

#### INTERNATIONAL CENTRE FOR DIFFRACTION DATA



- Standardized data
- More Coverage
- All data sets are evaluated for quality
- Reviewed, edited and corrected prior to publication
- Targeted for material identification and characterization

## Make the SMART move

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

### The Powder Diffraction File (PDF)

PDF-2 Release 2014 274,443 material entries 354,264 material entries PDF-4+ 2014 354,264 material entries WebPDF-4+ 2014 PDF-4/Minerals 2014 41,423 material entries

PDF-4/Organics 2015 494,966 material entries





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#### LET OUR TEAM OF EXPERTS HELP YOU TAKE YOUR SKILLS TO THE NEXT LEVEL!

#### Practical X-ray Fluorescence: 27 April-1 May 2015

From theory to hands-on exercises, this course offers techniques and skills to improve lab performance. Discover the latest in cutting-edge instruments such as TXRF, hand-held devices, energy dispersive and wavelength dispersive spectrometers through live demonstrations.

The XRF course covers the basics of X-ray spectra, instrumentation design, methods of qualitative and quantitative analysis, specimen preparation and applications for both wavelength and energy dispersive spectrometry. The course emphasizes quantitative methods, use of automated X-ray spectrometers, review of mathematical matrix correction procedures and new developments in XRF. Submit your samples for analysis by the XRF experts. Selected results will be the basis for class discussion!



#### Fundamentals of X-ray Powder Diffraction: 1–5 June 2015

For the novice with some XRD knowledge or for the experienced with an interest in the theory behind XRD, this clinic offers a strong base for increased lab performance.

The clinic covers instrumentation, specimen preparation, data acquisition and qualitative phase analysis. Hands-on use of personal computers for demonstration of the latest software; data mining with the PDF. The powder diffractometer: optical arrangement, factors affecting instrumental profile width, choice and function of divergence slit, detectors, X-ray optics, calibration and alignment.



#### \*Advanced Methods in X-ray Powder Diffraction: 8–12 June 2015

For the experienced XRD scientist, this clinic offers enhanced analysis skills through intense problem solving, as well as an introduction to the Rietveld Method. Computer-based methods of data collection and interpretation, both for qualitative and quantitative phase analysis is also emphasized.

The advanced clinic covers factors affecting d-spacing of crystals: unit cell, crystal structure, and solid solutions, as well as factors affecting diffraction-line intensities: relative and absolute intensities, structure-sensitive properties (atomic scattering and structure factors), polarization effects, and multiplicity, specimen-sensitive effects (orientation, particle size), measurement-sensitive effects (use of peak heights and peak areas), and choice of scanning conditions.



### \*Rietveld Refinement & Indexing Workshops:

#### Basic: 28–30 September 2015 / Advanced: 1–2 October 2015

Powder Pattern Indexing and Rietveld structural refinement techniques are complementary and are often used to completely describe the structure of a material. Successful indexing of a powder pattern is considered strong evidence for phase purity. Indexing is considered a prelude to determining the crystal structure, and permits phase identification by lattice matching techniques. This workshop introduces the theory and formalisms of various indexing methods and structural refinement techniques. One unique aspect of this workshop is the extensive use of computer laboratory problem solving and exercises that teach method development in a hands-on environment.



Take the three-day basic workshop, the two-day advanced workshop or both together for a full week of hands-on training. The ICDD basic Rietveld workshop is a pre-requisite for attending the advanced workshop. A basic understanding of crystallography is also required.

Don't miss the opportunity to meet with our faculty, offering knowledge in a wide range of industries and applications. You'll meet seasoned professionals with experience in metals, microelectronics, thin films, indexing, polymers, organic chemistry and much more. Featuring live instruments for the XRF & XRD Clinics!

#### Register Today at WWW.ICDD.COM/EDUCATION

\* See the ICDD web site for prerequisites for advanced courses.

FOR MORE INFORMATION CONTACT Eileen Jennings, Education Coordinator Tel: 610.325.9814 Fax: 610.325.9823 Email: clinics@icdd.com



## ICDD:

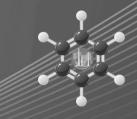




#### LOCATION

ICDD Headquarters, 12 Campus Boulevard Newtown Square, Pennsylvania 19073-3273 U.S.A.

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# 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

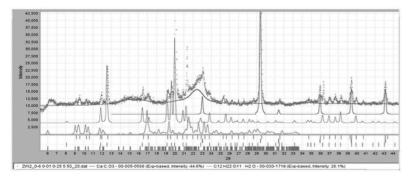
Enhanced identification for crystalline, nano and amorphous materials

Trade names for over 9,000 bioactive/pharmaceutical entries

Integrated data mining software

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.

## **COMPREHENSIVE ❖ STANDARDIZED ❖ QUALITY REVIEWED**









with quality marks and quality review processes that are ISO certified.

Standardized data

More coverage

All data sets are evaluated for quality

Reviewed, edited and corrected prior to publication

Targeted for material identification and characterization

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



