# INTERNATIONAL CENTRE FOR DIFFRACTION DATA

# SALES CATALOG





# THE POWDER DIFFRACTION FILE™ JADE® SOFTWARE

### Lu<sub>0.5</sub>Y<sub>0.5</sub>VO<sub>4</sub> - PDF<sup>®</sup> Entry 00-070-0358

Submitted by ICDD Distinguished Grantee, L. Vasylechko L'viv Polytechnic National University L'viv, Ukraine ICDD Grant-in-Aid

# OUR COLLABORATIVE PARTNERS INCLUDE:

# Cambridge Crystallographic Data Centre (CCDC)

Cambridge, UK Cambridge Structural Database (CSD)

### Fachinformationszentrum Karlsruhe (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 without being an expert in the field
- New data is contributed annually by highly qualified grantees from around the world
- PDF® products are compatible with major diffraction vendor's software



# 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 our website at www.icdd.com. Our goal is to help you solve your material analysis problems. We provide reference articles, technical bulletins, tutorials, and instructional videos. Many tutorials focus on capabilities of the database and others illustrate methods used to analyze pharmaceuticals, polymers, and minerals. Search and browse documents from ICDD's Pharmaceutical Powder X-ray Diffraction Symposium and the ICDD Spring Meetings for free. We also provide open access to over 1,000 full publications from Advances in X-ray Analysis (AXA) – the proceedings of the Denver X-ray Conference (DXC).



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# Announcing our new partnership with the Cambridge Crystallographic Data Centre (CCDC)!

# See the power of powder and single crystal data combined.

Two of the largest chemical data repositories have announced a new partnership which will allow greater utility and insights in the development of new drugs and materials. The International Centre for Diffraction Data, ICDD, publishes the PDF (Powder Diffraction File) and has managed the curation, publication and distribution of X-ray powder diffraction data for 80 years. The Cambridge Crystallographic Data Centre, CCDC, curates and maintains the CSD (Cambridge Structural Database) – the world's repository for small-molecule organic and metal-organic crystal structures. Both non-profit organizations have a strong focus on data quality, with entries edited and verified to ensure accuracy and standardized format.

The partnership will see the ICDD calculate and publish diffraction patterns, including atomic coordinates, from structures found in the CSD. By combining powder and single crystal data in this manner, the ability to match samples to known structures will be enhanced – enabling, for example, rapid analysis in the pharmaceutical industry from API discovery through drug delivery formulation.

"This collaboration between our two organizations is a win for the scientific community. Materials characterization is enhanced by this symbiotic relationship, particularly in the areas of phase identification and quantitative analysis. The goal is straightforward, to get more data into the hands of more analysts to help them get the right answer."

Tom Blanton, Executive Director ICDD "CCDC and ICDD have a common aim of collating, enhancing and making high-quality structural chemistry data available to scientists across the world. I am delighted that this collaboration helps extend our commitment to the FAIR data principles increasing the findability, accessibility, interoperability and reusability of this important dataset."

Juergen Harter, CEO CCDC

As discoveries and developments made using or even exclusively by informaticsbased approaches continue to rise, this partnership could open further opportunities for innovative research in the ever-changing pharmaceutical and organic materials landscape.



# LICENSE OPTIONS TO FIT YOUR BUDGET!



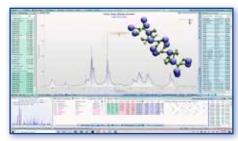
- **NEW**—Extended multiyear license terms— Let us know what you need!
- We will customize the license for a 1 to 9-year license term.
- 15% discount for new PDF-4 and JADE Pro Bundles
- One stop shopping—align PDF and JADE renewals for one billing and shipment
- **Save Money!** Combine a new license for PDF-4+ and PDF-4/Organics
- PDF-2 10-year license prepaid package
- PDF-4+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-4 Subscriptions
  - ICDD's subscriptions keep your database up-to-date with renewal pricing
  - ICDD offers automatic PDF-4 renewal shipments for convenience
  - Can't accept automatic shipments? ICDD will send a PDF-4 renewal reminder to keep you up-to-date with your subscription



# WORKING TOGETHER FOR YOU THE (deg)



JADE Pro is all-inclusive! It includes all of the features of JADE Standard, plus batch processing Whole Pattern Fitting (WPF) and Rietveld refinement tools. JADE Pro features a floating network license that allows access on one concurrent system at a time, so when you aren't using it, someone else in your organization can access it. Discounted additional seats create access to more concurrent shareable licenses.



### **Bundle License Options**

PDF-4+ and JADE Pro Bundle	DVD Code:	USB Code:	2020 – 2021 LIST \$	2020 - 2021 ACADEMIC \$
New - Single License	BUJPF4D21	BUJPF4S21	\$15,648	\$10,986
PDF-4/Organics and JADE Pro Bun	dle			
New - Single License	BUJPOR4D21	BUJPOR4S21	\$15,648	\$10,986

Please contact MDI for more licensing options

# **JADE STANDARD**

JADE Standard is a powerful, all-purpose powder XRD pattern viewer, processing and analysis program with great emphasis on quantification and phase ID. JADE Standard makes the task of processing and understanding your collected data simple and your results concise and easy to understand.

#### SIMULATION AND VISUALIZATION

#### All Levels of JADE Standard

Simulate 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.

#### WHOLE PATTERN FITTING + RIETVELD

#### JADE Standard Level 2B or Level 3

Quantify weight percentages and identify minor phases quickly and easily. JADE Standard can automate these tasks as soon as you load your pattern.

#### PHASE ID (S/M)

#### JADE Standard Level 2A or Level 3

Whole pattern-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.



