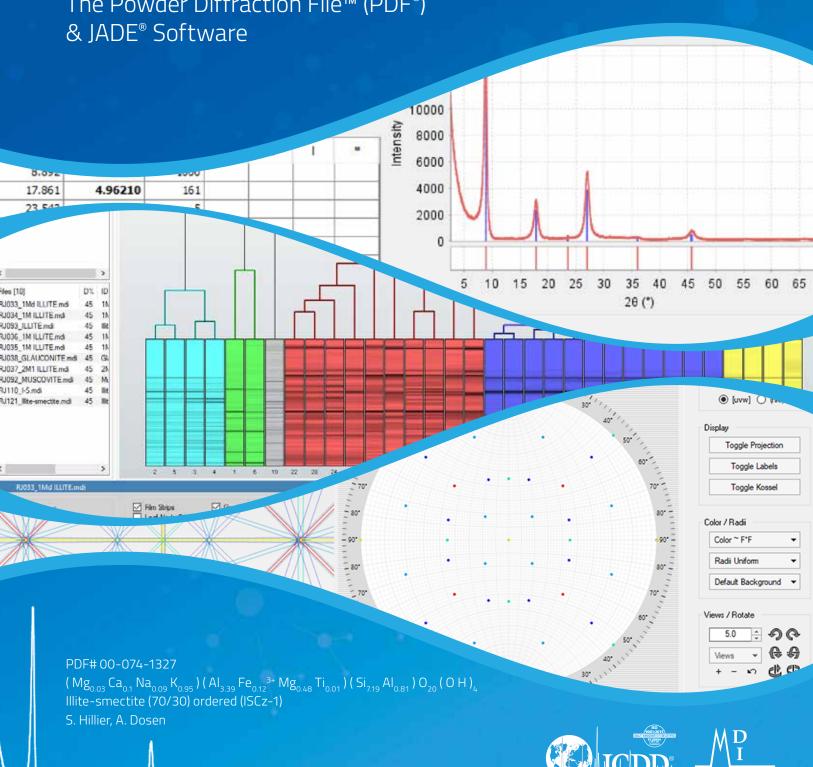
# 2024 - 2025 Sales Catalog

The Powder Diffraction File™ (PDF®)



# Our collaborative partners include:

Cambridge Crystallographic Data Centre (CCDC) Cambridge, UK - Cambridge Structural Database (CSD)

# FIZ Karlsruhe - Leibniz Institute for Information Infrastructure (FIZ)

Karlsruhe, Germany - Inorganic Crystal Structure Database (ICSD)

# National Institute of Standards and Technology (NIST)

Gaithersburg, Maryland, USA

## **Material Phases Data System (MPDS)**

Vitznau, Switzerland - Linus Pauling File (LPF)

# PDF Databases - Why We Are The Best!

- More data, higher quality, more content, many types of solid-state reference data
- The world's largest solid-state collection of minerals, metals and alloys, polymers, active pharmaceuticals, and commercial materials
- The world's largest and most diverse (by formula) collection of inorganic structures
- The world's largest collection of modulated structures
- Extensive bibliographic collections thousands of journals, hundreds of thousands of authors
- Standardized data, nomenclature, and structural classifications plus brand names, trade names, mineral names, zeolite names, and common names of commercial materials
- Identify materials accurately by utilizing the PDF's extensive subfile system that classifies materials by chemistry and application
- New data is contributed annually by highly qualified grantees from around the world
- PDF products are compatible with major diffraction vendor's software



Quality Management System Certified to ISO 9001:2015 by DEKRA

ICDD, the ICDD logo, PDF, Materials Data, JADE, Denver X-ray Conference, Denver X-ray Conference logo, and Materials Data-JADE-SM-WPF logo are registered in the U.S. Patent and Trademark Office. Powder Diffraction File, MDI, and the MDI-Materials Data logo are trademarks of the JCPDS-International Centre for Diffraction Data. ©2024 JCPDS-International Centre for Diffraction Data.

# THE INTERNATIONAL CENTRE FOR DIFFRACTION DATA (ICDD®)

is a non-profit scientific organization dedicated to collecting, editing, publishing, and distributing powder diffraction data for the identification of materials. The membership of the ICDD consists of worldwide representation from academe, government, and industry.

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# **ONLINE RESOURCES**

Visit www.icdd.com. Learn from reference articles, technical bulletins, tutorials, and instructional videos. Some tutorials and webinars focus on the capabilities of the PDF database, while others illustrate methods used to analyze pharmaceuticals, polymers, and minerals. It is free to search and browse documents from ICDD's Pharmaceutical Powder X-ray Diffraction Symposium (PPXRD) and the ICDD Spring Meetings. You get open access to over 1,000 full publications from Advances in X-ray Analysis (AXA) - the proceedings of the Denver X-ray Conference® (DXC). Try the Powder Diffraction File (PDF) Search and search using chemical name, formula, and elements to suggest which ICDD database product is right for you.





# THE POWDER DIFFRACTON FILE IS AVAILABLE FOR

# **DOWNLOAD!**

GET YOUR 2025 PDF DATABASE BY DOWNLOADING FROM THE CLOUD

BENEFIT FROM NO SHIPPING COST AND REDUCED DELIVERY TIME!





