The 2nd Pharmaceutical Powder X-ray Diffraction Symposium
PPXRD-2

8-12 December 2002
Organized by the International Centre for Diffraction Data
ICDD

- Powder Pattern Indexing
- Acquisition and Use of X-ray Powder Diffraction Data
- Polymorph Characterization by XRPD
- Structure Determination, Molecular Modeling & Pattern Matching
- Pharmaceutical Materials Characterization by SAXS
- Regulatory and Patent Issues
The 2nd 
Pharmaceutical Powder X-ray Diffraction Symposium
Best Western Concordville Hotel and Conference Center
Concordville, Pennsylvania, U.S.A.
8–12 December 2002

Sponsored and Organized by
the International Centre for Diffraction Data
E-mail: ppxrd@icdd.com
Telephone: 610.325.9814

PPXRD Symposium Scientific Organizing Committee

Dr. John Faber, Chair, International Centre for Diffraction Data, Newtown Square, PA, U.S.A.
Dr. Thomas Blanton, Eastman Kodak Company, Rochester, NY, U.S.A.
Dr. Harry G. Brittain, Centre for Pharmaceutical Physics, Milford, NJ, U.S.A.
Prof. Noriaki Hirayama, Tokai University, Shizuoka, Japan
Dr. Arnt Kern, Bruker AXS GmbH, Karlsruhe, Germany
Prof. Daniel Louër, University of Rennes I, Rennes cedex, France
Dr. Peter Munk, Philips Analytical B.V., Almelo, The Netherlands
Dr. Fangling Needham, International Centre for Diffraction Data, Newtown Square, PA, U.S.A.
Dr. Richard B. Ortega, Rigaku/MSC, Inc., The Woodlands, TX, U.S.A.
Prof. Peter W. Stephens, State University of New York, Stony Brook, NY, U.S.A.
Dr. Gregory A. Stephenson, Eli Lilly and Company, Indianapolis, IN, U.S.A.
Dr. Peter G. Varlashkin, GlaxoSmithKline, Research Triangle Park, NC, U.S.A.

Special thank you to
PANalytical (formerly Philips Analytical) for sponsoring Monday’s coffee breaks.

The information contained in this program is current as of 1 October 2002. Changes will be communicated at the Symposium.
Symposium Program
Best Western Concordville • Gold Ballroom

MONDAY, 9 DECEMBER

ACQUISITION AND USE OF X-RAY POWDER DIFFRACTION DATA

8:30-9:00 WELCOMING REMARKS & INTRODUCTIONS DR. JOHN FABER, ICDD

MORNING

WHAT IS IN YOUR PILL? WHAT ABOUT THEIRS?—Invited
Peter Stephens, State University of New York, Stony Brook, NY

AUTOMATION OF XRPD DATA ACQUISITION AND PATTERN ANALYSIS
Barbara C. Stahl, Igor Ivanisevic, David E. Bugay, Jesse R. Miller, Brett D. Bobzien, Leonard J. Chyall, SSCI Inc., West Lafayette, IN

HIGH THROUGHPUT SCREENING: DIFFRACTION ANALYSIS OF BRAND NAME DRUGS AND THEIR GENERIC COUNTERPARTS
J. Brian Litteer, Bruker AXS Inc., Madison, WI
Stefan Haaga, Bruker AXS GmbH, Karlsruhe, Germany

NON-INVASIVE X-RAY POWDER DIFFRACTION QUANTITATION OF GLYCINE POLYMORPHS IN INTACT COMPACTS AND MODELING OF INTENSITY VARIATIONS WITH SAMPLE THICKNESS AND SOLID FRACTION
Wenjin Cao, Kenneth R. Morris, Department of Industrial & Physical Pharmacy, Purdue University, West Lafayette, IN
Simon Bates, Bede Inc., Englewood, CO
Bruno C. Hancock, Matthew P. Mullarney, Pfizer Global Research & Development, Groton, CT

