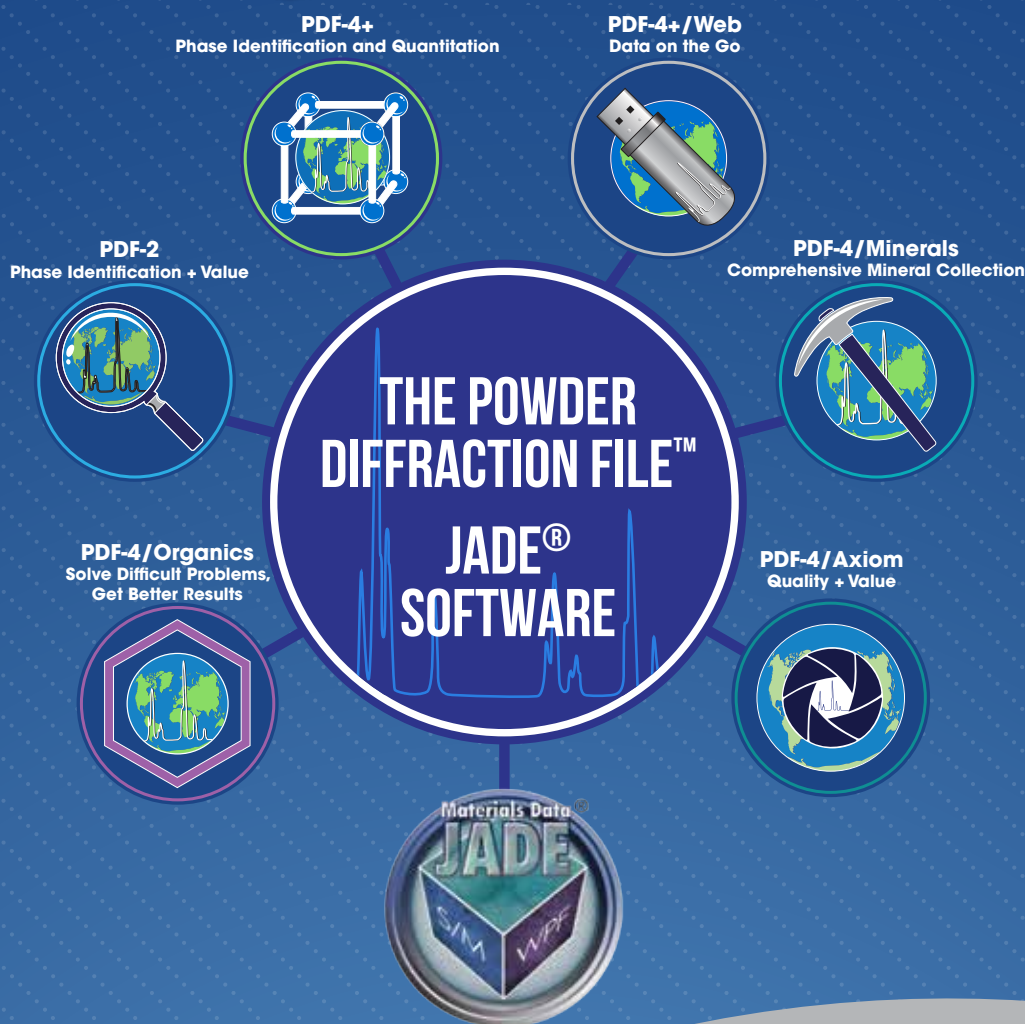




# Powder Diffraction File™ 2023 Databases & JADE® Software

## DIFFRACTION DATABASES AND ANALYSIS SOFTWARE

*You Can Trust*





## JADE Pro

### JADE Pro is all-inclusive!

JADE Pro includes all of the features of JADE Standard, plus batch processing Whole Pattern Fitting (WPF) and Rietveld refinement tools that go beyond what is available in JADE Standard. JADE's One-Click-Analysis™ and the JADE Toolkit are only found in JADE Pro. Additionally, JADE Pro features a unique floating network license that allows access on one concurrent system at a time, so when a license is not in use, it is available to someone else in your organization. Discounted additional seats create access to more concurrent shareable licenses that work together.

## KEY POINTS

- All-inclusive - Everything in JADE Standard and so much more
- Phase ID (Search/Match)
- Batch processing Whole Pattern Fitting (WPF) and Rietveld
- One-Click-Analysis™ for Whole Pattern Fitting (WPF)
- Pattern Indexing (All Crystal Systems)
- Rietveld Structure Refinement (Atomic Parameters)
- Ab Initio Tools (Charge Flipping +)
- Cluster Analysis of Powder Patterns
- Hardware Independent - supports a wide range of diffractometers
- Floating Network License - can work as a shareable multi-seat license
- Discounted Additional Seats Available

## JADE Standard

JADE Standard provides a more limited set of tools than JADE Pro but without the annual updates and renewal costs. Available in three levels -

1. Basic Level
2. Add either Phase ID (S/M) or WPF + Rietveld
3. Add both Phase ID (S/M) and WPF + Rietveld.

Simulation and Visualization - All levels of JADE Standard Simulate powder patterns to create your own custom database. Visualize a structure in 3D with motion. Visual cues throughout to better help you and your team understand the materials you are analyzing.

