

PPXRD-3

23-25 February 2004

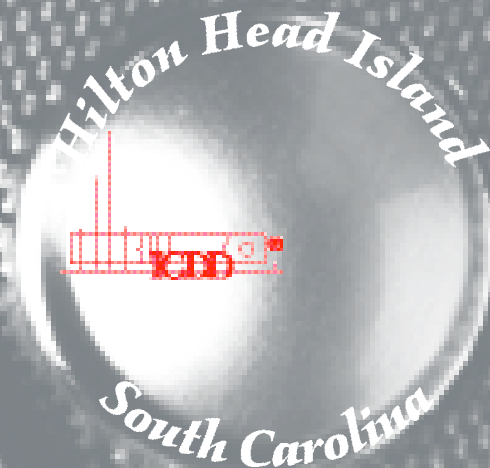
The International Centre for Diffraction Data

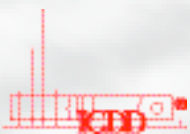
is pleased to announce....

The 3rd Pharmaceutical Powder X-ray Diffraction Symposium Program

Make the most of your XRPD data!

- ▼ Secure fast development of drug candidates ▼
- ▼ Obtain reliable data for regulatory submissions ▼
- ▼ Provide the right data to support patent development ▼





PPXRD-3

1

The 3rd Pharmaceutical Powder X-ray Diffraction Symposium 23-25 February 2004

**Crowne Plaza Resort
Hilton Head Island
South Carolina, USA**

Experience all that Hilton Head Island has to offer ...

- Spectacular island setting
- White-sand beaches
- Ocean-view dining
- Championship golf courses
- Lush tropical gardens

The PPXRD-3 Symposium has a special focus. We have organized topics to deal with making the most of your XRPD data. How do I determine crystallinity? How do I support the physiochemical team during solubility determinations? Is my material in a single crystalline phase? Can I use XRPD to determine stoichiometry during formulation processes? Do I need XRPD for stability studies? How can I prepare XRPD data for regulatory submissions? What XRPD data do I need to construct a good patent? The goal of PPXRD-3 is to create a venue to discuss and address these issues.

Scientific Organizing Committee

Dr. John Faber, Chair, *International Centre for Diffraction Data*, Newtown Square, PA, USA

Dr. Detlef Beckers, *PANalytical*, Almelo, The Netherlands

Dr. Harry G. Brittain, *Center for Pharmaceutical Physics*, Milford, NJ, USA

Dr. Julien Giovannini, *AstraZeneca*, Lund, Sweden

Dr. Jun Han, *Abbott Laboratories*, Abbott Park, IL, USA

Dr. Arnt Kern, *Bruker AXS GmbH*, Karlsruhe, Germany

Dr. Daniel Louër, *University of Rennes I*, Rennes cedex, France

Dr. Fangling Needham, *International Centre for Diffraction Data*, Newtown Square, PA, USA

Dr. Peter W. Stephens, *State University of New York*, Stony Brook, NY, USA

Dr. Gregory A. Stephenson, *Eli Lilly and Company*, Indianapolis, IN, USA

Dr. Raj Suryanarayanan, *University of Minnesota*, Minneapolis, MN, USA

Dr. Peter G. Varlashkin, *GlaxoSmithKline*, Research Triangle Park, NC, USA

Dr. Shawn Yin, *Bristol-Myers Squibb Company*, New Brunswick, NJ, USA

Special **Thank You** to our coffee break sponsors:



