

PURCHASE ORDER
INDUSTRIAL TECHNOLOGY DEVELOPMENT INSTITUTE

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|---|---|
| Supplier : MOLAVE TRADING INC. | P.O. No. : 23-977 # GIAE-PO-2023-09-0931 (EBD) |
| Address : Acero Building, 891 E. Delos Santos Ave., Quezon City | Date : September 4, 2023 |
| TIN : | Mode of Procurement : Public Bidding |

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| Place of Delivery : Metrology Building | Delivery Term : 120 calendar days |
| Date of Delivery : | Payment Term : |

| Stock/ Property No. | Unit | Description | Quantity | Unit Cost | Amount |
|---------------------|------|---|----------|---------------|---------------|
| | lot | Supply, Delivery, Installation and Commissioning of One (1) unit X-ray Crystallography Brand: D8 Quest Eco The D8 QUEST Eco is full-featured, easy-to-use research instrument providing fast 3D structures, complementary to NMR and mass spectroscopy, enabling the full range of service crystallography. The D8 QUEST Eco chemical crystallography X-ray system is capable of high-speed data collection with the latest photon-counting CPAD detector ensuring excellent data quality and unprecedented data acquisition efficiency. | 1 | 19,998,000.00 | 19,998,000.00 |
| | | Inclusions: | | | |
| | | Basic System | | | |
| | | Standard cabinet, enclosure, controller | 1 | | |
| | | 1kW Generator, tube housing, with internal cooling unit | 1 | | |
| | | Tube mount adapter for single source sealed tube, monochromator adapter plate Mo | 1 | | |
| | | Horizontal Goniometer | 1 | | |
| | | Configuration tested PC - Windows, 64 bit, English | 1 | | |
| | | 200-230V 1p 50/60Hz, for 1μS 2kVA and ECO 3kVA (all) | 1 | | |

EMAILED

Recipient: _____
Date: 09-27-23

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| D10-AJB-6 | | D8 QUEST ECO | 1 | | |
| D10-543 | | Triumph Monochromator Mo | 1 | | |
| D10-556 | | Beamstop, first source, 2.0 mm | 1 | | |
| D10-442 | | Fixed Chi Stage | 1 | | |
| D10-444 | | Goniometer Head Manual | 2 | | |
| D10-021 | | PHOTON III C7 | 1 | | |
| D10-1190 | | Mount for PHOTON detector, measurement height 214mm | 1 | | |
| D10-K94 | | Two Pinhole Collimator 0.6/21mrad | 1 | | |
| D10-R09 | | X-ray Tube, KFF Mo 1KC, 2.0 kW Mo point | 1 | | |
| D10-503 | | 4-axes motor driver board | 1 | | |
| D10-ER2 | | 10m power cable for 200-230V 1p 50/60Hz, for IMS 2kVA and ECO 3kVA (all) | 1 | | |
| D10-V29 | | Detector Track, manual, distance detection system | 1 | | |
| D10-V33 | | Video microscope SCD, standard definition | 1 | | |
| D10-711 | | Reference crystal Ylid for SCD | 1 | | |
| | | Steel Ball for SCD | 1 | | |
| 843-027000 | | APEX4 w. SHELXTL S/W, Win (site lic. Suppl.w. D8 QUEST / D8 VENTURE) | 1 | | |
| 123-028000 | | *Magnet Base to mount on XYZ-Goniom. head (9.3mm, 9000 Gauss) | 2 | | |
| K430C14 | | Crystalpin ⁿ ALS HT HR8-204, 0.1 - 0.2 MM (30 pack) | 1 | | |
| K430C16 | | Crystalpin ALS HT HR8-208, 0.3 - 0.4 MM (30 pack) | 1 | | |
| K410C312 | | *Oil for Crystal mounting - NVH | 1 | | |

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| | 700 | Application Training for two endusers at Bruker Singapore | 1 | | |
| | | Continuous ink printer (colored and black) and UPS with AVR function for PC system | 1 | | |
| | | UPS, 10kVA | 1 | | |
| | | AVR, 10kVA | 1 | | |
| | | Detailed Description of Items | | | |
| | | Basic Systems | | | |
| | DD, MDLD | Standard cabinet, enclosure, controller | 1 | | |
| | | Compact Radiation Safety Enclosure The small footprint radiation safety enclosure combines a maximum of operating convenience and ergonomics with excellent goniometer and sample visibility. The large swing door provides excellent access to the goniometer. Clearly visible LED lights indicate the X-ray status. Smart screen key displays show the status of the instrument and ensure an intuitive operation. The enclosure is illuminated by a series of dimmable white LED's. Depending on configuration racks mounted inside the enclosure provide easy access and storage space for optics and accessories. The enclosure offers an X-ray tight labyrinth for feeding-through cables and hoses. | | | |

