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**[RSD product category B]**

## ***X-ray Diffraction Station***

***TP16\_027***



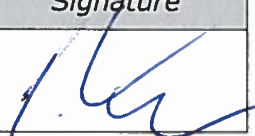
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## 1. Introduction

### 1.1. Purpose

This Requirements Specification Document (RSD) lists the technical requirements and constraints on the planned X-ray diffractometer setup for the RA4 experimental programme (Applications in molecular, biomedical, and material sciences) at the ELI Beamlines facility.

### 1.2. Scope

This RSD contains all of the technical requirements (functional, performance, operational, design, transportation & installation, safety, quality and verification) for the following product: **X-ray diffractometer setup** (PBS code: *E.E1.HXRS.XRDS*). This product is intended for use as an experimental end-station in the E1 experimental hall of the ELI Beamlines building.

This Product is a **product Category B** according to the ELI Beamlines RSD categories. Category B is an Off-the-shelf Product with customization (e.g., product performance) that does not require substantial design modifications to the product. Test programs shall be decided and performed on a case-by-case basis.

### 1.3. Terms, Definitions and Abbreviations

For the purpose of this document, the following abbreviations apply:

Abbreviation	Meaning
ELI	Extreme Light Infrastructure
RA4	Research activity 4
E1	Experimental hall 1
L1	Laser Hall 1
ASCII	American Standard Code for Information Interchange
RSD	Requirements Specification Document
VTC	Video Teleconferencing
W x L x H	Width x Length x Height

### 1.4. Reference documents

Number of document	Title of document
RD-01	00112523/A - E1 Room datasheet



## 2. General Functional, Performance and Design requirements

REQ-016502/A

### For the diffractometer

The diffractometer shall include the following elements:

- A 2 circle goniometer with motorized linear detector stage;
- An open Eulerian cradle;
- A head unit for single crystals mounting on the Eulerian cradle;
- A CCD microscope with light source for sample observation;
- A sealed tube X-ray source with optic;
- Pinhole units;
- Calibration samples;
- Cryo cooler unit (Low temperature device);
- Software and hardware for system control, measurements and data analysis.

*NOTE: The diffractometer set up does not include a radiation safety enclosure. This enclosure at the Contracting Authority site will be provided by the Contracting Authority.*

REQ-016503/A

### The 2-Circle Goniometer with motorized linear detector stage shall conform to:

External Diameter of the 2 circle goniometer < 55 cm

Utilized angular region:

2Theta: at least 240°

Omega: at least 200°

Accuracy: at least 0.005°

Reproducibility: at least 0.0002°

Stepper motors with optical encoders that remember the last position on power shutdown or failure.

Lifting eyes for movement by a crane.

Possibility for small manual positioning ( $\pm 5$  mm) of the goniometer base in xyz directions by screws.

REQ-016513/A

### Motorized linear detector stage shall conform to:

Motorized Detector linear stage compatible with DECTRIS Eiger X 1M.  
Motorized Detector linear stage distance travel: To position the detector surface between 40-400 mm from the sample point.

Motorized Detector linear stage motor: possibility to remember the last motor position on power shutdown or power failure.

Motorized Detector linear stage motor: limits on the operational range that prevents the detector from going out of the stage.

Motorized Detector linear stage mounted on the outer circle of the 2 circle goniometer.

REQ-016504/A

**The Open Eulerian Cradle shall conform to:**

Method of attachment: above the inner circle of the 2-circle goniometer.

Utilized angular region:

Chi: at least 90°

Phi: 360°

Position accuracy < 0.001°

"Sphere of confusion" < 0.01 mm

Allowed weight load at least 2 kg

Distance from the sample point to the table < 60 cm.

REQ-016505/A

**The Single Crystal Head Unit shall conform to:**

Easily mountable on the Eulerian cradle.

Weight compatible with the Eulerian cradle load allowance.

REQ-016506/A

**The video CCD microscope shall conform to:**

Mounted on the diffractometer and used for sample alignment.

Include a light source that can be turned on and off through the local control system

REQ-016507/A

**The sealed tube X-ray source shall conform to:**

Cu K $\alpha$  compatible with the DECTRIS Eiger X 1M.

Power consumption <200W.

Computer controlled startup and shutdown.

Computer controlled shutter.

Beamstop with either X-ray pindiode or another automated way for measurement of the sample transmission.

No rotating anodes.

REQ-016508/A

**The optic for the sealed tube X-ray source shall conform to:**

Effective Brilliance when used with the supplied X-ray source (ph/s/mm<sup>2</sup>/mrad<sup>2</sup>) => 1•10<sup>9</sup>.

Provide beamsizes on the sample <= 0.5 mm.

Be easily mountable and removable from the sealed tube X-ray source.

REQ-016514/A

**Multiple Pinhole Single Unit shall conform to:**

Moves the pinhole plate in XY direction parallel to the beam.

The plate can hold 5 pinholes.

Positioning Resolution ~1 micron.

The quantity of multiple pinhole single units shall be two.

REQ-016509/A

**Calibration samples shall conform to:**

Sample for sample-detector distance calibration.

Sample for absolute scattering intensity calibration: glassy carbon or another standard.

REQ-016515/A

**The low temperature device shall conform to:**

Delivers highly stable temperature control in the range: 80K-400K.

Liquid nitrogen consumption &lt;0.65 litres/hour at 5.5 litres/minute laminar gas flow.

Thermal stability &lt;0.15 Kelvin.

Easy mounting and removing.

Temperature and flow control via software.

REQ-016510/A

**The control and data acquisition systems shall conform to:**

Control all motorized and electronic parts of the diffractometer set up.

