Date: 13-12-2024

Prebid meeting for the Purchase of Single Crystal X-ray Diffractometer

Prebid meeting for the purchase of Single Crystal-X-RAD system is conducted on 13-12-2024 and Two firms [M/S IR technology services Pvt. Ltd. and M/S Bruker India Scientific Pvt. Ltd] have participated online. M/S IR technology services Pvt. Ltd.and M/S Bruker India Scientific Pvt. Ltd have presented details of their instrument online and suggested some point in written *via* email. The committee has considered all the points critically and responses to all points are attached with this note and shared with both the firms. Based on suggestion from the vendors the tender specifications has also been revised and same has been attached herewith.

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Response to M/S Bruker India Scientific Pvt. Ltd. Prebid queries/suggstions

The T&PC have considered all the queries/suggestions critically and accordingly the response to all queries are as follows.

Query/suggestion	Response
5. X-ray optics 2) Beam divergence: For Mo ≤ 5 mrad; For Cu ≤ 14 mrad (variable) or better 3) Target focus size ≤80 micrometer 4) Flux density: Mo ~$3x10^9$; Cu ~$5x10^{10}$ photons s/sq.mm or higher	**5.X-ray optics** 2)Beam divergence: For Mo ≤ 5 mrad; For Cu ≤ 14 mrad (variable) or better 3)Target focus size ≤120 micrometer 4) Flux density: Mo ~3 $x10^9$; Cu ~5 $x10^{10}$ photons s/sq.mm or better
6. Detector 1) Shutter less, air/water-cooled and maintenance free operation 3) Point spread function (PSF): ≤ 1 pixel (FWHM) or better 5) High detective quantum efficiency: ≥90% for both (Cu and Mo) radiation or better 6) Active area: 100 x 69 mm^2 or larger	**7.Detector** 1) Shutter less, air/water-cooled and maintenance free operation 3) Point spread function / parallax : ≤ 1 pixel or betterr 5) High detective quantum efficiency: ≥90% (for Cu); ≥60% (for Mo) or better 6)Active area: 69 x 80 mm^2 or larger
14.Control computers **Bruker provides below Factory tested PC specification for Controlling the SCD system:** 13th Gen Intel Core i9-13900K -16 GB RAM -256 GB SSD -2.0 TB SSD -27" LED monitor -US/INT-keyboard -Optical mouse -SATA DVD-RW Operating System: Windows 10 IoT Enterprise SAC, English, 64 bit	**14.Control computers** The system should be supplied with a desktop PC with factory-loaded software with following configuration or better. 13th Gen Intel Core i9 - 16 GB RAM - 256 GB SSD - 2.0 TB HDD - 27" LED monitor - Operating System: Windows 10 or latest.

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Response to IR Technology Services Pvt. Ltd. Prebid queries/suggstions

The T&PC have considered all the queries/suggestions critically and accordingly the response to all queries are as follows.

Query/suggestion	Response
Firm suggested to delete following point from the specification. **5. X-ray optics** 4) Flux density: Mo ~$1x10^9$; Cu ~$1x10^{10}$ photons s/sq.mm or higher	This is important point for targeted applications and cannot be deleted.
Firm suggested to delete following point from the specification. **6. Detector** 5) High detective quantum efficiency: ≥95% for (Cu) and ≥60% for Mo radiation or better	This is important point for targeted applications and cannot be deleted.