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| | | <p>The enclosure hosts the controller interface to the goniometer and offers room for additional 19" control electronics. A series of eight internal sockets assures a safe and clean cable management.</p> <p>Safety: The instrument complies with the requirements of the Machinery Directive 2006/42/EC. In addition, the instrument is in conformity with the directives 2014/35 EU relating to electric equipment and 2014/30/EU relating to electromagnetic compatibility.</p> <p>Maximum X-ray safety is guaranteed due to two independent fail-safe safety circuits. The maximum radiation level is significantly below 1 micro-Sievert/h under measurement conditions.</p> <p>Dimensions: Height x Width x Depth: 187 cm x 130 cm x 114 cm 73.5 inch x 51.2 inch x 44.7 inch</p> <p>Weight: Approximately 750 kg (depending on configuration and accessories)</p> | | | |

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| Stock/ Property No. | Unit | Description | Quantity | Unit Cost | Amount |
| | | <p>1 kW Generator, tube housing with internal cooling unit</p> <p><i>DID-ASZ</i> 1 KW GENERATOR WITH INTERNAL COOLING UNIT</p> <p>High stability, medium frequency design high voltage volume power supply for the X-ray tube. The generator is provided with a routine for the automatic-burn-in of X-ray tubes to facilitate maximum tube lifetime.</p> <p>The internal cooling units fits into the enclosure and requires no external water cooling. The water unit is equipped with a deionization filter to avoid the growth of algae.</p> <p>Technical data:</p> <ul style="list-style-type: none"> - Maximum continuous power: 1 kW - High voltage: 20-50 kV, adjustable in steps of 1 kV - Current: 5-60 mA, adjustable in steps of 1 mA - Stability: <0.005% for high voltage and current with 10% variation of main supply | 1 | | |
| | | <p><i>DID-ASZ</i> Tube mount adapter for single source sealed tube, monochromator adapter plate Mo</p> | 1 | | |

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| | | <p>BEAM PATH FOR SEALED TUBE WITH MONOCHROMATOR FOR MOLYBENUM RADIATION The solid beam path unit mounts directly into the groove ring of the D8 goniometer and features an ultimately user-friendly down-stream alignment. It is manufactured with smallest backlash for highest accuracy and accommodates the tube mount including the support for the graphite or TRIUMPH monochromator. The magnetic SNAP-IN coupling mounts and positions the collimator. Mounting bays for the video microscope and the primary beam stop complete the assembly.</p> <p>Sample Illumination For sample illumination a high brilliance, high intensity via LED is provided. The LED produces strong white light, which is remotely dimmable.</p> <p>Horizontal Goniometer</p> <p>HORIZONTAL GONIOMETER Highly-accurate, high-precision, two-circle goniometer with independent stepper motors and optical encoders.</p> | 1 | | |

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| | | <p>Technical data: Horizontal goniometer Angular range: 360°C (without accessories) Angular positioning: stepper motors with optical encoders Smallest addressable increment: 0.0001°C Maximum angular speed: 20°C/s (depending on accessories) Accuracy; 0.0005° Reproducibility: 0.0002°</p> <p>Bruker provides a ten-year warranty on the goniometer.</p> | | | |
| | | <p><i>DJO-AB-7</i> Configuration tested PC - Windows, 64 bit, English</p> <p>English</p> <p>Dedicated, configuration tested tower PC for instrument control: Intel Core i7-8700 16 GB RAM 256 GB SSD 2.0 TB hard disk drive 27" LED monitor US/INT-keyboard Optical mouse SATA DVD-RW Operating System: Windows 10 Pro, IoT EnT CBB High End EPKEA (ESD) COA, English MS Office 2019/2021</p> | 1 | | |

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| | | <p>Technical changes are possible, features may be upgraded at time of delivery.</p> <p><i>DIO-107-7</i> 200-230V 1p 50/60Hz. for IuS 2kVA and ECO 3kVA (all)</p> <p>ELECTRICAL SUPPLY</p> <p>Electrical supply: 200-230 V, 50/60Hz, single-phase Maximum power consumption: 2 kVA for IuS-based systems Maximum power consumption: 3 kVA for D8 ADVANCE ECO and D8 QUEST ECO systems</p> | 1 | | |
| | | <p><i>DIO-108-G</i> D8 QUEST ECO</p> <p>D8 QUEST ECO SYSTEM FOR CHEMICAL CRYSTALLOGRAPHY</p> <p>The D8 QUEST ECO is a fully featured research instrument. The D8 QUEST ECO diffractometer is housed in a compact X-ray safety enclosure requiring minimal installation requirements.</p> <p>Full compatibility with the D8 diffractometer family provides flexibility for the future as the system can be easily upgraded with high performance source and detector options. Crystal centering can be made even easier by adding the AGH.</p> | 1 | | |