# LICENSE OPTIONS TO FIT YOUR BUDGET!

- Extended multi-year license terms -Let us know what you need!
- Customized license for a 1 to 9-year license term
- 15% discount for new PDF-5+ and IADE Pro Bundles
- One-stop shopping: align PDF and JADE renewals for one billing and shipment
- PDF-2 10-year license prepaid package
- PDF-5+Scholar -10-year license for Academics
- PDF-4/Axiom 6-year and 9-year license prepaid packages
- SAVE time and money with ICDD's PDF-5+ and PDF-4/Minerals Subscriptions
  - ICDD's subscriptions keep your database up-to-date with renewal pricing
  - ICDD offers automatic PDF-5+ and PDF-4/Minerals renewal shipments for convenience
  - Can't accept automatic shipments?
     ICDD will send a PDF-5+ or
     PDF-4/Minerals renewal reminder to keep you up-to-date with your subscription

# **WHAT'S NEW FOR 2024-2025**











# Introducing Release 2025 of the Powder Diffraction File

PDF-5+

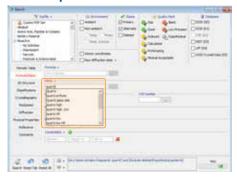
PDF-5+/Server Edition

PDF-4/Axiom

PDF-4/Minerals

PDF-2

## **Autocomplete Name Search**



Automatically suggests names based on user input using two methods:

- 1. Uses substring search to suggest similar names
- 2. Uses machine learning to suggest alternate spellings (if misspelled)

### **New Mineral Classifications**



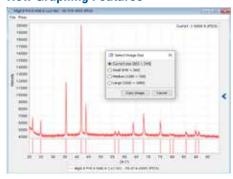
- IMA mineral symbols
- IMA mineral classifications
- Strunz-mindat classifications

### **Dynamic Hit Counts**



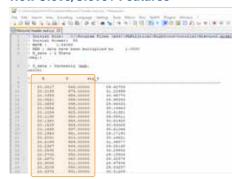
- Displays search hit counts based on selected criteria
- · For data mining searches
- · For matches filters

### **New Graphing Features**



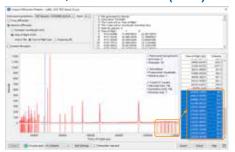
- Unzoom button on right side of all x-y graphs
- Quickly save any graph using the right-click menu
  - » Includes 2D > 1D diffraction integration\*
- Select image resolution when copying or saving a graph image

### **New Sleve/Sleve+ Features**



- Supports importing STOE files
  - » 1D diffraction patterns
- Supports importing MarCCD image files\*
  - » 2D diffraction patterns
- Supports importing CIF's exported from Jana
- Automatically detects 20 and intensity data if file format is not recognized

### **New Sleve/Sleve+ Features (cont.)**



- Bulk peak edit: Remove peaks directly from the peaks table using a right-click menu
- Add or remove peaks without having to reset the session
- Zoom to peak option for trace phase analysis
- Add phases to a Custom PDF Set
- Sleve+ project files now save and restore all simulation settings\*
  - » Geometry settings
  - » Profile settings
  - » Preferred orientation settings
  - » Internal standard settings
  - » Isotopic substitutions (neutrons)

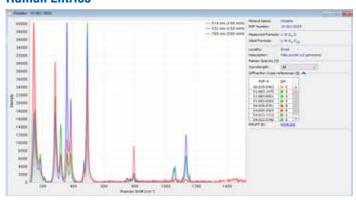


### Raman Search\*



- · Dynamic searches for new Raman data
  - » Periodic table search
  - » Mineral name search
  - » Formula search
  - » Locality search
  - » Description search
- · Search values highlighted in table
- · Save and retrieve searches
- Import Raman spectra for single-phase ID
  - » Supports data processing

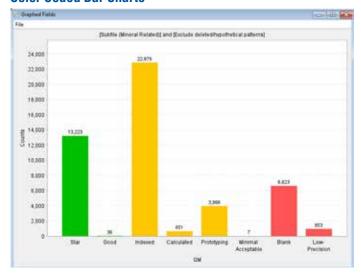
## **Raman Entries\***



- Displays Raman data
  - » Mineral name
  - » Measured formula
  - » Ideal formula
  - » Locality
  - » Description
  - » Set 10-xxx-xxxx
- Displays Raman spectra
  - » Supports multiple wavelengths (user-selectable)
- Displays cross-references
  - » Raman patterns linked to XRD patterns
  - » RRUFF ID

# **Color Coded Features**

## **Color Coded Bar Charts**



## **Color Coded Similarity Indexes\***



<sup>\*</sup> PDF-5+/PDF-4 only feature

# PDF-5+ 2025

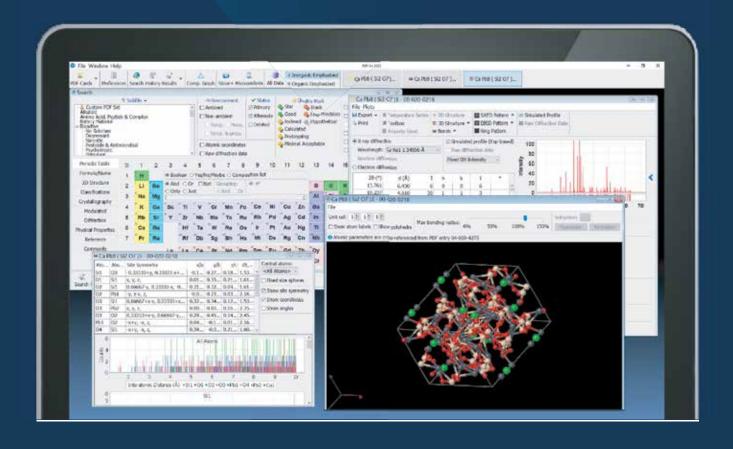
## THE POWDER DIFFRACTION STANDARD

Inorganic & Organic entries are combined into one powerful database with 1,104,100+ entries.



www.icdd.com/pdf-5

- 626,100+ entries with atomic coordinates
- Features 457,800+ entries for inorganic materials and 650,200+ entries for organic materials
- All entries have digital patterns for use in total pattern analysis
- 997,300+ entries have I/I<sub>c</sub> 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

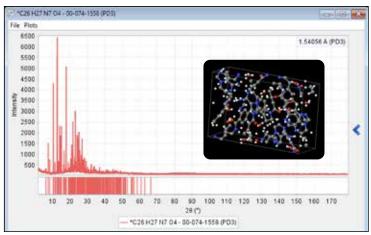




# PDF-5+ 2025

# The Powder Diffraction Standard

PDF-5+ combines the world's largest sources of inorganic and organic diffraction data from crystals and powders into a single database.