Symposium Program

Monday, 23 February

Morning

- 8:30–9:00 **Welcoming Remarks & Introductions: Dr. John Faber, ICDD**
ACQUISITION and USE OF X-RAY POWDER DIFFRACTION DATA
Session Chair: Dr. Detlef Beckers, PANalytical B.V., Almelo, The Netherlands
- 9:00–9:45 ACCURACY IN POWDER DIFFRACTION MEASUREMENTS—Invited
Robert L. Snyder, Georgia Institute of Technology, Atlanta, GA, USA
- 9:45–10:10 IN-SITU VARIABLE TEMPERATURE POWDER X-RAY DIFFRACTION AND THERMAL ANALYSIS
Shawn X. Yin, Raymond P. Scaringe, Jack Z. Gougoutas, Bristol-Myers Squibb Company, New Brunswick, NJ, USA
- 10:10–10:35 GENERATION OF ACCURATE X-RAY POWDER DIFFRACTION DATA OF A PHARMACEUTICAL COMPOUND FOR INCLUSION INTO THE INTERNATIONAL CENTRE FOR DIFFRACTION DATA (ICDD) POWDER DIFFRACTION FILE (PDF)
Gerald Monger, Peter Varlashkin, GlaxoSmithKline, Research Triangle Park, NC, USA
- 10:35–11:05 **BREAK**
- 11:05–11:30 FORMULATION ANALYSES OF OFF THE SHELF PHARMACEUTICALS
Timothy G. Fawcett, John Faber, International Centre for Diffraction Data, Newtown Square, PA, USA
C.R. Hubbard, Oak Ridge National Laboratory, Oak Ridge, TN, USA
- 11:30–11:55 RAPID COMBINATORIAL SCREENING BY TWO-DIMENSIONAL XRD
Bob B. He, Lutz Brügemann, Uwe Preckwinkel, Kingsley L. Smith, Bruker AXS, Inc., Madison, WI, USA
- 11:55–1:25 **LUNCH**

Afternoon: Continued: ACQUISITION and USE OF X-RAY POWDER DIFFRACTION DATA

- 1:25–1:50 ON THE OPTIMUM OPTICAL SETUP FOR MEASURING PHARMACEUTICAL SUBSTANCES
Martijn Fransen, Detlef Beckers, PANalytical B.V., Almelo, The Netherlands
(Detlef Beckers will be speaking on behalf of Martijn Fransen)
- 1:50–2:15 NEW DETECTOR TECHNOLOGY FOR SUPER SPEED X-RAY DIFFRACTION
Lutz Brügemann, A. Kern, H.-G. Krane, Bruker AXS GmbH, Karlsruhe, Germany
R. Durst, B. He, Y. Diawara, Bruker AXS, Inc., Madison, WI, USA
- POWDER PATTERN INDEXING AND PATTERN MATCHING**
Session Chair: Dr. Daniel Louër, University of Rennes, Rennes cedex, France
- 2:15–3:00 INDEXING: ALGORITHMS, ACCURACY, AND AB INITIO—Invited
James A. Kaduk, BP Chemicals, Naperville, IL, USA
- 3:00–3:30 **BREAK**
- 3:30–3:55 ADVANCES IN INDEXING OF POWDER DIFFRACTION PATTERNS: ITERATIVE USE OF LEAST SQUARES AND MONTE-CARLO BASED WHOLE POWDER PATTERN DECOMPOSITION
A.A. Coelho, Arnt Kern, Bruker AXS GmbH, Karlsruhe, Germany
(Arnt Kern will be speaking on behalf of A.A. Coelho)
- 3:55–4:20 INDEXING POWDER DIFFRACTION PATTERNS WITH THE DICHOTOMY ALGORITHM
Daniel Louër, University of Rennes, Rennes cedex, France
A. Boultif, Mentouri University, Constantine, Algeria

Symposium Program

Tuesday, 24 February

Morning

STRUCTURE DETERMINATION, RIETVELD REFINEMENT AND MOLECULAR MODELING

Session Chair: Dr. Peter Stephens, State University of New York, Stony Brook, NY, USA

8:30–9:15

IDENTIFICATION AND CRYSTAL STRUCTURE SOLUTION OF STABLE AND METASTABLE PHARMACEUTICAL COMPOUNDS USING X-RAY POWDER DIFFRACTION DATA—Invited

W.I.F. David, **K. Shankland**, CCLRC Rutherford Appleton Laboratory, Oxon, England, U.K.
C.R. Pulham, The University of Edinburgh, Edinburgh, Scotland, U.K.

9:15–10:00

CRYSTAL STRUCTURE SOLUTION AND REFINEMENT OF A SERIES OF D₂/□₂ RECEPTOR AGONISTS USING LABORATORY X-RAY POWDER DIFFRACTION DATA—Invited

A. Johnston, **A.J. Florence**, **N. Shankland**, Strathclyde University, Glasgow, Scotland, U.K.
K. Shankland, **A.J. Markvardsen**, W.I.F. David, CCLRC Rutherford Appleton Lab., Oxon, England, U.K.

