

**FEATURES:**

|  | PDF-4+ 2011    | PDF-2 RELEASE 2011 |
|--|----------------|--------------------|
| <b>Total entries</b>   | <b>316,291</b> | <b>243,911</b>     |
| <b>Inorganic entries</b>   | <b>285,883</b> | <b>213,584</b>     |
| <b>Organic entries</b>   | <b>35,923</b>  | <b>35,775</b>      |
| <b>Entries with atomic coordinates</b>                                 | <b>160,183</b> | <b>0</b>           |
| <b>Search Classifications:</b>   |                |                    |
| <b># of searches</b>   | <b>55</b>      | <b>51</b>          |
| All Names Search for compounds: plus nomenclature fields               | X              | X                  |
| Ambient/Non-ambient  | X              | X                  |
| ANX Structural Formula search (ICSD entries only)                      | X              | X                  |
| Atomic Coordinates   | X              | PDF-4*             |
| <b>Atomic Coordinates – Cross-Referenced</b>                           | <b>New</b>     | <b>PDF-4*</b>      |
| Atomic Environment Type  | X              | PDF-4*             |
| Author's Cell Axial Ratio search                                       | X              | X                  |
| Author's Cell Molecular Volume/Formula Unit Volume                     | X              | X                  |
| Bibliographic: Author, Journal, Title, Year, CAS No., Codens, Volume   | X              | X                  |
| Cell/Volume: Author's, Crystal, Reduced (including ESDs)               | X              | X                  |
| Color  | X              | X                  |
| Comments   | X              | X                  |
| Composition Search: weight & atomic percentages                        | X              | X                  |
| Cross-references page with each entry display                          |                |                    |
| NIST/ICSD to LPF   | X              | PDF-4*             |
| Experimental to LPF  | X              | PDF-4*             |
| Alternate patterns from Primary & Primary from Alternate               | X              | X                  |
| Crystal Data Axial Ratio Search  | X              | X                  |
| Crystal Symmetry   | X              | X                  |
| Density: Calculated & Measured   | X              | X                  |
| Density: Structure-derived density for LPF entries                     | X              | PDF-4*             |
| Search on any combination of Dmeas, Dcalc, and Dstruc                  | X              | X                  |
| Empirical Formula  | X              | X                  |
| Estimated Standard Deviation (ESD) available for most numeric searches | X              | X                  |
| I/I <sub>c</sub>   | X              | X                  |
| Integral Index   | X              | PDF-4*             |
| Lines: Long and Strong   | X              | X                  |
| LPF Prototype Structure search   | X              | X                  |
| Chemical Formula order   | X              | X                  |
| Alphabetical order   | X              | X                  |
| Melting Point  | X              | X                  |
| Mineral Classification, Mineral Name                                   | X              | X                  |
| Mineral subclasses: Gem, Natural, Synthetic                            | X              | X                  |
| Number of Elements   | X              | X                  |
| Organic Functional Group   | X              | X                  |
| PD3 Pattern  | X              | PDF-4*             |
| Pearson Symbol Code  | X              | X                  |
| Periodic Table   | X              | X                  |
| <b>Yes/No/Maybe Search</b>   | <b>New</b>     | <b>New</b>         |
| Property Sheet   | X              | PDF-4*             |
| Prototype Structure: Alphabetical order, Chemical Formula order        | X              | X                  |
| Quality Mark   | X              | X                  |
| R-factor   | X              | X                  |
| Reduced Cell: Cell Axes, Cell Volume                                   | X              | X                  |
| Smith-Snyder Figure of Merit (SS/FOM)                                  | X              | X                  |
| Space Groups: Author-Defined SPG, International Table SPG              | X              | X                  |
| <b>Structural Formula</b>  | <b>New</b>     | <b>New</b>         |
| <b>Subfile</b>   | <b>X</b>       | <b>X</b>           |
| <b>Modulated Structure</b>   | <b>New</b>     | <b>New</b>         |
| <b>Thermoelectric Material</b>   | <b>New</b>     | <b>New</b>         |
| <b>Organic Subfiles</b>  | <b>New</b>     | <b>New</b>         |
| Zeolite Classification   | X              | X                  |

