



Product Sheet XRD 50

DIFFRAC.DQUANT

- Software Feature Overview

DIFFRAC.DQUANT is the BRUKER software for quantitative phase analysis from X-ray diffraction data. It uses one or more individual peaks, to establish calibrations from standard reference samples.

DQUANT is a complete package that covers calibration models, data correction and evaluation routines. It is fully integrated in the DIFFRAC.SUITE software package for measurement, data evaluation and reporting.

Modes of operation

- Interactive workflow to set-up data evaluation methods in the graphical user interface
- Operator mode for interactive analysis of one or several unknown samples without the need to access the calibration
- Fully automated analysis of unknown samples as part of DIFFRAC.SUITE jobs or push-button solutions after the end of the measurement
- File based operation
- Support of DIFFRAC.SUITE database operation for measurement data, DQUANT methods storage and results export

Analytical models

- Calibration method
- Addition method
- Ratio method
- Simultaneous analysis of XRD and Calcium XRF data
- Chung methods (Reference Intensity Ratio)

Intensity models

- Manual (via keyboard)
- Single numeric (Calcium XRF data, measured at a fix position)
- Integrative (numeric integration by summation over a user defined range)
- Interface to peak-fit results from DIFFRAC.TOPAS or DIFFRAC.TOPAS BBQ

Intensity corrections

- Drift correction of primary XRD intensity and XRF proportional counter
- Tabular and graphical monitor history
- Absorption correction for thin specimen (filter papers)
- Background correction

Standards

- Number of standards not restricted by the DQUANT software
- Addition of new standard to calibrations without re-measuring older standards

Data types for calibration and unknowns

- Concentration of phases, the element Calcium, and concentration modules (value calculated from concentration via built-in formula editor)
- Number of peak intensities per compound not restricted by the DQUANT software

- Calibratable intensity module = values calculated from intensities via built-in formula edito

Calibration models and tools

- Regression curves up to 3rd order (constant, slope, square, cube)
- All parameters selectable: used/unused and fix/refine
- Weighting schemes: Unit weights, 1/sigma, 1/sigma squared
- Linear multivariate regression
- Intensity, concentrations and residuals chart
- Calibration table with selectable standards for outlier elimination
- Sequences (conditional calibration programs)

Unknowns calculation

- Number of unknowns in batch operation not restricted by DQUANT software
- Single file or batch processing

Reporting

- Individual or combined reports for the calibration and the results of unknown samples
- Connection to 3rd party laboratory information systems via proprietary exchange format
- Results export to DIFFRAC.SUITE database for reporting in Results Manager

Supported computer operation systems

- Windows 8.1 and 10 (32 and 64 bit)

Language support

- English, French, German, Japanese, Chinese

Compliance

- DQUANT is part of the DIFFRAC.SUITE Part 11 package. The software fully complies with the cGxP/21 CFR Part 11 requirements of the pharmaceutical industry.

Update and upgrade policy

- Free maintenance updates (without access to new features) are available from brukersupport.com
- Bug fixes are cumulative and can be applied via maintenance update to any previous version
- Upgrades are paid versions with a higher license level that provide new functionality

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