

University of Alabama X-ray Diffraction Laboratory
 Shelby Hall 3034, Department of Chemistry and Biochemistry

Single Crystal Submission Form (revised 5-14-2019)

Please carefully fill out one form for each sample and bring your sample(s) to

Dr Fengrui Qu, Shelby Hall 3056, Tel: 205-348-0074

Please **e-mail a copy of this form** to fqu@ua.edu

Sample name/code:	date:
Submitting Person:	e-mail:
	phone:
Research Advisor:	e-mail:

O ₂ Sensitive? (Yes/No. Same below)	Cryst. Solvents:	
Moisture Sensitive?	Solvent Loss Possible?	
Radiation Sensitive?	Expected Sum Formula:	
Temp. Sensitive? Note: Data will be collected at 100K unless otherwise stated.	Expected Moiety Formula:	
Light Sensitive?		
Absolute structure req. (chiral samples)?:	Purity (%) or Elem. Anal.:	
Other Analyses Performed (Please circle): NMR (list which nuclei: _____) IR MS	Other methods: Note: If none done, the sample will be lower priority, unless none of the other methods are applicable. If other methods cannot be used, please list the reason here:	
Has the compound been characterized before by SC XRD? If Yes, please give CSD number or unit cell:	Please circle one Unit Cell only Data collection only Full analysis	
	Potentially useful info, e.g. possible unit cells to look for:	

Continue on next page

Chemdraw Sketch of Synthetic Procedure (include all reagents and solvents used):

Chemdraw Sketch of Proposed Structure

(3D drawing of expected isomer for chiral compounds, include **atom numbering scheme**, or it will be assigned by the crystallographer):

Other Notes:

Continue on next page

Biological Macromolecules Section (all others can skip):

Cryopreservation conditions details if known: _____

Space group if known: _____

Molecular Weight: _____

Location of sample: Attached: Please call for when ready:

Action taken: Crystal do not diffract/diffract poorly: Data set collected:

Unit cell only determined: Data set number: _____

XRD Facility Policies and Procedures: While it is very exciting to see our new XRD instrument finally is here, we do need to stipulate a few rules to ensure a pleasant, smooth and productive use of the instrument.

- 1) Normally the samples are analyzed in the order they come into the queue. Samples will be analyzed on a first come, first served basis, with exceptions made in extenuating circumstances.
- 2) If you need to use the instrument yourself for specialized experiments, please arrange this with Dr. Qu and ensure that all students and PIs are trained prior to using the instrument. Please clean the area after use (including the microscope and benchtop), put away all equipment, and please shut off items once you are done (light bulbs, etc.).
- 3) The sample waits in the queue, not the person. Meaning that multiple samples submitted by the same person on different dates will be analyzed at different times. When each sample gets to the front of the queue it will be analyzed.
- 4) *Please fill out the sample submission forms carefully and diligently.* Other forms of characterization (NMR, IR, MS, etc) should be conducted beforehand. The crystallographer, Dr. Fengrui Qu, has the right to move your samples to the bottom of the queue while waiting for you to fill out the missing information. Oftentimes, the analysis may indicate to you that your synthesis resulted in a different molecule than you first expected, and this may cause you to revise the proposed structure.
- 5) Please only submit the amount of sample you are willing to dispose of. The crystallographer will need use the whole sample in order to do a good job. Do NOT bring all your precious sample if you cannot afford losing all, or it being contaminated. If you need the sample back, please note on the form and talk with me directly in advance.
- 6) Typically, the crystallographer will introduce Paratone to the sample container when transferring the sample out of the container onto the glass slide. So, your sample will be contaminated with Paratone. Only under rare circumstances, and with your special request in advance, I can try my best to avoid Paratone. But there is no guarantee of that.
- 7) Please remember to pick back your sample vials after your sample has been processed.
- 8) Please remember to acknowledge the new Rigaku instrument when you publish and include this information: "We thank NSF CHE MRI 1828078 and UA for the purchase of the single crystal X-Ray diffraction instrument". Please let Drs. Qu and Papish know when the paper is published so we can keep a list of papers that acknowledge the new instrument.