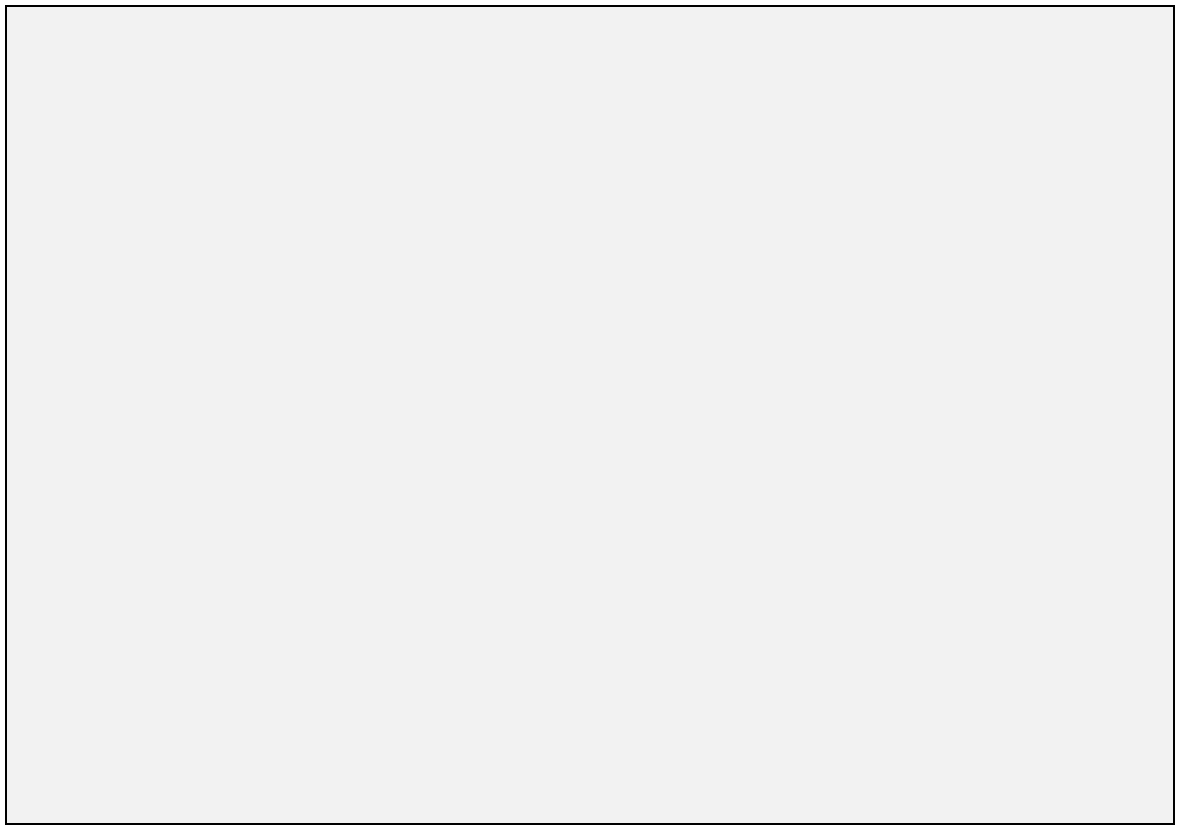
Results

Decay (%) _____ *R(int)* _____ *Absorption correction:* ☐*Multi-scan* ☐*None* ☐*Other*
Total refls. _____ *Refls. F>4σ(F)* _____ *Trans. min.* _____ *Trans. max.* _____
Space group _____ *(no. ___)* *Solution method:* ☐*Direct* ☐*Patterson* ☐*Other*
R1 _____ *wR²* _____ *Goof* _____ *Resolution (Å):* ☐*0.84* ☐*0.77* ☐*Other* _____
Parameters _____ *Restraints* _____ *Flack parameter* _____ *Notes:* _____

Sample History Record

Sample submitted on *(/ / 2005)* *Applicable codes:*_____
Sample initiated on *(/ / 2005)* ***A**bandoned, **C**ompleted, **D**ata only, **K**nown, **P**ublishable,*
Report completed on *(/ / 2005)* ***Q**uestionable, **S**upercell, **T**winned, **U**npublishable*
Work billed on *(/ / 2005)* *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 has been completed will cost an additional $75.*



Notes:

Policies:

1) Report files are sent as attachments via email unless requested otherwise. These include a CIF (crystallographic information file), which is required by most journals, and a full report with diagrams. Additional diagrams and / or alternative file formats are available upon request.

2) All samples will be disposed of after one month unless specified otherwise.

3) Most submissions are completed within two weeks of receipt of the crystals unless additional crystallographic challenges are present, at which point the crystal submitter will be informed.