QUANTITATIVE EVALUATION OF AN ACTIVE PHARMACEUTICAL INGREDIENT IN TABLETS
Detlef Beckers, PANalytical (formerly Philips Analytical), Almelo, The Netherlands
Ingeborg Fix, K.-J. Steffens, University Bonn, Institute for Pharmaceutical Technology, Bonn, Germany

SIMULATED PXRD PATTERNS IN STUDIES OF THE PHASE COMPOSITION AND THERMAL BEHAVIOR OF BULK CRYSTALLINE SOLIDS
Shawn Yin, Raymond P. Scaringe, John Dimarco, Jack Z. Gougoutas, Solid State Science Group, Pharmaceutical Research Institute, Bristol-Myers Squibb Company, New Brunswick, NJ

THE NEW ORGANIC POWDER DIFFRACTION FILE, PDF-4/ORGANIC 2003, WITH INTEGRATED SEARCH AND RETRIEVAL FUNCTIONS
John Faber, Fangling Needham, ICDD, Newtown Square, PA

AFTERNOON

POWDER PATTERN INDEXING

POWDER PATTERN INDEXING—Invited
Daniel Louër, Universite de Rennes 1 Laboratoire de Chimie du Solide et Inorganique Moléculaire Cristallographie des Poudres et Réactivité des Solides, Rennes cedex, France

ADVANCES IN INDEXING OF POWDER DIFFRACTION PATTERNS: ITERATIVE USE OF SINGULAR VALUE DECOMPOSITION AND MONTE-CARLO BASED WHOLE POWDER PATTERN DECOMPOSITION
A.A. Coelho, A. Kern, Bruker AXS GmbH, Karlsruhe, Germany
Tuesday, 10 December

Morning

Polymorph Characterization by XRPD

Structural DSC Exploiting Time-Resolved Powder Diffraction—Invited

W.I.F. David, A.J. Markvardsen, K. Shankland, Rutherford Appleton Laboratory, Oxon, United Kingdom

P. Fernandes, Rutherford Appleton Laboratory, Oxon, United Kingdom and Department of Pharmaceutical Sciences, University of Strathclyde, Glasgow, Scotland, U.K.

A. J. Florence, N. Shankland, Department of Pharmaceutical Sciences, University of Strathclyde, Glasgow, Scotland, U.K.

Application of XRD in Polymorph Identification During High Throughput Screening for Pre-Formulations

Li Song, Anny Tangkilisan, Quyen Ng, Thomas Kudla, Symyx Technologies, Santa Clara, CA

High-Throughput Screening in Solid Form Selection

Arjen van Langevelde, Erwin Blomma, Crystallics BV, Amsterdam, The Netherlands

Crystal Structures and Bonding in Cellulose Polymorphs

James A. Kaduk, BP Chemicals, Naperville, IL

Paul Langan, Los Alamos National Laboratory, Los Alamos, NM

High Throughput Powder Diffraction—The Search for Polymorphs—Invited

Chris Gilmore, Gordon Barr, University of Glasgow, Glasgow, Scotland, U.K.

The Elucidation of the Tetramorphism of Fananserine with XRPD: From Phase Characterization to Phase Diagram

J. Giovaninni, Institute of Chemistry of Rennes, LCSIM-CNRS, University of Rennes, France and Aventis Pharma, Laboratoire de Physique Appliquée, Vitry-sur-Seine, Rennes cedex, France

M. A. Perrin, F. Leveiller, Aventis Pharma, Laboratoire de Physique Appliquée, Vitry-sur-Seine, France

D. Louër, Institute of Chemistry of Rennes, LCSIM-CNRS, University of Rennes, Rennes cedex, France

Toscani, R. Ceolin, Laboratoire de Chimie Physique, University of Paris V, Paris, France

