

Pharmaceutical Powder X-ray Diffraction Symposium 27-29 September 1999

PPXRD Symposium Scientific Organizing Committee

Dr. John Faber, ICDD
Dr. Ron Jenkins, ICDD
Dr. Raj Suryanarayanan, University of Minnesota
Dr. Marek Zakrzewski, Rhone-Poulenc Rorer
Dr. Peter Varlashkin, Glaxo Wellcome, Inc.
Mr. Chris Kidd, Glaxo Wellcome, Inc.
Terry Maguire, ICDD

The Pharmaceutical Powder X-ray Diffraction Symposium targeted the special issues and techniques of X-ray diffraction relating to the pharmaceutical fields and was held at the International Centre for Diffraction Data Headquarters, 12 Campus Blvd., Newtown Square, PA 19073, U.S.A. **The pages relating to the PPXRD Symposium are held here for archival purposes. For more information contact Terry Maguire at ICDD. Phone: +1-610-325-9814, Fax +1-610-325-9823, E-mail maquire@icdd.com.**

PROGRAM:

[Monday](#)

[Tuesday](#)

[Wednesday](#)

[Poster Sessions](#)

[Structural Determination Workshop](#)

[Special Events](#)

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[See/Download the PPXRD Program in Adobe PDF form](#)

SCHOOLS:

An optional one-day school on [Structure Determination from Powder X-ray Patterns](#) will be held on September 30th.

SPONSORS:

Corporations and manufacturers are invited to sponsor a social function during the symposium. For more information contact Terry Maguire at ICDD. Phone: +1-610-325-9814, Fax +1-610-325-9823, E-mail maquire@icdd.com.

ACCOMMODATIONS:

The PPXRD Symposium will be held at the ICDD Headquarters at 12 Campus Boulevard, Newtown Square, PA 19073, U.S.A. The Sheraton Great Valley, located at 707 East Lancaster Pike, Frazer, PA 19355, U.S.A., is the designated host hotel for the PPXRD Symposium.

Tel: 610-524-5500, Fax: 610-594-8060.

A block of rooms is reserved for Symposium guests for the nights of 26-29 September 1999. Rates are 123.00 \$US for a standard room, plus 6% tax. An upgraded room on the Executive Level is 143.00 \$US, plus 6% tax. Reservations must be made by 1 September 1999. Please mention PPXRD when you make your reservation. Check-in time is 4:00 p.m., and checkout is 12:00 noon. You must advise the hotel at least 24 hours in advance of a cancellation to avoid a charge of one night's room and tax.

All guest rooms offer the following amenities: coffee maker, hair dryer, iron & ironing board, work desk, two telephones, voice mail, computer access, nightly turndown service, and a daily newspaper delivered to your room. The Executive Level features upgraded room amenities (such as a bathrobe), use of the club lounge and complimentary wine and hors d'oeuvres in the evenings, and a continental breakfast in the mornings. The indoor swimming pool is open daily until 9:00 p.m., and the exercise facility is open 24 hours. The Sheraton offers same day

dry cleaning, a self-serve guest laundry, safe deposit boxes, a gift shop, and complimentary local transportation (upon availability).

TRANSPORTATION:

During the Symposium and Workshop, the Sheraton will provide transportation to the ICDD each morning and return transportation to the Sheraton at the conclusion of each day's session.

Ground Transportation from Philadelphia Airport to Sheraton Great Valley:

Paoli Airport Limousine: 23.00 \$US per person each way; no reservation necessary; leaves 15 minutes after the hour until 10:15 p.m. Dial 11 from the Ground Transportation counter, located in the Baggage Claim area of the airport, or call 610-647-5466 from outside the airport.

Super Shuttle: 29.00 \$US for one passenger, 11.00 \$US each additional passenger; no reservation required; leaves frequently. Dial 43 from the Ground Transportation counter, located in the Baggage Claim area of the airport, or call 800-258-3826 from outside the airport.

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.

DIRECTIONS:

Directions to ICDD from Philadelphia International Airport

Take Airport Exit towards Delaware, merging onto I-95 South. Follow I-95 South for 5 miles to Exit 7 (I-476 North.) Follow I-476 North for 9 miles, and at Exit 4 turn left onto Route 3. Follow Route 3 for 4 miles, turning left onto Campus Boulevard at the traffic light, into the Newtown Square Corporate Campus. The ICDD is on the right at 12 Campus Boulevard.