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Revised Technical specification for the "Single-crystal X-ray Diffractometer and Accessories"

Name of Specifications / Parts / Accessories of Tender Enquiry
1. Brief description An advanced single crystal X-ray diffraction system with the Highest level of safety design for data collection and structural determination of molecules with all the software and peripherals required to fully integrate the system. Sensitive, noise-free, fast, accurate, versatile, and reliable X-ray diffraction system with the following specifications. The system offered should be complete with all respect. The instrument should be compatible with Indian power supply (220-240V/ 50 Hz). Quoted SCXRD model should have minimum 20 installations worldwide and minimum 5 installations in India.
2. Desired applications SCXRD system should be capable of performing 1) Accurate crystal structure determination of small organic/inorganic/organometallic compounds. 2) Absolute structure/configuration determination of organic compounds. 3) High-resolution charge density studies with sufficient data completeness. 4) SCXRD data collection under non-ambient conditions (80 to 400 K). 5) Studies small and/or weakly diffracting crystals. 6) Crystals with large unit cells (~50 Å). 7) Studies on complex multi-domain/modulated crystals. 8) It should have the facility to do Powder X-Ray Analysis.
3. X-ray Generator Fully automatic computer-controlled system 1) Max. Voltage: 50 kV or better 2) Max. Current: 1 mA or better 3) Output stability: ±0.1% or better
4. X-ray Tube 1) Sources: Cu and Mo (both) 2) Micro-focus X-ray Tube. 3) Max Power: 50 W or better
5. X-ray optics 1) Multilayer optics and collimators of suitable size 2) Beam divergence: For Mo ≤ 5 mrad; For Cu ≤ 14 mrad (variable) or better 3) Target focus size ≤120 micrometer 4) Flux density: Mo ~3 x10^9; Cu ~5 x10^{10} photons s/sq.mm or better
6. Goniometer 1) Type: 4-circle or kappa goniometer with four axis 2) Detector distance range: 32-200 mm or better 3) Sphere of confusion: ≤ 7 micrometer 4) Equipped with sample illuminator, video image camera and external LCD monitor for crystal mounting
7. Detector A state-of-the-art high-resolution hybrid photon counting pixel detector (HPC) or Charge-Integrating Pixel Array Detector (CPAD) for diffraction high pixel counts rate linearity for both Mo and Cu radiation, low dead time and low background noise. 1) Shutter less, air/water-cooled and maintenance free operation 2) Low noise, high dynamic range high count rate linearity 3) Point spread function / parallax : ≤ 1 pixel or better

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4) Count rate per pixel: ≥ $1x10^6$ cps/pixel or better
5) High detective quantum efficiency: ≥90% (for Cu); ≥60% (for Mo) or better
6) Active area: 69 x 80 mm^2 or larger

8. Software

A WINDOWS or LINUX-based user-friendly GUI software for instrumental control, data collection and analysis with the following features:

1) Data acquisition, integration, scaling, absorption correction, space group determination, auto as well as manual structure determination and final report generation for publication purpose.
2) Functionality for designing the data collection strategies for optimized image scans with desired exposure, redundancy, resolution and completeness.
3) Morphology/face indexing measurements of crystals.
4) Identification, indexing, and structure solution for complex (twin and modulated) crystals.
5) Functionality to allow the collection of powder diffraction data, analysis and plotting for the PXRD pattern generated from the measurements. Software for functional display and intelligent data processing of powder diffraction images and cylindrical Debye-Scherer view to analyze complete powder patterns from multiple frames.
6) The offered software must-have functionality for the structure determination functionality of both small and large molecules.
7) The data collection refinement and analysis software should be provided with unlimited site licence with free updates so that can be installed in any number of PCs

9. Polarizing microscope

A suitable latest generation Stereo Zoom microscope with the LED illumination and Polariser/ Analyser for crystal selection should be quoted with the following specifications or higher:

1) Zoom range: minimum 8:1 (0.6X – 5.0X) or better
2) Magnification range: minimum 6.3X to 50X or better
3) Working distance: 80-92 mm or better.
4) High-resolution digital camera (resolution 6MP or better) with USB interface
5) A compatible latest Windows OS based PC (intel i7, 1TB SSD) for image capture and recording., 27 inches 4K or better LED Monitor.