Calquence®, acalabutinib dihydrate Form III, used to treat various types of non-Hodgkin lymphoma.

# **(1)** KEY POINTS

- Rapid phase identification designed to support automated quantitative analyses
- Features 1,104,100+ entries with over 626,100+ having atomic coordinates
  - > 457,800+ entries for inorganic materials
  - > 650,200+ entries for organic materials
- Integrated data mining software
- All entries have digital patterns for use in total pattern analysis
- More than 997,300+ entries have I/I<sub>c</sub> values for quantitative analysis by Reference Intensity Ratio (RIR) method
- Combines powder and single crystal data
- Includes crystalline, semi-crystalline, and amorphous solid-state materials
- World's largest and most diverse collection of structures for inorganic and organic materials
- Extensive data mining is facilitated with 139 display fields coupled with 85 searches
- LPF entries have a link to mpds.io
- One (1) year license serviced by subscription

PDF-5+ Purchase Options	1	1	2024-2025	2024-2025
PDF-5+ 2025	USB CODE	DOWNLOAD CODE	2024-2025 LIST\$	ACADEMIC \$
New - Single License	P5S25	P5L25	\$9,395	\$6,265
Renewal from 2024 to 2025	P5RS25	P5RL25	\$2,115	\$1,375
PDF-5+ and JADE Pro bundle*				
New - Single License	BUJPP5S25	BUJPP5L25	\$16,310	\$11,465
*Purchase a new license for PDF-5+ and JADE Pro				
PDF-5+ 2025 Multi-year License*				
Renewal – 3 year License	P5S26MR28	P5L26MR28	\$5,710	\$3,715
Renewal – 5 year License	P5S26MR30	P5L26MR30	\$8,990	\$5,845
PDF-5+ Scholar 2025 (10-Year License Package)*				
PDF-5+ New - Single License	P5S25	P5L25		\$6,265
Scholar Multi-year	P5SPS26MR30	P5SPL26MR30	NA	\$5,845
				\$12,110

## Save Money! Take advantage of ICDD's Site License - Request a quote today!

PDF-5+ 2025 Site License*	USB CODE	DOWNLOAD CODE	2024-2025 LIST \$	2024-2025 ACADEMIC \$
New - Master License	P5S25M	P5L25M	\$9,395	\$6,265
New - additional License, each	P5S25C	P5L25C	\$2,115	\$1,375
Renewal - Yearly Master License	P5RS25M	P5RL25M	\$2,115	\$1,375
Renewal - additional License, each	P5RS25C	P5RL25C	\$855	\$590
PDF-5+ 2025 Site/Multi-year License*				
Renewal - 3 year Master Site License	P5S26MR28M	P5L26MR28M	\$5,710	\$3,715
Renewal - 3 year additional Site License, each	P5S26MR28C	P5L26MR28C	\$2,565	\$1,770
Renewal - 5 year Master Site License	P5S26MR30M	P5L26MR30M	\$8,990	\$5,845
Renewal - 5 year additional License, each	P5S26MR30C	P5L26MR30C	\$4,275	\$2,950
PDF-2 to PDF-5+ Conversion				
PDF-2 2024 to PDF-5+ 2025	P2524RSU25	P2524RLU25	\$2,115	\$1,375
PDF-2 2023 to PDF-5+ 2025	P2523RSU25	P2523RLU25	\$4,230	\$2,750
PDF-2 2022 to PDF-5+ 2025	P2522RSU25	P2522RLU25	\$6,345	\$4,125
PDF-2 2021 to PDF-5+ 2025	P2521RSU25	P2521RLU25	\$8,460	\$5,500

<sup>\*</sup>Please see product policies on pages 18 and 19



# **Extend the Power of Your Database**Built for Teams of Ten or More

Workplaces and work habits have evolved from just a few years ago, and this database licensing model provides the flexibility that large organizations and academics need to meet the varying demands of clients, teams, and students.

Install on your server and as many computers as you wish. A 10-User license provides access to 10 computers at a time and floats among an unlimited number of systems. Deployment to new hires is seamless. When it's time for the latest database, your renewal is simplified with one single product. Ensure everyone in your organization is using the latest set of data with one shared floating 10 or more seat license. Additional benefits occur when access is granted to occasional use individuals without any added cost to your bottom line.

Your IT department will be happy as updates are streamlined, all while offering savings for your budget. If you need to provide access to 10 or more systems, please contact us at <a href="mailto:sales@icdd.com">sales@icdd.com</a> to consider how our new Server License would work best for your team.



# PDF-5+ 2025 The Powder Diffraction Standard

PDF-5+ combines the world's largest sources of inorganic and organic diffraction data from crystals and powders into a single database.

PDF-5+ contains 457,800+ inorganic and 650,200+ organic entries to ensure that you have the data you need for all of your phase identification needs. Every entry is editorially reviewed and assigned quality marks, so the curated PDF-5+ database allows users to do quantitative analysis by any of three methods: Rietveld Analysis, Reference Intensity Ratio (RIR) method, or Whole Pattern Fitting.



# **JADE Pro**

# The Analysis Software Professionals Choose

You need data you can trust, AND you need to find the best way possible to analyze your data. Now you can extend the power of your ICDD PDF-5+ Server Edition by including the highly regarded data analysis software JADE Pro. We created JADE to provide independent, unbiased results for peak search, whole pattern fitting, and Rietveld. JADE gets daily improvements and has grown to include an enormous list of valuable tools for your materials research and exploration. The power of JADE combined with the PDF-5+ Server Edition means a team can easily share a 10-seat license. The Server Edition can result in cost savings for your organization and a chance for you to extend the power to your team by providing access to BOTH the PDF database and JADE to as many individuals as you need. The database and software products offer the same functionality as the individual products. In coupling them in a 10 or more user server license, important resources are available to more team members, and everyone is in sync, all while reducing costs.



- 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<sup>™</sup> 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





# **JADE Pro**

# **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<sup>TM</sup> 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.

