

14th Pharmaceutical Powder X-ray Diffraction Symposium PPXRD-14 summary

Theresa Maguire

International Centre for Diffraction Data, Newtown Square, Pennsylvania 19073, USA
maguire@icdd.com

The 14th Pharmaceutical Powder X-ray Diffraction Symposium (PPXRD-14) once again provided a friendly forum for the exchange of knowledge and cutting-edge ideas among those interested in the combined fields of XRD and pharmaceutical sciences. This year, the symposium returned to Fort Myers, Florida, with the scenic Sanibel Harbour Marriott as our host, during the week of 6–9 June 2016. Nearly 40 attendees from ten countries were in attendance.

The symposium began with an optional, full-day workshop on Monday, focusing on *Quantitative Phase Analysis by XRPD*, chaired and instructed by **Arnt Kern**, Bruker AXS, Germany; **Fabia Gozzo**, Excelsus Structural Solutions SPRL, Belgium; and **Mathilde Reinle-Schmitt**, Paul Scherrer Institute, Switzerland. The workshop discussed the basis for quantitative phase analysis (QPA) for both single-peak and whole-pattern-fitting approaches. Discussions

focused on how to select and apply the QPA methods, particularly in the context of the derivation of absolute phase abundances. The presence of poorly crystalline or amorphous content requires extension of the basic methods, but once these are established, they can be shown to produce QPA to similar lower limits of detection as obtained for crystalline materials.

Two and a half days of technical sessions followed, with the topics of:

- Patent Issues
- Amorphous, Activated, and Nano Materials
- Qualitative and Quantitative Analysis
- PXRD Techniques/Rietveld Refinement/Crystal Structure Prediction/Crystal Structure Verification
- New Frontiers in X-ray Diffraction for Pharmaceutical Research and Development
- Formulation & Product Development/Polymorph, Salt & Co-crystal Screening.

Within these technical sessions there were 10 invited presentations at PPXRD-14. “Using X-ray Powder Diffraction and Other Solid-State Data to Protect Pharmaceutical Inventions” Eyal Barash (Barash Law LLC); “Characterization of Spatial Phase Heterogeneity in Tablets by X-ray Diffractometry” Raj Suryanarayana (University of Minnesota); “Instrumentation and Applications of 2D XRD for Pharmaceuticals”, Bob He (Bruker); “Crystal Structures of Large-Volume Commercial Pharmaceuticals”, James Kaduk (Illinois Institute of Technology); “Transmission Non-Ambient X-ray Powder Diffraction as a Means to Study Liquid-Solid Transformations”, Simon Bates (Triclinic Labs); “Strategies to Expand Solid-state Landscapes of Drugs to Enable Successful Tablet Formulation Development”, Chanquan Sun (University of Minnesota); “Two-Dimensional X-ray Diffractometry in Pharmaceutical Product and Process Development”, Naveen Thakral (Amgen Inc.); Capturing the Significance of X-ray Crystallography in Pharmaceutical Field: The Application to Characterize New Salt, Co-Crystal and Co-Amorphous”, Etsuo Yonemochi (Hoshi University); Characterization of Active Pharmaceutical Ingredients and Excipients in Commercial Formulations and Preparations of New Crystal Forms by Crystallization and Heat Treatment”, Graciela Diaz de Delgado.

In addition to the oral technical sessions, an evening Poster Session and reception were held, hosted by ICDD, in conjunction with a vendor exhibition. We thank the following organizations that participated: Bruker AXS; International Centre for Diffraction Data; PANalytical; Rigaku Americas Corporation; and STOE & Cie GmbH.



Photo 1. (Color online) Quantitative phase analysis by XRPD – Workshop Instructors (L to R -Fabia Gozzo, Arnt Kern, Mathilde Reinle-Schmitt).



Photo 2. (Color online) Bob He presenting his lecture on the use of 2D detectors for XRD analysis.

The complete program, including abstracts, is available for viewing at <http://www.icdd.com/ppxrd/14/program.htm>.

This event provided the perfect opportunity for attendees to network with colleagues, peruse the scientific posters, and discover the latest tools for XRD analysis as displayed by the vendors. The exhibition was held during the first two days of the symposium. We wish to thank DECTRIS for sponsoring a full day of coffee breaks during the symposium. We are also thankful for the efforts of the PPXRD Organizing Committee

who created a successful program filled with presentations covering fundamentals, as well as cutting-edge developments! If you have an idea for future symposiums, please feel free to contact any member of the *Organizing Committee*.

Don't miss the next PPXRD, scheduled for **18–21 August 2017**. PPXRD-15 is being held as a satellite meeting to the Twenty-Fourth Congress and General Assembly of the International Union of Crystallography, in Hyderabad, India. Stay informed by visiting www.icdd.com/ppxrd.