X-RAY DIFFRACTION

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, or the entire diffraction scan in the case of Partial Least Squares Regression (PLSR), 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 (*.raw, *.brml)
- 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)
- **New V2: Partial Least Square Regression (PLSR)**

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
- **New V2: Profile fit of individual peaks with optional use of area or amplitude in the calibrations**

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 editor
- Properties not directly related to an individual phase but showing correlation to the XRD scan for PLSR

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 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 10 and 11 (64 bit)

Language support:

- English
- French
- German
- Japanese

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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