

## Rapid Access for Beamtime on I19

Researchers wishing to run samples via rapid access mode must submit a Rapid Access Proposal using the Diamond UAS system <https://uas.diamond.ac.uk>. Once you are set up, select Create New Proposal at the top of the list of Useful Links on the Home page. Select Rapid from the list of options. Under Science Overview, there is the option download the template for the proposal – please include any relevant space group and unit cell information you already have. The completed form should be saved as a pdf and uploaded and then the remaining sections need to be filled in before submitting the proposal.

*These are guidelines only, and applicants with proposals or experiments that lie outside of these are encouraged to contact I19 beamline staff to discuss their requirements.*

### 1. Arrangements

Samples for successful rapid access proposals will be run when time permits. Therefore, there will not be a call for proposals with set deadlines. Applicants can expect to be informed of the outcome within a week of submission, but successful applicants may only be informed of the date of their beamtime 2 weeks before. Once the visit has been scheduled, please submit the relevant investigators and ERA via the UAS as soon as possible.

**Please Note:** It is not feasible to guarantee that samples will be run at the scheduled time due to the possibility of unforeseen machine or beamline problems. If this occurs, samples that have been allocated time will be run during the next available rapid access period.

### 2. Objectives

Rapid Access Mode is to provide a route for data collection on samples that are timely and of high scientific interest. It is **not** to be used for the routine measurement of samples, for large numbers of samples, or for lengthy experiments – these should be applied for using other access modes.

Currently, it is intended that users will **not** need to visit I19 for rapid access experiments. The samples should be sent to Diamond by post or courier, they will be run by I19 staff and the results made available by remote access.

### 3. Criteria

1. Rapid Access mode is available for academic use only; industrial users should contact the Industrial Liaison Office.
2. Applications will not be accepted from research groups who have scheduled beamtime in the same AP for the same/very similar proposals.
3. As soon as a proposal has been deemed successful, the sample(s) will be scheduled in the next available rapid access slot.
4. The normal maximum number of samples allowed per application is 2. (However, if more than 2 samples are required, please ensure the reasons are very clear.)
5. If possible, up to 3 crystals of each sample should be sent.
6. Only low risk materials (as assessed by the DLS health and safety group) are allowed.
7. All samples received, must be accompanied by data safety sheets and handling information otherwise they will be treated as potentially hazardous waste and disposed of immediately.

8. Samples can be returned if requested, unless the crystals have been sent to Diamond pre-mounted on I19 sample mounts.

All conditions for acceptance of beamtime, by the users, are the same as for other access routes.

#### **4. Safety Considerations**

Full hazard declarations must be included (the ERA) at the time of submission of the proposal and a copy of all relevant MSDS's must be included with the samples sent to DLS.

Generally, only low-risk materials will be accepted for this access mode and samples that can be considered one of the following:

- Radioactive
- Highly reactive, e.g. explosive
- Biohazardous

will only be considered on a case-by-case basis, with special arrangements being made for these exceptions.

#### **5. Data Collection**

A standard data collection protocol will be used:

1. The energy of the X-ray beam will be ~18 keV ( $\lambda = 0.6889 \text{ \AA}$ )
2. Unless otherwise specified, data will be collected at 100 K
3. A sphere of data will be collected – the standard collection should give data complete to ~0.6  $\text{\AA}$  resolution, if the sample is capable.
4. Data may only be collected on the crystal judged to be the “best” for each sample

Once the data has been collected, it will be made available for the user to access remotely for processing etc., please see the guidelines regarding data retrieval sent from the user office. Results should also be available to view in real time via ISPyB: <https://ispyb.diamond.ac.uk>.

See also: <https://www.diamond.ac.uk/Instruments/Crystallography/I19/Manual/EH1/ISPyB>

#### **6. Sample Mounting**

Samples will be stored at room temperature open to the air and, therefore, samples stable to these conditions will be considered first for rapid access beamtime. However, if time permits, more sensitive samples will also be considered.

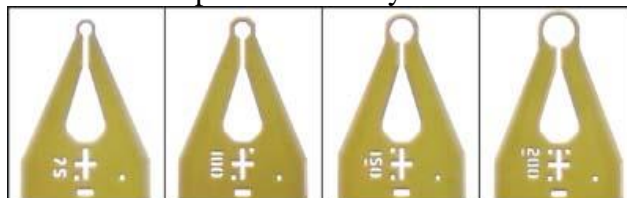
Samples should be delivered to DLS by post or courier (see Section 7 for the postal address). If samples are being shipped in solvents, it is recommended to use a minimum amount of solvent, and to ensure the vial is completely sealed and protected appropriately prior to posting.

For pre-mounted samples, up to 3 crystals of each sample should be sent, covering a variety of sizes, no bigger than 50 x 50 x 50 microns. If more than 3 crystals are sent, it is possible that time constraints will mean only 3 crystals can be screened. For sensitive samples, several crystals should be sent and I19 staff will pick the 3 crystals.

No liability will be accepted by DLS or I19 for any damage to, or loss of, sample during transit or mounting/dismounting onto the instrument.

### 6.1. Air Stable Samples

For air stable samples, crystals should be sent pre-mounted using either MiTeGen loops (<https://www.mitegen.com/product/dual-thickness-micromounts>) or another suitable loop on SPINE (17.6 mm) length pins. The size of the loop should closely match that of the crystal.



A2 assortment: 75, 100, 150 and 200 micrometer apertures



The pins should be glued into cryocaps, e.g.,

It is important to adhere to these guidelines in order for the robot and auto centring software to work. Please contact a member of I19 staff if further details are required.

It is preferable for the user to have their own supply of mounts; if the users own mounts are used, the mounts and samples will be returned. Prepared mounts can be supplied by I19 if required but, in this case, the sample(s) will **not** be returned to the user. If mounts are required, please specify this in the proposal.

The crystal should be mounted within/on the loop because it is difficult to see the crystal if it is not within the loop area. It is recommended that crystals should be glued onto the mount to ensure they remain intact during transit.

If sending pre-mounted crystals please fill in the form (which will be sent once time has been allocated), indicating where the sample is on the loop, and which sample it is.

### 6.2. Sensitive Samples

If the samples are more sensitive, then these can be sent to DLS still contained within their mother liquor in a vial or Schlenk tube, where I19 staff will mount the crystals just before the data collections are carried out. Please try to send the samples in a container with a neck wide enough to accommodate a micro-spatula.

## 7. Rapid Access Postal Address

All prepared samples must be packaged appropriately and sent in advance to:

Dr. Sarah Barnett  
Beamline I19 - Rapid Access Facility  
Diamond Light Source  
Harwell Science & Innovation Campus  
Didcot  
Oxfordshire OX11 0DE  
United Kingdom

If required, please request sample return once the data collections are complete, including the address and contact phone number.

## **8. Important Notes**

Full safety information (MSDS's where appropriate) must be enclosed with all samples.

All samples must arrive at DLS **at least** 3 working days prior to the date of scheduled beamtime.

Delivery/postal arrangements and associated costs are the responsibility of the applicant.

No responsibility is accepted by DLS for the loss or damage of samples in transit.

Samples not conforming to the preparation guidelines will not be run.