Directions to ICDD from Sheraton Great Valley Hotel

Take 202 South to the Route 3 East (Newtown Square) exit. Follow Route 3 east for approximately 8.5 miles. Turn right (at traffic light) into the Newtown Square Corporate Campus on Campus Boulevard. ICDD is located on right at 12 Campus Boulevard.

Directions to Sheraton Great Valley Hotel from Philadelphia International Airport

Take I-95 South approximately 5 miles to Route 322 West. Take 322 West approximately 5 miles, turn left onto Route 1 South. Follow Route 1 South for ½ mile and turn right onto 202 North. Take Route 202 North 12 miles to Route 30 East (Frazer Exit). Turn right at end of ramp onto Route 30 East. Sheraton Great Valley will be on your left. Caution: Routes 202/322 separate just past the Holiday Inn. Make sure to go right. Also, do not take Route 30 West Exit which comes before the Route 30 East Frazer Exit.

Directions to Sheraton Great Valley Hotel from:

North - NJ Turnpike South to PA Turnpike West. Take Exit 24 from Turnpike to 202 South 12 miles to Route 30 Exit. Hotel is on left ½ mile.

South - Take I-95 North to Wilmington/West Chester 202-North Exit. Continue on 202 North to Route 30 Exit. Turn right off exit. Hotel is on immediate left.

East - From PA Turnpike West take Exit 24. Then take Route 202 South 12 miles to Route 30 East. Hotel is on left ½ mile.

West - From PA Turnpike East, take Exit 23 to 100 South. Take 100 South 4 miles to Route 30 East. Hotel is on left 2 miles.

[SEE MAP OF AREA](#)

ATTIRE:

Attire is informal for most activities.

CLIMATE:

Average range of temperatures is 55 to 75° F.

TRAVEL:

The official travel agency for the Symposium is Kitty Ward Travel. For assistance contact Maureen Ward at 1-800-752-3718.

For the latest conference information, call Terry Maguire, Corporate Secretary, at ICDD, Phone: +1-610-325-9814, Fax +1-610-325-9823, E-mail maguire@icdd.com.

[See/Download the PPXRD Brochure in Adobe PDF form](#)

[See/Download the PPXRD Program in Adobe PDF form](#)

Symposium Program

Monday 27 September 1999

Morning	Acquisition and Use of X-ray Powder Diffraction Data Chris Kidd, Chair
8:30- 9:00	Welcoming Remarks & Introductions R. Jenkins, International Centre for Diffraction Data, Newtown Square, PA
9:00- 9:45	The Role of XRPD in the Characterization of Pharmaceutical Materials – Invited J. Bernstein, Ben-Gurion University of the Negev, Beer Sheva, Israel
9:45-10:30	On the Obtaining of High Quality Experimental Data with Pharmaceutical Specimens – Invited R. Jenkins, International Centre for Diffraction Data, Newtown Square, PA
10:30-11:00	Break
11:00-11:45	The Effect of Different Preparations of XRD Specimens on the Quality of the Diffraction Data – Invited D. K. Smith, Emeritus, The Pennsylvania State University, University Park, PA
11:45-12:30	Investigation of Reactions in Pharmaceutical Solids by Temperature and Humidity Controlled XRD – Invited S. Rastogi, R. Suryanarayanan, University of Minnesota, Minneapolis, MN, and M. Zakrzewski Philips Analytical X-ray, The Netherlands. Present address: Rhône-Poulenc Rorer, Collegeville PA
12:30-1:30	Lunch
Afternoon	Polymorph Characterization by XRPD Peter Varlashkin, Chair
1:30-1:55	Rapid Screening of Polymorphs by Diffraction Methods C. Lehmann, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany
1:55-2:20	Characterization of Multiple Polymorphs / Pseudomorphs of a Developmental Pharmaceutical Using Thermal and X-ray Powder Diffraction Methods R. Newman, D. Miller, Dow Chemical U.S.A., Midland, MI
2:20-2:45	Characterization and Interconversion of the Polymorphs of an IP Receptor Antagonist Z. Chen, J. Lang, Roche Carolina Inc., Florence, SC
2:45-3:15	Break

