SUCCESS IS BEING EXCELLENT AT WHAT YOU DO

Learn how to get the most from your PDF-4 database from the database experts.

Join ICDD at our free PDF-4 users meeting during the 64th Annual Denver X-ray Conference!

Users Meeting

Sunday, 2 August 2015
Denver X-ray Conference 2015
Westminster, Colorado
10:00 am–4:00 pm

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Register by 24 July 2015

Participants are encouraged to bring their laptops to this workshop. ICDD will install a trial version of the PDF-4+ or PDF-4/Organics to facilitate a hands-on workshop.

Getting Started Tutorial

This tutorial will discuss and demonstrate the basic functions of PDF-4 data mining, thus enabling the user to distill the huge number of entries in PDF-4 to a manageable selected subset.

- Selecting search criteria for >60 unique Search Fields
- Viewing/analyzing search results
- Using History to optimize your searches
- Using digital patterns for data simulations and analysis

Advanced Features Tutorial

This tutorial focuses on the power of PDF-4 data mining and Sleve+ for phase identification, simulation of X-ray, neutron, and electron diffraction patterns, and retrieval/use of PDF-4 database information for advanced analyses.

- Performing neutron and electron diffraction simulated profiles, electron backscattering patterns, simulated electron (spot) patterns, and ring patterns
- Advanced data mining — tools to extract the data you need
- Using Sleve+ — choosing the appropriate search criteria and strategies for identification and problem analysis
- Interfaces — Using PDF-4 information as input for advanced analyses (whole-pattern fitting, structure analysis, molecular visualization, cluster analysis)
- Similarity indexes — their use and value
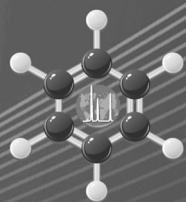- How to choose coordinate structures for Rietveld Refinement

Register online at www.icdd.com/education/usersmeeting.asp
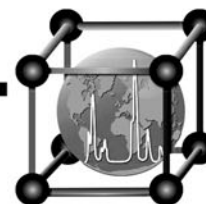
PDF-4/Organics 2015
Solve Difficult Problems, Get Better Results

Comprehensive materials database featuring 494,000+ organic and organometallic compounds

Features the largest collection of pharmaceuticals, excipients and polymers

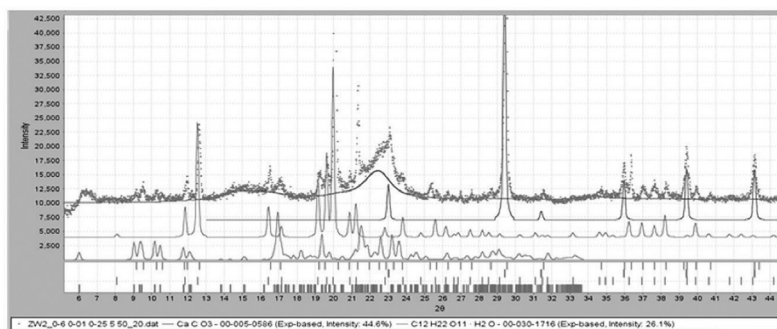Highly targeted collection, with special focus on materials used in commercial and regulatory fields

Enhanced identification for crystalline, nano and amorphous materials

Trade names for over 9,000 bioactive/ pharmaceutical entries

Integrated data mining software

SIeve+ Search-indexing Software (included as an added-value)

Combines powder diffraction and crystal structure reference data

ZW2_0-6 0-01 0-25 5 50_20.dat — Ca C O3 - 00-005-0586 (Exp-based, Intensity: 44.6%) — C12 H22 O11 · H2 O - 00-030-1716 (Exp-based, Intensity: 26.1%)

The four phase identification of the formulation of Lipitor uses references from a single crystal determination, an experimental powder pattern of cellulose Iβ, 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.

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Make the **SMART** move
to PDF-4+

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

S	Standardized data
M	More coverage
A	All data sets are evaluated for quality
R	Reviewed, edited and corrected prior to publication
T	Targeted for material identification and characterization

PDF-4+ 2014 features over 354,000 entries including 239,000+ entries with atomic coordinates.

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