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Fundamentals of X-ray Powder Diffraction:

5 – 9 June 2017

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 through live demonstrations. It also covers hands-on use of personal computers for demonstration of the latest software including data mining with the Powder Diffraction File (PDF) and use of the powder diffractometer: optical arrangement, factors affecting instrumentation profile width, choice and function of divergence slit, calibration and alignment, detectors, and X-ray optics.

Advanced Methods in X-ray Powder Diffraction:

12 – 16 June 2017

For the experienced XRD scientist, this session offers enhanced analysis skills through intense problem solving, as well as an introduction to the Rietveld Method. The course emphasizes computer-based methods of data collection and interpretation, both for qualitative and quantitative phase analysis.

The advanced clinic covers factors affecting d-spacings of crystals, as well as factors affecting diffraction-line intensities; structure-sensitive properties (atomic scattering and structure factors), polarization effects, and multiplicity. Additionally, the clinic covers specimen-sensitive effects (orientation, particle size), measurement-sensitive effects (use of peak heights and peak areas), and choice of scanning conditions will also be addressed.

Rietveld Refinement & Indexing Workshop:

Basic Workshop: 25 – 27 September 2017
***Advanced Workshop: 27 – 29 September 2017**

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 along with quantitative analysis. 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.

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Eileen Jennings, Education Coordinator
Tel: 610.325.9814 **Fax:** 610.325.9823
Email: clinics@icdd.com

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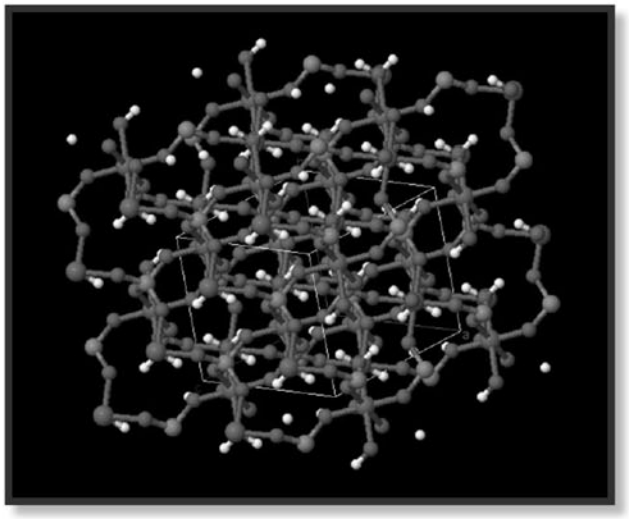
PDF-4+ 2016

Designed for phase identification and quantitative analysis

Comprehensive materials database featuring 384,000+ entries



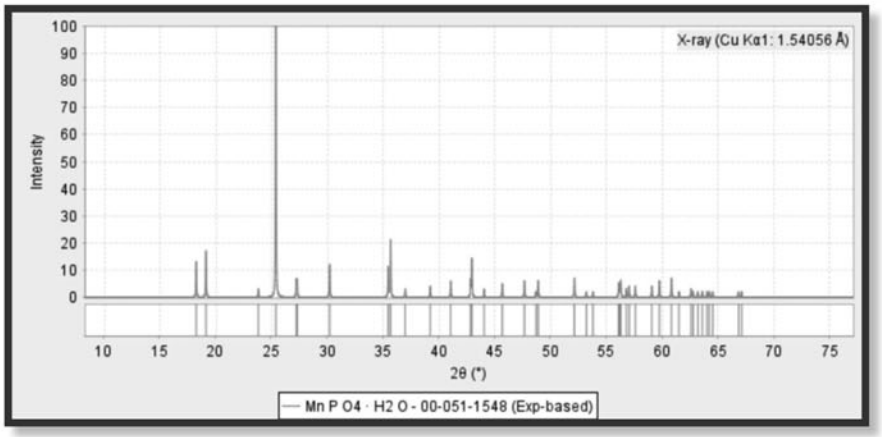
All entries have digital patterns for use in total pattern analysis

271,449 entries with atomic coordinates

286,885 entries have I/I_c 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



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AS A MEMBER OF THIS ELITE GROUP, YOU WILL RECEIVE THE FOLLOWING BENEFITS:

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- Publication of pattern(s) in the Powder Diffraction File™ (PDF®)
- Receive calibration standards
- Purchase certain ICDD products at reduced prices
- Web-based access to the list of compounds in the ICDD master database – includes published patterns, as well as patterns still in the editorial process
- First-time grantees receive a complimentary one-year subscription to Powder Diffraction

For over 50 years, ICDD has supported a well-developed program of grants to researchers around the world. One of our main objectives is to expand the range of reference materials by producing and cataloging high-quality diffraction patterns in our internationally renowned database, the Powder Diffraction File. Thanks to the longevity of this program, these contributions account for approximately a quarter of the current experimental file. ICDD awards financial support to qualified investigators in the form of grant-in-aid on a competitive proposal basis. The duration of a grant is 12 months with two cycles per year. Cycle I begins 1 April and Cycle II begins 1 October.

