X-RAY DIFFRACTION

D6 PHASER AUTOLOADER

Automated Benchtop Powder XRD

The Power of Automation

Automated X-ray diffraction provides accurate and comprehensive data collection and evaluation. From pharmaceuticals to construction materials, data-driven decisions enhance overall production quality and ensures that products meet stringent quality standards.

In today's fast-paced industrial landscape, quality and process control plays a pivotal role in ensuring product consistency, safety, and compliance. Whether you're managing a laboratory, overseeing production processes, or handling critical materials, the shift toward automated quality control offers substantial advantages.

When it comes to X-ray diffraction, the D6 PHASER AUTOLOADER provides a state-of-the-art solution for analysis ranging from positive material identification to phase and structure quantification. Access to these fast and reliable measurements is ideal for big data initiatives.

Laboratory managers face the challenge of optimizing resources while maintaining quality. Automated quality control reduces labor costs by minimizing manual tasks. Efficient resource utilization translates to cost savings and streamlined operations. Moreover, consistent handling and reduced variability enhance data quality, contributing to reliable results. Managers can rest assured that their processes meet the quality control protocols.

Key features

The D6 PHASER AUTOLOADER is a dedicated X-ray powder diffractometer with external sample loader featuring:

- Industry-standard specimen rings
- Up to 5 magazine positions
- Manual loading position for priority samples
- Optional position for sample transit from/to conveyor belt
- Support for up to 96 mm wide conveyor belts
- Sample pre-loading
- Specimen rotation during measurement
- Optional workbench

Technical Excellence, Efficiency and Versatility

Powerful Performance

The D6 PHASER is engineered to meet the rigorous demands of quality control engineers and laboratory supervisors. It features an X-ray source power of up to 1.2 kW, the highest available on the market, ensuring efficient sample analysis. The system's short beam path contributes to its superior performance compared to many floor-standing systems. The tailored beam optics are designed for precision, providing optimal intensity and accuracy. Additionally, the D6 PHASER AUTOLOADER benefits from industry leading hardware such as Dynamic Beam Optimization (DBO) and advanced detectors, ensuring data quality on par with Bruker's floor-standing instruments. This integration facilitates a high level of analytical performance in quality control processes.

Sample Handling and Automation

The D6 PHASER AUTOLOADER is designed to streamline sample handling. It accommodates up to five sample positions, providing flexibility for a variety of holders. A precision mechanical gripper ensures safe and efficient handling. Samples are preloaded on an externally accessible sample swing, while maintaining X-ray safety for the operator. This allows a continuous measurement workflow with minimal downtime by exchanging a processed sample for the next one in the queue while a measurement is running. The loading position also allows manual sample introduction, ideal for priority measurements. Sample size compatibility includes both 51.5 mm steel rings and smaller 40 mm holders made from boric acid.

Once loaded into the measurement position, the sample is rotated, a critical feature that contributes to improved particle statistics. By continuously rotating the sample, data accuracy is improved, resulting in more precise and statistically robust results.

Seamless Integration

- **Stand-Alone Operation**: the D6 PHASER AUTOLOADER operates independently, without direct connectivity to an automated sample preparation system. Users can run predefined analysis recipes using pushbutton templates. These templates encapsulate the necessary steps for data acquisition, including parameters like exposure time, scan range, and detector settings. Once the measurement is complete, the AUTOLOADER follows the template instructions to evaluate the data.

- **Online Operation**: the analyzer is part of a larger automated system within the plant. The AUTOLOADER interfaces directly with the plant's control center, which oversees various processes, including sample preparation machines, transport conveyors, and the analyzer. The well-established AXSCOM software (already utilized for floor-standing XRD and XRF analyzers) serves as the bridge between the D6 PHASER AUTOLOADER and external control systems.

Efficiency and Accessibility Redefined. The D6 PHASER AUTOLOADER isn't just another benchtop X-ray diffractometer — it's streamlining your workflow, enhancing safety, and maximizing efficiency.