# **P** 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



# **SO MANY ADDITIONAL TOOLKIT FEATURES!**

**Only Found in JADE Pro** 



# **▼ED-XRF**

For manual or automatic identification of elements and minerals.

# **XRD Digitizer**

Take a picture of an XRD plot and this tool will convert it to a digital format that you can now work with in JADE. Use advanced image editing options to tweak any imperfections or remove artifacts from your image.

# **Charge Flipper + Solve Structure**

For structure solution using the charge flipping method.

# **Regression Analysis**

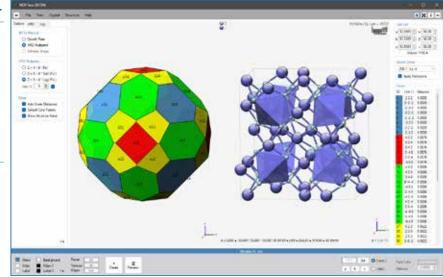
Easily perform regression analysis on data without leaving JADE Pro's Toolkit.

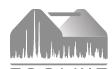
# **BFDH Morphology** ►

Create predicted crystal shapes based on the Bravais-Friedel-Donnay-Harker model. Other options include ability to promote the presence of certain (hkl)-faces by applying XRD multipliers from calculated structure intensities or calculating a Scherrer shape from fitted profiles.

## **Microstructure Tool**

Provides methods for the analysis of the residual stress and microstructure defects for various diffraction geometries and is applicable to cubic phases (FCC, BCC) following a profile fitting in JADE (D. Rafaja).





# **EVEN MORE TOOLKIT FEATURES**

**Toolkit is found only in JADE Pro** 



# ◆ For Oriented Clays - ClaySim

For (001)-patterns. Performs simulations and analyses of oriented clays based on structure types introduced by R.C. Reynolds.

## **MDI SizeStrain**

Designed for crystallite size and micro-strain analysis using X-ray powder diffraction data. This Toolkit supports both Warren-Averbach and Williamson-Hall methods for crystallite size determination.

## **3D Scatter Plot**

A scatter plot tool for xyz data sets from columnar data files.

## Raman Mineral >

Designed for the mineral phase ID from Raman Stokes spectra. Whole spectra correlation functions are used for finding similarity matches for single-phase and multi-phase spectra.

# **Pattern Matching**

Try the full Pattern Matching method used in both ROCKJOCK and ClaySim.

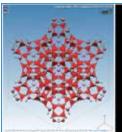


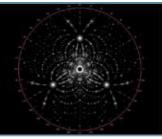
# **◄ Cluster Analysis with Dendrograms**

View your clusters with automatic cluster color coding with Principal Component or Fuzzy Clustering. Streamline your analysis by adding reference patterns as cluster markers, recalling setup protocols for reproducibility and other correlation functions for determining pattern similarities.

## **Area Detector Tool**

Built to extract powder patterns from images obtained with flat area detectors, so that they can easily be analyzed in JADE Pro.





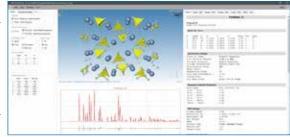
# **<b>◄** Laue Visualization

Simulations, alternative structure visualizations and stereographic projections with the ability to export Adobe PDF booklets.

# Simulated Annealing ►

An alternative direct space

structure solution method (SA) designed for inorganic structures applying Coulomb interactions and repulsive potentials.



# **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 -

Level 1: Base

Level 2: A - Phase ID (S/M)

B - WPF + Rietveld

Level 3: Add both Phase ID (S/M) and WPF + Rietveld

Included with all levels of IADE Standard -

Simulation and Visualization - 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.

# **REY 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

# WPF + RIETVELD

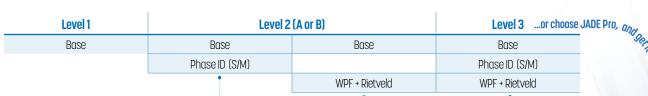
Found in Levels2B: Whole Pattern Fitting (WPF)3: Search/Match and WPF











## 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**

A special build meant 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.





# **Get More Power With JADE Pro**

# JADE is available in Pro and Standard

JADE FEATURE LIST	Pro	1	2A	2B	3
Intuitive, State-of-the-Art UI	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>
Reads All Vendor Pattern Files	<b>✓</b>	<b>✓</b>	<b>~</b>	<b>✓</b>	<b>√</b>
Smart Column Data Importer	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>	<b>√</b>
Merge Multi-Scans/Segments	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>
1, 2, and 3D Pattern Overlay	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>
Déjà Vu ID Similar Pattern Files	<b>✓</b>	<b>✓</b>	<b>~</b>	<b>✓</b>	<b>√</b>
Handles Variable/Fixed-Slit Data	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>
Multiple Display Axes and Any Diffraction Wavelength	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>
Zero Offset Correction and Theta Calibration	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>
Background Fitting/Batch Fitting/Removal	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>	<b>√</b>
Auto Peak Search and Multi-Filter Search	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>
Wide Variety of Report and Print Options	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>
Includes Starter Database	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>
ICDD PDF Database Access (as well as other databases)	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>
Multitude of Data Choices for Database Retrieval	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>
View Crystal Structures and Reflection Planes	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>
View Polyhedra, Calculate Bond Distances and Angles	<b>✓</b>	<b>✓</b>	<b>√</b>	<b>√</b>	<b>√</b>
Simulate Powder Patterns from Crystal Structures	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>
Individual Analyst/Shared Work Environments	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>
Support for Custom d-1% list for Phase Overlay	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>
Excellent Profile Fitting and Batch Profile Fitting	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>
RIR Quant, Size & Strain and Residual Stress	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>
Quantitative Analysis	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>
Line-Based Unit Cell and Batch Refinement	<b>✓</b>	<b>✓</b>	<b>✓</b>	<b>√</b>	<b>√</b>
Structure Database Manager	<b>✓</b>		<b>✓</b>	<b>✓</b>	<b>√</b>
Profile Based Search/Match (S/M)	<b>✓</b>		<b>✓</b>		<b>√</b>
Subfile + Chemistry + Unit Cell Filters in S/M	<b>✓</b>		<b>✓</b>		<b>✓</b>
Minor and Trace Phase ID	<b>✓</b>		<b>✓</b>		<b>✓</b>
Single Peak and Severely-Orientation S/M	<b>✓</b>		<b>✓</b>		<b>✓</b>
Solid-Solution and Isotypical Phase ID	<b>✓</b>		<b>✓</b>		<b>✓</b>
Auto-S/M in background thread on loading a pattern file	✓		<b>✓</b>		<b>✓</b>
Full pattern S/M on PD3 phases by correlation & similarity	<b>✓</b>		<b>✓</b>		<b>✓</b>
WPF and Rietveld Refinement (Unlimited Phases)	<b>✓</b>			<b>✓</b>	<b>✓</b>
Gold Standard Quantitative Analysis	<b>✓</b>			<b>✓</b>	<b>✓</b>
Seamless Integration with Database Retrieval	<b>✓</b>			<b>✓</b>	<b>✓</b>
Auto-Loading of Structure Data from Database	✓			<b>✓</b>	<b>✓</b>
Combination of Phases with/without Structure Data Weight%	<b>✓</b>			<b>✓</b>	<b>✓</b>
Linking of Unit Cell, Phase Broadening Parameters	<b>~</b>			<b>✓</b>	<b>✓</b>
Custom d-1% (hkl, FWHM, Skew) to Fit Clay Phases	<b>~</b>			<b>✓</b>	<b>√</b>
March-Dollase and Spherical Harmonics Orientation Function	<b>✓</b>			<b>✓</b>	<b>✓</b>
Amorphous Content with/without Internal Wt% Standards	<b>✓</b>			<b>✓</b>	<b>✓</b>
Atomic Occupancy and Bond Distance Constraints	<b>✓</b>			<b>✓</b>	<b>√</b>
Polynomial and Spline Curve Background Fitting	<b>✓</b>			<b>✓</b>	<b>√</b>

