Request for Crystal Structure Determination

UM# _____

SUBMITTED ON: _____

User Name: _____

E-mail, *Phone**: _____

Advisor Name: _____

E-mail, *Phone*: _____

Signature: _____

Organization: _____

Department: _____

Address: _____

KFS#, PO#, etc For internal use only

Billing contact: _____

E-mail, *Phone*: _____

Signature: _____

* *Items in italic are optional,* **in bold – mandatory.** For more info check tooltips.

Chemical Formula or possible **Chemical Elements**:

Graphic/Structural Formula:

Privide ◯ on next page or ◯ in the link below:

Solvents *and compounds used in the synthesis:*

Stability *& other relevant properties of samples, etc:*

Unwanted or Desired structures UM#, CCDC#, or Unit Cell(s):

Repeating structure determination for UM#

☐ "Powder" Diffraction Pattern
☐ Unit Cell ONLY, ☐ High precision
☑ Search CCDC, ICSD
☐ Data Collection ONLY
☐ Confirm Preliminary Structure
☐ Confirm Atom Labeling
☑ Full Structure Determination
☑ Full Report + ☐ CheckCIF report
☐ Simulated Precession 2D images

Change only if needed

Radiation	◉ MoK_α	○ CuK_α	○ :	
Resolution d(Å)	◯ 0.8 Å	◯ 0.7 Å	◯ max possible	◯ :
Glove box use:	◉ No	◯ Store only	◯ Mount & Store	◯ :
Special conditions	◉ No	◯ Refrigerator	◯ Freezer	◯ :
Mounting in	◉ Oil (regular)	◯ Fluorinated oil	◯ Air	◯ :
Mounting on	◉ Nylon loop	◯ Glass fiber	◯ Capillary	◯ :
Temperature	◉ [-123°C/150K]	◯ [-153°C/120K]	◯ [-173°C/100K]	◯ :
Unit cell vs Temp.	Start:	End:	Stop:	
	Start:	End:	Stop:	

For XCC use only

Data Collection: Conducted on:

Crystal	Shape: prism		Color: colourless		Size:
Detecor	SDD (mm): 50		2θ°: -31		Total time (h): 8.75
Scan:	Start, °	Step, °	# frames	τ, sec	Positions
ω	-31	-0.36	508	10	φ: 90, 210, 330
φ	0	-0.36	1000	10	ω: -211

Structure Determination. Completed on:

Unit Cell			
Search-match	☐ none	:	
Integration			
Space Group			
Solving	◉ XT, ◯ XS, ◯ XM, ◯ :		
Twinning, type	◉ none, ◯ regular, ◯ split crystal, #twins:		
	◯ mero-, ◯ non-mero-, ◯ pseudo-merohedral		
Absorption	◉ Sadabs, ◯ Twinabs, ◯ Face-index, ◯ none		
	◯ Ellipsoid, ◯ Lamina ( ), ◯ :		
Squeeze	☐ Yes	# electrons:	Vol:
Disorder	☑ none, ☐ tails, ☐ solvent, ☐ WMD, ☐ OD		
Quality	R1:	☐ Publ. ☐ Connect. ☐ Low.res./qual.	
Status			

Peter Y. Zavalij
pzavalij@umd.edu
http://www.chem.umd.edu/facility/xray/

X-ray Crystallographi Center
Deprtment of Chemistry & Biochemistry
Univeristy of Maryland

091 Chemistry Bldg. / College Park, MD 20742
Office: (301)405-1861
Lab: (301)405-3230