- All-inclusive Phase ID, batch processing Whole Pattern Fitting (WPF) and Rietveld
- Floating network license can work as a shareable multi-seat license
- Discounted additional seats
- One-Click-Analysis<sup>™</sup> for Whole Pattern Fitting (WPF) automates your analysis
- Pattern Indexing (All Crystal Systems)
- Rietveld Structure Refinement (Atomic Parameters)
- Ab Initio Tools (Charge Flipping +)
- Cluster analysis of powder patterns
- Hardware independent application supports a wide range of diffractometers



- Reads all vendor pattern files
- Handles variable/fixed-slit data
- Auto peak search and multi-filter search
- Simulate patterns from crystal structures
- Available in three levels:
  - Level 1: Base
  - Level 2A: Search-match
  - Level 2B: Whole Pattern Fitting (WPF)
  - Level 3: Search-match and Whole Pattern Fitting (WPF)
- Phase identification (Level 2A and 3)
- Minor and trace phase ID
- WPF Rietveld refinement (Level 2B and 3)
- No annual renewal fee
- Used on a single workstation
- Hardware independent application supports a wide range of diffractometers

	Т	HRFF	LEVEL	ς	
<b>JADE</b> Standard	1	24	2B	3	
Intuitive, State-of-the-Art UI	•	•	•	•	
Reads All Vendor Pattern Files	•	•	•	•	
Smart Column Data Importer	•	•	•	•	
Merge Multi-Scans/Segments	•	•	•	•	
1, 2 and 3D Pattern Overlay	•	•	•	•	
Déjà Vu ID Similar Pattern Files	•	•	•	•	
Supports Multiple Axes/Wavelengths	•	•	•	•	
Handles Variable/Fixed-Slit Data	•	•	•	•	
Zero Offset and Theta Calibration	•	•	•	•	
Background Fitting/Batch Fitting/Removal	•	•	•	•	
Auto Peak Search and Multi-Filter Search	•	•	•	•	
Wide Variety of Report and Print Options	•	•	•	•	
Includes Starter Database	•	•		•	
ICDD PDF Database Access and Others	•	•			
Multitude of Choices for Data Retrieval		•	•		
View Crystal Structures and Reflection Planes	•		•		
Simulate Patterns from Crystal Structures	•	•			
Individual Analyst/Shared Work Environments		•			
Supports Custom d-I% list for Phase Overlay		•		•	
Profile Fitting with RIR Quant, Size and Strain		•		•	
Batch Profile Fitting		•		•	
Whole Pattern Based Search/Match (S/M)	JADE Base	•			
Use Chemistry and Unit Cell Data in S/M	•				
Solid-Solution and Isotypical Phase ID	Star	•		•	
Preferred-Orientation Data and Single Peak S/M	Standard	•		•	
Minor and Trace Phase ID		•		•	
Structure Database Manager				•	
•					
WPF-Rietveld Refinement (Unlimited Phases) Gold Standard Quantitative Analysis		JADE with :		•	
		E Standard 1 S/M	•	•	
Seamless Integration with Database Retrieval		dard	•	•	
Auto-Loading of Structure Data from Database					
Combination of Phases with/without Structure Data					
Linking of Unit Cell, Phase Broadening Parameters					
Custom d-1% (hkl, FWHM, Skew) to Fit Clay Phases					
Amorphous Content with/without Internal wt% Standards       •       •         Atomic Occupancy and Bond Distance Constraints       •       •					
				•	
Polynomial and Spline Curve Background Fitting			<b></b>		
RECOMMENDED CONFIGURATION			ADE	ADE vith b	
Intel® Core™ i7, i5 or i3, 8GB RAM, 24" or larger monitor, V			Star. NPF	Star. oth S	
10 (or Windows 8 or 7) JADE has been written to take full adv the Windows environment and ever more powerful hardware of			JADE Standard with WPF	IADE Standard vith both S/M a	
today. JADE makes many calculations and provides a tremend			<u></u>	JADE Standard with both S/M and WPF	
of information back to the user. Your JADE experience will be r				VPF	

# **RECOMMENDED CONFIGURATION**

Intel® Core™ i7, i5 or i3, 8GB RAM, 24" or larger monitor, Windows 10 (or Windows 8 or 7) JADE has been written to take full advantage of the Windows environment and ever more powerful hardware available today. JADE makes many calculations and provides a tremendous amount of information back to the user. Your JADE experience will be richer on a larger screen. JADE can read all current data formats from Synchrotron Beamlines, Rigaku, Bruker (Siemens), Malvern Panalytical (Philips), ARL Thermo Fisher Scientific (Scintag), Shimadzu, Proto, XOS, X-Y data and other formats. JADE also understands the many reference patterns and structure databases and their formats including ICDD products (PDF-4+, PDF-4+/ Web, PDF-4/Axiom, PDF-4/Minerals, PDF-4/Organics, PDF-2), NIST Crystal Data, AMCSD \*.amc CIF, MOL, PDB, and others, including custom databases.

# JADE Pro

# The Professional Version of JADE Includes everything found in JADE Standard and much more.

# JADE Pro is constantly adding features.

New this year, JADE Pro has added a toolkit, which includes items such as size/strain, an area detector reader, structure solver, laue simulation, charged flipper, an XRD pattern digitizer as well as cluster analysis visualization tools. Additionally JADE Pro & Standard has been translated to both Chinese and Japanese.

JADE Pro has a low buy-in with updates serviced by subscription. One of the most valuable benefits of software as subscription is that your software is always up to date. All new features are included, which helps you expand the capabilities of your lab and expand knowledge of your particular science and appreciation of your data sets. JADE Pro can be used as a shareable floating-seat license. For example, a group of 5 people can share 3-seat license which would provide for 3 systems running JADE Pro concurrently.

For most of our customers, the Professional version of JADE is the most logical path to provide the most features for the least cost. If you have any questions at all as to what path may be best for your lab or organizaion, please contact us - we always love to hear from our fellow XRD Scientists!

In addition to all the features found in JADE Standard, below is a highlight of some additional features found only in JADE Pro.

One-Click Phase ID and Rietveld Analysis
Size and Strain Analysis (Warren-Averbach)
Pattern Indexing (All Crystal Systems)
Line-Based Cell Refinement
Simulate Series of Powder Patterns from Crystal Structures
WPF and Rietveld Batch Processing
Rietveld Structure Refinement (Atomic Parameters)
Fourier Map Tools
Ab Initio Tools (Charge Flipping +)
Cluster Analysis of Powder Patterns
Floating (Shareable) Network License
Future Feature Updates via Subscription
Floating (Shareable) Network License

# **INTRODUCING JADE QA**

JADE QA was created for production line XRD needs and is designed to extend the power of Rietveld Quantitative Analysis (QA) to those in your organization responsible for overseeing consistencies in production.

JADE QA works in union with a specialist who knows how to analyze site specific samples and is able to create a setup file in a separate higherlevel version of JADE geared for the analytical scientist. A JADE QA setup file (or WPF control file), can be modified and updated by the specialist at any time. There is no limit to the number of setup files that can be handed off to JADE QA. Alongside its main task of performing production-level quantitative analysis, once JADE QA has a setup file, technicians can perform the following in a real time production setting:

illicovite-31 . La Te

Clinker Mix (8 Phases)

Tuesday, June 16, 2020 3:17

Hatrurite • Ca35iO6 • | Pe... Tuesday, June 16, 2020 3:1...

