

**Institute of Chemical Research of Catalonia Foundation**

**TECHNICAL SPECIFICATIONS FOR THE CONTRACTING, BY OPEN PROCEDURE, SUBJECT TO HARMONIZED REGULATION, OF THE SUPPLY AND INSTALLATION OF A SINGLE-CRYSTAL X-RAY DIFFRACTOMETER FOR THE INSTITUTE OF CHEMICAL RESEARCH OF CATALONIA.**

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# **TECHNICAL SPECIFICATIONS FOR THE CONTRACTING, BY OPEN PROCEDURE, SUBJECT TO HARMONIZED REGULATION, OF THE SUPPLY AND INSTALLATION OF A SINGLE-CRYSTAL X-RAY DIFFRACTOMETER FOR THE INSTITUTE OF CHEMICAL RESEARCH OF CATALONIA.**

## **1. Object of the contract**

The object of this contract is the supply of a complete single crystal X-ray diffraction system for the determination of crystalline and molecular structures. The equipment must have two radiation sources (Cu and Mo), a detector, a goniometer and a crystal cooling system. It must also have an automatic robotic system for screening plates with sample wells in the form of crystalline powder or single crystals. It must also have a workstation and software for the management of the equipment and the processing of the data.

The equipment must be installed in a radiation protection cabin with all the components necessary for the operation of the equipment with the properties described. The main components of the equipment are described in section 2 (technical characteristics).

The purchase is necessary to improve the X-ray Diffraction service and thus provide better quality in the research process of the different groups of ICIQ Researchers.

## **2. Technical characteristics**

The minimum technical characteristics required for the subject of the contract are specified below.

### **2.1. Generalities**

- The equipment subject to the contract must have CE marking.
- The main parts of the equipment must be installed inside a radiation protection cabin.
- The equipment must be approved according to the current ionizing radiation regulations defined by the Spanish Government's Nuclear Safety Council. It should be able to operate in an uncontrolled space.
- It must be able to be installed in a space with dimensions: 250 cm x 250 cm x 250 cm.

### **2.2. X-ray radiation sources:**

- Radiation sources based on high-brightness molybdenum and copper rotating anodes that provide X-rays with wavelengths of 1.54178 Å and 0.71073 Å. The equipment must allow easy and automated switching between copper and molybdenum radiation.

### **2.3. Optics:**

- High flux confocal optical system for copper and molybdenum K $\alpha$  radiation with smart optics for continuous self-alignment of X-ray radiation under optimal conditions.

### **2. 3. Goniometer:**

- Four circle Kappa goniometer.

#### 2.4. Detector:

- Curved hybrid photon counting X-ray detector with a minimum angular resolution of 100°.

#### 2.5. Software and equipment control:

- The equipment must have software that allows the measurement and processing of data from the measured crystals (a minimum of 10 licenses).
- The team must have software that allows refining and processing the single crystal data until obtaining a publishable CIF (a minimum of 10 licenses).
- The equipment must have software that controls the automatic robotic system for screening well plates.
- The equipment must have software with the necessary licenses (a minimum of 10 licenses) that allows the processing of powder diffraction data to obtain publishable level powder diffractograms.
- The equipment must have software that allows Rietveld refinements with the aim of making quantifications, detection limit determinations and structural determinations (resolution and refinement) from powder diffraction data (a minimum of 2 licenses).

#### 2.6. Accessories

- Cryogenic system that allows controlled measurements to be made in the range between -173 °C and 227 °C. This accessory must be redundant and ensure the operation of the measurements at a temperature of -173 °C.
- Automatic robotic system for screening plates with sample wells containing samples in the form of crystalline powder or single crystals.
- If necessary, the equipment must have a refrigerator to cool the generator and other equipment components.

### 3. Equipment Capacity

The bidding company must attach to the technical report the results of the measures requested in sections 3.1 and 3.2.

3.1. The equipment must be capable, using copper and molybdenum radiation, and the conditions described in this section, of measuring a **sucrose single crystal**.

#### Measurement conditions for the single crystal test (3.1):

Sample: Sucrose (monoclinic,  $P2_1$ ). Crystal size: less than 40 µm in any direction or volume less than 0.00007 mm<sup>3</sup>. Mount: MiTeGen MicroLoop or MicroMount double-thickness 50 µm or smaller, so that crystal size can be easily compared to the size of the loop. (A picture of the crystal without the loop, a video of the crystal, and the size of the mount must be provided.)

Objectives of the measure:

- Scanning width of 0.5° per frame.
- Full completeness in space group symmetry down to 0.60 Å (Mo) or 0.81 Å (Cu) resolution.

- Minimum average redundancy of 5 in the spatial group. (Documentation of strategy calculation must be provided.)