Afternoon

Structure Determination, Molecular Modeling & Pattern Matching

Structures and Transformations in Pharmaceuticals—Invited

K. Shankland, W.I.F. David, A.J. Markvardsen, N. Shankland, Rutherford Appleton Laboratory and Crystallografx Ltd., Oxon, United Kingdom

Structure Determination of Caffeine Anhydrous C₈H₁₀N₄O₂ from Powder Diffraction Data with TOPAS

A. Kern, F. Stowasser, Bruker AXS GmbH, Karlsruhe, Germany

C. Lehmann, Max-Planck-Institut fuer Kohleforschung, Mulheim an der Ruhr, Germany

Influence of Powder Diffractometer Geometry on the Results of Structure Determination Process of New Polymorph of p-Methyl-Ketoprofen Derivative

S. Prugovečki, PANalytical (formerly Philips Analytical) B.V, Almelo, The Netherlands

A. Danilovski, Z. Sljiković, M. Oresić, M. Dumić, PLIVA d.d., Prilaz baruna Filipovica, Zagreb, Croatia

B. Prugovečki, Faculty of Science, University of Zagreb, Zagreb, Croatia

Solving Crystal Structures with Molecular Orientational Disorder Using XRPD and Simulated Annealing Methods

Ashfia Huq, Peter W. Stephens, Department of Physics and Astronomy, State University of New York, Stony Brook, NY
Symposium Program

Best Western Concordville • Gold Ballroom

Wednesday, 11 December

Morning  REGULATORY AND PATENT ISSUES

PATENT LITIGATION AND X-RAY POWDER DIFFRACTION: SWIMMING WITH THE SHARKS—Invited

Harry G. Brittain, Center for Pharmaceutical Physics, Milford, NJ

POLYMORPHISM AND DRUG DEVELOPMENT: A REGULATOR’S VIEWPOINT—Invited

Wilson H. DeCamp, Division of New Drug Chemistry III, Food and Drug Administration, Rockville, MD

PROSECUTING AND LITIGATING PXRD PATENTS—Invited

Steven Lee, Kenyon & Kenyon, New York, NY

Afternoon  PHARMACEUTICAL MATERIALS CHARACTERIZATION BY SAXS

THE APPLICATION OF SMALL-ANGLE SCATTERING TECHNIQUES IN THE DESIGN AND CHARACTERIZATION OF PHARMACEUTICAL MATERIALS—Invited

Rex Hjelm, Los Alamos Neutron Science Center, Los Alamos National Laboratory, Los Alamos, NM

NANOSTRUCTURE ANALYSIS OF PHARMACEUTICAL APPLICATIONS USING 2D SMALL ANGLE X-RAY SCATTERING

K. Erlacher, R. Gorgl, Material Center Leoben GmbH, Austria and Erich Schmid Institute, Austrian Academy of Sciences and University of Leoben, Leoben, Austria

P. Doppler, H. Jakob, Bruker AXS, Austria

SMALL- AND WIDE-ANGLE X-RAY SCATTERING IN PHARMACEUTICAL RESEARCH AND INDUSTRIAL PRACTICE

Peter Laggner, Austrian Academy of Sciences, Austria, Hecus M. Braun-Graz X-Ray Systems, Graz, Austria
XRD Tutorial
Best Western Concordville • Victoria Room
Sunday, 8 December 2002
6–9 pm

A three-hour introductory tutorial on X-ray powder diffraction, at which a light dinner will be served.

Poster Session, Reception & Exhibits
Best Western Concordville • Gold Ballroom & Courtyard
Monday, 9 December 2002

Manufacturers’ Exhibits and Poster Session • 6-9 pm
Reception • 6:30–8:30 pm
Two hour social with carving station, hot and cold hors d’oeuvres, crudites, wine, beer & sodas.