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| | | <p>Chemical Crystallography The D8 QUEST ECO covers applications in organic and inorganic chemistry, metal-organic and solid-state chemistry as well as mineralogy and pharmacy. It is configurable for the investigation electron densities or measurements under non-ambient conditions, such as high- or low-temperature studies or the investigation of phase-transitions.</p> <p>1 kW Sealed tube X-ray source with TRIUMPH monochromator The 1 kW Mo sealed tube source features a long tube lifetime and internal water chiller. With the TRIUMPH monochromator, the source delivers a high-flux X-ray beam ideally suited for a wide variety of applications in chemical crystallography.</p> <p>3-axis goniometer The D8 QUEST ECO features the highly accurate, high-precision, fixed-chi goniometer with optical encoders. Large scan range continuous rotation about omega, phi, and 2-theta axes provides full experimental flexibility and delivers complete data sets down to 0.4 Å resolution.</p> | | | |

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| | | <p>PHOTON III 7 detector The PHOTON III 7 is a large area (7,000 mm²) detector using state-of-the-art photon counting CPAD technology. The air-cooled PHOTON III 7 delivers excellent spatial accuracy and exceptional sensitivity to Mo radiation, enabling high quality structure determination from a broad range of crystal types.</p> <p>The crystal-detector distance is fully adjustable between 35-240 mm to allow optimal spatial resolution of the diffraction pattern.</p> <p>APEX Software Suite A site license is provided for the full APEX suit of software including the STRUCTURE NOW automation routine. The APEX suites provides an intuitive user interface which includes plug-ins for instrument control, data collection and processing, structure determination and report generation. A plug-in for collecting and processing powder diffraction data is also included as standard.</p> <p>Manuals The system is shipped with a comprehensive package of operation manuals for software and hardware (on CD-ROM).</p> | | | |

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| | D10-543 | Triumph Monochromator Mo TRIUMPH MONOCHROMATOR FOR MOLYBDENUM RADIATION Curved crystal X-ray monochromator for the generation of monochromatic Mo-K (alpha) radiation from a sealed X-ray tube. The TRIUMPH monochromator provides a top hat shaped beam profile, which makes it ideal for research dealing with a variety of crystal sizes. The TRIUMPH monochromator delivers an up to 3 times higher intensity compared to a flat graphite X-ray monochromator. | 1 | | |
| | D10-552 | Beamstop, first source, 2.0 mm BEAM STOP FOR SINGLE/FIRST SOURCE, 2.0 MM Beam stop, including magnetic SNAP-IN mount with 3-point support and component recognition. | 1 | | |
| | D10-442 | Fixed Chi Stage FIXED-CHI SAMPLE STAGE The fixed-chi sample stage 3-axis mounts on the omega axis of the horizontal goniometer and supports a 360° phi drive | 1 | | |

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| | | <p>mounted in the magic angle of 54.7 degrees. The open geometry has minimal obstruction and allows mounting of additional crystal conditioning devices easily. This enables for efficient data collection with the smallest possible number of scans and a minimized total data collection time - even for samples with low symmetry. The fixed-chi stage can be used with a manual or a motorized detector track. The fixed-chi stage has a minimum of moving parts which makes it very stable and robust.</p> <p>Technical data: Stepper motor with optical encoders Phi: Angular Range: n*360° Speed: 0.00°/min - 1500°/min Accuracy: 0.025° Reproducibility: 0.001° Magic Angle: 54.7°</p> <p>Sphere of confusion: 7 micrometer Half-beam alignment tool included.</p> <p><i>DIO, P44</i> Goniometer Head Manual</p> <p>XYZ GONIOMETER HEAD</p> <p>The XYZ-goniometer head is required for manual sample mounting on Bruker SC-XRD systems. The goniometer head</p> | 2 | | |

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| | | meets the IUCR standard. An adjustment pin allows changing the standard height from 49 mm to 64 mm. | | | |
| | | X, Y, Z translations can be adjusted by 2.7 mm each. | | | |
| | | The weight of the XYZ goniometer head is 120 g. | | | |
| | | Sample mounting pins, goniometer-head key, and a storage box are included as accessories. | | | |
| | D17-D21 | PHOTON III C7 | 1 | | |
| | | PHOTON III C7 CPAD AREA DETECTOR (7X10) | | | |
| | | The PHOTON III is the first pixel array detector to support both photon counting and charge integration for the best sensitivity and dynamic range. This 'Mixed Mode' operation dramatically improves both productivity and data quality. | | | |
| | | The PHOTON III C7 features high quantum efficiency across a wide energy range. By design the PHOTON III is charge sharing noise free and does not suffer from count rate saturation. The PHOTON III detector features 14 milliseconds frame read out as well as | | | |

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| | | <p>zero dead time between frames for fast data collection. The detector supports destructive read out (DR) and non-destructive read out (NDR). Adaptive oversampling (AO), an extension of the measurement of correlated frames, uses varying combinations and DRs and NDRs to match detector operation to the diffraction properties of the sample.</p> <p>The PHOTON III incorporates a powerful Digital Signal Processing (DSP) unit for real time data processing and is operated in shutterless data acquisition mode. The PHOTON III is a low maintenance, low power consumption detector that is air cooled. Sensitive parts are sealed under atmospheric pressure and the detector does not require any dry air gas purge. The use of dedicated, high resolution rare-earth scintillators ensures that the Shannon-Nyquist sampling criterion is fully satisfied.</p> <p>Up to high energies the PHOTON III achieves negligible parallax error.</p> <p>Technical data: - Detector type: 4th generation Charge Integrating Pixel Array (CPAD), latest pixel array detector technology - Active area: 69 x 104 mm²</p> | | | |