10:00–10:30

BREAK

10:30–10:55

ANALYSIS OF SHORT RANGE ORDER IN X-RAY AMORPHOUS INDOMETHACIN USING X-RAY POWDER DIFFRACTION AND PAIR-WISE DISTRIBUTION FUNCTIONS

Simon Bates, SSCI, Inc., West Lafayette, IN, USA
George Zograf, University of Wisconsin-Madison, Madison, WI, USA
Kieran Crowley, Cardinal Health Inc., Somerset, NJ, USA

10:55–11:20

RECENT ADVANCES IN STRUCTURE SOLUTION FROM POWDER DIFFRACTION DATA

Cikui Liang, Accelrys, Inc., San Diego, CA, USA

11:20–11:45

CRYSTAL STRUCTURE OF D-MANNITOL HEMIHYDRATE

Cristian E. Botez, **Peter W. Stephens**, Stony Brook University, Stony Brook, NY, USA and Brookhaven National Laboratory, Upton, NY, USA
Cletus Nunes, **Raj Suryanarayanan**, University of Minnesota, Minneapolis, MN, USA

11:45–1:15

LUNCH

Afternoon

Continued: STRUCTURE DETERMINATION, RIETVELD REFINEMENT AND MOLECULAR MODELING

1:15–1:40

STRUCTURE DETERMINATION OF AMBUIC ACID WITH SYNCHROTRON POWDER DIFFRACTION AND SOLID-STATE NMR

Yuegang Zhang, **Peter L. Lee**, **Robert Von Dreele**, Argonne National Laboratory, Argonne, IL, USA
James K. Harper, **David M. Grant**, University of Utah, Salt Lake City, UT, USA

1:40–2:05

THE CRYSTAL STRUCTURE OF GUAIFENESIN, 3-(2-METHOXYPHENOXY)-1,2-PROPANEDIOL

James A. Kaduk, BP Chemicals, Naperville, IL, USA

PROCESS ANALYTICAL TECHNOLOGY

Session Chair: Dr. Peter Varlashkin, GlaxoSmithKline, Research Triangle Park, NC, USA

2:05–2:50

USE OF X-RAY POWDER DIFFRACTOMETRY TO MONITOR PHASE TRANSITIONS DURING PHARMACEUTICAL PROCESSING—Invited

Raj Suryanarayanan, University of Minnesota, Minneapolis, MN, USA

2:50–3:20

BREAK

3:20 - 3:45

POLYCAPILLARY X-RAY OPTICS ENABLED DIFFRACTION-BASED PROCESS DIAGNOSTICS AND CONTROL

Walter M. Gibson, **Huapeng Huang**, X-ray Optical Systems, Inc., East Greenbush, NY, USA

3:45 - 4:10

IN SITU XRPD OF COMPACTS AS A POTENTIAL NON-DESTRUCTIVE ANALYTICAL TECHNIQUE FOR DETECTING PROCESS INDUCED PHASE CHANGES

Peter L.D. Wildfong, **Nicole A. Morley**, **Kenneth R. Morris**, Purdue University, West Lafayette, IN, USA

Symposium Program

Wednesday, 25 February

Morning

POLYMORPH CHARACTERIZATION BY XRPD

Session Chair: Dr. Shawn Yin, Bristol-Myers Squibb, New Brunswick, NJ, USA

8:30-9:15

POLYMORPHS AND OTHER CRYSTAL FORMS: WHAT'S IN THAT POWDER?—Invited
Raymond P. Scaringe, Bristol-Myers Squibb, New Brunswick, NJ, USA

9:15-9:40

PHARMACEUTICAL POWDER X-RAY DIFFRACTION: FROM DESIGN TO FINAL SELECTION OF A DEVELOPABLE MATERIAL
Julien Giovannini, AstraZeneca R&D, Lund, Sweden

9:40-10:05

IDENTIFICATION OF POLYMORPH TYPE AND PREDICTION OF MATERIALS PROPERTIES FROM LABORATORY X-RAY POWDER PATTERNS USING INDEXING AND ELECTRON DENSITY CALCULATIONS

Simon Bates, Igor Ivanisevic, Barbara Stahly, SSCI, Inc., West Lafayette, Indiana, USA

10:05-10:35

BREAK

10:35-11:00

POLYMORPHIC FORM SCREENING USING X-RAY POWDER DIFFRACTION

Gregory A. Stephenson, Gregory S. Clanton, Benjamin A. Diserod, Eli Lilly and Company, Indianapolis, IN, USA

