



Product Sheet XRD 51

DIFFRAC.EVA

● Software Feature Overview

DIFFRAC.EVA provides tools for the analysis of one- and two-dimensional diffraction data. It supports all kinds of Bruker detectors and scan types. The EVA functionality covers a broad analytical spectrum from data reduction, basic scan evaluation and presentation, detailed peak analysis, phase identification and quantification, to the determination of crystallinity and crystallite size. EVA interfaces with all relevant databases for phase ID but may additionally use crystal structures and complementary information from e.g. XRF based chemical analysis for its award-winning species identification.

Furthermore, DIFFRAC.EVA supports the evaluation of large amounts of data that originate from today's state-of-the-art fast detectors, the use of in-situ

environments, or high-throughput screening studies. The software provides specific chart types, but also advanced chemometrics tools for cluster analysis and pattern-matching based species identification and phase quantification.

It fully supports conventional file-based tasks but also integrates the DIFFRAC.SUITE database infrastructure for daily work, even in controlled environments as required by the 21 CFR Part 11 regulations for the pharmaceutical industry. Finally, DIFFRAC.EVA is used for the preparation of publication ready graphs and user specific reports, either directly in EVA or using the DIFFRAC.SUITE RESULTS-MANAGER and the instrument database.

General data evaluation options

- Scan arithmetic (add, subtract, combine, normalize, merge, re-bin)
- Peak search and creation of peak lists, e.g. for phase identification
- Manual and fully automatic background determination
- Data smoothing (Savitzky-Golay method or Fourier filtering)
- $K\alpha_2$ -stripping (enhanced Rachinger method)
- 2theta-offset and sample displacement corrections
- Peak/Background and Signal/Noise calculation (new V6)
- Calculation of mass absorption coefficients and corresponding X-ray penetration depth into the specimen
- Calculation of profile parameters such as line position, center of gravity, integrated area, half width and more (area tool)
- Analytical profile analysis for single peaks and patterns (fit tool)
- Automatic 2theta-offset detection (new V6)
- Crystallite size determination (Scherrer method)
- Simultaneous evaluation of multiple scans
- Undo / redo of view operations

Advanced XRD2 data evaluation and display options

- Single 2-D frame integration over gamma and 2Theta with full frame, wedge, ring and line cursor
- Integration on merged 2-D frames with slice, wedge and ring cursor
- Multiple integrations on stackable 2-D frames with one click
- User configurable masks with angular or pixel coordinates
- "Rocking curve analysis" on stackable 2-D frames with various frame properties
- Frames are automatically grouped into mergeable or stackable lists
- For large zoom factors the 2-D view displays the number of counts inside the pixel areas

Cluster analysis

- Combine up to four datasets: XRD, XRF, IR, Raman, TGA/DSC, numeric data (new V6)
- Automatic Weighting Scheme
- Five clustering methods
- Cluster Validation Tools
- Customizable Analysis Methods
- Re-run selected analysis

- Interactive Dendrograms
- Cell view
- 3-D MMDS and PCA plots
- 6-D plots of sample prep info
- Numerical Results
- Amorphous Phases Identification
- Reference patterns for mixtures
- Quality Control mode
- Report Writer
- Online documentation, Program Tutorial
- SQUALL: semi-quantitative analysis based on reference scans
- PMI: Positive Materials Identification (new V6)

Species identification and quantitative phase analysis options

- Supports ICDD PDF2, PDF4 plus, Web PDF and PDF4 AXIOM, user databases and the COD reference database
- User update of COD search and structure database (new V6)
- Search by various selection criteria such as chemical composition, card quality marks, subfiles, and more
- Simultaneous search in multiple reference databases
- Search on full-scan or individual peak data
- Search for solid solutions and isostructural phases
- Highly sophisticated residual search with Match peaks supporting the identification of minor phases
- Wavelength cursor for interactive identification of spectral aberrations (tungsten, $K\beta$ lines)
- Consideration of 2theta-offset and sample displacement errors
- Graphical adjustment of peak positions via tuning of lattice parameters e.g. to describe solid solutions
- hkl-generator for calculating peak positions based on lattice parameters and space group to aid identification of missing or redundant specimen peaks
- Interactive overlay of the search results with the measurement data for easy evaluation
- Display of stick patterns or "Rietveld-type" tick marks with hkl-indices, if available
- Display of calculated profiles of the individual species in a mixture
- Quantitative analysis based on RIR (reference intensity ratio) and spiking methods
- Matching lines view for individual peak analysis (new V6)
- Degree of crystallinity determination

- “Combined XRD-XRF analysis”: Validation and improvement of search as well as quantitative phase analyses results using elemental analysis results; direct access to Bruker XRF databases, formatted ASCII-files, and more
- Support of variable counting time data
- Use of crystal structures (cif- and DIFFRAC.TOPAS str-format) for pattern generation
- TOPAS connectivity (STR export of the selected candidates)
- Create PRO file (new V6)
- STR information added to COD und User DB (new V6)
- Auto phase ID

Data display options

- Self-explaining user interface, fully customizable by each individual user (dockable panels, configurable tool-bars; save/load general settings, tool-bar layouts and application specific screen layouts)
- Advanced picture-in-picture (PIP) and vertical-in-place (VIP) zoom options
- Customizable 2-D and 3-D multi-scan representations (iso-intensity plots, waterfall plots)
- Free customization of graphics and text properties for creation of publication-ready figures
- Side view to for charting additional information (non-ambient properties, time, crystallinity) to combine with multi-scan presentations
- Bragg 2D: Two-dimensional visualization of sample inhomogeneities (large crystallites, preferred orientation), measured with a 1-dimensional detector

Data exchange and reporting options

- Creation of customizable, high quality analysis reports including charts, tables, and complimentary information
- Data exchange options to and from any other Windows application: copy and paste, Windows bitmaps and metafiles
- Display and printout of all reference database patterns
- Data conversion from/to Bruker’s proprietary file format to ASCII single Y, 2 column XY file or a 3 column XYE file
- Comprehensive measurement parameters reporting
- Predefined and customizable table layouts
- Connection to DIFFRAC.SUITE instrument database for multi-sample reporting of scan, peak and pattern properties via RESULTS-MANAGER

- LabNotes (new V6)
- User defined pattern color schemes to match with complimentary techniques (SEM, microXRF) (new V6)

Compliance

- DIFFRAC.EVA 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

Multilanguage support

- English, French, German, Japanese

Supported computer operation systems

- Window 8.1 and 10 (32 and 64 bit)
- Supporting multi-core CPUs

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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