



## X-RAY DIFFRACTION

# DIFFRAC.DQUANT V2

Simplifying Advanced Quantitative Phase Analysis  
for Crystalline and Amorphous

### Streamlined Workflow and User-Friendly Options

DQUANT, the latest BRUKER software for quantitative phase analysis from X-ray diffraction data, revolutionizes the field of X-ray powder diffraction. Utilizing one or more diffraction peaks, DQUANT establishes highly accurate calibrations based on standard reference samples.

With support for various quantitative procedures, including the ratio, addition, and Chung internal reference methods, DQUANT offers a comprehensive solution. Seamlessly integrated into the DIFFRAC. SUITE software package for measurement and data evaluation, it covers everything from calibration models to data correction and evaluation routines. Designed to cater the users of all skill levels, DQUANT provides a guided workflow from method definition to the presentation of final results. Whether interactive or fully automated analysis is preferred, DQUANT empowers the user with a single-button operation.

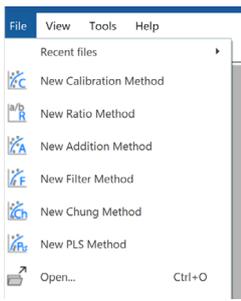
Ideal for both seasoned lab managers and daily operators, DQUANT combines innovative software, streamlined workflows, and method architecture to deliver maximum flexibility with unparalleled simplicity. Experience the new benchmark in quantitative crystalline-phase analysis through X-ray diffraction with DQUANT.

Innovation with Integrity

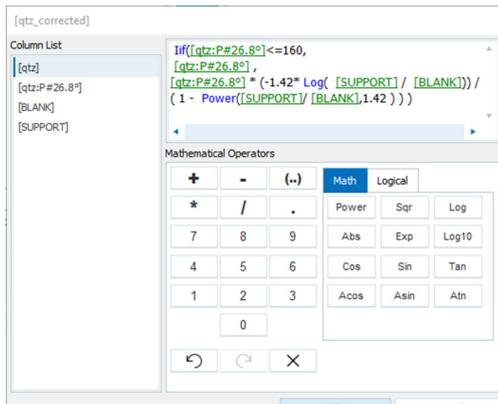
### Introducing Version 2

DQUANT now incorporates an advanced peak profile fitting capability for precise intensity determination, especially beneficial when dealing with overlapping peaks. Amplitude and peak area, are available for subsequent calibrations. A consistent fit model is established using reference scans, ensuring accuracy, and reliability. This model is then used for the automatic evaluation of unknown samples.

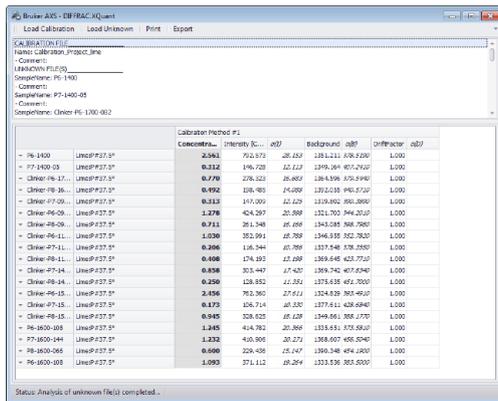
Version 2 includes Partial Least Squares regression, a powerful technique for extracting sample properties, such as concentrations, from X-ray powder diffraction data. Two validation methods, test set validation or cross-validation, are offered during the training step to ensure model robustness. The software also identifies outliers and evaluates scan data that may not improve the results.



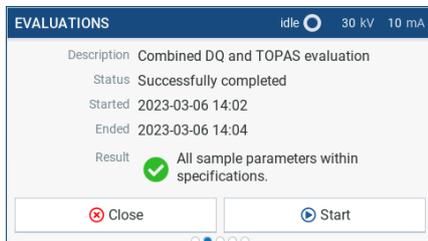
**Figure 1** Predefined calibration methods create data trees, specific to the analysis. To customize the method simply work your way through the data tree from top to bottom.



**Figure 2** Expression editor with syntax highlighting for defining concentration and intensity modules.



**Figure 3** While the expert mode allows access to the full functionality of DQUANT, the operator mode is limited to the evaluation of unknown samples.



**Figure 4** DQUANT is seamlessly integrated with DIFFRAC.SUITE for automated data evaluation.

## Simplified Workflow and Flexible Options: Effortless Analysis for All Users

DQUANT is designed to provide a seamless analysis experience for laboratory supervisors and operators with varying levels of expertise. Here is how DQUANT simplifies the workflow and offers flexible options:

### 1. Calibration and Interactive Analysis

DQUANT serves as an expert system for laboratory supervisors, guiding them in setting up calibration methods. With its intuitive graphical user interface and pre-configured data trees, the software streamlines the process for different analytical tasks. Calibration curves and intensity-drift correction can be established and verified directly in the user interface mode. Experienced users also have the option to analyze unknown samples interactively.

### 2. Tailor-Made Reporting and Analytical Flexibility

Concentration-modules in DQUANT allow for customized reporting of results based on calibrated concentrations. For maximum analytical flexibility, intensity-modules are available. The built-in formula editor enables easy column arithmetic of intensities, providing access to user-defined intensity corrections, peak overlap correction, and averaging techniques to reduce preferred orientation effects.

### 3. Drift Monitoring and Absorption Correction

DQUANT supports the establishment of drift monitors to keep calibrations up-to-date. Drift history is recorded from the initialization date, allowing additional standards to be added without re-measuring other standards. Additionally, the software supports absorption correction for samples of finite thickness, ensuring accurate determination even for micrograms of material.

### 4. Streamlined Data Evaluation and Results Presentation

DQUANT leverages the power of the DIFFRAC.MEASUREMENT package to simplify quantitative analysis. Measurement jobs link scan and evaluation conditions to sample IDs, including unknown samples, standards, and drift monitor samples. The data evaluation and results presentation can be triggered automatically or performed manually by the operator. The process is as simple as pushing a button.

### 5. Automation and Simplified Interface

For users who prefer more control, DQUANT offers a simplified user interface. Verified calibrations can be loaded, and batches of unknown samples can be analyzed without modifying the calibration. Results for multiple samples can be generated in a single run and presented according to the defined layout in the calibration project file. Various table layouts are provided, with customizable options for further export, printing, or generating documents in PDF or XPS formats.



## DQUANT: Empowering Industries with Advanced Analytical Capabilities

DQUANT, the powerful software solution within the DIFFRAC.SUITE, offers a range of applications across diverse industries. Here's how DQUANT can transform your operations:



### Minerals and Metals Industry:

- Accurate determination of Fe<sup>2+</sup>/Fe<sup>3+</sup> in iron ore
- Quantification of retained austenite in steel
- Electrolytic bath control for aluminum production



### Chemistry:

- Differentiation between white pigment rutile/anatase
- Precise analysis of fertilizers and other chemical compositions



### Construction Materials:

- Quantification of free lime in clinker for construction materials



### Workers Health Surveillance:

- Detection of breathable silica dust or asbestos deposited on filters



### REACH Compliance:

- Concentration analysis of minerals like quartz in filter dust or materials such as limestone

### Pharmaceutical Industry:

- Identification of amorphous and crystalline forms without crystal structure requirements
- Full compliance with cGxP/21 CFR Part 11 regulations for pharmaceutical industry needs

With its wide range of applications and compliance with industry standards, DQUANT empowers businesses across various sectors to achieve accurate and reliable analysis, ensuring optimal efficiency and regulatory compliance.