All levels of JADE Standard are perpetual licenses and sold without the benefit of updates or any of JADE Pro's extensive set of extra

features, like the ability to share a license. Since it is a subscription, JADE Pro has a lower buy-in than JADE Standard.

> If you have JADE Classic, there still may be trade-in value towards the purchase of a current version of JADE Standard or JADE Pro.

Additional JADE Features Only Available in JADE Pro	Pro
One-Click-Analysis™ - Phase ID and WPF/Rietveld Analysis	<b>✓</b>
Size and Strain Analysis (Warren-Averbach & Williamson Hall)	<b>✓</b>
Pattern Indexing (All Crystal Systems)	<b>✓</b>
Simulate Series of Powder Patterns from Crystal Structures	<b>✓</b>
WPF and Rietveld Refinement Batch Processing	<b>✓</b>
Rietveld Structure Refinement (Atomic Parameters)	<b>✓</b>
Atomic Occupancy and Bond Distance Constraints	<b>✓</b>
Fourier Map Tools	<b>✓</b>
Ab Initio Tools (Charge Flipping +)	<b>✓</b>
Cluster Analysis of Powder Patterns	<b>✓</b>
Floating (Shareable) Network License	<b>✓</b>
All Updates via Subscription	<b>✓</b>
Extract Patterns from Area Detector 2D Images	<b>✓</b>
Digitize Any XRD Plot Image	<b>✓</b>
Cluster Analysis Visualization Dendrograms	<b>✓</b>
Toolkit App Version of ClaySim	<b>✓</b>
Toolkit App for Microstructure Analysis	<b>✓</b>
Toolkit App for Structure Solver Workflow	<b>✓</b>
Laue Simulations and Visualization	<b>✓</b>
Toolkit App for Simulated Annealing	<b>✓</b>
Toolkit App for Regression Analysis	<b>✓</b>
Toolkit App for Pattern Matching	<b>✓</b>
Toolkit App for 3D Scatter Plot	<b>✓</b>

# **Multiple Languages!**

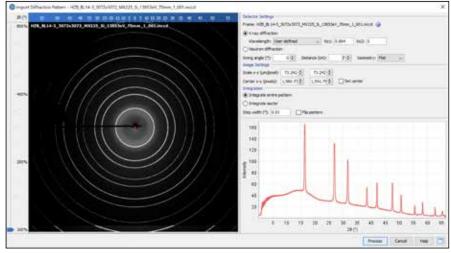
To better support diverse teams sharing a license of JADE Pro across their organization and to ensure consistent results regardless of language, JADE can switch on the fly to Chinese or Japanese languages.



# Sleve/Sleve+ 2025

# Search and Identify

ICDD's search identification programs, Sleve for PDF-2 and Sleve+ for PDF-5+ and PDF-4, are designed to search and identify unknown materials. Sleve/Sleve+ are integrated into the ICDD databases to allow the use of the extensive data mining interfaces, searches, and sorts available to improve the accuracy and precision of the phase identification process.

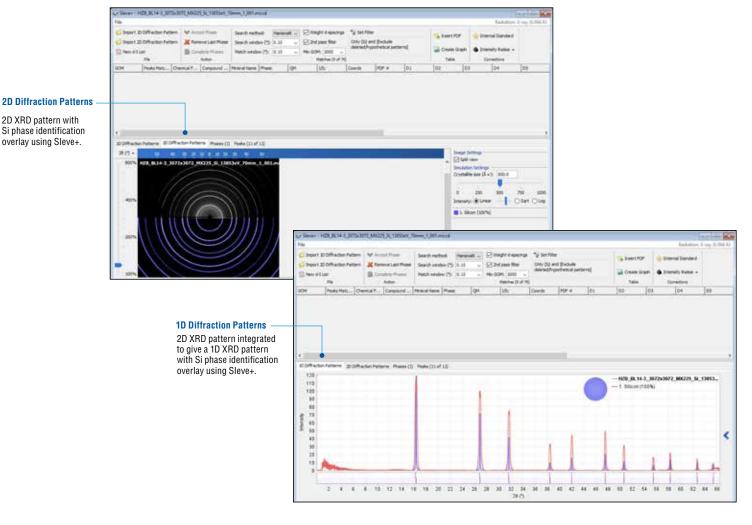


2D XRD data provided by Dr. Manfred Weiss, HZB

# **(1)** KEY POINTS

- · Included free in all PDF databases
- Designed to search and identify unknown materials
- Complementary with most commercial software programs
- Match filter algorithms better results, more accuracy
- Identify non-crystalline materials and complex multi-phase specimens
- Strength of Sleve/Sleve+ is evident in the analysis of minor and trace phases
- Supports X-ray, synchrotron, electron\*, and neutron\* data
- "Intelligent" RIR for semi-quantitative analysis\*
  - \* PDF-5+/PDF-4 only feature (Sleve+)