- 3:15-3:40 **Polymorph Determination of GP IIB/IIIA Antagonist, Roxifiban, Using a Combination of Electron Diffraction and Synchrotron X-ray Powder Diffraction Techniques**
Z. Li, R. Harlow, C. Foris, DuPont Company, Central Research & Development, Wilmington, DE, and
H. Li, P. Ma, R. Vickery, M. Maurin, DuPont Pharmaceuticals Company, Wilmington, DE
- 3:40-4:05 **Quantitation of Two Polymorphic Forms Using Rietveld Analysis, Synchrotron X-ray Powder Diffraction, and Traditional X-ray Powder Diffraction**
A. Newman, M. Andres, G. Stahly, A. Thomas, Solid State Chemical Information, Inc., West Lafayette, IN, and P. Stephens, State University of New York, Stony Brook, NY
- 4:05-4:30 **Powder X-ray Diffraction Methods to Find Various Hydrates of a Drug Substance**
M. Davidovich, J. Gougoutas, J. DiMarco, R. Mueller, I. Vitez, Bristol-Myers Squibb Pharmaceutical Research Institute, New Brunswick, NJ, and A. Newman, Solid State Chemical Information, Inc., West Lafayette, IN

Tuesday 28 September 1999

- Morning** **Indexing, Structure Determination, and Molecular Modeling**
Marek Zakrzewski, Chair
- 8:10- 8:55 **Dealing with Materials that Contain Crystalline and Amorphous Constituents – Invited**
J. Faber, International Centre for Diffraction Data, Newtown Square, PA
- 8:55- 9:40 **Molecular Structures from Powders: Global Rietveld Analysis – Invited**
B. David, Rutherford Appleton Laboratory, Oxon, United Kingdom
- 9:40-10:00 Break
- 10:00-10:45 **Terephthalate Salts. Salts of Monopositive Cations – Invited**
J. Kaduk, BP Amoco PLC, Naperville, IL
- 10:45-11:30 **Application of Structure Solution from Powder Patterns – Invited**
G. Stephenson, Eli Lilly and Company, Fishers, IN
- 11:30-11:55 **30 Years of Rietveld Analysis: The Next Generation**
A. Kern, A. Coelho, Bruker-AXS GmbH, Karlsruhe, Germany
- 11:55-12:20 **Powder Solve - A New Method for Crystal Structure Determination from Powder Data**
M. Wahle, G. Engel, S. Wilke, F. Leusen, Molecular Simulations Inc., San Diego, CA
- 12:20-12:45 **Solution of Flexible Molecular Structures from Powder Diffraction Data Using Simulated Annealing**
Y. Andreev, P. Bruce, University of St. Andrews, Fife, Scotland
- 12:45-1:45 Lunch
- Afternoon** Marek Zakrzewski, Chair
- 1:45-2:30 **Polymorphs and Salt Forms of Pharmaceuticals Solved from Powder Diffraction Data – Invited**
K. Shankland, Rutherford Appleton Laboratory, Oxon, United Kingdom
- 2:30-2:55 **A Systematic Search Strategy for Structure Determination from X-ray Powder Diffraction Data: Application to Anhydrous Theophylline**
E.D.L. Smith, R. Hammond, K. Roberts, Heriot-Watt University, Edinburgh, United Kingdom, and
J. Cherryman, Zeneca Specialties Research Centre, Manchester, United Kingdom
- 2:55-3:20 **Do Microcrystal Diffraction Facilities Make Structure Solution from Powder Diffraction Data Obsolete?**
C. Frampton, Roche Discovery Welwyn, Hertfordshire, United Kingdom
- 3:20-3:40 Break

- 3:40-4:25 **Application of Synchrotron Radiation to Problems in the Pharmaceutical Sciences – Invited**
P. Stephens, State University of New York, Stony Brook, NY
- 4:25-5:10 **Powder Diffraction from Biological Macromolecules Using Synchrotron Radiation – Invited**
F. Rotella, Argonne National Laboratory, Argonne, IL

Wednesday 29 September 1999

- Morning** **Preformulation, Formulation, Regulatory & Patent Issues**
John Faber, Chair
- 8:30-9:15 **New Methods for PercentAGE Crystallinity Determination – Invited**
S. Bates, Kratos Analytical, Chestnut Ridge, NY
- 9:15-10:00 **Applications of X-ray Powder Diffractometry in Preformulation and Formulation – Invited**
R. Suryanarayanan, University of Minnesota, Minneapolis, MN
- 10:00-10:30 Break
- 10:30-11:15 **The Impact of Polymorphism on Drug Development: A Regulator's Viewpoint – Invited**
W. DeCamp, Food and Drug Administration, Rockville, MD
- 11:15-12:00 **XRD Data and Patents – Invited**
G. Geist, US Patent & Trademark Office, Washington, DC
- 12:00-1:00 Lunch
- Afternoon** Ron Jenkins, Chair
- 1:00-1:45 **PPXRD: Swear by Your Results, Not at Them – Invited**
S. Tarling, Birkbeck College, London, United Kingdom
- 1:45-2:30 **The Role of the Organic Powder Diffraction File in the Provision of Pharmaceutical Data – Invited**
J. Faber, R. Jenkins, R. Snyder, International Centre for Diffraction Data, Newtown Square, PA
- 2:30-3:15 **XRPD Patents in Litigation – Invited**
S. Lee, Kenyon & Kenyon, New York, NY
- 3:15-3:35 Break
- 3:35-4:15 **Question and Answer Session**
- 4:15-4:45 **Future Topics and Wrap-up:** Chris Kidd, Chair

Poster Session
Sheraton Great Valley, Regency Ballroom
Monday, 27 September 1999
5:30 - 9:00 p.m.