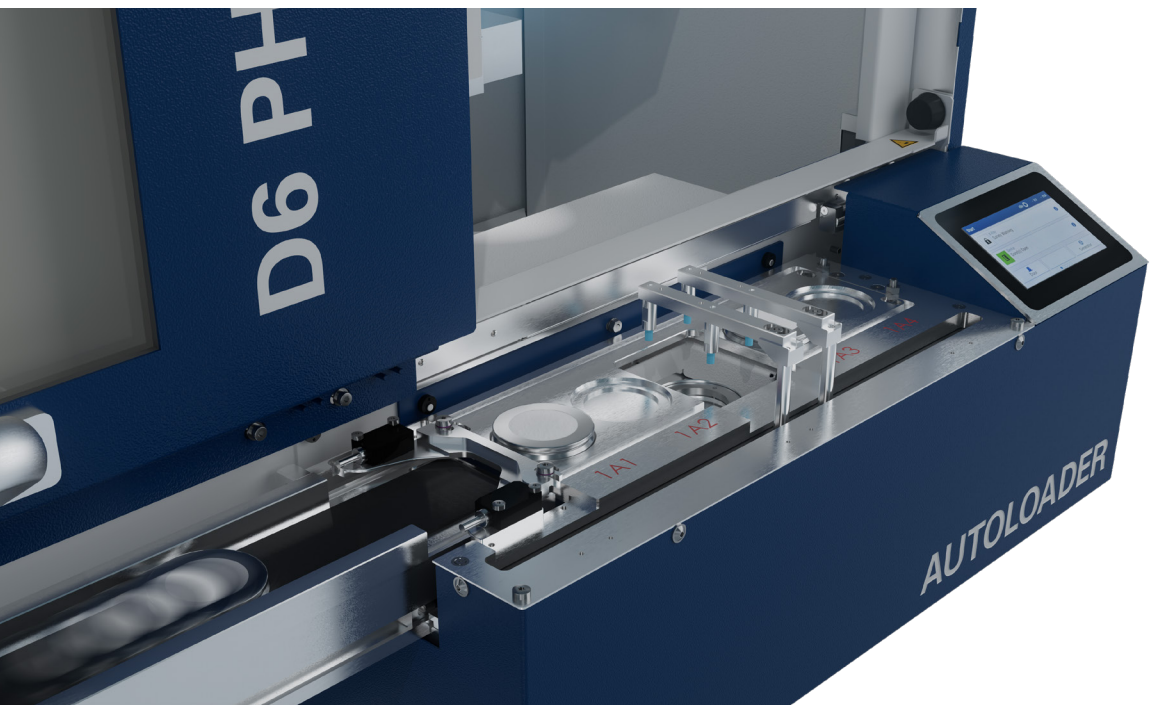

Figure 1
D6 PHASER X-ray powder diffractometer equipped with AUTOLOADER for online operation.

The **DIFFRAC.SUITE** provides comprehensive analytical capabilities when it comes to automated powder diffraction data analysis.

- **DIFFRAC.DQUANT** offers two distinct approaches for automated quantification of sample composition. The first method, Classic Single Peak Calibration-Based Quantification, evaluates single peaks using calibration curves and reference standards, making it ideal for rapid routine analysis and straightforward tasks with low quantification limits. On the other hand, the **Full Pattern Calibration-Based** Partial Least Squares (PLS) method utilizes regression to analyze the entire diffraction pattern. This approach models complex relationships between the diffraction pattern and composition, enabling accurate quantification of properties, even those not directly related to concentrations. Both methods are integral to DIFFRAC.DQUANT, catering to different analytical needs.

- The Rietveld method, in **DIFFRAC.TOPAS BBQ**, is a technique for phase analysis by crystal structure-based quantification. It uses detailed crystallographic information to fit the entire diffraction pattern of a sample. This comprehensive approach allows precise determination of quantitative phase composition, ensuring that calculated phase fractions are accurate and reliable. It's a established tool for researchers and industrial users who require detailed phase analysis in their work. With pre-built application packages for construction materials, aluminum, pharmaceutical or battery materials markets, it's easy to implement.

- **DIFFRAC.EVA** offers two different methods of automated material analysis. Positive Materials Identification (PMI) is a correlation-based analysis that identifies the type of material by matching measured reference scans with unknown sample scans. It's a fast method of material identification without the need for detailed analysis of the components of a mixture. Conversely, SQUALL (semi-quantitative analysis of all materials) provides automatic identification of the phases present in a sample. This is achieved by matching reference scans and using Reference Intensity Ratios (RIR) to provide a more detailed understanding of the phase composition of the sample, particularly useful for phases where an accurate or well-defined crystal structure is not available or a good analytical description of the peak profiles does not exist (e.g. clays).

Data Management:

The **DIFFRAC.SUITE** is designed for efficient data management. All measurement and evaluation results are stored in the instrument's internal database. This centralized storage not only makes data easy to access, but also helps to maintain and manage data integrity. The system can also integrate smoothly with a plant's Laboratory Information Management System (LIMS). This integration is critical because it ensures traceability, quality control, and compliance with industry standards. This increases the reliability and accountability of the analytical processes within the plant.

cGxP Solutions:

The 21 CFR Part 11 compliant version of the DIFFRAC.SUITE has been carefully designed to ensure the integrity and security of the data in a regulated environment. It stores measured data and reports as electronic records for efficient retrieval and archiving. The software also provides a secure and verifiable record of operations by capturing electronic signatures associated with method execution, data evaluation and reporting. Critical for compliance and oversight, detailed audit trails are maintained to record any changes, accesses, or modifications to the electronic records. To protect sensitive data from unauthorized access, robust security controls are implemented, including access controls, user authentication, and authorization mechanisms. Taken together, these features help to ensure compliance with regulatory standards and provide a trusted framework for the management of critical data.

Figure 2
Results manager view, showing selected results of TOPAS quantitative phase analysis results from a cement plant.

Technical specifications

Geometry	Theta/Theta (sample always horizontal)
Max. usable angular range	-3 to 152 ° 2θ
Accuracy	± 0.01° through entire measuring range
Achievable peak width	< 0.03° FWHM
X-ray wavelengths	Cu, Co, Cr standard ceramic sealed tube (others on request)
X-ray generator options	540 W (30 kV, 18 mA) 600 W (40 kV, 15 mA) 1.2 kW (40 kV, 30 mA)
Detector options	SSD 160-2 LYNXEYE-2 LYNXEYE XE-T
Sample stage	Rotating sample of 51.5 or 40 mm diameter
AUTOLOADER	Mechanical gripper for up to 5 positions and 1 manual position. Optional belt connection
Stage attachments	Fixed or motorized air-scatter screen
Primary optics	Fixed or motorized, divergence slit, Soller collimators
Cooling options	Internal water-to-air cooling (540 W, 600 W, 1.2 kW) Connection to laboratory supply, 3.6 l/min at 3 – 4.5 bar
Exterior dimension (h x d x w)	70.0 cm (27.6") x 75 cm (29.5") x 88.5 cm (35.0"), width 110 cm (43.3") with open door
Max. weight	160 kg (353 lbs)
Power supply	100 V – 240 V (600 W and 540 W), 200V – 240 V (1.2 kW)
Computer	PC connected via LAN interface

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