

Instructions For X-ray Data Collection with Shamrock

Summary: This document provides guidance as to cryo-mount and shipping dewar recommendations for optimally utilizing Shamrock Structures CrystalEXPRESS™ data collection service. The document also details information that critically needs be shared with Shamrock Structures before initiation of actual data collection

Details:

Cryo-Mounts

- Magnetic base/caps
 - Hampton Research: http://hamptonresearch.com/product_detail.aspx?cid=24&sid=135&pid=378
 - Preferred:
 - CrystalCap Magnetic ALS (pack of 60): HR4-779
 - Also needed if shipping on canes: CrystalCap Magnetic Vial: HR4-904
 - Acceptable:
 - Any CrystalCap Magnetic or “ALS style” cap, but preferably NOT CrystalCap Copper Magnetic.
- Cryo-loops
 - Preferred:
 - Molecular Dimensions:
http://www.moleculardimensions.com/us/merchant.ihml?new_id=199&step=2
 - Mounted Litholoops: packs of 20 mounted on 18mm microtubes
 - Size according to crystal need.
 - Acceptable:
 - Hampton Mounted CryoLoop™ – 20mm:
http://hamptonresearch.com/product_detail.aspx?cid=24&sid=136&pid=384
 - Size according to crystal need.
 - Hampton Mounted CryoLoop™ – 10mm:
http://hamptonresearch.com/product_detail.aspx?cid=24&sid=136&pid=383
 - Size according to crystal need.
- Assembled Cryomount
 - Preferred:
 - Overall length: “ALS standard” or “18mm” = 22mm from bottom of magnetic cap to center of loop.
 - Mounted Litholoop: insert intact loop assembly into magnetic cap and affix with super glue or 5-minute epoxy (latter is more durable under LN2 temperatures during shipping)
 - Mounted CryoLoop™: snap microtube at pre-notched second notch from bottom (18mm length) and insert into magnetic cap and affix as above.
 - Acceptable:
 - Premounted CrystalCap™ Copper Magnetic ALS HT:
http://hamptonresearch.com/product_detail.aspx?cid=24&sid=152&pid=570
 - Size according to crystal need.

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- Premounted CrystalCap™ HT:
http://hamptonresearch.com/product_detail.aspx?cid=24&sid=152&pid=445
 - Size according to crystal need.

Shipping Dewars:

- Preferred:
 - Dewar: Taylor –Wharton CX100:
<http://www.discountcryo.com/ProductDetails.asp?ProductCode=CX100>
 - Dewar: Taylor-Wharton CXR100:
<http://www.discountcryo.com/ProductDetails.asp?ProductCode=CXR100>
 - Shipping Case for Either above Dewar:
<http://www.discountcryo.com/ProductDetails.asp?ProductCode=CX10%2D8C00>

CRITICAL INFORMATION FOR DATA COLLECTION

- Obtain from Shamrock
 - Shamrock_DataCollectionForm.pdf:
 - “Notebook” or “Experimental Page” that will be filled out by Shamrock for each crystal upon which data were collected.
 - Review form to ensure that sufficient information to meet internal requirements will be recorded: notify Shamrock if other information needs to be recorded.
 - Shamrock_DataSummary.xls:
 - Customer Sample Information and Overall Summary document for experiment
 - Customer fills out the following fields (green highlighted fields on form) and provides back to Shamrock prior to data collection:
 - Protein: protein name or “code” name for sample
 - Customer Cane/Puck Name: the name of the cryo-cane or puck in which the sample resides
 - Customer Cane/Puck Slot: the position on the cane or in the puck in which the sample resides.
 - Compound: Name (usually coded) of compound present in sample unless customer has it otherwise coded sufficiently into the position or “Protein” field name to guarantee customer’s internal records keeping needs.
 - Comments: Any pertinent comments about the crystal. Such information might include:
 - Expected Space Group
 - Expected Unit Cell Constants
 - Go-No Go resolution for data collection: i.e., what is the minimum acceptable resolution to trigger data collection.
 - Any other special instructions.
 - Shamrock fills out the following fields and returns completed form to customer at end of data collection:

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- Comments: replace customer comments in this field with brief description of diffraction quality or pertinent observations about crystal for every sample examined
 - ALL OTHER FIELDS
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- Information that is critical or helpful to Shamrock prior to data collection
 - Go-No Go (minimum) resolution acceptable to trigger data collection for each sample.
 - Any specific data processing preferences:
 - Desired “highest resolution shell” $I/\sigma I$
 - Desired “highest resolution shell” R-merge
 - High-resolution shell cutoff triggered by one or both of the above?
 - High-resolution shell cutoff determined by Shamrock, based upon “expected trends” in the data.
 - Mandated output file names:
 - Typically same as “Data Set” field name from Shamrock_DataSummary.xls
 - Can be coded, sequential name (e.g., x08-103, exp000371, X2008_171) the first of which in the series must be provided by customer.
 - Expected space group and unit cell constants
 - Expectation for twinning, cracking, space group transitions, etc.
 - Shamrock Deliverables
 - Merged intensity, statistical log, and Shamrock_DataCollectionForm.pdf files for each sample for which data are collected.
 - Uploaded for each sample within 15-20 minutes of completion of data collection to S-cubed (Shamrock Secure Server) and available for customer download.
 - S-cubed login procedure, individual secure account, and password provided by Shamrock before data collection initiation.
 - Full data archive copy of all data collected and processing
 - Provided on customer supplied USB2.0 compatible disk as part of sample return shipment.
 - With prior arrangements (and return shipment to Shamrock by customer in a timely fashion), Shamrock can provide a loaner disk of this type.

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