Environmentally-Controlled Sample Stage for Scintag's Six-Position XRD Sample Changer
C. Buckner, C. Kidd, S. Long, P. Varlashkin, J. Zhu, Glaxo Wellcome, Inc., Research Triangle Park, NC

Pitfalls in the Availability of Multiple PDF Entries
R. Jenkins, International Centre for Diffraction Data, Newtown Square, PA

Powder Diffraction at a Synchrotron Source

A. Mehta, J. Arthur, Stanford Synchrotron Radiation Laboratory, Stanford, CA

Traditional Equipment for the Measurement of Powder Patterns

R. Jenkins, International Centre for Diffraction Data, Newtown Square, PA

Non-Traditional Equipment for the Measurement of Powder Patterns

J. Faber, International Centre for Diffraction Data, Newtown Square, PA

The ICDD Grant-In-Aid Program

T. Kahmer, R. Jenkins, International Centre for Diffraction Data, Newtown Square, PA

Crystal Structures of Small Organic Monomers

J. Kaduk, BP Amoco PLC, Naperville, IL

Structural Determination of Sodium Phenoxyacetic Acid Hydrate

J. Evans, K. Roberts, G. White, G. Rosair, Heriot-Watt University, Edinburgh, Scotland, and A. Kapitan, A. H. MARKS Ltd., West Yorkshire, England

Powder XRD in the Pharmaceutical Industry - An Overview

S. Robie, Scintag, Inc., Cupertino, CA

Review of Widely Used Indexing Techniques

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

X-ray Powder Diffractometry and Other Methods to Establish the Pharmaceutical Quality of Generic Drug Raw Materials Available in South Africa

M. De Villiers, W. Liebenberg, E. Swanepoel, E. Van Tonder, T. Dekker, Potchefstroom University for CHE, Potchefstroom, South Africa

Structure Determination Workshop**ICDD Headquarters****Thursday, 30 September 1999****9:00 a.m. – 4:00 p.m.**

Lecturers Include: John Faber, ICDD, Jason Hanko, Molecular Simulations, Inc., James Kaduk, BP-Amoco PLC, Stev Maginn, Cambridge Crystallographic Data Centre, Frank Rotella, Argonne National Laboratory, Peter Stephens, State University of New York at Stony Brook, Mark Wahle, Molecular Simulations, Inc.

The Structure Determination Workshop is oriented to the elucidation of pharmaceutical materials. The workshop will be hands-on with the use of Cerius2 (Molecular Simulations, Inc.). In addition to display and the determination of molecular structures, current plans are to use the new simulated annealing Monte Carlo module called Powder Solve. Do's and Don'ts for solutions to problems will be discussed.

Special Events**Sheraton Great Valley, Regency Ballroom****Monday, 27 September 1999**

5:30-9:00 p.m.

Manufacturers' Exhibit and Poster Session

6:00-8:00 p.m.

Reception – Sponsored by Bruker AXS, Inc.
Two hour social with carving station, hot and cold hors d'oeuvres, trays of cheese, vegetables and fruits, wine, beer and sodas.
Held in conjunction with Exhibit and Poster Session.

Exhibitor Information

Exhibits will be located in the Regency Ballroom on the Ground Floor of the Sheraton Great Valley on Monday, 27 September from 5:30-9:00 p.m. The following is a list of exhibitors registered to date:

[Bruker AXS, Inc](#)

[Cambridge Crystallographic Data Centre \(CCDC\)](#)

INEL, Inc.

[International Centre for Diffraction Data \(ICDD\)](#)

[Kratos Analytical, Inc.](#)

[LND, Inc.](#)

[Molecular Simulations, Inc.](#)

[Philips Analytical](#) B.V.

[Rigaku/USA, Inc](#)

[Scintag, Inc.](#)

[Solid-State Chemical/Pharmaceutical Information, Inc. \(SSCI\)](#)

[SPEX CertiPrep, Inc.](#)

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