- Read and import all types of XRD patterns
- Overlay patterns in 2D and 3D
- Save and browse work files and browse pattern files
- Print patterns and peaks
- Perform pattern processing via
  - Background fitting
  - Peak search
  - Data cursor tools

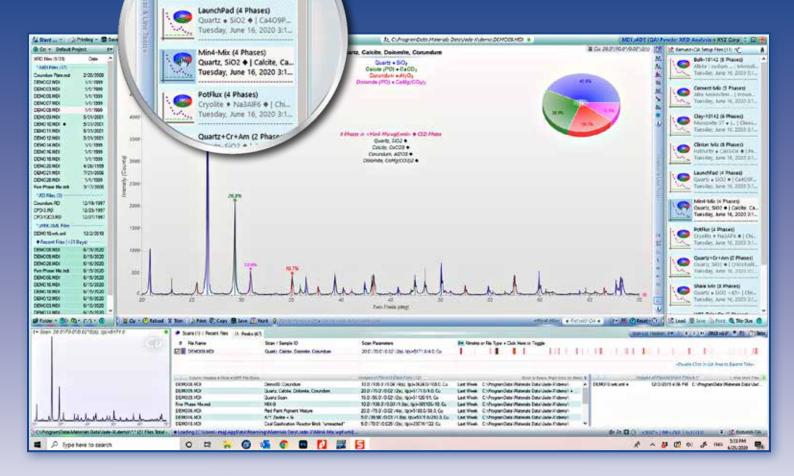
JADE QA's tailored user interface echoes the well-established and intuitive JADE Pro interface. The JADE QA setup files carry their own phase data for the intended analysis, and do not allow the following:

- Access to the ICDD PDF database for phase identification (S/M)
- Ability to create custom crystal structure data for phase overlays and S/M
- Ability to view crystal structures and simulate powder patterns from them
- Profile fitting tools and those related functions.

Once a setup file has been created and passed to JADE QA, simply select a setup file to compare and run the refinement. The results of a JADE QA refinement show both a difference plot and a QA chart. The plot shows a difference plot for the observed & fitted patterns so that a technician can evaluate the goodness of fit. The QA chart shows the Whole Pattern Fitting refinement progress with weight percentages. Once JADE QA has run, you may print the fitted pattern plot and QA chart and if you wish you may copy the QA phase list for use in a spread sheet like Excel.

JADE QA supports batch processing for up to 16 similar scans. JADE QA will automatically analyze each scan with a QA setup file and compile a summary QA phase list along with a QA report for each individual scan.

JADE QA - built for production line quantitative analysis carried out by a technician and backed by the support of an analytical scientist running a higher-level version of JADE Standard that supports both S/M and WPF or all the power of JADE Pro.



JADE IS MULTILINGUAL!

JADE has been localized for both China and Japan.



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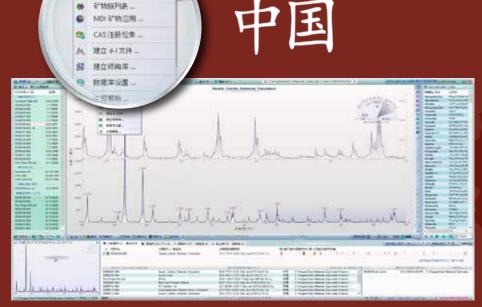
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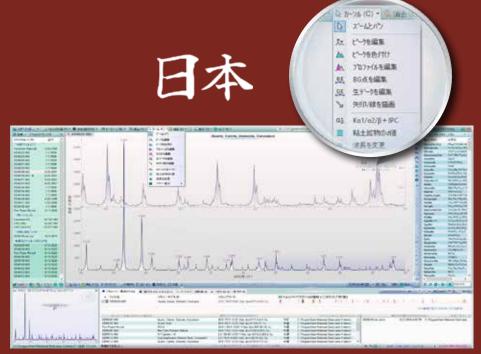
JADE is now available in both Chinese and Japanese as well as English. If Windows is running one of these languages, JADE will install in that language. Alternate language selection is made within JADE and may be changed at any time on the fly.

A multi-language version of JADE provides flexibility for a language-diverse team. Individuals sharing a JADE Pro license may choose which language they prefer to use without impacting another team member sharing the same license but preferring a different language.

For global entities with diverse geographic locations, a unified XRD analysis platform, independent of equipment or language, ensures consistent results throughout the organization.

JADE is relied upon for unbiased results around the world, and to reflect that global embrace, JADE has recently been translated to both Chinese and Japanese. Same product, same product number, now multilingual.







# Introducing Release 2021 of the Powder Diffraction File

# THE PRODUCT LINE INCLUDES:

PDF-4+	•
2021	

PDF-4+/Web 2021

PDF-4/Axiom 2021

PDF-4/Minerals 2021

PDF-4/Organics

PDF-2 2021



# **Intensity Scaling for 2D** Multiphase Analysis (Sleve+ only)

2021

 Intensities are now scaled for ring pattern simulations when doing 2D multiphase analysis.

Sleve+ search results for a three phase unknown.



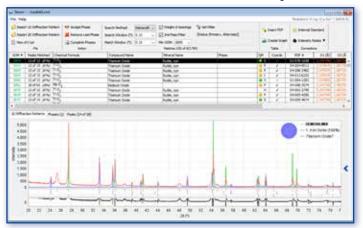
# **New Searches and Display Fields** (all products)

- Refined Formula A formula derived from the occupancies and site multiplicities of the elements in the atomic coordinates.
- Wyckoff Sequence

Data mining search results for the Wyckoff sequence "d2 c14"

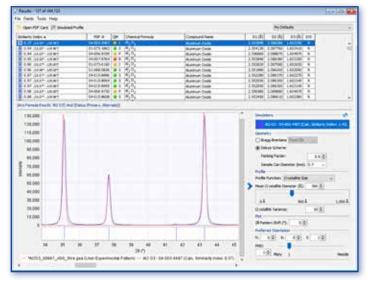


# Import JADE Projects Directly into Sleve+ for Phase Identification (Sleve+ only)



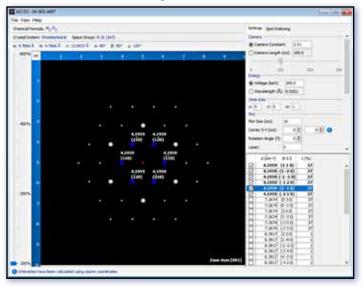
Experimental data that was imported and processed in JADE, can now be imported into Sleve+ for complimentary phase identification.