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| | | <ul style="list-style-type: none"> - Read out frequency: 70 Hz - Maximum count rate: 4×10^6 counts/pixel-sec - Read out dead time: 0 sec (full shutterless operation) - Dimension: Width: 152.0mm Height: 161.5mm Depth: 156.3mm - Size of dead areas: zero, single monolithic sensor - Dynamic range: > 200,000 - 100% of the pixel area is fully sensitive to X-rays - Charge sharing noise: 0 electrons, by design - Shannon-Nyquist sampling criterion is fully satisfied - Parallax at high incident angle: < 1 pixel (for Ag and Mo) - Count-rate nonlinearity: < 1% (up to full count rate) - High defective quantum efficiency (DQE): Quantum Efficiency vs. Energy 100% @ 8.1 KeV (Cu) 100% @ 12.4 KeV (1 Angstrom) 92% @ 17.5 KeV (Mo) 73% @ 22.2 KeV (Ag) 65% @ 24.2 KeV (In) Weight: ~3.5 Kg - Cooling water or operating gas requirements: not required, completely sealed design, air-cooled | | | |

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| | | - Warranty: 3 years | | | |
| | <i>DIO-M30</i> | Mount for PHOTON detector, measurement height 214mm | 1 | | |
| | | MOUNT FOR PHOTON DETECTOR Mount for PHOTON detector, measurement height 214mm | | | |
| | <i>DIO-K94</i> | Two Pinhole Collimator 0.6/21mrad | 1 | | |
| | | TWO PINHOLE COLLIMATOR 0.6MM/21 MRAD | | | |
| | | Two pinhole collimator, including magnetic SNAP-IN mount with 3-point support and component recognition. | | | |
| | <i>DIO-RO9</i> | X-ray Tube, KFF Mo 1KC, 2.0 kW Mo, point | 1 | | |
| | | X-RAY TUBE, KFF MO 1KC, 2.0 KW, POINT | | | |
| | | Fine focus tube with Mo-anode and ceramic insulation body | | | |
| | | Technical data: Point focus Maximum power load: 2.0 kW Standard settings: 50KV, 40mA Optical focus at 6 degrees take off angle: 0.4 x 0.8 mm | | | |

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| | D10-ED3 | 4-axes motor driver board 4-AXES MOTOR DRIVER BOARD Stepper motor controller with encoder readout for a maximum of four motors. | 1 | | |
| | D10-ED2 | POWER CABLE 10 m power cable for 200-230 V, 50/60Hz, single-phase For IuS-based systems (2 kVA), and D8 ADVANCE ECO and D8 QUEST ECO (3 kVA) | 1 | | |
| | D10-U29 | DETECTOR TRACK WITH DISTANCE DETECTION SYSTEM The track mounts on the theta axis of a horizontal goniometer and allows for a manual positioning of the detector. The detector position is constantly read by the distance detection system, and the instrument software is updated on-line. Technical data: Sample to detector distance: 35-240mm Distance detection system | 1 | | |
| | D10-U33 | Video microscope SCD, standard definition | 1 | | |

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| | | <p>INTEGRATED VIDEO MICROSCOPE</p> <p>Video microscope for live image of the sample on the screen of the control terminal. Control software provides crosshair and optional grid for crystal centering and monitoring. Camera is fully integrated for semi-automated face indexing crystal description for integrated numerical absorption correction. The 1000baseT interface supports remote streaming and multicasting.</p> <p>Technical data: Magnification: 4 x (optical), 1245488x (electronical) Field of vision: 1.2 mm Resolution: 1292*964 pixel Max. frame rate: 30 fps Working distance: 65 mm Aperture: F27.0</p> | | | |
| | 010-Y11 | Reference crystal Ylid for SCD | 1 | | |
| | | <p>TEST SAMPLE MOUNTED ON PIN</p> <p>A magnetic-base mounted Sulphonium Ylid crystal (sample), is used for the factory's system test procedure. The identical sample will be delivered with the system.</p> | | | |

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| | | <p>collimators and beamstops automatically. Obscuration of the detector by components of the goniometer is minimized and collisions are made impossible APEX4 controls all instruments running Bruker Instrument Service (BIS) while data from previous generations and numerous third party equipment can be processed off-line.</p> <p>The package comprises of an easy-to-use graphical user interface (GUI) with extensive feedback and on-line help. The suite offers a wealth of tools for basic operations and automation, such as remote control of the X-ray generator (s) from standby to full power and back, control for driving the diffractometer and shutter operations. Optional low-temperature devices, such as the Cryostream 800, Cobra or N-HELIX can be also controlled remotely. Suitable defaults and valid ranges of values are calculated and suggested wherever possible throughout the course of the structure determination. In dual source configurations the package supports multiple wavelengths with an automated switch and subsequent automated collection of the complete data.</p> <p>The entire package can handle twinned or intergrown samples with up to eight individual domains simultaneously.</p> | | | |

