

# ICDD 2011 Product Summary

		<u>PDF-2</u> <u>2011</u>	<u>PDF-4+</u> <u>2011</u>	<u>PDF-4/Minerals</u> <u>2011</u>	<u>PDF-4/Organics</u> <u>2012</u>
<b>Entries</b>	<b>Total No. of Data Sets</b>	243,911	316,291	37,642	470,181
<b>Source Distribution</b>					
	00-Experimental	106,997	106,997	11,456	32,878
	01-FIZ	126,847	60,633	11,343	5,905
	02-CCDC	0	0	0	431,359
	03-NIST	10,067	3,297	216	39
	04-MPDS	0	145,364	14,627	0
<b>Subfile Distribution</b>					
	Inorganic	213,584	285,883	37,562	8,496
	Organic	35,775	35,923	612	467,134
<b>Fundamentals</b>					
	No. of Binaries	37,432	56,326	6,373	5,204
	No. of Ternaries	81,255	109,072	7,416	45,449
	No. of Quaternaries	67,115	83,122	8,439	113,728
	≥5 Elements	56,049	64,486	14,574	305,544
<b>Quantitative Analysis Parameters</b>					
	RIR—No. with I/I <sub>c</sub>	148,722	221,102	26,870	441,891
	Rietveld - Total No. with Atomic Coordinates	0	160,183	17,646	31,650
	Pattern Fitting—Digital Patterns	0	316,291	37,642	470,181
<b>Crystallographic and Bibliographic Data</b>					
	Unit Cells - Author, Crystal and Reduced	212,714	285,094	36,197	452,825
	Reference Citations	301,625	362,335	46,576	481,627
	Journals	2,376	2,392	1,133	1,595

## PDF-2 Release 2011

- designed for rapid material identification
- New for 2011—data mining software is integrated into PDF-2, free of charge!
- licensed for 5 years; customer may upgrade database any time during the license period; if customer chooses not to upgrade the database at the end of the license period, ICDD will renew the license for one (1) additional 5 year license term
- single user, single PC license
- multiyear and site licenses available

## PDF-4+ 2011—Quantitative Analysis

- largest inorganic database
- advanced database designed for rapid materials identification and capability for quantitative analysis
  - Rietveld Analysis—largest collection of inorganic atomic coordinates with 160,183 entries
  - Reference Intensity Ratio—221,102 data sets having I/I<sub>c</sub> values
  - Total Pattern Analysis—316,291 data sets with full digital patterns
  - 5,625 full digital raw data scans, including 100 clays
- data mining software integrated into the database
- licensed for one year by subscription with required annual renewals
- WebPDF-4+—access PDF-4+ via the Internet
- single user, single PC license (WebPDF-4+ is single user, single hardware key)
- multiyear and site licenses available

## PDF-4/Minerals 2011

- minerals subset of PDF-4+, which includes the features incorporated into PDF-4+
- licensed for one year by subscription with required annual renewals
- single user, single PC license

## PDF-4/Organics 2012

- targeted to the pharmaceutical industry, consumer products, catalysis, forensic science, analytical labs, combinatorial analysis, drug discovery and production
- designed to identify organic and organometallic materials
- contains a few thousand inorganic materials, primarily pharmaceutical excipients to help with formulation analysis and identification
- applications include material identification, quantitative analysis, formulation analysis, polymorph identification, salt, solvate and hydration analyses and crystallite size analysis
- data mining and search-indexing software (Sieve+) integrated into the database
- licensed for one year by subscription with required annual renewals
- single user, single PC license
- multiyear and site licenses available

A multiyear license offers customers who are concerned about PDF-4 annual renewals, the ability to prepay for future licenses and alleviate the concerns with yearly budgets.

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