X-RAY POWDER DIFFRACTION (XRPD) LIKE TOOL IN THE CHARACTERIZATION OF SOLID STATE PHARMACEUTICAL PRODUCTS, INNOVATIVE VS GENERIC
A. Devia, Y. C. Arango, Universidad Nacional de Colombia Sede Manizales, Manizales, Columbia
C. I. Salazar, Unisalud, Manizales, Columbia

CONVOLUTION BASED PROFILE FITTING
A. Kern, A.A. Coelho, Bruker AXS GmbH, Karlsruhe, Germany
R.W. Cheary, University of Technology Sydney, Sydney, Australia

APPLICATIONS OF X-RAY POWDER DIFFRACTION IN PHARMACEUTICAL ANALYSIS
Tomikatsu Kubo, Application Laboratory, Rigaku Corporation, Osaka, Japan
Akira Kishi, Product Planning and Marketing, Rigaku Corporation, Tokyo, Japan

NEW POLYMORPH SCREENING APPROACHES
Barbara C. Stahly, Leonard J. Chyall, G. Patrick Stahly, SSCI Inc., West Lafayette, IN

CRYSTAL STRUCTURE OF 8-MANNITOL
Cristian E. Botez, Peter W. Stephens, Department of Physics, Stony Brook University, Stony Brook, NY
Cletus Nunes, Raj Suryanarayanan, College of Pharmacy, University of Minnesota, Minneapolis, MN

MONOPOTASSIUM DIHYDROGEN CITRATES
James A. Kaduk, BP Chemicals, Naperville, IL

Instrument Calibration & Indexing Workshop
Best Western Concordville • Victoria Room
Thursday, 12 December 2002
8am–4pm

Does your instrument produce good data?
Instrument calibration and indexing will be covered in this hands-on workshop.
Exhibitor Information

Exhibits will be located in the Courtyard outside of the Gold Ballroom
Best Western Concordville Conference Center

**Exhibit Hours:**
Monday, 9 December 8 am–9 pm
Tuesday, 10 December 8 am–3:30 pm

A diagram of the exhibit locations will be available in the Book of Abstracts.

**Exhibitors:**
Bede Scientific Incorporated
Bruker AXS, Inc.
Cambridge Crystallographic Data Centre (CCDC)
Hecus M. Braun-Graz X-ray Systems
INEL, Inc.
International Centre for Diffraction Data (ICDD)
PANalytical (formerly Philips Analytical)
Rigaku/MSC, Inc.
SPEX CertiPrep, Inc.
SSCI, Inc.
Thermo ARL
X-ray Optical Systems
Accommodations & Travel

The PPXRD Symposium will be held at the Best Western Concordville Hotel and Conference Center in Concordville, Pennsylvania, U.S.A.

**Hotel Information**

Best Western Concordville Hotel  
Route 322 & U.S. Route 1  
Concordville, Pennsylvania 19331 U.S.A.  
Telephone: 610.358.9400; Hotel Reservations Only +1.800.522.0070  
Fax: 610.358.9381  
Web: www.concordville.com

A block of rooms is reserved for Symposium guests for the nights of 8–11 December 2002. The special PPXRD rate of 105.00 $US for a standard room, plus 8% tax includes hot breakfast buffet in the hotel lobby second floor. Check-in time is 3:00 p.m., and checkout is 12:00 noon. Reservations must be made by **27 October 2002**. You will not be guaranteed a room or the special PPXRD rate after this date. Please mention PPXRD when you make your reservation.

All guest rooms offer the following amenities: hair dryer, in-room minibar, iron and ironing board, coffee maker, two telephones, data port, voice mail, and complimentary USA Today delivered to your room. The Best Western Hotel also invites you to the nightly complimentary Managers’ Reception Monday–Thursday 5–6:30 p.m. Other hotel amenities include on-site Business Center, complimentary local transportation, same day dry cleaning, laundry facilities, heated indoor pool and steam sauna, fitness center, and game room.