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| | 010-713 | Steel Ball for SCD STEEL BALL FOR SC-XRD Steel Ball for instrument alignment - Mounted on magnetic pin - Diameter: 0.381mm micrometer | 1 | | |
| | 843-02900 | APEX4 w. SHELXTL S/W, Win (site lic.suppl. W. D8 QUEST / D8 VENTURE) APEX4 SOFTWARE SUITE INCLUDING SHELXTL (SUPPLIED WITH AN INSTRUMENT), WINDOWS Workgroup license to use the APEX4 software suite on a user owned computers running Windows 10 IoT Ent CBB High End EPKEA (ESD) COA, English The APEX4 software suite provided with the system consists of a comprehensive suite of reliable routines for the collection and integration of CMOS, CCD and IP frame data from single crystals, and for solving, refining, displaying and publishing of structural results. Systems with DAVINCI.DESIGN (D8 QUEST, D8 VENTURE, D8 QUEST ECO) benefit from the unique 3D robotic path planning, where the path planning routine continuously checks the validity of the experimental setup. Hardware recognition identifies components like mirrors, | 1 | | |

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| | | <p>Modulated structures are fully supported for further processing in dedicated programs such as JANA. Powder samples can be evaluated in transmission mode as flat samples or in capillaries ^{capillaries}. *</p> <p>Within the suite all input and output parameters are stored in an integrated PostgreSQL data base (online lab journal). This ensures complete integrity of all user-selected and program-determined experimental values within the system. Furthermore, information from the database avoids the unintended measurement of structures, which have been measured before. The data base organizes data storage and backup, take care of individual user configuration and provides a comprehensive overview of projects on the individual computer. In a multi-user, multi-computer environment the installation is expandable to provide a site overview. The integration into an existing LIMS is facilitated.</p> <p>The IDEAL module is latest addition to the suite. The module is exclusive to Bruker and leads to more accurate models:</p> <p>The current Independent Atom Model (IAM) is insufficiently suited to handle the electron density information included in high resolution data (0.6 A and beyond). *</p> | | | |

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| | | <p>IDEAL is an easy-to-use extension to the IAM to tackle this problem. IDEAL offers a new way to take electron density from bond electrons and the lone pairs into account and uses pre-calculated fragment-based information applying extremely fast fragment matching algorithms to make computing most efficient.</p> <ul style="list-style-type: none"> - IDEAL adds and refines bond-oriented deformation density from the Generalized Invariom Database (GID) to the IAM - The GID contains transferable pseudoatom parameters of the Hansen-Coppens multipole model and associated local atomic coordinate systems from almost 3000 model compounds - IDEAL works for small-molecule and macromolecular diffraction data - IDEAL is fast as it relies on pre-computed database parameters avoiding long-time quantum chemical computations - Compatible with CHECKCIF <p>A fully automated pipeline (STRUCTURE NOW) is provided, which follows the natural flow of the structure determination process from the initial crystal quality assessment through data collection, data processing, structure solution and refinement, finalizing with a publication-ready report.</p> | | | |

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| | | <p>Outside of STRUCTURE NOW, the APEX4 suite offers all of the manual adjustments the expert requires for advanced crystallography. A dropdown menu bar with seven main categories provides guidance through the crystallographic experiment, from sample information to report generation:</p> <ul style="list-style-type: none"> - Set-up of the Experiment - Sample Quality Evaluation - Data Collection - Data Reduction - Data Examination - Structure Solution and Refinement - Report and Publication <p>The suite offers dedicated tools for archiving all data and experimental results on DVD or external, user-defined network shares to guarantee data security.</p> <ul style="list-style-type: none"> - The Set-up category features: <ul style="list-style-type: none"> - User-friendly input of sample related information, such as sample identification code, sample color, chemical formula, and crystal parameters - User-selectable and user-configurable mounting positions of the sample for easy sample mounting and alignment - Data acquisition routines for single frames, single runs, multiple runs, and rotation images - Launch of the fully automated structure determination pipeline (STRUCTURE NOW) | | | |

