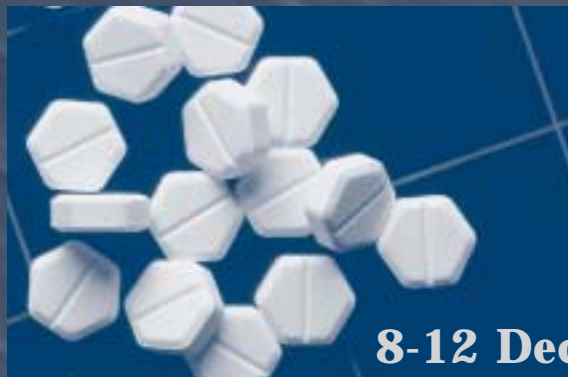


PPXRD

Program

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



8-12 December 2002

*Organized by the International
Centre for Diffraction Data*



- 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/MSI, 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.



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. Stahly, 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, Université 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

Symposium Program

Best Western Concordville · Gold Ballroom

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 Ung, Thomas Kudla, Symyx Technologies, Santa Clara, CA

HIGH-THROUGHPUT SCREENING IN SOLID FORM SELECTION

Arjen van Langevelde, Erwin Blomsma, 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

S. Toscani, R. Céolin, 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 $C_8H_{10}N_4O_2$ 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. Šiljković, M. Orešić, 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 Hug, 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 δ -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.

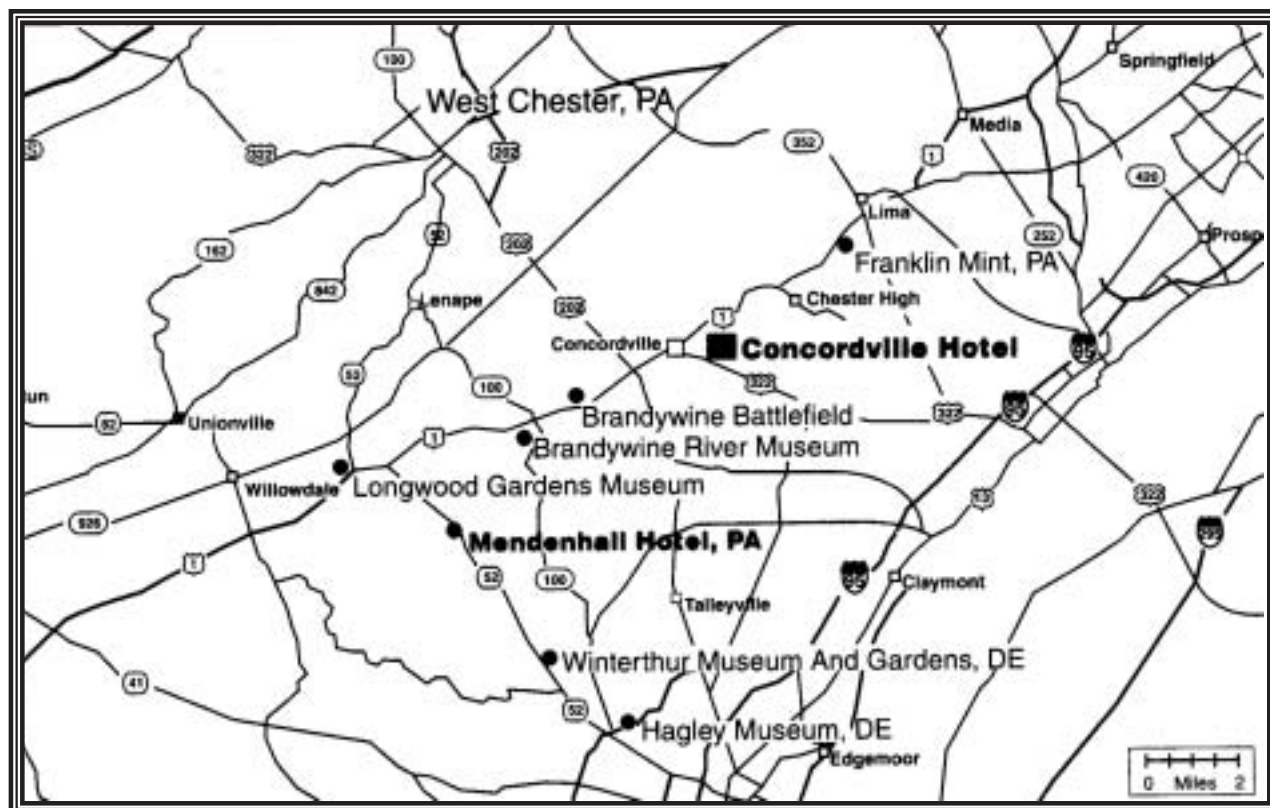
From PA Turnpike: Take Exit 25A (new Exit 20) for Route 476 toward Chester, follow 476 South to Exit 3 (new Exit 5) Lima/Springfield, follow Route 1 South; hotel is 12 miles from Exit 3 (new Exit 5) on left behind Concordville Inn Restaurant (before Route 322)

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

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

Total: _____

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.
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- 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)