11:00-11:25

INFLUENCE OF EXPERIMENTAL CONDITIONS ON THE PHASE TRANSITIONS OF α , β -TREHALOSE
D. Beckers, S. Prugovečki, PANalytical B.V., Almelo, The Netherlands

11:25-12:55

LUNCH

Afternoon

REGULATORY AND PATENT ISSUES

Session Chair: Dr. Julien Giovannini, AstraZeneca R&D, Lund, Sweden

12:55-1:40

APPLICATIONS OF X-RAY POWDER DIFFRACTION TO REGULATORY ISSUES—Invited
Stephen R. Byrn, Purdue University and SSCI, Inc., West Lafayette, IN, USA

1:40-2:25

PHARMACEUTICAL SOLID POLYMORPHISM—THE FDA VIEW—Invited

Andre S. Raw, Lawrence X. Yu, Food and Drug Administration—Center for Drug Evaluation and Search, Rockville, MD, USA

2:25-2:50

21CFR PART11—WHAT'S LEFT (FOR XRPD)?

Arnt Kern, Bruker AXS GmbH, Karlsruhe, Germany

2:50-3:10

BREAK

3:10-3:55

POLYMORPHS AND PURITY AND PATENTS; OH MY—Invited

Michael H. Teschner, Esq., Lerner, David, Littenberg, Krumholz & Mentlik, Westfield, NJ, USA

3:55-4:15

Q&A/Closing Remarks

Poster Session, Reception and Exhibits

23 February 2004
Crowne Plaza Resort
Manufacturers' Exhibits and Poster Session
6–9 pm

PREPARATION AND CHARACTERIZATION OF GLIMEPIRIDE SOLID DISPERSIONS BY POWDER X-RAY DIFFRACTION AND DIFFERENTIAL SCANNING CALORIMETRY

S. M. Al-Saidan, Y.S.R. Krishnaiah, Kuwait University, Safat, Kuwait

DETERMINING THE RELATIVE SENSITIVITY OF X-RAY POWDER DIFFRACTION FOR IDENTIFYING AND MONITORING CRYSTAL FORM CHANGES OF ACTIVES IN SOLID DOSAGE FORMULATIONS

Gerald Monger, GlaxoSmithKline, Research Triangle Park, NC, USA

ANALYSIS OF MANNITOL X-RAY DIFFRACTION PATTERNS

J. Faber, T.G. Fawcett, F. Needham, International Centre for Diffraction Data, Newtown Square, PA, USA

J. Kaduk, BP Chemicals, Naperville, IL, USA

A. Kern, Bruker AXS GmbH, Karlsruhe, Germany

D. Louër, University of Rennes, Rennes cedex, France

R.B. Ortega, Rigaku/MSC, Inc., The Woodlands, TX, USA

P.W. Stephens, State University of New York at Stony Brook, Stony Brook, NY, USA

G. Stephenson, Eli Lilly and Company, Indianapolis, IN, USA

P.G. Varlashkin, GlaxoSmithKline, Research Triangle Park, NC, USA

AUTOMATIC PROCESSING AND PERFORMANCE QUALIFICATION (PQ) IN PHARMACEUTICAL APPLICATIONS

Jeffrey P. Nicolich, PANalytical, Natick, MA, USA

Wenjin Cao, AMGEN, Thousand Oaks, CA, USA

SINGLE CRYSTAL STUDIES OF MEFENAMIC ACID AS A TOOL TO UNDERSTAND POLYMORPHISM

Vrushali Waknis, Neeraj Kumar, P.V. Bharatam, C.L. Kaul, Ramesh Panchagnula, National Institute of Pharmaceutical Education & Research (NIPER), Punjab, India

T.N. Guru Row, Deepak, Solid State Structural Chemistry, IISc, Bangalore, India

SAXSess—AN ANALYTICAL TOOL FOR BIOMATERIALS

Heimo Schnablegger, Anton-Paar GmbH, Graz, Austria

Alexander Bergmann, Otto Glatter, University of Graz, Graz, Austria

X-RAY POWDER DIFFRACTION AND SORPTION-DESORPTION INVESTIGATIONS OF INDAPAMIDE

Matej Smrkolj, Andrej Gartner, Marija Grčman, Krka, d.d., Novo Mesto, Slovenia

Anton Meden, University of Ljubljana, Ljubljana, Slovenia

APPLICATION OF HIGH THROUGHPUT SCREENING TO THE STUDY OF THE CONFORMATIONAL POLYMORPHS OF "ROY"