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| | | <p>The Evaluation category features:</p> <ul style="list-style-type: none"> - Visualization of frames with numerous options, e.g. zoom, contrast control, color schemes, movie mode - Various tools for frame analysis, including 2D- and 3D- reflection profiles, rocking curves, resolution circles, overlays of predicted peak positions - Mouse-driven numerical output of relevant parameters, such as pixel intensity, resolution (Theta and Angstrom), background and integrated intensities, integer and non-integer hkl-values - unit cell determination based on reflections from phi, omega or phi/chi scans using up to three fast and reliable automated indexing routine: Fast Fourier Transformation, Difference Vector algorithms and Least-Square Methods. Prior to least-squares cell refinement and Bravais lattice determination routines a consistency check is applied. - Discrimination of reflections used for indexing through various filters and manual selection. - User-friendly routines for unit cell comparison to determine rotation angles or twin laws - Extensive orientation-matrix manipulation tools for unit-cell transformation and comparison in crystallographic standard and non-standard settings | | | |

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| | | <ul style="list-style-type: none"> - Extensive graphical display of the undistorted reciprocal space and indexing of twinned and modulated samples - User-controlled or automated 3D orientation to display the undistorted diffraction pattern with numerous tools for grouping and ungrouping reflections, e.g. to apply a maximum intensity threshold, visually index modulated structures (q-vector) and visually verify the Laue symmetry (e.g. for educational purposes) - Graphical feedback on crystal degradation or slippage for each scan - CellCheckCSD, to avoid the accidental data collection of an already published structure from a starting material, product or by-product while the crystal is on the diffractometer - Lattice parameters, space group and molecular formula of unknown structures are provided for a comparison with the given sample. <p>The Collect category features:</p> <ul style="list-style-type: none"> - Strategy planner for fast and efficient automated data collection based on previously determined data collection parameters - 3D visualization of the measurement strategy and reflection dependent redundancy | | | |

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| | | <ul style="list-style-type: none"> - Suggestion of the ideal data collection time based on extrapolated intensity information - Suggestion of the most useful scan-width and the best crystal-to-detector distance, based on beam divergence, lattice parameters, and mosaic spread - Suggestion of the maximum useful resolution (maximum diffraction angle) - The user can specify parameters, such as overall data collection time, data completeness and data redundancy - During data collection a moving crystal video stream or a series of crystal images is recovered for further processin in a user friendly, intuitive routine which allows the semi-automated determination of the face indices and corresponding vector length - Friedel pairs can be measured in the same image, which avoids incorrect determination of the anomalous signal in case of decaying crystal (exploiting Kappa geometry) - Shuttered Mode: Automated re-takes are triggered to maximize the instrument's dynamic range by automatically reducing exposure times and/or applying a built-in attenuator - Shutterless Mode: Fast data collection of inner shells to maximize the instrument's dynamic range. The approach also allows a quick structure solution in only a couple of minutes - On-the-fly data integration while data collection is ongoing | | | |

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| | | <ul style="list-style-type: none"> - Multiple data collections at various temperatures or temperature ramping - Scans from oriented samples, which allows retrieval of information on the Laue symmetry prior to a data collection (exploiting Kappa geometry) - Inspection of reflections in bisecting mode at user-selectable psi positions, e.g. for Renninger contribution (exploiting Kappa geometry) - E-mail messaging service, e.g. on the completion of the experiment - A routine to integrate data from powder samples: <ul style="list-style-type: none"> - Combination of multiple frames collected with varying incidence angle - Cylindrical Debye-Scherrer view to analyze complete powder pattern from multiple frames - Easy data integration to Intensity vs. 2-Theta scan - Capability to handle flat detector data with variable sample detector distance for optimum peak solution. - Easy data processing using DIFFRAC.SUITE (optional) The Reduce Data category for data integration and scaling features: <ul style="list-style-type: none"> - Accurate determination of reflections intensifies and background preserving the information on reflections' three-dimensional intensity distribution from fine- or wide- | | | |

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| | | <p>sliced diffraction images.</p> <ul style="list-style-type: none"> - Learned profile method is applied also for twinned, split, or modulated crystal data - Automated control and adjustment of the crystal orientation matrix - Automatic exclusion of obscurations, e.g. caused by beam stop shadows - Exclusion of user define areas (e.g. for the exclusion of ice-rings in proteins or gasket scatter from high-pressure cells) - Accurate handling of $K(\alpha) / K(\alpha)^2$ splitting for all resolutions and wavelength - Incident and oblique beam correction for best data quality at short, most efficient detector distances - Final lattice parameters and orientation matrix refined using all reflections collected - Systematic error estimation based on modern Monte Carlo simulation methods - Data scaling and absorption correction based on the intensities of symmetry-related reflections measured at different angular settings (SADABS & TWINABS) - Numerical absorption correction using face indices determined from the video analysis of the crystal can be carried out. - The routine supports processing of modulated structure data resulting in data sets ready for further processing in JANA - Empirical absorption on samples of as many as eight domains. Overlapping reflections from multiple-domain samples are not rejected | | | |

