## 2018 Powder Diffraction File™ **Diffraction Data You Can Trust**

ICDD databases are the only crystallographic databases in the world with quality marks and quality review processes that are ISO certified.

#### PDF-4+ **Phase Identification and Quantitate** 398,726 Entries

295,309 Atomic Coordinates

PDF-2 **Phase Identification** + Value 298.258 Entries





WebPDF-4+ Data on the Go 398,726 Entries 295,309 Atomic Coordinates



**PDF-4/Organics** Solve Difficult Problems, **Get Better Results** 526,126 Entries 106,369 Atomic Coordinates

# 871,758



**PDF-4/Minerals Comprehensive Mineral** Collection 45,497 Entries

37,210 Atomic Coordinates

Standardized Data

More Coverage

All Data Sets Evaluated For Quality

Reviewed, Edited and Corrected Prior To Publication

Targeted For Material Identification and Characterization



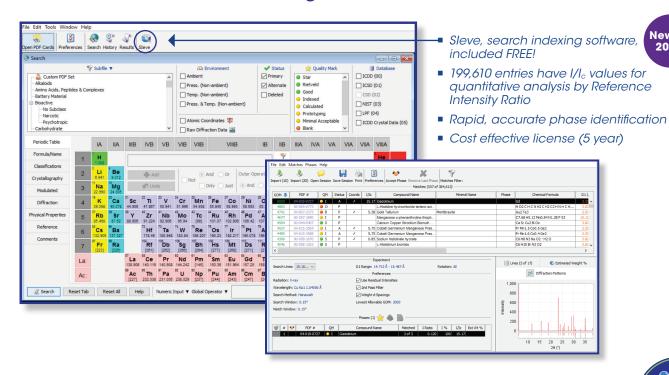
www.icdd.com/products/







### Featuring over 298,000 entries



PDF-4+ 2018

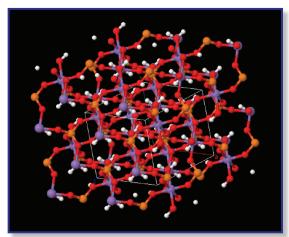


New for

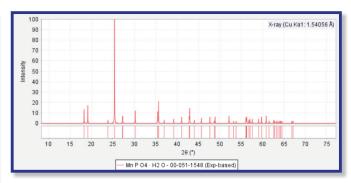
2018!

#### Phase Identification and Quantitate

# Featuring 398,000+ entries 295,309 entires with atomic coordinates



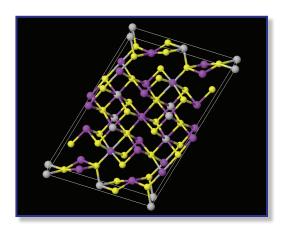
For PDF-4+ "Data on the Go" ask ICDD about WebPDF-4+



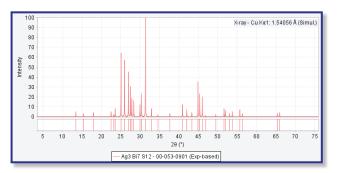
- All entries have digital patterns for use in total pattern analysis
- 295,309 entries with atomic coordinates
- 298,663 entries have I/I, values for quantitative analysis by Reference Intensity Ratio
- All entries are stored in a standardized format for easy search and interpretation
- All entries go through a rigorous editorial process to ensure quality



## Featuring 45,000+ entries 37,210 entries with atomic coordinates



- All entries have digital patterns for use in total pattern analysis
- 37,210 entries with atomic coordinates
- 34,434 entries have I/I<sub>c</sub> values for quantitative analysis by Reference Intensity Ratio
- Classified by IMA designations
- A subset of the PDF-4+ database with all of the features and capabilities, targeted toward minerals and mineral related compounds



## PDF-4/Organics 2018



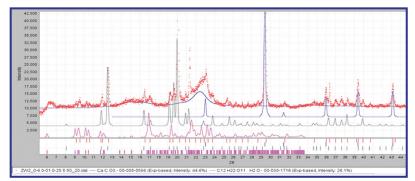
Solve Difficult Problems, Get Better Results

## Featuring 526,000+ organic & organometallic compounds 106,369 entries with atomic coordinates

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

## Combines powder diffraction and crystal structure reference data

The four phase identification of the formulation of Lipitor uses references from a single crystal determination, an experimental powder pattern of cellulose I $\beta$ , a calculated powder pattern and pattern extracted from the patent literature. The identification required an inorganic excipient, polymer excipient and two organic compounds. A variety of reference materials and sources enabled the identification.



## **ICDD 2018 Product Summary**

Data Entry Source	PDF-2 2018	PDF-4+ 2018 WebPDF-4+ 2018	PDF-4/ Minerals 2018	PDF-4/ Organics 2018
00- ICDD	116,613	116,613	12,140	40,154
01- FIZ	170,778	69,655	12,907	12,658
02- CCDC	0	0	0	431,359
03- NIST	10,067	2,917	213	282
04- MPDS	0	208,741	20,175	0
05- ICDD Crystal Data	800	800	62	41,673
Total No. of Data Sets	298,258	398,726	45,497	526,126
Subfile Distribution:				
Inorganic	264,876	365,291	45,441	39,355
Organic	42,478	43,515	711	515,458
New Entries	7,139	14,113	1,156	10,072
Rietveld—No. with atomic coordinates	0	295,309	37,210	106,369
Reference Intensity Ratio (RIR)—I/I	199,610	300,078	34,434	493,521
Experimental Digital Patterns	0	12,396	131	6,639
Pattern Fitting—Calculated Digital Patterns	0	398,726	45,497	526,126

All ICDD databases combine the power of both powder diffraction and crystal structure reference data. We are the only crystallographic database in the world with quality marks and quality review processes that are ISO certified. Each PDF database includes our integrated data mining software.

#### PDF-2 2018

Sleve included **FREE** 

#### Phase Identification + Value

- Designed for rapid, accurate phase identification
- Cost effective license (licensed for 5 years)

#### PDF-4+ 2018

#### Phase Identification and Quantitate

- Designed for phase identification and quantitative analysis
- Features digitized patterns, molecular graphics, and atomic coordinates
- Data simulation programs enables the analysis of X-ray, neutron, electron, and synchrotron data

#### WebPDF-4+ 2018

#### Data on the Go

- Provides portability to the PDF-4+ via the internet
- Equivalent to PDF-4+

#### PDF-4/Minerals 2018

#### **Comprehensive Mineral Collection**

- The most comprehensive collection of mineral data
- 45.497 minerals and related materials
- Includes all the features of PDF-4+

#### PDF-4/Organics 2018

#### Solve Difficult Problems, Get Better Results

- Highly targeted collection of materials used in commercial and regulatory fields
- Largest collection of pharmaceuticals, excipients, and polymers
- Includes ICDD's search-indexing software, Sleve+, as an added value

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