# Quick Settings Panel for Pattern Simulations (PDF-4 only)



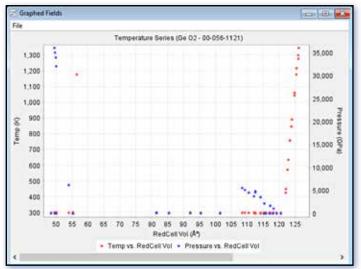
Quick settings panel allows the user to dynamically change various simulation settings directly on the graph.

# d-spacings Table in SAED Simulation Window (PDF-4 only)



New table displays the d-spacings, HKL's, and intensities for all spots in the SAED pattern simulation window. Spots can be highlighted by clicking on them in the table or directly in the simulation.

# Plot Left and Right Y-axes of Data Mining Searches (PDF-4 only)



Temperature series graph for  $GeO_2$  displaying both temperature (left y-axis) and pressure (right y-axis) as a function of reduced cell volume.

# WHICH ICDD DATABASE IS RIGHT FOR YOU?

	PDF-4+ 2021	PDF-4+/ WEB 2021	PDF-4/ AXIOM 2021	PDF-4/ MINERALS 2021	PDF-4/ ORGANICS 2021	PDF-2 2021
I WORK PRIMARILY WITH INORGANIC COMPOUNDS	<b>~</b>	<b>~</b>	<ul> <li>Image: A second s</li></ul>			¥
I WORK PRIMARILY WITH ORGANIC COMPOUNDS					~	
I WORK PRIMARILY WITH MINERALS				~		
I WORK WITH ELECTRON DIFFRACTION/SYNCHROTRON	~	~		~	~	
I NEED TO WORK AT THE OFFICE AND HOME		<b>v</b>				
I NEED TO DO QUANTITATIVE ANALYSIS						
RIETVELD	✓ *	✓ *	✓ *	✓ *	✓ *	
REFERENCE INTENSITY RATIO (RIR)	✓ †	✓ †	✓ *	✓ †	✓ †	✓ †
PATTERN FITTING	✓ *	✓ *	✓ *	✓ *	✓ *	
I NEED A DATABASE WITH ATOMIC COORDINATES	<ul> <li>Image: A second s</li></ul>	<b>~</b>	<b>~</b>	~	<b>~</b>	
HOW MANY ENTRIES ARE IN THE DATABASE?	444,133	444,133	97,789	48,946	547,295	316,820
HOW MANY ENTRIES ARE NEW?	17,944	17,944	5,184	1,777	8,791	5,259
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. You need to check with your software vendor for compatibility.	~	~	~	~	~	~
WHAT IS THE LICENSE TERM FOR THE DATABASE?	1 YEAR	1 YEAR	3 YEAR	1 YEAR	1 YEAR	5 YEAR
MULTI-YEAR LICENSE AVAILABLE	~	~		~	~	
SITE LICENSE AVAILABLE	<b>~</b>	<b>~</b>			<b>~</b>	<ul> <li>Image: A second s</li></ul>

\* Using diffraction equipment manufacturer or vendor software.

 $\dagger$  Using Sleve or Sleve+, diffraction equipment manufacturer or vendor software.

NEW~ Extended multi-year license terms – let us know what you need!



# Preferred Computer Specifications for PDF Databases

- Hard disk space requirements:
  - PDF-2 2021 4 GB
  - ◆ PDF-4+ 2021 10 GB
  - PDF-4+/Web 2021 0.5 GB
  - PDF-4/Minerals 2021 1.5 GB
  - PDF-4/Organics 2021 19 GB
  - PDF-4/Axiom 2021 3 GB
- Intel<sup>®</sup> Core<sup>™</sup> 2 Duo processor or better
- NTFS file system required
- 4 GB system memory



# Supported Microsoft® Operating Systems:

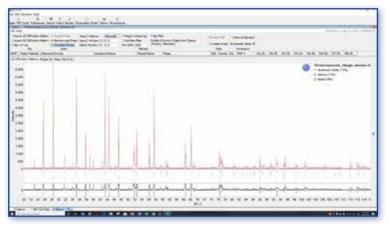
- Windows<sup>®</sup> 7 SP1
- Windows<sup>®</sup> 8
- Windows® 8.1
- Windows<sup>®</sup> 10



# PDF-4+ 2021

### Phase Identification and Quantitation

PDF-4+ combines the world's largest sources of inorganic diffraction data from crystals and powders into a single database.



# KEY POINTS

- Rapid phase identification designed to support automated quantitative analyses
- Features 444,100+ entries with over 336,500+ having atomic coordinates
- 47,100+ entries for organic materials
- Integrated data mining software
- All entries have digital patterns for use in total pattern analysis
- More than 343,400 entries have I/I<sub>c</sub> values for quantitative analysis by Reference Intensity Ratio (RIR)
- 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 materials
- Extensive data mining is facilitated with 131 display fields coupled with 77 searches
- One (1) year license serviced by subscription