**General Information**

Attire: Attire is informal for most activities  
Climate: The average temperature in December is 33° F  
Time Zone: EST  
Airport: Philadelphia International
Finding Your Way Around

Directions to Best Western Concordville Hotel and Conference Center

From Philadelphia International Airport: Take I-95 South to Exit 3A (new Exit 3) Route 322 West; hotel is located 8 miles on right

From Delaware & Maryland: Take I-95 North to Exit 8 Route 202 North, Right on Route 1 North, go past junction of Route 1 and Route 322; hotel is located 25 yards on right.

From PA Turnpike: Take Exit 25A (new Exit 20) for Route 476 toward Chester, follow 476 South to Exit 3 (new Exit 5) Lima/Springfield, follow Route 1 South; hotel is 12 miles from Exit 3 (new Exit 5) on left behind Concordville Inn Restaurant (before Route 322)

From NJ Turnpike: Take Exit 2, follow Route 322 West, over the Commodore Barry Bridge to I-95 South to Exit 3A (new Exit 3) Route 322 West; hotel is 8 miles on right.

Ground Transportation from Philadelphia Airport to Best Western Concordville Hotel:

Delaware Express Shuttle: 28.00 $US per person each way; reservations strongly suggested. Dial 24 from the Ground Transportation counter, located in the Baggage Claim area of the airport. Call for reservations at 302-379-5906.

Taxi: Available outside the Baggage Claim area. Fares are not regulated and vary widely with each driver. This mode of transportation is not recommended unless traveling to Center City Philadelphia.
2002 PPXRD-2 Symposium Registration Form

- XRD Tutorial 8 December 2002 PPXRDT02 $50.00
- Symposium only 9-11 December 2002 PPXRD02 $1,200.00
- Symposium & Workshop 9-12 December 2002 PPXRDWS02 $1,450.00
- Yes, I would like to receive samples to measure in my lab for discussion during the Symposium (no additional fee)

The easiest way to register

Online at: www.icdd.com/ppxrd
Fax to: +610.325.9823
Mail to: ICDD, Attn: Leah Mooney
12 Campus Boulevard
Newtown Square, PA 19073-3273 U.S.A.

Dr. Mr. Mrs. Ms.

First Name ________________________________ Middle Initial ___ Last Name ________________________________

Preferred Badge Name (if different)____________________________________________________________________________

Company/Organization______________________________________________________________________________________

Business Address (street) ____________________________________________________________________________________

City __________________________________________ State ________ Zip ____________ Country ____________________

Business Phone ____________________ Fax __________________________ Business Web Site ________________________

E-mail ________________________________________ Home Phone (in case of emergency) ____________________________

Method of payment:
- Enclosed is a check for $__________, payable to ICDD in U.S. dollars and drawn on a U.S. bank
- Please bill: Name ____________________________________________Title ______________________________________
  Address (if different from above) ______________________________________________________________________________
  Phone ____________________________ P.O. # ________________

Charge: Visa Mastercard American Express

Cardholder's Name ________________________________________________________________________________________

Credit Card # ______________________________________________________ Expiration Date ______________________

Cardholder's Signature ____________________________________________________________________________________

Please note any needs related to disabilities.

Special needs ______________________________________________________________________________________________

Hotel Registration—Best Western Concordville Hotel

Direct to: Best Western Concordville Hotel Organization: International Centre for Diffraction Data (ICDD)—PPXRD
Attention: Reservations
P.O. Box 607
Rte. 322 & U.S. Rte. 1
Concordville, PA 19331 U.S.A.
TEL: +800.522.0070 FAX: +610.358.9381 Web site: www.concordville.com

Please reserve Smoking Nonsmoking

Arrival (Day-Date) ________________________________ Departure (Day-Date)______________________________

Name ________________________________________________________________________________________________

Address ______________________________________________________________________________________________

City __________________________________________ State ________ Zip ____________ Country ____________________

Telephone _____________________________________________________________________________________________

Credit Card Type and Number ____________________________ Exp. Date ______________________
(to guarantee reservation)