10. Low Temperature Attachment or (Cooling Facility and Sample Temperature)

1) The diffractometer shall be equipped with a low-temperature device based on the use of liquid nitrogen (LN2), which must be capable of maintaining a stable sample temperature of 80 to 400 K, with an error not larger than ±1 K over the whole temperature range and should be complete with 60 Litre liquid Dewar and its peripherals.
2) Further, it should be possible to set the sample temperature (for fixed low-temperature experiments) through the instrument control software.
3) A liquid nitrogen storage Dewar for 150 liters capacity with auto refill accessory and necessary valves, regulators, transfer line and other accessories should be included. Dewar should be provided with a suitable trolley for easy movement.

11. System Video Microscope & Illumination

1) A good quality microscope with the highest possible magnification to view the crystal while mounting and centering in line with the X-ray beam i.e. alignment, monitoring, and face-absorption corrections.
2) Coupled with software for the required video capturing of color images of the crystal mounted on the goniometer platform.
3) Additionally, provision to transfer and store images should be provided.

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12. Consumables-

1) Goniometer Heads: 3 No's with strong magnetic bases
2) Test crystals: 1 No.
3) Reusable Goniometer Bases – 40 No's
4) Dual-Thickness Micro Mounts™ with 5 each of 10, 20, 30, 50, 75, 100, 150, and 200 µm apertures - 80 No's
5) Magnetic Cryovials – 20 No's
6) NVH Oil 1 liter – 2 No's
7) Base holder and Protective Storage Case – 2 No's
8) Heavy-duty tweezers - 2 No's
9) Quartz Capillary Size 0.3mm - 25 pack
10) Quartz Capillary Size 0.5mm - 25 pack
11) Capillary Wax 40 G pack – 1 No.
12) Tool kit 1no.

13. UPS

A branded ISO-9001 certified IGBT-based online UPS of 10 kVA capacity suitable to the quoted system with an in-built isolation transformer and SMF Batteries including all accessories for providing minimum of 30 minutes backup on full load.

14. Control computers

The system should be supplied with a desktop PC with factory-loaded software with following configuration or better.

13th Gen Intel Core i9

- 16 GB RAM
- 256 GB SSD
- 2.0 TB HDD
- 27" LED monitor
- Operating System: Windows 10 or latest.

15. Computer for structure solution and refinement

The configuration of the desktop PC should be equivalent or better to the following specs: latest Intel Core i7 (10th generation or higher) processor, 32 GB RAM, 2TB SSD, 27" LED professional monitor, compatible latest licensed Windows operating system (64 bit)., graphic Card, CD-DVD read-write drives, USB ports, LAN connectivity, and wireless keyboard and mouse.

16. Manuals and Documentation

All operational manual, maintenance and calibration procedure documentations shall be provided in English language. In addition to the hard copies, soft copies of the manuals shall also be provided in CD/DVD/USB

17. Warranty

Minimum 5-year unconditional comprehensive on-site warranty on the complete system including accessories should be provided for the continuous operation of the machine.

Commitment is also sought for ensuring spare parts availability for at least 10 years from OEM after successful installation and or 10 years after discontinuation of the system/model. An undertaking in this regard should be submitted with the quotation.

One PM kit for complete system per year must be quoted for warranty period of 5 years.

Separate list of consumables which are required to be replaced during PM to be provided.

18. After Sales Service

The supplier should provide a prompt after-sales service such as regular instrument maintenance, troubleshooting and fixing.

19. Installation and Commissioning

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1) Installation and commissioning should be at CSIR-IHBT site. The expenditure involved in it will be borne by the supplier only suitable room will be provided. 2) Suitable tables - 2 nos 3) Chairs - 2 nos 4) Hot and Cold Split AC (1.5 Ton with 5-star rating) - 2 Nos. 5) Necessary pre-installation advice should be enclosed along with the technical bid.
20. Application Training On-site training (from operating the instrument to complete structure determination) for a minimum of four working days after the successful installation should be provided. This training must be provided by an application scientist having expertise in X-ray crystallography and the training must be split in to 2 separate sessions of 2 days each with basic and advance capabilities.

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