PDF-4+ Purchase Options				
PDF-4+ 2021	DVD CODE	USB CODE	2020 –2021 LIST \$	2020 -202 ACADEMIC S
New - Single License	F4D21	F4S21	\$8,910	\$5,925
Renewal from 2020 to 2021	F4RD21	F4RS21	\$1,960	\$1,250
PDF-4+ and JADE Pro Bundle*				
New - Single License	BUJPF4D21	BUJPF4S21	\$15,648	\$10,986
*Purchase a new license for PDF-4+ and JADE Pro				
PDF-4+ 2021 Multi-year License*				
Renewal - 3 year license	F4D22MR24	F4S22MR24	\$5,290	\$3,375
Renewal - 5 year license	F4D22MR26	F4S22MR26	\$8,330	\$5,315
PDF-4+Scholar 2021 (10-Year License Package)*				
PDF-4+ New – Single License	F4D21	F4S21	NA	\$5,925
Sleve+ – New Single License	SWS421N	SWS421N	NA	\$500
Scholar Multi-year	F4SPD22MR26	F4SPS22MR26	NA	\$6,125
Save Money! Take	advantange of ICDD's Com	bo Site License – Reau	vest a auote todav!	\$12,550
PDF-4+ 2021 Site License*		-		
New Master License	F4D21M	F4S21M	\$8,910	\$5,925
New - additional licenses, each	F4D21C	F4S21C	\$1,960	\$1,250
Renewal - Yearly Master License	F4RD21M	F4RS21M	\$1,960	\$1,250
Renewal - additional licenses, each	F4RD21C	F4RS21C	\$750	\$495
PDF-4+ 2021 Site/Multi-year License*				
Renewal - 3 year Master Site License	F4D22MR24M	F4S22MR24M	\$5,290	\$3,375
Renewal - 3 year additional licenses, each	F4D22MR24C	F4S22MR24C	\$2,250	\$1,485
Renewal - 5 year Master Site License	F4D22MR26M	F4S22MR26M	\$8,330	\$5,315
Renewal - 5 year additional licenses, each	F4D22MR26C	F4S22MR26C	\$3,750	\$2,475
PDF-2 to PDF-4+ Conversion				
PDF-2 2020 to PDF-4+ 2021	F2420RDU21	F2420RSU21	\$1,960	\$1,250
PDF-2 2019 to PDF-4+ 2021	F2419RDU21	F2419RSU21	\$3,920	\$2,500
PDF-2 2018 to PDF-4+ 2021	F2418RDU21	F2418RSU21	\$5,880	\$3,750
PDF-2 2016 to PDF-4+ 2021	F2416RDU21	F2416RSU21	\$7,840	\$5,000
* Please see product policies on pages 16 and 17			V	

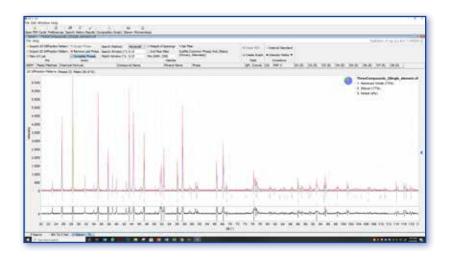
# PDF-4+ Purchase Options



# PDF-4+/WEB 2021

#### Data on the Go

PDF-4+/Web provides portability to the PDF-4+ database via the internet. It enables access to the entire suite of programs and data files, so that it is equivalent to PDF-4+ 2021.



# KEY POINTS

- PDF-4+ database via the Internet
- Access to the entire suite of PDF-4+ programs and data files
- Can be used on any computer that meets the specifications
- Requires access to a high-speed internet connection Delivered as a USB compatible dongle\*
- Installation and renewals are handled via the internet
- One (1) year license serviced by subscription



PDF-4+/Web 2021 requires a fully-powered USB port, web browser, and ability to open TCP/IP ports through any existing firewalls. Connectivity speed should be at least 10 Mbps or higher.\*

\*see Preferred Computer Specifications, page 8

Explorer



# PDF-4+/Web Purchase Options

PDF-4+/Web 2021	DONGLE CODE	2020 –2021 LIST \$	2020 –2021 ACADEMIC \$
New - Single License	W421	\$8,910	\$5,925
Renewal from 2020 to 2021	W4R21	\$1,960	\$1,250
PDF-4+/Web 2021 Multi-year License*			
Renewal - 3 year license	W422MR24	\$5,290	\$3,375
Renewal - 5 year license	W422MR26	\$8,330	\$5,315
PDF-4+/Web 2021 Site License*			
New Master License	W421M	\$8,910	\$5,925
New - additional licenses, each	W421C	\$1,960	\$1,250
Renewal - Yearly Master License	W4R21M	\$1,960	\$1,250
Renewal - additional licenses, each	W4R21C	\$750	\$495
Save Mo. PDF-4+/Web 2021 Site/Multi-year License*	ney! Take advantange of ICDD's Combo	Site License – Reque	est a quote today!
Renewal - 3 year Master Site License	W422MR24M	\$5,290	\$3,375
Renewal - 3 year additional licenses, each	W422MR24C	\$2,250	\$1,485
Renewal - 5 year Master Site License	W422MR26M	\$8,330	\$5,315
Renewal - 5 year additional licenses, each	W422MR26C	\$3,750	\$2,475
PDF-4+/Web Conversion			
PDF-2 2020 to PDF-4+/Web 2021	W2W2ORU21	\$1,960	\$1,250
PDF-2 2019 to PDF-4+/Web 2021	W2W19RU21	\$3,920	\$2,500
PDF-2 2018 to PDF-4+/Web 2021	W2W18RU21	\$5,880	\$3,750
PDF-2 2016 to PDF-4+/Web 2021	W2W16RU21	\$7,840	\$5,000
PDF-4+ 2020 to PDF-4+/Web 2021	W4W2ORU21	\$1,960	\$1,250

10 INTERNATIONAL CENTRE FOR DIFFRACTION DATA

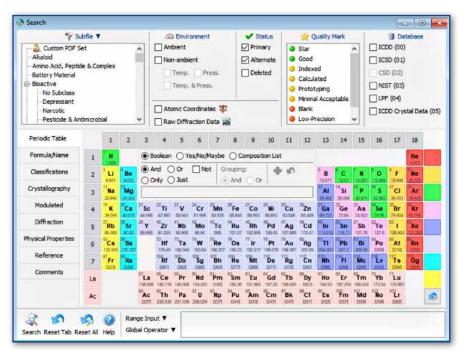
\* Please see product policies on pages 16 and 17



# **PDF-4/AXIOM 2021**

### **Quality plus Value**

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



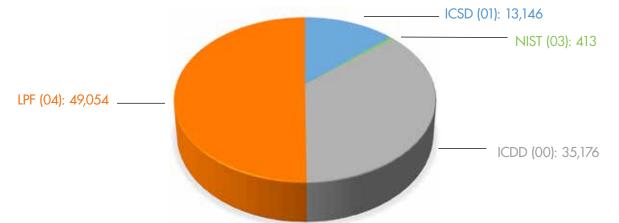


- Cost effective
- Single License: Three (3) year license term
- Optional: Two additional seats (three (3) year license term)
- NEW Six (6) year and nine (9) year prepaid packages
- No subscription
- Featuring 97,700+ entries, including inorganic and organic entries
- 69,700+ entries with atomic coordinates
- Data focused on ambient entries
- Fundamental mineral entries
- ICDD data mining software
- ICDD's search identification software is not included (available with PDF-4+)