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| | | <p>but properly processed and kept in the data set</p> <p>The Examine Data category features:</p> <ul style="list-style-type: none"> - XPREP for interactive space-group determination and statistics routine. - Routines to scale, sort, merge and normalize datasets - Extensive statistics are provided for evaluation of the data quality. - Powder pattern simulation from single crystal data for comparison with the bulk powder sample - Generation of pseudoprecession images from data collection frames for the detection and verification of twinning, superstructures, modulated structures and diffuse scattering - Diffraction space viewer for the undistorted investigation of textured samples. Fibers and non-Bragg diffraction - Search and display of user defined reflections and its symmetry equivalents in data frames for detailed visual analysis <p>The Find Structure category features:</p> <ul style="list-style-type: none"> - AUTOSTRUCTURE, for fully automated structure solution and completion. This routine works efficiently for samples from organic, metal-organic and inorganic chemistry as it uses several powerful routines: - Intrinsic Phasing (XT) for initial structure solution, element assignment and space group determination | | | |

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| | | <ul style="list-style-type: none"> - Various tests are applied to identify and correct imperfections in the initial structure model: - Hirshfeld rigid body test, where 1,2 and 1, 3 distances are checked to determine if atoms constituting a bond have sufficiently equal vibrational amplitudes in the direction of the bond - Valence-Bond method, taking into account that the valence of an atom as a function of the bond length - Integration of the electron density around an atom after anisotropic refinement - Final results are checked for consistency against a subset of the Crystallography Open Database (COD) - Interactive structure solution using the Intrinsic Phasing (IP) routine by default: - Powerful, robust and easy to use engine for structure solution and space group determination based on Laue group information - High success rate even on weak and incomplete data → Automated element assignment and initial structure refinement ✓ - Automated transfer of the initial structure model for further model building and refinement (based on SHELXL) - The structure refinement on data from regular and multiply twinned samples based on F² (XL) - Graphical Interface with direct interaction to the Interactive Editor - Mono or stereo visualization of the three-dimensional structure | | | |

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| | | <ul style="list-style-type: none"> - Interactive display of mesh-style isosurfaces based on Fo and Fo-Fc calculations - Interactive display of maxima in the electron density map, highlighting same height peaks - Addition of Hydrogen atoms at idealized positions using Fo-Fc map for optimization - Mouse over help on XL commands and command auto-completion - Interactive, graphical refinement history function with return to previous refinement steps - Mouse- or editor driven atom labelling and renaming mode - Automated transformation of atom coordinates to the asymmetric unit - Interactive refinement of the structure model via function key - Interactive Editor window providing full functionality of the structure refinement program (XL) - Highlighting in editor mouse-selected atoms from the Graphical User Interface - Easy setting of restraints and constraints for simplified treatment of disordered groups or side chains - Convenient residue naming scheme; rigid-group constrains; distance, anti-bumping, planarity and chiral-volume restraints; restraints on H-atom positions and isotropic and anisotropic displacement parameters (including solvent/ water) | | | |

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| | | <ul style="list-style-type: none"> - Flack's x and Parson's Q parameters are refined to determine the absolute configuration - Graphical routine to display the current structure model in various models, such as wire, ball-and-stick, pipes, thermal ellipsoids (banded or sliced) - Structure models can be rotated interactively in three directions and stored in user selectable OpenGL resolution modes or as a POV-Ray input file - Interface to third party software such as Olex2 <p>Although XT typically outperforms established structure solution methods requiring space group information, multiple Direct-, Patterson-, or Dual-Space routines and search methods with known fragments, such as automatic superposition, Patterson interpretation and Patterson routines (XM, XS, XPS) are provided within the package.</p> <p>The Report category features:</p> <ul style="list-style-type: none"> - PLATON's CIFCHECK-routine to ensure crystal structure consistency and integrity through tiered alerts on potential pitfalls and shortcomings - Automated generation of fully publication ready CIF-file - Easily sharable HTML report providing a complete, easy-to-read overview of the results obtained including a Jmol-applet | | | |

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| Supplier : MOLAVE TRADING INC. | | P.O. No. : GIAE-PO-2023-09-0931 (EBD) | | | |
|---|------|--|----------|-----------|--------|
| Address : Acero Building, 891 E. Delos Santos Ave., Quezon City | | Date : September 4, 2023 | | | |
| TIN : | | Mode of Procurement : Public Bidding | | | |
| Gentlemen: Please furnish this Office the following articles subject to the terms and conditions contained herein: | | | | | |
| Place of Delivery : Metrology Building | | Delivery Term : 120 calendar days | | | |
| Date of Delivery : | | Payment Term : | | | |
| Stock/ Property No. | Unit | Description | Quantity | Unit Cost | Amount |
| | | <ul style="list-style-type: none"> - The report delivers a detailed analysis of the structure with respect to configuration including bonding geometry, torsion angles and packing in the crystal: - HTML format - Experimental details, such as project name, structural formula, crystal size, data collection and processing details, reliability criteria for intensity data and crystal structure - Interactive graphics (JMOL) - Tables with structural information - Bond lengths and distances <p>Up to six times per year expert-tested updates of the software package are released with latest features.</p> <p>Manuals</p> <ul style="list-style-type: none"> - Comprehensive package of operation manuals (software and hardware, on CD-ROM) <p>Updates are free-of charge and registered users can download the package and all related documentation from www.brukersupport.com</p> <p>cat. No, 843-027000</p> | | | |