Phase ID (S/M) - JADE Standard Level 2A or Level 3 Profile-based Search/Match with minor and trace phase ID or search on a single peak. Ability to include chemistry filters and unit cell data as well as preferred-orientation.

WPF + RIETVELD - JADE Standard Level 2B or Level 3 Quantify weight percentages and identify minor phases quickly and easily.



## JADE QA

Built for production line Quantitative Analysis (QA) typically carried out by a technician. Requires a setup file created by an analytical scientist using JADE Pro. JADE QA runs independently of JADE Pro and was designed to extend the power of Rietveld Quantitative Analysis (QA) to those in your organization responsible for overseeing consistencies in production who may or may not have a background in XRD.

Level 1	Level 2 (A or B)		Level 3
Base	Base	Base	Base
	Phase ID (S/M)		Phase ID (S/M)
		WPF + Rietveld	WPF + Rietveld

## KEY POINTS - ALL LEVELS

- Reads all vendor pattern files
- Handles variable/fixed-slit data
- Auto peak search and multi-filter search
- Simulate powder patterns from crystal structures
- No annual renewal fee
- Individually licensed for workstations
- Hardware Independent - supports a wide range of diffractometers

### PHASE ID (SEARCH/MATCH)

- Found in Levels  
2A: Search/Match  
3: Search/Match and Whole Pattern Fitting
- Phase Identification (S/M)
- Minor and Trace Phase ID

### WPF + RIETVELD

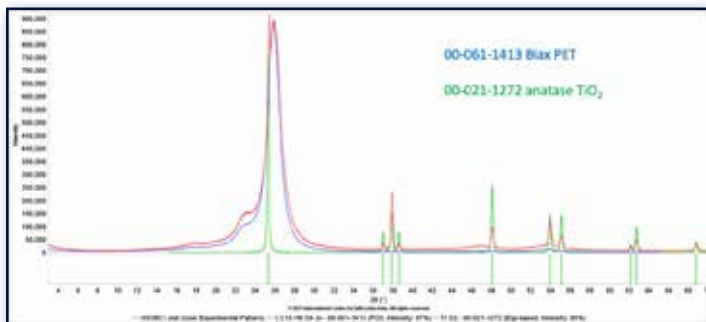
- Found in Levels  
2B: Whole Pattern Fitting (WPF)  
3: Search/Match and WPF
- WPF & Rietveld Refinement



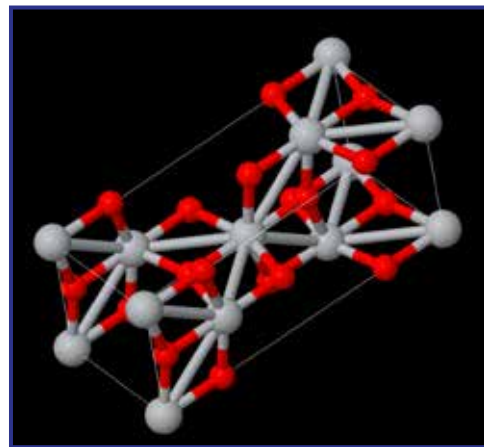
# PDF-4+ 2023

Phase Identification and Quantitation

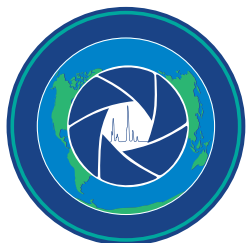
Featuring 480,300+ entries  
369,500+ entries with atomic coordinates



- All entries have digital patterns for use in total pattern analysis
- 376,300+ entries have  $I/I_c$  values for quantitative analysis by Reference Intensity Ratio
- All entries are stored in a standardized format for easy search and interpretation
- All entries go through a rigorous editorial process to ensure quality