### Requires diffraction equipment manufacturer or vendor software for phase identification applications

# **Database Sources**

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



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

PDF-4/Axiom 2021	DVD CODE	USB CODE	2020 –2021 LIST \$	2020 –2021 ACADEMIC \$
New License - 3 years	AX4D21	AX4S21	\$3,550	\$2,550
Two Additional Seats (each seat: single PC installation)	AX4D21MS	AX4S21MS	\$1,000	\$500
PDF-4/Axiom 2021 Packages*				
PDF-4/Axiom - 6 years	AX4D6YR	AX4S6YR	\$7,100	\$5,100
PDF-4/Axiom - 9 years	AX4D9YR	AX4S9YR	\$10,650	\$7,650

\*Purchase two or three Single Licenses (Release 2021, Release 2024, and Release 2027)

- Each PDF-4/Axiom product is licensed for three (3) years

Shipping fees for all databases billed on the original invoice

\* Please see product policies on pages 16 and 17



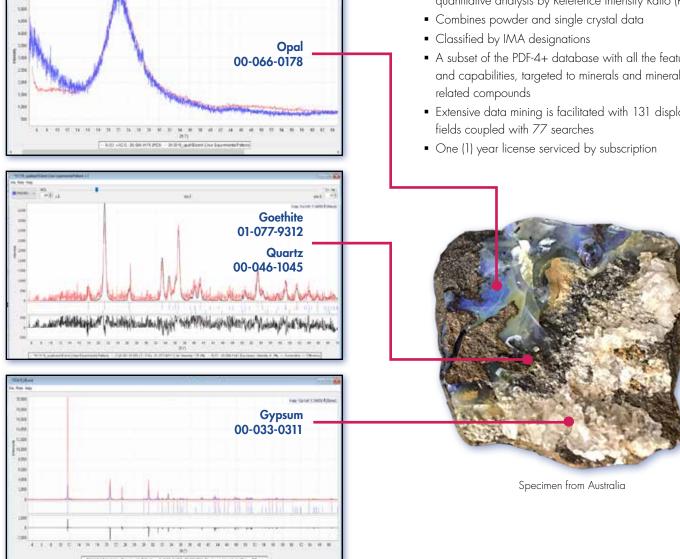
# PDF-4/MINERALS 2021

### **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.



- Rapid phase identification, plus support for automated quantitative analyses
- Features 48,900+ entries, including 40,300+ entries with atomic coordinates
- Integrated data mining software
- All entries have digital patterns for use in total pattern analysis
- More than 37,500 entries have I/I<sub>c</sub> values for quantitative analysis by Reference Intensity Ratio (RIR)
- A subset of the PDF-4+ database with all the features and capabilities, targeted to minerals and mineral related compounds
- Extensive data mining is facilitated with 131 display fields coupled with 77 searches



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

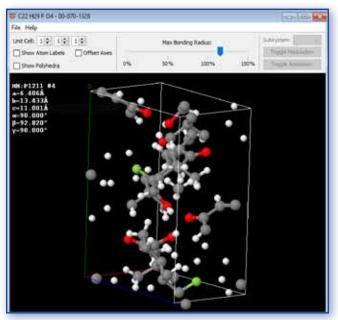
PDF-4/Minerals 2021	DVD CODE	USB CODE	2020 –2021 LIST \$	2020 –2021 ACADEMIC \$
New - Single License	MN4D21	MN4S21	\$1,720	\$1,170
Renewal from 2020 to 2021	MNR4D21	MNR4S21	\$935	\$610
PDF-4/Minerals 2021 Multi-year License*				
Renewal - 3 year license	MND422MR24	MNS422MR24	\$2,805	\$1,830
Renewal - 5 year license	MND422MR26	MNS422MR26	\$4,675	\$3,050



# PDF-4/ORGANICS 2021

### Solve Difficult Problems, Get Better Results

PDF-4/Organics database is a highly targeted collection, with special focus on materials used in commercial and regulatory fields. It provides the best of both worlds by including single crystal and powder diffraction data together in a single, edited, and standardized database.



PDF Entry 00-070-1328 3D Structure

# KEY POINTS

- Largest collection of pharmaceuticals, excipients, and polymers
- Features 547,200+ entries and 126,900+ entries with atomic coordinates
- Integrated data mining software
- Sleve+ search-indexing software included as an added value
- Combines crystalline, semi-crystalline, and amorphous solid state materials
- Combines powder and single crystal data
- 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 9,100 bioactive/pharmaceutical entries
- One (1) year license serviced by subscription

# Includes 5,400+ new CSD entries from our new partnership with Cambridge Crystallographic Data Centre

# **REQUEST A QUOTE TODAY!**

PDF-4/Organics Purchase Options				
PDF-4/Organics 2021	DVD CODE	USB CODE	2020 –2021 LIST \$	2020 –2021 ACADEMIC \$
New - Single License	OR4D21	OR4S21	\$8,910	\$5,925
Renewal from 2020 to 2021	OR4RD21	OR4RS21	\$2,660	\$1,400
PDF-4/Organics and JADE Pro Bundle*				
New - Single License	BUJPOR4D21	BUJPOR4S21	\$15,648	\$10,986
*Purchase a new license for PDF-4/Organics and JADE Pro				
PDF-4/Organics 2021 Multi-year License*				
Renewal - 3 year license	OR4D22MR24	OR4S22MR24	\$7,180	\$3,780
Renewal - 5 year license	OR4D22MR26	OR4S22MR26	\$11,300	\$5,950
PDF-4/Organics 2021 Site License*				
New Master License	OR4D21M	OR4S21M	\$8,910	\$5,925
New - additional licenses, each	OR4D21C	OR4S21C	\$2,660	\$1,400
Renewal - Yearly Master License	OR4RD21M	OR4RS21M	\$2,660	\$1,400
Renewal - additional licenses, each	OR4RD21C	OR4RS21C	\$1,600	\$750
PDF-4/Organics 2021 Site/Multi-year License*				
Renewal - 3 year Master Site License	OR4D22MR24M	OR4S22MR24M	\$7,180	\$3,780
Renewal - 3 year additional licenses, each	OR4D22MR24C	OR4S22MR24C	\$4,800	\$2,250
Renewal - 5 year Master Site License	OR4D22MR26M	OR4S22MR26M	\$11,300	\$5,950
Renewal - 5 year additional licenses, each	OR4D22MR26C	OR4S22MR26C	\$8,000	\$3,750