G.A. Stephenson, G.S. Clanton, B.A. Diseroad, R.M. Goodwin, Eli Lilly and Company, Indianapolis, IN, USA

LAYERED STRUCTURE OF A MULTIPLE HYDRATE-FORMING PHARMACEUTICAL COMPOUND

Y.-H. Kiang, Wei Xu, Laura A. DeBusi, Merck and Co., Inc., West Point, PA, USA

Nancy Tsou, Richard G. Ball, Nobuyoshi Yasuda, Merck and Co., Rahway, NJ, USA

Peter W. Stephens, State University of New York, Stony Brook, NY, USA

Instrument Calibration & Indexing Workshop

Thursday, 26 February, 8am–4pm

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

To participate in the hands-on exercises, all workshop attendees must bring their own laptop computer, Windows®-based with Windows® 98 or later, to the workshop. **PPXRD-3** will provide the data analysis software for use on your laptop computer throughout the workshop.

Exhibitor Information

*Exhibits will be located in Salon D
Crowne Plaza Resort*

Exhibit Hours:

Monday, 23 February 10 am–9 pm
Tuesday, 24 February 10 am–3:30 pm

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

Exhibitors:

Accelrys
Bruker AXS, Inc.
Hecus X-ray Systems
INEL, Inc.
International Centre for Diffraction Data (ICDD)
PANalytical (formerly Philips Analytical)
Rigaku/MSK, Inc.

Accommodations & Travel

The PPXRD Symposium will be held at the **Crowne Plaza Resort**,
Hilton Head Island, South Carolina, USA

Hotel Information

Crowne Plaza Resort
130 Shipyard Drive, Shipyard Plantation
Hilton Head Island, South Carolina 29928, USA
Web site: www.cphiltonhead.com

To make your reservation see options below. Please reference the International Centre for Diffraction Data or PPXRD group to receive the reduced group rate of \$110, plus resort fee (currently \$8), and 10% tax. The deadline for reservations is 1 February 2004. You will not be guaranteed a room after that time. Please contact the hotel for the policy on cancellation of reservations. For your convenience, reservations can be made at the Crowne Plaza Resort with these easy options:

Internet: www.cphiltonhead.com	Group Booking Code: ICD
Telephone: 1.800.334.1881 or +843.842.2400	Group Name: International Centre for Diffraction Data or PPXRD
Fax: +843.842.6503	

Reservation deadline for group rate: 1 February 2004

General Information

Attire: Attire is informal for most activities
Climate: The average temperature in February is 61°F
Time Zone: EST
Airports: Savannah International Airport, Savannah, Georgia, USA
Hilton Head Island Airport, South Carolina, USA

2004 PPXRD-3 Symposium Registration Form

- | | | | |
|---|---------------------|---------------|-------------|
| <input type="checkbox"/> Symposium only | 23-25 February 2004 | PPXRD04 | \$ 1,200.00 |
| <input type="checkbox"/> Symposium & Workshop | 23-26 February 2004 | PPXRDWS04 | \$ 1,500.00 |
| <input type="checkbox"/> Symposium only Student fee | 23-25 February 2004 | PPXRDSTUD04 | \$ 400.00 |
| <input type="checkbox"/> Symposium & Workshop Student fee | 23-26 February 2004 | PPXRDWSSTUD04 | \$ 700.00 |

Total: _____

The easiest way to register



Online at:

www.icdd.com/ppxrd



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Mail to: ICDD, Attn: Leah Mooney

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Newtown Square, PA 19073-3273 USA

Dr. Mr. Mrs. Ms.

First Name _____ Middle Initial _____ Last Name _____

Preferred Badge Name (if different) _____

Company/Organization _____

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Home Phone (in case of emergency) _____

Business web site _____

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 _____



Cancellation Policy

Cancellations must be submitted in writing to ICDD. A full refund will be issued, less a \$50 processing fee, if the cancellation is received at least two weeks before the symposium (Monday, 9 February 2004). No refunds will be issued for cancellations received after 9 February 2004.