Run on a personal computer with 24" flat screen monitor.

Compatibility with the DECTRIS Eiger X 1M detector.

Have routines for accurate instrument calibration.

Have automatic data collection and diffractometer control.

Have data treatment including automated peak indexation, integration, elimination of redundancies, powder diagrams, creation, automatic spacegroup determination, absorption corrections. The software should be suitable for protein crystallography.

System shall be delivered with all necessary motor drivers, controllers, EU compatible power supplies and cables.

The control interfaces should be equipped with an Ethernet port, that will allow communication with the ELI Beamline computer. The communication should be performed on a standard protocol, which can be implemented on the Linux based control system. The company providing the diffractometer should help to integrate the instrument into the ELI Beamline network environment

**NOTE:**     *The RJ45 socket can be provided by extender/convertor or by mounting on a DIN rail.*

### 3. Building and Environmental conditions

REQ-016496/A

All elements of the X-ray Diffractometer and optics shall be suitable for operation in the building and environmental conditions of the Contracting Authority.

*NOTE: For further information regarding building and environmental conditions see the document "E1 room datasheet" (RD-01).*

### 4. Transportation and Installation requirements

REQ-016497/A

All elements of the X-ray Diffractometer and optics shall be delivered in protective package preventing damage and contamination. The package shall have a minimum of two plies separate clean packaging.

REQ-016498/A

Each item shall be cleaned and packaged in clean environment of class 7 according to ČSN EN ISO 14644 or cleaner. If the Supplier cannot fulfill class 7 cleanliness requirements, the Supplier and Contracting Authority shall agree on the cleaning method to be used to clean devices without decreasing the devices' performance and to avoid contamination of the clean space of the Contracting Authority.

REQ-016518/A

The installation and verification of the Product (X-ray diffractometer setup) shall be conducted by the Supplier.

*NOTE: The product shall be installed in the radiation safety enclosure provided by the Contracting Authority.*

REQ-017823/A

All transportation and installation tools and equipment entering the clean room areas of the Contracting Authority shall be cleaned and reviewed by the Contracting Authority's approved methods. The Supplier and Contracting Authority shall agree on the cleaning method to clean tools and equipment used at the installation without decreasing their performance or safety.

*NOTE: Some tools can be provided by the Contracting Authority upon agreement.*

REQ-017826/A

The transportation and installation procedures shall be compliant with the Contracting Authority's installation regulations.



REQ-017824/A

All participants to the installations shall undertake a lecture by the Contracting Authority regarding safety, cleanliness, protection of the environment and working methods before starting their activities on the premises. The content of the lecture shall be adequate to the working area and the work activities expected.

REQ-017825/A

The Supplier shall allow supervision of the activities related to the transportation and installation by the Contracting Authority.

*NOTE: Any acts of supervision shall not mean that the Contracting Authority assumes additional liability of any kind exceeding its liabilities according to the contract.*

## 5. Safety Requirements

REQ-017822/A

The diffractometer set up shall be compatible with the radiation safety enclosure of the Contracting Authority.

*NOTE: Details of the radiation safety enclosure will be provided on request.*

## 6. Quality Requirements

### 6.1. General Quality Requirements

REQ-016500/A

The supplier shall provide a Product User Manual as part of the delivered Device. The Manual shall include the instructions and descriptions regarding the following procedures:

- transport;
- handling;
- storage;
- installation and verification;
- safe operation and maintenance procedures.

*NOTE: The Manual shall be approved by the Contracting Authority.*

REQ-016501/A

Supplier shall provide a declaration of conformity with technical requirements defined by the product RSD and ensure completeness of the product.

REQ-016517/A

The Supplier shall establish and maintain a non-conformance control system compatible with CSN EN ISO 9001: 2010 edition 2 or equivalent.

## 6.2. Specific Quality Requirements

REQ-016511/A

The Supplier shall provide a final design suggestion of the complete X-ray diffractometer setup that is to be accepted by the Contracting Authority before manufacturing starts.

REQ-016512/A

The unit system of the mounting holes, sizes and layout shall be metric.

REQ-016519/A

Supplier shall provide basic training at ELI premises on how to operate the Product (X-ray diffractometer setup). This training shall take place after the successful acceptance of the product (see section 6.3.1).

*NOTE1: Minimal duration of the training shall be 2 working days with possibility for further training via VTC (e.g. by Skype) or another convenient way.*

REQ-018214/A

In case of a warranty repair of the instrument by the Supplier, the Supplier shall redo necessary parts of the verification procedure. The results of this process shall be provided to the Contracting Authority.

## 7. Verification requirements

### 7.1. Acceptance

Acceptance of the product shall be performed according to the relevant sections in the contract and follow the successful outcome of a verification process.

The verification process shall demonstrate the following:

- That the delivered product is free of fabrication errors and is ready for the intended operational use;
- That the functions of the instrument meet the relevant performance requirements;
- Detected non-conformities (if any) have been solved in accordance with the non-conformance control system defined by REQ-016517/A.

#### REQ-016520/A

The verification process shall consist of a series of tests where the following functionalities must be verified and/or results obtained.

- Safety circuit operational test;
- Verification of the sphere of Confusion (SoC);
- X-ray Flux measurement and stability test;
- Beam alignment according to the goniometer centre;
- Calibration of the Sample to Detector Distance (SDD);
- At least one single crystalline sample tests.

#### REQ-016521/A

The verification process shall be carried out on the delivered final product.

#### REQ-016522/A

The results from the verification process shall be documented in a test report that is to be approved by the Contracting Authority before acceptance.