

Single Crystal X-ray Diffractometer

Minimum Specification (Mandatory Requirements)

1. Capabilities:

- Dual Source:
- Molybdenum Microfocus X-ray Source and Copper Microfocus X-ray Source.
 - Switching between these sources must be possible for a standard user (e.g. a first year PhD student without a background in crystallography) and should take no more than 10 minutes.
- Must be able to accommodate and measure large samples with a minimum diameter of 100 μm .
- Must be able to switch collimator to allow for:
 - Large sample environments, especially Diamond Anvil Cells. This may require short collimators to be installed.
 - The system must be able to accommodate and measure a Diamond Anvil Cell. Setting up a loaded Diamond Anvil Cell for measurement on the system must be possible for users
 - Different collimator apertures to allow for the measurement of a range of different crystal sizes.
- Switching between collimators must take no more than 30 minutes.
- The system must be able to work as a function of temperature between 300 K and 90 K with an uncertainty of no more than ± 1 K, and a maximum rate of at least 2 K/minute.
- Capable of measuring a full sphere of data on an Ylid sample a resolution of 0.8 \AA and an I/σ value of at least 3 within 1 hour.
- Video camera for modelling crystal shape for use in absorption correction.
- Ability to modify distance between the sample and detector ('detector distance') between at least 40 mm and 135 mm
- Sphere of confusion $< 7 \mu\text{m}$
- Angular resolution:
 - Omega ≤ 0.00125 degrees
 - Theta ≤ 0.00125 degrees
 - Kappa ≤ 0.0025 degrees
 - Phi ≤ 0.005 degrees
- Scanning speed range: 0.005 to 3.0 degrees/second

2. Test Samples:

- 5 test samples (commercially available crystals) will be issued by UKRI, the samples will all be supplied from the same batch and will be screened before being sent
- Request for test crystals must be made to UKRI within 10 calendar days of your registration within Emptoris. Requests must be submitted via the Emptoris e-Sourcing messaging system and clearly state your full organisation details, address, contact name etc
- These samples will be crystals of:
 - Aragonite – Twinned Orthorhombic (often appears hexagonal)
 - Boric Acid – Trigonal planar
 - Sodium Acetate Trihydrate – monoclinic with many hydrogen bonds
 - Vanadinite
 - Cerussite
- A measurement of each of these samples will be taken by the Supplier. During each of these measurements, the whole process from mounting the sample through to data reduction will be recorded in real time.

- All of these recordings will include showing the PC screen to allow determination of the use of software.
- All of these recordings will show the alignments necessary for a good measurement.
- One of these recordings will show the process for starting the system up from being off, showing the system being totally powered up through to data collection and data reduction.

3. System:

- Suitable for constant use at full power for at least 20 days per month
- The goniometer must hold at least 2 Kg
- Air cooled system with no external chillers required for full operation
- Collision detection/avoidance system to prevent goniometer damage
- Maximum size 2 m width, 1.8 m depth, 2.65 m height, not including desk space
- Intuitive controls; intuitiveness of controls will be judged based on video submission from sample tests (see above)
- Calibration needed no more frequently than 6 months and without company engineer.
- Should accommodate standard Huber heads
- Should produce <80dBa accumulated noise from all running equipment

4. Detector Type:

- Area/2D detector,
 - Hybrid Pixel or Charge-Integrating Pixel
- Active area of at least 70 x 70mm²
- Pixel size no larger than 180 x 180 μm²
- At least 18-bit dynamic range
- Adjustable thresholds for XRF suppression
- Free from bloom and flare and streaking and afterglow

5. Support:

- At least 2 years' warranty, including any additional options purchased
- During warranty:
 - Maximum response time for remote support is 24 hours from notification of a fault
 - Maximum on site attendance time of 48 hours from notification of a fault is expected
 - Maximum on site fix time of 4 days after diagnosis is expected.
 - In the event equipment cannot be fixed on site:
 - Expected that it will be fixed and returned within a 2 week timescale.
 - If this is not possible, whether expected to take longer or unexpected delays make the repair take longer than expected, it is expected that a replacement or loan system/demo system can be made to continue operational functionality where possible, free of charge.
- Full & Comprehensive Maintenance, Service & Support coverage for the System. This will be available in the UK and will be for the following 7 years. This must include a help line and email contacts.
- Annual preventative maintenance performed under warranty.
- All spare parts, such as fuses, likely to be needed during the warranty period must be included.
- Cleaning and maintenance of the system must take no longer than 1 hour per week.