\* Please see product policies on pages 16 and 17



# PDF-2 2021

### 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.

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	Zooke Name Attende Name CALI Number Brity Cate Mudification Date	26/04/202			



- Features 316,800+ entries
- 216,100+ entries have I/I<sub>c</sub> values for quantitative analysis by Reference Intensity Ratio (RIR)
- Integrated data mining software
- Sleve search-indexing software included as an added value
- Combines powder and single-crystal data
- Rapid data mining with our 57 display fields coupled with 71 searches
- Five (5) year license

# Take Advantage of ICDD's PDF-2 10-Year License Package REQUEST A QUOTE TODAY!

PDF-2	Purchase	<b>Options</b>
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			2020 - 2021	2020 -2021
PDF-2 2021: 5 (five) year License	DVD CODE	USB CODE	LIST \$	ACADEMIC \$
New - Single License	C2D21PN	C2S21PN	\$8,910	\$5,925
Renewal - from 2020 to 2021	C2D20PU21	C2S20PU21	\$1,960	\$1,250
Renewal - from 2019 to 2021	C2D19PU21	C2S19PU21	\$3,920	\$2,500
Renewal - from 2018 to 2021	C2D18PU21	C2S18PU21	\$5,880	\$3,750
Renewal - from 2016 to 2021	C2D16PU21	C2S16PU21	\$7,840	\$5,000
PDF-2 2021: 10 (ten) year License Package				
New licenses (2021 and 2026)	PD2D10YR	PD2S10YR	\$17,820	\$11,850
Purchase Two (2) New PDF-2 Single Licenses (Release 2021, Release 2026)				
PDF-2 2021 Site License*				
New Master License	C2D21PNM	C2S21PNM	\$8,910	\$5,925
New - additional licenses, each	C2D21PNC	C2S21PNC	\$1,960	\$1,250
Renewal - Yearly Master License	C2D20PU21M	C2S2OPU21M	\$1,960	\$1,250
Renewal - additional licenses, each	C2D20PU21C	C2S2OPU21C	\$750	\$495
PDF-2 to PDF-4+ Conversion				
PDF-2 2020 to PDF-4+ 2021	F2420RDU21	F2420RSU21	\$1,960	\$1,250
PDF-2 2019 to PDF-4+ 2021	F2419RDU21	F2419RSU21	\$3,920	\$2,500
PDF-2 2018 to PDF-4+ 2021	F2418RDU21	F2418RSU21	\$5,880	\$3,750
PDF-2 2016 to PDF-4+ 2021	F2416RDU21	F2416RSU21	\$7,840	\$5,000

\* Please see product policies on pages 16 and 17

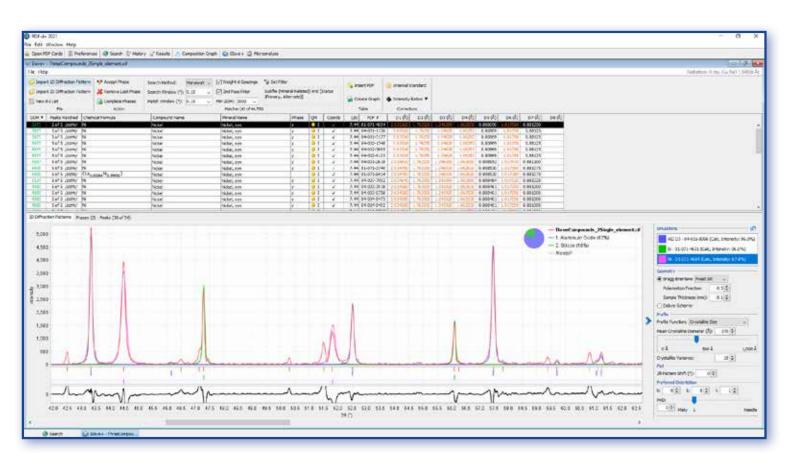
# SIEVE/SIEVE+ 2021

### Search and Identify

ICDD's search identification programs, Sleve for PDF-2 and Sleve+ for 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 accuracy and precision of the identification process.



- 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 multiphase specimens
- Strength of Sleve/Sleve+ is evident in the analysis of minor and trace phases
- Supports X-ray, synchrotron, electron<sup>+</sup>, and neutron<sup>+</sup> data
- "Intelligent" RIR for semi-quantitative analysis†
   † PDF-4 only



# **Sleve+ Purchase Options**

Sleve+ 2021	CODE	2020 – 2021 LIST \$	2020 - 2021 ACADEMIC \$
New - Single License	SWS421N	\$760	\$500
Renewal	SWS421U	\$450	\$280
Sleve+ 2021 Multi-year License*			
Renewal - 3 year license	SWS422MR24	\$1,215	\$760
Renewal - 5 year license	SWS422MR26	\$1,915	\$1,190

\*Please see product policies on page 16 - 17.

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**PRODUCT LICENSE POLICIES** 

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A site license includes the purchase of a Master License, and the

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PDF-2: The license term for PDF-2 and Sleve is five (5) years.

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# **RELEASE 2021**

LICENS	SE TERMS
Product	License Term
PDF-2 with Sleve	5 years
PDF-4/Axiom	3 years
PDF-4 products*	1 year
Sleve+*	1 year

\* Serviced by subscription featuring automatic annual renewals.

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# Note: PDF-4/Axiom and PDF-4/Minerals are excluded from site license options.

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# LICENSING CONTINUED

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Note: PDF-2 can only be combined with PDF-4+ or PDF-4+/Web.

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Note: (PDF-2, PDF-4/Axiom, and PDF-4/Minerals databases are not eligible).

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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 11 for PDF/Axiom and page 14 for PDF-2. (See below)

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

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### Fundamentals of X-ray Powder Diffraction

17 - 21 May 2021 www.icdd.com/xrd/

### Advanced Methods in X-ray Powder Diffraction

24 - 28 May 2021 www.icdd.com/xrd/

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FALL 2021 www.icdd.com/rietveld/



#### 18 INTERNATIONAL CENTRE FOR DIFFRACTION DATA

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www.icdd.com  $\rightarrow$  Conferences

# **70TH DENVER X-RAY CONFERENCE**

www.dxcicdd.com

The Westin Chicago Lombard, Yorktown Center Lombard, Illinois, USA 2 - 6 August 2021

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.

# PHARMACEUTICAL POWDER X-RAY DIFFRACTION SYMPOSIUM

www.icdd.com/ppxrd/

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.