Sleve+ offers a variety of algorithms and options that allow users to optimize results for particular chemistries for both standard and non-standard diffraction systems.

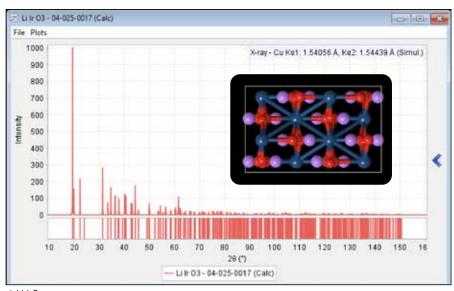




# PDF-4/Axiom 2025

# Quality Plus Value

PDF-4/Axiom is focused on identification and quantitation with data entries selected for benchtop users.



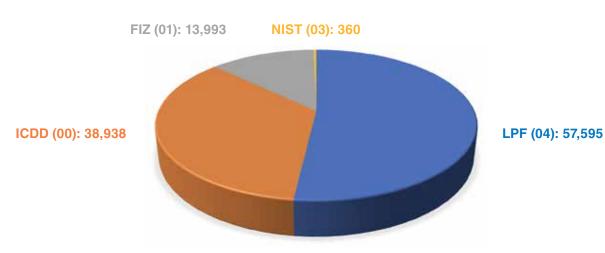
 $\beta\text{-Li}_2IrO_3$ 

# **(1)** KEY POINTS

- · Cost-effective
- Single License: Three (3) year license term
- Optional: Two (2) additional seats (three (3) year license term)
- Six (6) year and nine (9) year prepaid packages available
- New license available after term expires
- Featuring 110,800+ entries, including inorganic and organic entries
- 80,700+ entries with atomic coordinates
- Number of entries with I/I<sub>c</sub> values: 79,500+
- Extensive data mining is facilitated with 139 display fields coupled with 82 searches
- · Data focused on ambient entries
- · Fundamental mineral entries
- ICDD data mining software Sleve+ Included

# **Database Sources**

(See inside front cover for ICDD's collaborative partners)



# **Axiom Purchase Options**

PDF-4/Axiom 2025	USB CODE	DOWNLOAD CODE	2024-2025 LIST \$	2024-2025 ACADEMIC \$
New - Single License	AX4S25	AX4L25	\$3,715	\$2,665
Two Additional Seats (each seat: single PC installation)	AX4S25MS	AX4L25MS	\$1,050	\$540
PDF-4/Axiom 2025 Packages*				
PDF-4/Axiom - 6 years	AX4S6YR	AX4L6YR	\$7,430	\$5,330
PDF-4/Axiom - 9 years	AX4S9YR	AX4L9YR	\$11,145	\$7,995

- \* Purchase two or three Single Licenses
- (Release 2025, Release 2028, and Release 2031)
- Each PDF-4/Axiom product is licensed for three (3) years
   Shipping fees for all databases billed on the original invoice

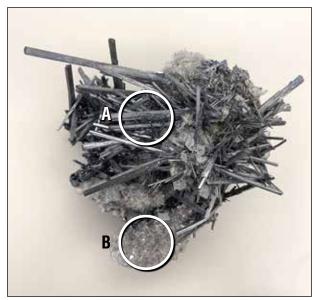
<sup>\*</sup>Please see product policies on pages 18 and 19



# PDF-4/Minerals 2025

# Comprehensive Mineral Collection

PDF-4/Minerals is the most comprehensive collection of mineral data in the world! Ninety-seven percent of all known mineral types, as defined by the International Mineralogical Association (IMA), are represented in the database

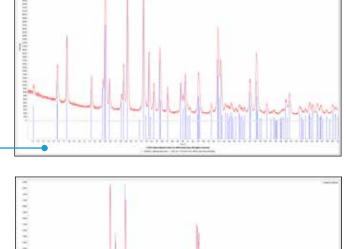


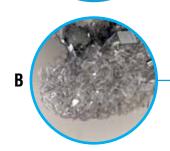
Dark needles (Stibnite, Sb<sub>o</sub>S<sub>o</sub>) on a matrix of clear platy crystals(Barite, BaSO<sub>d</sub>)

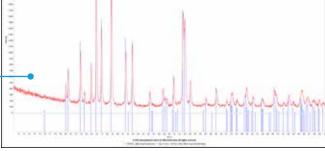
# **(1)** KEY POINTS

- Rapid phase identification, plus support for automated quantitative analyses
- Features 53,400+ entries, including 43,900+ entries with atomic coordinates
- · Integrated data mining software
- All entries have digital patterns for use in total pattern analysis
- More than 41,300+ entries have I/I<sub>c</sub> values for quantitative analysis by Reference Intensity Ratio (RIR)
- · Combines powder and single crystal data
- · Classified by IMA designations
- A subset of the PDF-5+ database with all the features and capabilities, targeted to minerals and mineral related compounds
- Extensive data mining is facilitated with 139 display fields coupled with 84 searches
- One (1) year license serviced by subscription

