



## X-RAY DIFFRACTION

# DIFFRAC.BBE – Black Box Evaluation

## Software Feature Overview

### What is DIFFRAC.BBE?

DIFFRAC.BBE (Black Box Evaluation) is a Windows console application that automates XRD data evaluation tasks. It can be triggered automatically from DIFFRAC.MEASUREMENT CENTER after a measurement or manually from the command line. This software automates data evaluation tasks through “workers,” offering expanded functionality and integration with other evaluation programs, the BRUKER instrument database, and LIMS systems.

### How does DIFFRAC.BBE work?

DIFFRAC.BBE operates primarily through macro scripts written in the YAML language. These scripts act as instructions for the software, detailing the evaluation tasks to be performed. A macro archive containing the instructions macro file and all other necessary input files can also be utilized.

This archive is automatically unpacked at runtime into a secure, tamper-proof workspace that acts as a local file server to ensure data integrity throughout the evaluation process.

### DIFFRAC.BBE Key Features

- Integration with DIFFRAC.TOPAS
- Integration with DIFFRAC.TOPAS BBO
- Support for DIFFRAC.EVA (PMI, SQUALL, Workflows, EVA-Core)
- DIFFRAC.DQUANT
- DIFFRAC.STRESS
- UTF Script execution
- Database import and results export
- Batch processing. Synchronous or Asynchronous operation
- Integration with DIFFRAC.MEASUREMENT CENTER

## Workers Supported by BBE

### DIFFRAC.TOPAS

BBE's powerful automation capabilities, combined with the flexibility and analytical depth of TOPAS, provide a comprehensive solution for a wide range of XRD data analysis needs. BBE's integration with TOPAS facilitates various automated XRD applications:

- **Rietveld Refinement:** Automates execution and parameter extraction from Rietveld refinements for quantitative phase analysis, crystal structure determination, and microstructural analysis.
- **Batch Processing:** Enables processing multiple measurements with the same TOPAS refinement settings, streamlining the analysis of large datasets.
- **Parameter Monitoring:** Tracks specific parameters, such as lattice parameters, crystallite size, or phase concentrations, across multiple measurements.
- **Customizable Reporting:** Offers flexible output options (XML, CSV, database) for customized reporting and integration with LIMS systems.

### Benefits of Using TOPAS with BBE

- **Increased Efficiency:** Automates repetitive TOPAS refinements, saving time and effort.
- **Improved Reproducibility:** Ensures consistent application of refinement settings across multiple measurements.
- **Reduced Errors:** Minimizes potential errors associated with manual data processing.
- **Enhanced Data Management:** Streamlines data storage and reporting, facilitating integration with other systems.

BBE is compatible with DIFFRAC.TOPAS v6 or higher. TOPAS is executed in launch mode.

### DIFFRAC.TOPAS BBQ

TOPAS BBQ is an automated version of TOPAS dedicated to Black Box Quantitative analysis. DIFFRAC.BBE is compatible with DIFFRAC.TOPAS BBQ version 7 or higher. This version includes BBE as the automation engine of BBQ and the TOPAS v7 compute kernel. BBE supports both legacy mode and automatic mode for TOPAS BBQ integration.

- **Legacy Mode:** Designed for users with existing TOPAS BBQ installations, allowing them to upgrade to the latest TOPAS BBQ kernel easily without updating the Start Job templates. The reporting capability is limited, compared to Automatic Mode.
- **Automatic Mode:** Intended for fresh BBQ installations, enabling users to take advantage of the extended RESULTS MANAGER features introduced with MEASUREMENT CENTER 8.6.3 and 8.7. Existing application templates can be updated for automatic use easily.

### DIFFRAC.EVA

BBE simplifies the process of automated phase identification with EVA Core by using macro scripts to define the input data, filters, output options, and database selection. EVA Core is the automated phase identification component extracted from the full DIFFRAC.EVA software and is part of the EVA distribution. It supports chemical and database filters created in EVA. The supported search databases cover ICDD PDF2, PDF5+, PDF AXIOM, COD, and EVA User Databases.

Building on the automation capabilities of BBE version 1, DIFFRAC.EVA integration in version 2 introduces workflow execution, enabling seamless orchestration of evaluation tasks through structured EVA workflows. This enhancement allows users to define and run complex analysis sequences with minimal manual intervention.

Additionally, version 2 incorporates PMI (Positive Material Identification), a correlation-based method designed to assign material types to unknown samples where precise phase identification is not required. This approach is particularly useful in quality control and screening applications. The release also includes SQUALL, a semi-quantitative phase analysis module that leverages pattern matching against reference scans to identify and estimate the abundance of individual phases.

## Data Exchange, Storage, and Visualization Supported by DIFFRAC.BBE

### UTF Script Execution

BBE operates primarily through macro scripts written in a YAML-based language. Within the macro script, various analytical and data-handling tasks are defined. A key strength of the macro script is its ability to concatenate tasks in multi-step evaluations. BBE allows the execution of User Task File (UTF) scripts as part of a larger evaluation sequence.

These scripts, written in Windows Batch syntax, provide a high degree of customization and flexibility in the automation process.

### DIFFRAC.STRESS

BBE extends its automation capabilities to the DIFFRAC.STRESS package, streamlining the evaluation of residual stress measurements. Once the initial data evaluation is implemented, BBE executes the full analysis pipeline—covering data pre-processing, peak position determination, stress calculation, and results storage in the Bruker database. While command scripts are interactively developed within the STRESS software, BBE ensures consistent execution and integration into broader workflows. Results can be reviewed using STRESS's built-in report generator, or externally via RESULTS MANAGER or the ANALYSIS LIBRARY within the XRD ASSISTENT suite. This automated approach is especially valuable for users applying single push-button methods in routine quality control across industries such as metals, automotive, and precision-machined components, and also proves effective for evaluating coatings and layered materials.

### Data Exchange

- **Standardized Bruker Format:** DIFFRAC.BBE uses the same data exchange format (temp\_c.xml) as other Bruker DIFFRAC.SUITE software, including EVA in manual database mode, automated EVA (SQUALL and PMI), and DIFFRAC.DQUANT.
- **Legacy Bruker Format (temp\_c.dat):** BBE also supports the older ASCII file format (temp\_c.dat) for compatibility with existing automation systems in the field.
- **CSV Files:** BBE can generate CSV files, which can be read by common spreadsheet software and are suitable for LIMS connections.
- **Parameter Export:** BBE automates the export of TOPAS parameters into the instrument database.

### Data Storage

- **Instrument Database:** Evaluation results are automatically transferred to the instrument database, offering centralized storage, consistent presentation, flexibility for report generation, and review capabilities. DIFFRAC.BBE v.2 is compatible with MEASUREMENT CENTER v 8.8.

### Data Visualization

- **RESULTS MANAGER:** The instrument database's RESULTS MANAGER provides a common interface for visualizing evaluation results.
- **Post-Visualization:** TOPAS launch mode refinements can be visualized at any time in the instrument database.

In summary, DIFFRAC.BBE provides multiple data exchange formats, utilizes a robust database solution for storage, and offers visualization capabilities through the RESULTS MANAGER, ensuring efficient handling of evaluation results.

### Supported Computer and Operating Systems

- Windows 10 and 11 (64 bit)

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