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www.icdd.com  $\rightarrow$  Resources

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CDD.	$\underset{\text{Materials Data}^{\text{MD}}}{\bigwedge} \mathbf{D}$
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○ Order-Bill Me ○ Please Send Quotation ○	Please Send Proforma
End-User (where the database/software is installed	l and used; person responsible for license)
End-user Company	
End-User: First Name	Last Name
Department	
Street Address (No P.O. Boxes)	
Address (Building/Room No.)	
City Postal Code	State/Providence
Country	
Phone	Mobile Phone
Email	Website
ICDD Customer Account No. (If known)	
I currently use:  PDF-2  PDF-4+  PDF-4/Organics  PE	DF-4/Minerals  PDF-4+/Web  PDF-4/Axiom  None
Release Year	Product Serial No
I currently use: ] JADE Standard ] JADE Pro None	
Product Serial No	
$\Box$ Ship to address the same as End-User	
Ship To (if different from End-User)	
Organization	
Ship To: First Name	Last Name
Department	
Street Address (No P.O. Boxes)	
Address (Building/Room No.)	
City Postal Code	State/Providence
Country	
Phone	Mobile Phone
Email	Website

Order Details			
Items Ordered	Media Type	Quantity	Price (\$USD)
	O dvd O usb		
	O DVD O USB		
	O DVD O USB		
	O DVD O USB		
	O dvd O usb		
Company Classification			
O Book Dealer O Corporation O Degree-G	ranting-Institution $*$ $\bigcirc$ Vendo	or O Go	vernment
O Institute O Other			
*Academic Pricing Policy An academic price is awarded to degree-granting (A resources for student's course work that are affilitated to submit documentation to verify eligibility. Please cor	with the degree-granting instituti	on. Institutions	•
<b>Billing Address</b> (If different from End-User): If paying with credit card, address must be the bill	ing address.		
First Name	Last Name		
Organization			
Address			
Address (Building/Room No.)			
City	Postal Code		
State/Providence	Country		
Phone	Email		
Terms are net 30 days, unless order is Proforma/Prepay. Finar Shipping/handling charges will be added to your invoice. Du responsibility of the customer.			
<b>NOTE:</b> All ICDD Order/Quotations are processed in a first-in/fi in our queue for processing. If we need additional information		is been receive	d, it will be placed
Credit Card Payment			
Credit Card Type: O Visa O MasterCard	O American Express		
Name On Card (Please Print or Type)			
Signature	Date		
Credit Card No	Expiration Date	CVV No	
ICDD Quote-Order Form: Please submit by emailing to sales or faxing to 610-325-9823	@icdd.com		Experience Constructions Data RDER/QUOTE FORM - 06/01/20

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# **Contact Information**

phone	1.610.325.9814
toll free	1.866.378.9331 (USA & Canada)
fax	1.610.325.9823
email	info@icdd.com
registration	registration@icdd.com
sales	sales@icdd.com
technical support	support@icdd.com
web	www.icdd.com

# Four Easy Ways to Order

online	icdd.mybigcommerce.com
email	sales@icdd.com
fax	1.610.325.9823
mail	International Centre for Diffraction Data
	12 Campus Boulevard
	Newtown Square, PA 19073-3273 USA

Please send us a sales order via fax, email or mail. ICDD requires the name of the end user on all orders. Use product codes in your order, if possible. A convenient order/form can be found on our website at

www.icdd.com  $\rightarrow$  Products  $\rightarrow$  Purchase Products  $\rightarrow$  Order/Quote Form.

The Powder Diffraction File databases are licensed, copyrighted databases. In order to purchase an ICDD database license, an end-user must purchase the license directly through the ICDD or place an order directly through one of our licensed distributors (www.icdd.com/distributors).

# E-commerce

- Secure transmission using SSL encryption
- Customer online order history
- Online order tracking
- Email order confirmation
- Email shipping notification
- Customer satisfaction

# Pricing

The prices listed herein supersede all others previously published and are subject to change without notice. ICDD reserves the right to discontinue any product at its discretion. Visit our website at *www.icdd.com* or contact our Customer Service Department for the most recent product information and pricing.

# **Return Policy**

Products may be returned within 30 days from the invoice date for a full refund or credit (excluding shipping/handling). Products must be returned in original condition to qualify for a refund or credit. **Registered products cannot be returned.** Please complete a Return Merchandise Authorization (RMA) form to receive approval prior to returning product. Defective products will be replaced promptly, but must be returned for testing.

# Warranty Policy

Customers' sole remedy for any defective Licensed Product shall be replacement of the Licensed Product, which right must be exercised by written notice given within 30 days of purchase. Defective products will be replaced promptly, but must be returned for testing.

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.

# **Payment Terms**

Wire transfers, credit cards (MasterCard, Visa, American Express) and checks in USD and drawn on USA banks are acceptable forms of payment. Letters of credit will not be accepted. Payment is due within 30 days from invoice date. Finance charges of 1.5% per month (annual percentage rate of 18%) may be applied to overdue balances.

# Licensing

ICDD licenses the use of the Powder Diffraction File and software. Licensing for the Powder Diffraction File and associated software (Sleve and Sleve+) are packaged with the DVD, USB, and/or USB dongle. ICDD's product licenses are nontransferable and intended for use on a single computer. Please refer to the sales descriptions and product policies for further information on licensing.

\*Contact ICDD for PDF-4+/Web licensing.

# Orders

Orders which include terms and conditions are reviewed prior to order acceptance. Once orders are accepted, they are processed in a first-in/first-out basis.

Note: Customers in Japan, South Korea and Russia must order through an ICDD licensed vendor.

### Shipment

All orders shipped by ICDD are F.O.B. Newtown Square, PA, USA.

Import duties and all taxes are not included in pricing and are the sole responsibility of the customer. Shipment will be made by a commercial carrier chosen by ICDD. For your convenience, shipping charges will be added to all invoices. Shipments can be insured upon request; additional charges will apply.

# **ICDD Licensed Distributors**

www.icdd.com  $\rightarrow$  Products  $\rightarrow$  Purchase Products  $\rightarrow$  Distributors or

www.icdd.com/distributors/

# **Return Merchandise Authorization (RMA)**

www.icdd.com  $\rightarrow$  Products  $\rightarrow$  Ordering Information  $\rightarrow$  Return Policy  $\rightarrow$  ICDD\_RMA\_form.pdf

#### or

www.icdd.com/assets/files/ICDD\_RMA\_form.pdf



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