### Dark needle 04-016-4161 Sb<sub>2</sub>S<sub>3</sub>, Stibnite







Clear crystal 04-002-3304 BaSO4, Barite

# **PDF-4/Minerals Purchase Options**

PDF-4/Minerals 2025	USB CODE	DOWNLOAD CODE	2024-2025 LIST \$	2024-2025 ACADEMIC \$
New - Single License	MN4S25	MN4L25	\$1,840	\$1,250
Renewal from 2024 to 2025	MNR4S25	MNR4L25	\$985	\$650
PDF-4/Minerals 2025 Multi-year License*				
Renewal - 3 year license	MNS426MR28	MNL426MR28	\$2,955	\$1,950
Renewal - 5 year license	MNS426MR30	MNL426MR30	\$4,925	\$3,250

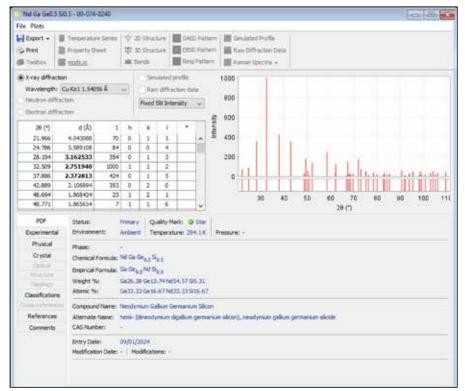
<sup>\*</sup>Please see product policies on pages 18 and 19



# PDF-2 2025

# Phase Identification + Value

PDF-2 is designed for inorganic materials analyses. In addition, common organic materials from ICDD are added to the database to facilitate rapid materials identification.



Intermetallic compounds display interesting physical and chemical properties. They are used in industry as shape memory alloys, as materials for hydrogen storage, catalysis, as well as magnetic, thermoelectric, or superconducting materials



- Features 359,400+ entries
- 252,600+ entries have I/I<sub>c</sub> values for quantitative analysis by Reference Intensity Ratio (RIR) method
- · Integrated data mining software
- Sleve search-indexing software included
- · Combines powder and single-crystal data
- Rapid data mining with our 60 display fields coupled with 75 searches
- Five (5) year license

Every Powder Diffraction File entry is editorially reviewed and assigned a quality mark.

We are proud to say ICDD's Quality Management System is ISO 9001:2015 certified by DEKRA



# **PDF-2 Purchase Options**

PDF-2 2025: Five (5) year License	USB CODE	DOWNLOAD CODE	2024-2025 LIST \$	2024-2025 ACADEMIC\$
New - Single License	C2S25PN	C2L25PN	\$9,395	\$6,265
Renewal from 2024 to 2025	C2S24PU25	C2L24PU25	\$2,115	\$1,375
Renewal from 2023 to 2025	C2S23PU25	C2L23PU25	\$4,230	\$2,750
Renewal from 2022 to 2025	C2S22PU25	C2L22PU25	\$6,345	\$4,125
Renewal from 2021 to 2025	C2S21PU25	C2L21PU25	\$8,460	\$5,500
PDF-2 2025: Ten (10) year License Package				
New - Licenses (2025 and 2030)	PD2S10YR	PD2L10YR	\$18,790	\$12,530
PDF-2 2025 Site License*				
New - Master License	C2S25PNM	C2L25PNM	\$9,395	\$6,265
New - additional licenses, each	C2S25PNC	C2L25PNC	\$2,115	\$1,375
Renewal - Yearly Master License	C2S24PU25M	C2L24PU25M	\$2,115	\$1,375
Renewal - additional licenses, each	C2S24PU25C	C2L24PU25C	\$855	\$590
PDF-2 to PDF-5+ Conversion				1
PDF-2 2024 to PDF-5+ 2025	F2524RSU25	F2524RLU25	\$2,115	\$1,375
PDF-2 2023 to PDF-5+ 2025	F2523RSU25	F2523RLU25	\$4,230	\$2,750
PDF-2 2022 to PDF-5+ 2025	F2522RSU25	F2522RLU25	\$6,345	\$4,125
PDF-2 2021 to PDF-5+ 2025	F2521RSU25	F2521RLU25	\$8,460	\$5,500

<sup>\*</sup>Please see product policies on pages 18 and 19

# Which ICDD Database is Right for You?

	PDF-5+ 2025	PDF-5+ Server Edition 2025	PDF-4/ Axiom 2025	PDF-4/ Minerals 2025	PDF-2 2025
I work primarily with inorganic compounds			-		
I work primarily with organic compounds					
I work primarily with minerals				-	
I work with electron diffraction/synchrotron					
I need to be flexible with my work location					
I need to do quantitative analysis					
Rietveld	•	•		•	
Reference Intensity Ratio (RIR)					
Pattern Fitting					
I need a database with atomic coordinates			-	•	
How many entries are in the database?	1,104,137	1,104,137	110,886	53,434	359,407
How many entries are new?	42,239	42,239	2,847	1,495	9,645
I am using vendor software for my analysis. Which databases will work with my vendor software?  Global software vendors provide search/match software that interfaces with our databases. Please check with your software vendor for compatibility.	•	•	•	•	•
What is the license term for the database?	1 year	1 year	3 years	1 year	5 years
Multi-year license available					
Site license available		<b>■</b> †			

<sup>†</sup> Requires a 10 concurrent user minimum license.

### **System Requirements:**

- Intel® Core™ 2 Duo processor (recommended minimum) or better
- 4 GB system memory

# JADE Standard/JADE Pro:

- Intel® Core™ i7, i5, or i3
- 8 GB system memory
- 24" or larger monitor Your JADE experience will be richer on a larger screen.

### **Hard Disk Space Requirements**

- PDF-2 2025 5 GB
- PDF-5+ 2025 38 GB
- PDF-5+ Server Edition 2025 38 GB
- PDF-4/Minerals 2025 2 GB
- PDF-4/Axiom 2025 4 GB
- JADE Standard/JADE Pro 400 MB

## Support Microsoft® Operating System:

- Windows® 7 SP1
- Windows® 8/8.1
- Windows® 10
- Windows® 11

Do you have 10 or more concurrent users on a network? See pages 6 - 7 for Server Edition details.