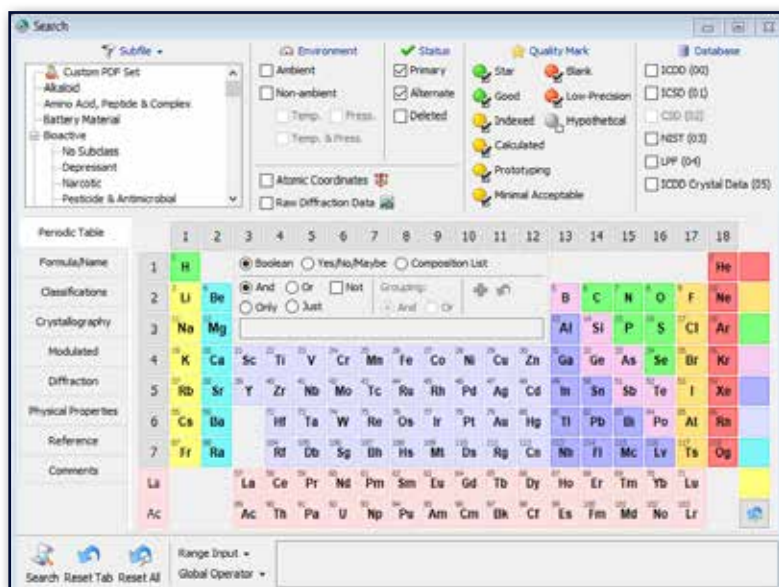
Need "Data on the Go"?  
Ask ICDD about PDF-4+/Web



# PDF-4/Axiom 2023

Quality Plus Value

Featuring over 105,200+ entries  
76,400+ entries with atomic coordinates



- Data focused on ambient entries
- Fundamental mineral entries
- (3) year license term
- Low cost additional license
- 6-year and 9-year prepaid packages

ICDD's Data Mining  
Software Included



# PDF-4/Minerals 2023

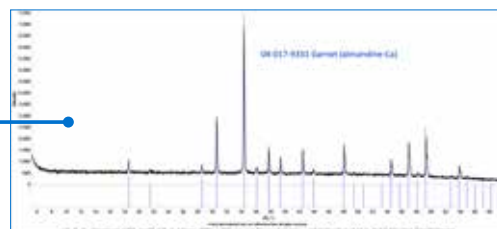
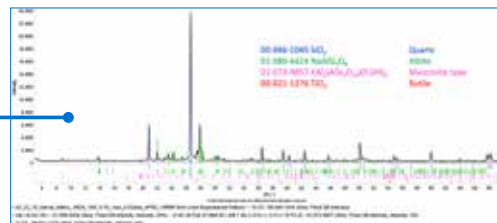
Comprehensive Mineral Collection

Featuring 50,900+ entries  
42,000+ entries with atomic coordinates



Caption????

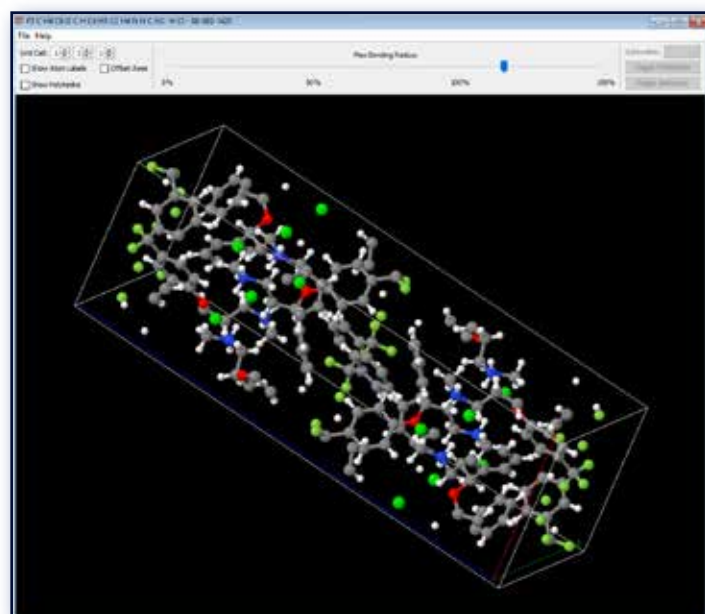
- All entries have digital patterns for use in total pattern analysis
- 39,200+ entries have  $I/I_0$  values for quantitative analysis by Reference Intensity Ratio
- Classified by IMA designations
- A subset of the PDF-4+ database with all of the features and capabilities, targeted toward minerals and mineral related compounds



# PDF-4/Organics 2023

Solve Difficult Problems, Get Better Results

Featuring 608,700+ organic & organometallic compounds  
204,200+ entries with atomic coordinates



- Features the largest collection of pharmaceuticals, excipients, and polymers
- Highly targeted collection with special focus on materials used in commercial and regulatory fields
- Enhanced identification for crystalline, nano, and amorphous materials
- Brand names for over 9,000 bioactive/pharmaceutical entries
- Integrated data mining software
- Sieve+ search-indexing software included as an added value

Contains entries from CCDC  
Cambridge Structure Database