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|---------------------|-------------------|---|----------|-----------|--------|
| | <i>123-012800</i> | <p>*Magnet Base to mount on XYZ-Goniom. head (9.3 mm, 9000 Gauss)</p> <p>MAGNETIC BASE FOR STANDARD PINS</p> <p>The magnetic base fits to goniometer head 87-000-088 and standard pins K430C39 or K430C40. The strength of the magnet is 9000 Gauss.</p> <p>cat. No. 123-012800</p> | 2 | | |
| | <i>K430C40</i> | <p>Crystalpin ALS HT HR8-204, 0.1 - 0.2 MM (30 PACK)</p> <p>CRYSTALPIN ALS HT HR8-204, 0.1 - 0.2 MM (30 PACK)</p> <p>The mount is designed for cryo-crystallography systems that accept ALS style sample mounts. It fits to a magnetic goniometer head base, such as provided by the AUTOMATED GONIOMETERHEAD (AGH). The conical shape is compatible with SCOUT gripper, ALS style grippers, auto mounters and sample handlers.</p> <p>The mount features a two dimensional (2D) alphanumeric 16 x 16 data matrix code on the underside. The mount is also color coded yellow. loop size 0.1 - 0.2 mm.</p> | 1 | | |

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| | <i>K430616</i> | Crystalpin ALS HT HR8-208, 0.3 - 0.4 MM (30 PACK) CRYSTALPIN ALS HT HR8-208, 0.3 - 0.4 MM (30 PACK) The mount is designed for cryo-crystallography systems that accept ALS style sample mounts. It fits to a magnetic goniometer head base, such as provided by the AUTOMATED GONIOMETERHEAD (AGH). The conical shape is compatible with the SCOUT gripper, ALS style grippers, auto mounters and sample handlers. The mount features a two dimensional (2D) alphanumeric 16 x 16 data matrix code on the underside. The mount is also color-coded blue/red, loop size 0.3-0.4 mm | 1 | | |
| | <i>K400312</i> | *Oil for Crystal mounting - NVH CRYOPROTECTANT OIL Viscous cryoprotectant oil for crystallography. The oil can be used to coat moderately air-unstable, small molecule samples under an inert atmosphere before transferring the sample into a gas stream of the low temperature device. | 1 | | |
| | <i>900</i> | Application Training for two end-users at Bruker Singapore | 1 | | |

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| Stock/ Property No. | Unit | Description | Quantity | Unit Cost | Amount |
| | | Continuous Ink Printer (color & black) UPS with AVR function will be provided for the PC system | 1 | | |
| | | UPS, 10kVA | 1 | | |
| | | AVR, 10kVA | 1 | | |
| | | Installation and Training: Offer includes installation by certified field service engineer and on-site training by Bruker certified applications specialist. Offer also includes training for two (2) end-users at Bruker Singapore. Warranty: One (1) year on parts and three (3) years on services (PMS) annually from the date of installation. <i>Supplier</i> We shall be notified in writing immediately on occurrence of a defect, informing us of the kind and the probable cause of the defect. <i>Supplier</i> We shall not be liable for consequential, indirect or incidental damages including without limitation loss of profit, production or data, with the exception of product liability claims for personal | | | |

PURCHASE ORDER
INDUSTRIAL TECHNOLOGY DEVELOPMENT INSTITUTE

23-978 TF

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| Stock/ Property No. | Unit | Description | Quantity | Unit Cost | Amount |
| | | injury or property damage to third persons. | | 19,998,000.00 | 19,998,000.00 |
| | |  END USER: ATHENA DANA V. CORTES-CHA | Less: VAT EWT | 892,767.86 178,553.57 | 19,998,000.00 |
| | | | | | <u>18,926,678.57</u> |
| (Total Amount in Words) Eighteen Million Nine Hundred Twenty Six Thousand Six Hundred Seventy Eight and Fifty Seven Centavos Only | | | | | |
| Conforme: | | Very truly yours, | | | |
|  <u>PINA ALCALA</u> Signature over Printed Name of Supplier | |  <u>DR. ANNABELLE V. BRIONES</u> Signature over Printed Name of Authorized Official | | | |
| <u>Sept. 27, 2023</u> Date | | Director Designation P 9/11 | | | |
| Fund Cluster : VIP Project 4: De Novo Synthesis of Non-infective Zika Pseudovirus as Reference for Diagnostics and Vaccines Funds Available : | | | ORS/BURS No. : <u>TF02023092371</u> | | |
| | | | Date of the ORS/BURS: _____ | | |
|  <u>PATRICIA ASHLEY M. MENDOZA</u> Signature over Printed Name of Chief Accountant/Head of Accounting Division/Unit | | | Amount : <u>19,998,000.00</u> | | |