# **ICDD's FREE Webinar Series** Mastering the PDF Database and JADE Software

Learn the potential of Powder Diffraction File and JADE from ICDD's and Materials Data's experts and developers. Take an hour to build your confidence and productivity.



# **Our Experts Teach You:**

**Quantitative Phase Analysis with Cements** Raman Search Match **Clay Analysis** 

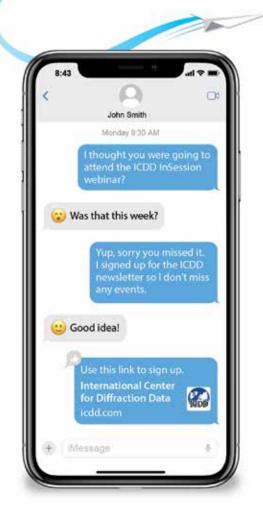
**Data Mining in the Powder Diffraction File Navigating a Powder Diffraction File Entry** and more



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## **RELEASE 2025**

LICENSE TERMS				
Product	License Term			
PDF-2	5 years			
PDF-4/Axiom	3 years			
PDF-5+*	1 year			
PDF-4/Minerals*	1 year			

<sup>\*</sup> Serviced by subscription featuring automatic annual renewals.

# **Product License Policies**

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An academic price is awarded to degree-granting (Assoc., B.S., M.S., Ph.D.) institutions and organizations that provide resources for student's course work that are affiliated with the degree-granting institution. Institutions may be required to submit documentation to verify eligibility. Please consult individual product pages for eligible products.

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ICDD's standard site license policy is designed for a multi-user laboratory to facilitate multiple licenses of the PDF-2 or PDF-5+ databases at a single site. A single site is defined by the building where the database will be installed. Multiple users in different buildings need to purchase separate site licenses for each building.

A standard ICDD site license includes the purchase of a Master License, and the purchase of Secondary Licenses (discounted additional licenses). Customers may purchase an unlimited number of additional licenses at discounted pricing. The number of computers that will be running the database in a single building determines the number of licenses.

ICDD multi-user server licenses are software products that include ICDD's JADE Pro and/or PDF-5+. The server licenses are scaled to serve high-volume research environments (10-concurrent user license minimum required) and is a floating, remotely accessible, and network shareable license.

**Note:** PDF-4/Axiom and PDF-4/Minerals are excluded from site license options. PDF-2 and PDF-5+ cannot be combined in a single site license.

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Customers with a single license may add additional licenses to create a site. To qualify for additional license pricing, the single license must be current. If necessary, customers may need to renew their single license to the current release, then add an additional license to create the site.



**PDF-5+** *The* Powder Diffraction Standard



PDF-5+ Server Edition
Extend the Power of Your Database –
Built for Teams of Ten or More



PDF-4/Axiom Quality plus Value



PDF-4/Minerals
Comprehensive Mineral Collection



**PDF-2**Phase Identification + Value

#### **Site License Renewals**

In order to take advantage of the site license renewal pricing, both the Master License and the Secondary Licenses of the database must be renewed yearly. To renew a site license, ICDD requires that the Master License and all Secondary Licenses be purchased concurrently on a single purchase order.

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Multi-year license renewal pricing for PDF-4/Minerals is offered as a convenience to our customers. It is not subject to the discount offered with our other multi-year licenses.

**Note:** PDF-2 and PDF-4/Axiom databases are not eligible for multi-year licensing options; however ICDD offers prepaid packages. Visit page 13 for PDF/Axiom and page 15 for PDF-2.

# PDF-5+Scholar Multi-year License for Academics 10-Year License



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product release), plus the PDF-5+Scholar multi-year license. During your 10-Year license, you will receive six (6) products of the newest release of the PDF-5+. The first five (5) PDF-5+ products will be licensed for one (1) year. The final sixth (6th) PDF-5+ product will be the PDF-5+Scholar product, which is licensed for five (5) years.

The 10-Year license is available on USB or download.

Like PDF-5+ and PDF-4/Minerals, the 10-Year license is handled by automatic subscription. The yearly automatic renewals will be shipped based on the anniversary of the original invoice for the 10-Year license. Shipping fees for all databases are billed on the original invoice.

# For more information, please visit: www.icdd.com/pricing-policies/

Product warranty is on the preferred computer specifications associated with the product release. If you need to change your computer specifications, ICDD recommends that you reference the ReadMe.txt or product insert for your product release to check for compatibility.

# Take advantage of ICDD's prepaid packages:

PDF-2: 10-Year license – Page 15

PDF-5+Scholar: 10-Year license for Academics – Page 5
PDF-4/Axiom: 6-Year and 9-Year license prepaid – Page 13

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24 – 28 March 2025 www.icdd.com/xrf

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XRD I: 2 – 6 June 2025 www.icdd.com/xrd

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XRD II: 9 – 13 June 2025 www.icdd.com/xrd

#### **Rietveld Refinement & Indexing**

Fall 2025

www.icdd.com/rietveld



\*Dates, location, and format of courses and conferences may be subject to change.

#### **CONFERENCES\***

#### www.icdd.com $\rightarrow$ Conferences

#### 74th Denver X-ray Conference

The Bethesda North Marriott Hotel & Conference Center, Rockville, Maryland, USA 4-8 August 2025

DXC is the world's largest annual conference dedicated to the fields of X-ray analysis. Experts in the fields of X-ray diffraction and X-ray fluorescence gather for a week of workshops, technical sessions, and manufacturer's exhibits. DXC attendees will have access to sessions on the latest advancements in XRD and XRF.

#### www.dxcicdd.com

# Pharmaceutical Powder X-ray Diffraction Symposium

XRD Training for the Pharmaceutical Scientist! ICDD sponsors this symposium designed to create a forum for the exchange of knowledge and cutting-edge ideas among those interested in the combined fields of XRD and pharmaceutical sciences. Visit the PPXRD website for news on the next symposium. Search and browse presentations from past PPXRD for free.

www.icdd.com/ppxrd

#### **RESOURCES**

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