- Remote support must be available to help with technical application support for the instrument. A response to the issue raised must be received within 24 hours of the issue with the system being raised.
- Training must take place at the installation site for up to 5 users, with emphasis on both theoretical and practical training.
 - Initial training will be a minimum of 2 day's
 - Further training will be provided for additional options if purchased.

6. IT:

- The system must come with a PC capable of controlling the hardware and suitable for all included hardware and software, allowing full operational functionality for a minimum of two years, assuming constant use at least 20 days per month.
- The system must come with software for processing/integrating/reducing the data.
- There must be provision for the processing of data away from the attached PC and site network. Data must be able to be processed off site.
- The reduced data must be exportable as a format which can be opened by non-proprietary software (.hkl files and associated file types such as .ins files)
- The sample temperature must be controllable through the software, which must be integrated into the control software.
- The system must output a human-readable log file.
- The system must have access to low level systems, such as direct control of the shutter and goniometer motors (such as x, y, z and phi motors), control over the generator including the ramp rate, control over camera position, both in angle and in detector distance and temperature control for the low temperature option.

7. Safety:

- Alarm and safety features compliant with IRR17, with "Safe systems of work" included in documentation and in training sessions. This must include an interlock system to British standard and lights should be clear and unambiguous.
- Train RPS on monthly interlock checks
- Critical exam before acceptance

8. General Environmental Conditions:

- The environment in which the Proposed System will be expected to operate has general environmental conditions which have been estimated as follows:
 - Humidity: 55% RH \pm 10% RH
 - Vibration: There are no known sources of local vibration
 - Temperature: 21°C \pm 3°C
 - Power Spike: There are no known sources of local power spikes/surges

9. Validation:

UKRI reserve the right to arrange a site visit during the standstill period to validate the information submitted before the contract is awarded. If the supplier has incorrectly disclosed information submitted as part of the bid, UKRI reserve the right not to award a contract to that supplier.

Validation shall include but limited to:

- The instrument must demonstrate its capabilities to meet all the requirements
- An acceptance test will be carried out by UKRI at the successful bidders premises, test samples will be provided so measurements can be taken.

List of samples:

- i. Raffinose – a large, twinned crystal
 - ii. Deuterated Prussian Blue - small, moisture sensitive crystal with diffuse scatter and superstructure
 - iii. Benzil – crystal with diffuse scatter
 - iv. ROY – Simple crystal system for absolute structure determination.
 - v. Ce_2PtGe_3 – Crystal with twinning, diffuse scatter and superstructure
- The use of the system to measure the sample, on the time necessary to acquire good quality data, on the maximum data quality obtained in a given time and a specific question for each sample will be validated during the visit:

Five tests will be performed to show case the range of science that UKRI require the system to cover:

- i) Twinning
- ii) Superstructure determination
- iii) Diffuse scatter test
- iv) Absolute structure determination
- v) All of the above (aside from ii)

10. Delivery, Installation and Commissioning:

- Delivery of the instrument must be made by 07/03/19
- Installation and commissioning plan to be proposed and must be completed within 4 weeks from delivery

11. Kick-Off Meeting:

- The successful bidder is required to visit UKRI at Rutherford Appleton Laboratory to review the proposed Operational Room ('Point of Use') to identify any potential causes of concern such as floor loading, dimensions of access route etc. in case any such risk is thus identified, appropriate items (such as Surge Protection System, Anti-Vibration Table, EMF Shielding etc.) should be included as an optional extra
- The successful bidder must assign and provide details of a key contact to discuss any issue (not covered by research confidentiality) and upon further request, be willing to allow STFC representatives to visit their location to observe the Proposed System in operation

12. List of Upgrades and Options (Not a Mandatory Requirement):

Costs provided are for information only and will not be scored as part of this tender. The cost of options are included in the estimated value of this contract, UKRI reserve the right to purchase any of the upgrades/options within this contract:

- High temperature stage/oven
- Low temperature stage (sub 90K)
- Autosampler Stage
- Auto focus goniometer head
- Consumables for 12 month period
- Spare parts to maintain full functionality