Measurement temperature: 100 K

Measurement time (including travel time): 1 h for Mo and 15 min for Cu, or as fast as possible. (This results in exposure times of the order of magnitude of 2 s/0.5° for Mo and 0.05 s/0.5° for Cu.)

Data processing: Standard integration; scaling; numerical and empirical absorption correction; without error model (experimental errors must be maintained to preserve data comparability) and with error model. Structure refinement with SHELXL using standard IAM. Complete meta-final files of data processing must be provided.

3.2. The device must be able to measure a sample of crystalline Cystine powder (orthorhombic phase P212121,  $a \approx 5.32 \text{ \AA}$ ,  $b \approx 12.14 \text{ \AA}$ ,  $c \approx 56.13 \text{ \AA}$ ,  $V 3620 \text{ \AA}^3$ ;  $Z = 8$ ) with molybdenum and copper radiation (one measurement in each radiation) and using a robotic system that gives a peak resolution as close as possible to  $0.05^\circ$  in  $2\theta$ .

#### Measurement conditions for the crystalline powder diffraction test (3.2):

The team must be able to measure a sample of crystalline **Cystine powder** (orthorhombic phase P212121,  $a \approx 5.32 \text{ \AA}$ ,  $b \approx 12.14 \text{ \AA}$ ,  $c \approx 56.13 \text{ \AA}$ ,  $V 3620 \text{ \AA}^3$ ;  $Z = 8$ ) with molybdenum and copper radiation (one measurement in each radiation) and using a robotic system that gives a peak resolution as close as possible to  $0.05^\circ$  in  $2\theta$ . The measurement range will be from  $4^\circ$  to  $40^\circ$  in  $2\theta$ .

## **4. Maintenance and after-sales service**

4.1. The bidding company must have a technical service and applications laboratory, in order to provide adequate technical and scientific support.

4.2 The bidding company must provide remote service to resolve possible doubts about the operation of the equipment, diagnose faults and be able to resolve certain faults.

4.3 The bidder shall submit a formal budget for an annual preventive and corrective maintenance contract covering all equipment and including:

- General equipment review
- Complete cleaning of the equipment
- Change of consumable material
- Labor
- Displacement
- Repair of any equipment failure
- Parts needed for any equipment repair

If you are the successful bidder, this budget will be considered binding throughout the life of the equipment, with the price varying only based on the variation in the CPI.

## **5. Improvements**

The following will be considered as an improvement in the offer:

- Offering complete preventive maintenance of the equipment during the warranty period. Preventive maintenance of the equipment is understood to be a general

inspection and cleaning of the equipment and the replacement of all consumables of the equipment, with travel and labor included.

- Training plan: basic operation of the equipment and advanced options.
- Providing an additional spare anode/tube.

## **6. Interlocutors**

- The successful bidder will appoint a valid interlocutor to resolve issues arising from the general operation of the supply.
- The ICIQ interlocutor will be the person designated for this purpose, belonging to the *Scientific Core Facilities*.

## **7. Warranty period**

Warranty for the entire equipment as a whole: minimum 1 year.

Warranty means the repair of the equipment at no cost as long as the repair is not necessary due to misuse of the equipment.

## **8. Delivery time**

The delivery period is set at a maximum of 24 weeks from the date of the signature of the contract.

## **9. Reducing the environmental impact of supply**

It will be assessed that the awarded company complies with the following environmental criteria:

- That the bidding company has an environmental policy implemented in the company that helps reduce the environmental impact of the supply subject to the contract. If it does, it must be attached.
- The materials used in the packaging, protection and transport of the supplies will preferably be recycled and recyclable or reusable. They will incorporate the prints strictly necessary to carry out the correct identification, traceability and transport of the supply and will not use inks that contain substances harmful to the environment or with metal content. This requirement will have to be proven by means of a responsible declaration prior to transport and may be verified during the supply.
- The unpacking and collection of waste generated during the supply and installation of the equipment will be the responsibility of the successful bidder. The successful bidder will remove the waste from the center and treat it responsibly in accordance with current legislation. This measure will be justified by providing a responsible declaration and, once the service has been carried out, by providing the corresponding identification of the accredited waste company or companies that will be responsible for its management.
- The land transport used during the transport of the supply will be low-emission. This measure will be justified by providing a responsible declaration and, once the service has been carried out, by providing the certification of the transport company

that accredits it or the technical sheet of the vehicle used in the supply where the engine generations and emission levels can be compared.

In the event of offering these measures and ultimately failing to comply with them, the corresponding penalties established in the Specific Clauses will be applied.

#### **10.- Tender budget**

The tender budget is 780.000,00 € (excluding VAT).

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#### **11. Place of delivery**

The successful bidder will install the supplied equipment in its final location within the ICIQ X-ray Diffraction laboratory.

Tarragona, January 14, 2026.

**Dr. Jordi Benet Buchholz**

Manager of the Diffraction Unit

Catalan Institute of Chemical Research Foundation