Geographic Locations of Grants for the Past 15 Years:

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Malaysia
Netherlands
P.R. of China
Poland
Portugal
Russia
Spain
Switzerland
Taiwan
Tunisia
Ukraine
United Kingdom
United States
Uruguay

Total Proposals Funded for the Past Fifteen Years: 682

THE FINER POINTS OF THE GRANT-IN-AID PROGRAM

- Grant-in-Aid funds can be used most effectively as supplements to existing research projects involving the preparation and characterization of new materials, using powder diffraction techniques.
- Grant-in-Aid proposals will be considered, on a competitive basis, from any qualified investigator (academic, government, or industry), around the world, who can demonstrate expertise in the preparation of high quality powder diffraction patterns.
- Proposals addressing current opportunities to extend and improve the usefulness of the Powder Diffraction File™ are given highest priority.
- The duration of a Grant-in-Aid is 12 months. Renewal for additional 12-month periods may be considered on a competitive basis. Grant recipients are required to submit biannual progress reports.
- Deadlines for receipt of Grant-in-Aid proposals are due either by 31 July or by 31 January, depending on the cycle. Prior to submitting a grant proposal to the ICDD, please review the detailed Grant-in-Aid guidelines. These guidelines are available from ICDD's website at www.icdd.com/gia or by emailing the Grant Coordinator.

Any questions or comments regarding the ICDD Grant-in-Aid Program should be directed to:

Denise DelCasale, *Grant Coordinator*
Email: delcasale@icdd.com

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MAKE THE **SMART** MOVE TO THE **POWDER DIFFRACTION FILE**

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

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 2016	291,119 material entries
PDF-4+ 2016	384,613 material entries
WebPDF-4+ 2016	384,613 material entries
PDF-4/Minerals 2016	44,341 material entries
PDF-4/Organics 2017	516,054 material entries

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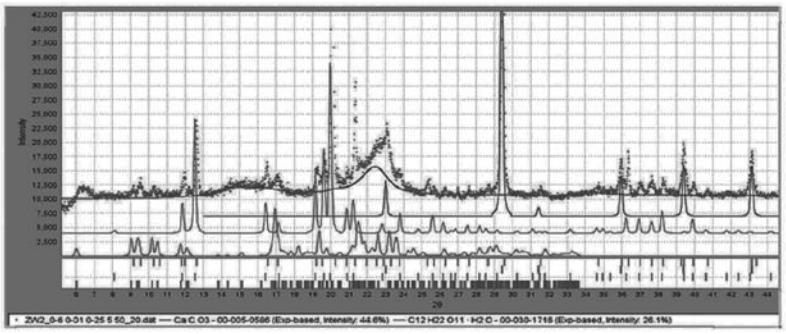
PDF-4/Organics 2017

Solve Difficult Problems, Get Better Results

Comprehensive materials database featuring 516,000+ 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 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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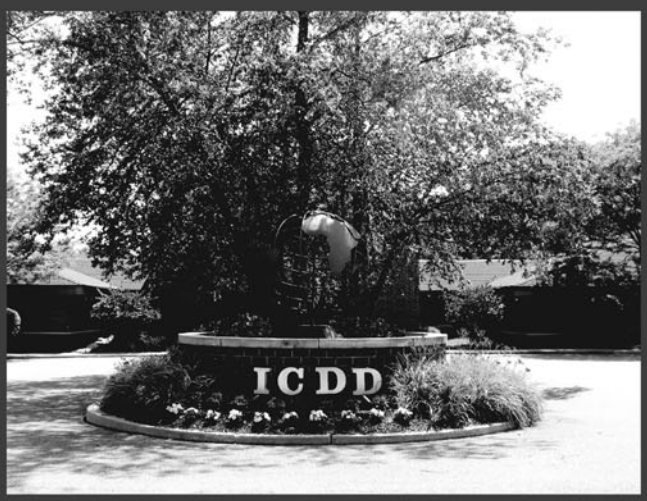

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The International Centre for Diffraction Data will continue to develop tools and support the education required for materials analyses of tomorrow.

ICDD's Mission

The International Centre for Diffraction Data will continue to be the world center for quality diffraction and related data to meet the needs of the technical community. ICDD promotes the application of materials characterization methods in science and technology by providing forums for the exchange of ideas and information.

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- PDF-4+
- WebPDF-4+
- PDF-4/Minerals
- PDF-4/Organics
- Sleve/Sleve+

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  - XRD
  - XRF
  - Specialized Workshops

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