\* Available only in PDF-4+

**Bolded items signify new features.**

## DISPLAY & CAPABILITIES:

|   | PDF-4+ 2011 | PDF-2 Release 2011 |
|---|-------------|--------------------|
| <b># of display fields</b>  | <b>91</b>   | <b>40</b>          |
| 2D structures for experimental organic entries                              | X           | X                  |
| 3D structures for LPF entries: unit cell views                              | X           | PDF-4*             |
| Bond Distances/Angles display   | X           | PDF-4*             |
| Database fields for display in search results, include, but not limited to: |             |                    |
| Ambient/Non-ambient   | X           | X                  |
| AuthorCell Z and XtlCell Z  | X           | PDF-4*             |
| Author's Cell Molecular Volume/Formula Unit Volume                          | X           | PDF-4*             |
| Author's cell and volume  | X           | PDF-4*             |
| Cross-Referenced Atomic Coordinates   | X           | PDF-4*             |
| Crystal data and volume   | X           | X                  |
| Crystal Data Axial Ratio  | X           | PDF-4*             |
| D4 to D10 and L4 to L10   | X           | PDF-4*             |
| Has Atomic Coordinates  | X           | PDF-4*             |
| Reduced cell and volume   | X           | X                  |
| Smith-Snyder Figure of Merit (SS/FOM)                                       | X           | PDF-4*             |
| <b>Structural Formula</b>   | <b>New</b>  | <b>PDF-4*</b>      |
| Digitized patterns for experimental & calculated entries:                   | X           | PDF-4*             |
| Calculated patterns: X-ray, electron and neutron                            | X           | PDF-4*             |
| Automatic patterns: X-ray, electron and neutron                             | X           | X                  |
| Automatic/manual experimental data import for known file types              | X           | X                  |
| Automatic/manual experimental data background subtraction                   | X           | X                  |
| Experimental data smoothing   | X           | X                  |
| Experimental data K $\alpha_2$ profile stripping                            | X           | X                  |
| Experimental data peak finding (2nd derivative algorithm)                   | X           | X                  |
| Experimental data manually add/remove peaks                                 | X           | X                  |
| <b>New wizard for processing experimental data</b>                          | <b>New</b>  | <b>New</b>         |
| Electron Diffraction Pattern: Simulated                                     | X           | PDF-4*             |
| <b>Spot size slider</b>   | <b>New</b>  | <b>PDF-4*</b>      |
| Electron Backscattering Pattern   | X           | PDF-4*             |
| Graphing Capabilities:  |             |                    |
| Advanced custom importing: Save custom settings                             | X           | X                  |
| Graph results (x-y plot, category plot, histogram)                          | X           | X                  |
| Profile functions: Crystallite size, Pseudo-Voigt, plus more                | X           | PDF-4*             |
| Geometry types: Debye-Scherrer, Bragg-Brentano                              | X           | PDF-4*             |
| 2-theta correction  | X           | PDF-4*             |
| Scale intensities to highest peak   | X           | PDF-4*             |
| <b>Unified Simulated Profile Preferences</b>                                | <b>New</b>  | <b>PDF-4*</b>      |
| <b>Greek Character Searches</b>   | <b>New</b>  | <b>New</b>         |
| "Not" operator available for every search                                   | X           | X                  |
| PD3 Patterns: Raw experimental data   | X           | PDF-4*             |
| PDF Entry Display:  |             |                    |
| <b>All References Table</b>   | <b>New</b>  | <b>New</b>         |
| Author's Cell Molecular Volume/Formula Unit Volume                          | X           | X                  |
| Crystal Symmetry  | X           | X                  |
| Footnotes for d-spacings  | X           | X                  |
| <b>Modulated Structures</b>   | <b>New</b>  | <b>New</b>         |
| User Comments Report - view all user comments                               | X           | X                  |
| View up to 3 intensities at one time: fixed slit, variable, & integrated    | X           | PDF-4*             |
| Ring Pattern  | X           | PDF-4*             |
| Search Results Capabilities:  |             |                    |
| Calculations for mean, median, and ESD                                      | X           | X                  |
| Ability to add any field directly to results from menu option               | X           | X                  |
| Flexible formulae sorting in search results                                 | X           | X                  |
| Open multiple PDF Cards at once   | X           | X                  |
| Total Pattern Analysis: Similarity Index                                    | X           | PDF-4*             |
| <b>Normalized R-index</b>   | <b>New</b>  | <b>PDF-4*</b>      |
| Integral Index  | X           | PDF-4*             |

\* Available only in PDF-4+

**Bolded items signify new features.**