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PR No. 1000020763 (Rfx No. 6100001021)

Detailed Technical Specifications for Wide angle X-ray diffractometer with high temperature and electrochemical attachment.

1. BASIC: Diffractometer cabinet (radiation enclosure) with suitable electronics rack and system controller for basic & additional electronics (e.g. non-ambient controllers), also equipped with suitable doors for easy access to the diffractometer. The cabinet complies to the regulations on X-ray, electrical and mechanical safety. The emission level is below 10 microSievert per hour at 10 cm distance from the system surface. Also included is suitable data acquisition software Data Collector that contains the following functionality such as: data acquisition based on suitable format,, measurement strategy determination tools, configuration and measurement management, automatic processing, data conversion and viewing functionality for X-ray diffraction systems.
2. X-RAY GENERATOR TUBE: The sealed tube X-ray generator (Copper) should be designed for an enhanced stability of the focal spot to use with various optics such as Slits, X-ray mirrors, Xray Multi graded Mirror, hybrid and Johansson monochromators etc. The X-ray tube should be equipped with one window for line focus and one for point focus. Minimum power of generator being 3 kW. Voltage not less than 20 kV.
3. SAMPLE STAGE:
   A. SPINNING SAMPLE & NON-SPINNING SAMPLE STAGE: Fixed WAXS stage and Spinning Sample stage for sample spinning with programmable phi-axis positioning or scanning for analysis of powders or solid samples
   B. AUTO SAMPLE CHANGING STAGE: An auto sample changing stage for powder samples is to be provided for a minimum of 6 samples and option for spinning.
   C. CIRCULAR HOLDERS FOR REFLECTION: Sample holder having both bottom and top plate used for the back-loading or front-loading of powder specimens, either manually or semi-automatically. 10 nos.
   D. LOW BACKGROUND SAMPLE HOLDER : low background or zero background sample holder for small sample quantity – 5 nos.
   E. CIRCULAR HOLDERS FOR TRANSMISSION: Sample holders for measurement of samples in transmission geometry.
   F. Powder Sample Preparation Kit.
4. INCIDENT BEAM OPTICS FOR LINE FOCUS BASED ON SLITS:
   A. Soller slit 0.02 radians or near about equivalent aperture in deg./mm for incident beam optics, exchangeable with Soller slit of 0.08 radians or near about equivalent aperture in deg./mm.

B. Divergent beam optic to perform Bragg-Brentano measurements.

5. GONIOMETER:
   A. Radius not less than 240 mm.
   B. Minimum step size of 0.0001 degrees
   C. Minimum range of 0 to 120 degrees in two theta
   D. Minimum scan speed of 0.05 degree per minute or less
   E. Maximum scan speed of 10 degree per minute or more

6. DETECTORS AND MONOCHROMATORS
   A. Semiconductor detector for both line and point detector X-ray diffraction applications having following features
      - Maximum global count rate of more than 1 X 10^8 (one hundred million) CPS
      - Active area more than 100 mm squared
      - Energy resolution around CuK better than 25 % or less than 2000 eV for Cu Kα at 25°C
      - 0D, scanning and static 1D functionality
   B. Ni Beta filter.
   C. Fixed Anti scatter slit assembly
   D. Diffracted beam linear detector (1D) monochromator
   E. Soller slit 0.02 radians or near about equivalent aperture in deg./mm, for large aperture it should be exchangeable with Soller slit 0.04 radians or near about equivalent aperture in deg./mm.

7. SOFTWARE

Performs data treatments and XRD phase identification on various systems. Allows installation of the software on one additional device. Includes the following features:

   A. Search-match algorithm uses peak and profile data
   B. Auto-residue scoring
   C. Advanced reporting functions
   D. Graphics for examining, displaying, and editing diffractograms
   E. Supports any number of user-defined reference databases
   F. Includes batch feature for auto function of a sequence
   G. Automation ready - can be launched from a command prompt
   H. Similarity analysis of scans (cluster analysis up to 50 scans)
   I. Referenced Intensity Ratio (RIR) for estimation of quantities of all identified phases
   J. Percent crystallinity
   K. Very fast profile fitting
   L. Line profile analysis, microstructure analysis by profile fits
   M. PLS partial least squares to determine/quantify one property directly from raw data
   N. 64 Bit Windows 10 Professional compliant
   O. Preparing automated Rietveld analysis
   P. Unit cell indexing and Unit cell refinement
   Q. Space group testing and unit cell transformation
   R. Structure reviewing, distances and angles
   S. Structure solution

T. Line profile analysis, microstructure analysis by profile and structure fits
U. Mixed fits from structure-, HKL- and profile data
V. The vendor must also provide the latest ICDD PDF4 database original license for search match functionality with 3 years validity from the date of purchase.

ADDITIONAL ATTACHMENTS/ACCESSORIES:

8. Sample heating stages capable of heating from ambient to 1500 ^{o}C in inert or vacuum with suitable software to collect XRD scans at intermittent temperature.
9. Electrochemical stage with electrical feedthrough through the X-ray chamber and potentiostat for in-situ analysis for aqueous electrochemistry applications.
10. Compatible Chiller unit, Suitable UPS for XRD as well as water chiller, branded computer & laser printer should be offered.
11. Warranty 1 year from date of successful installation.