

## BCA INDUSTRIAL GROUP AUTUMN MEETINGS AstraZeneca Pharmaceutical SIG - 7th Nov 2007

## At AstraZeneca - Macclesfield

09:15 REGISTRATION, COFFEE & PASTRIES.

Chair: Anne Kavanagh.

09:45 WELCOME.

09:50 Roger Davey Polymorphism in molecular crystals - how much have we learnt?

10:25 Gordon Barr (for Chris Gilmore) Is PXRD the Gold Standard in High Throughput Experiments?

**11:00 COFFEE** 

11:25 Tal Austin Understanding relative polymorph stability through structure and thermodynamics

12:00 Bill Jones Screening for New Crystal Forms Based on Mechanical Activation of Mixtures

**12:35 Jerry Heng** Crystal Engineering: The Importance of Surface Properties

13:10 LUNCH

Chair: Roy Copley.

**13:55 Fred Vogt** X-ray Diffraction, Computational Chemistry and Solid-state NMR: A Multi-disciplinary Approach to Understanding the Pharmaceutical Solid-state

14:30 Jonathan Burley Cocrystals and Other Complex Pharmaceutical Materials: Structure Solution from Powder Diffraction

**15:05 COFFEE** 

15:30 Jacco van de Streek Semi-automated Rietveld Refinement of Molecular Crystal Structures with DASH & TOPAS

**16:05 Maryjane Tremayne** Powders and 'Peer-Pressure': Pitfalls and Progress

16:40 CLOSE

## Local organiser:

Dr Anne Kavanagh, Tel:01625 517454 Email: IGChair.BCA@googlemail.com

More details at: <a href="http://bca.cryst.bbk.ac.uk/bca/ig/meet07AM.htm">http://bca.cryst.bbk.ac.uk/bca/ig/meet07AM.htm</a>



## BCA INDUSTRIAL GROUP AUTUMN MEETINGS Autumn Meeting - 8th Nov 2007



At AstraZeneca - Macclesfield

Morning Session - Rietveld applications.

09:15 REGISTRATION, COFFEE & PASTRIES.

Chair: Steve Norval. 09:45 WELCOME.

**09:50 Jeremy K. Cockcroft**, Rietveld: Pitfalls for the non-Expert.

10:30 Tony Bell, Time Resolved Synchrotron X-ray Powder Diffraction Study of Biogenic Nano-Magnetite.

11:00 COFFEE

Chair: Jeremy K. Cockcroft.

11:30 Steve Norval, Versatile Rietveld - Applications to Real Materials.

12:00 Michela Brunelli, Rietveld Refinement of organic molecules: investigation of hydrogen-bond patterns

12:30 Stuart Turner, Rietveld Fitting of High-throughput Data.

13:00 LUNCH

Afternoon Session - Crystallography in Industry

Chair: Judith Shackleton.

**13:50 Robert Hammond**, Application of X-Ray Diffraction In-line to Monitor Solution Mediated Phase Transformations between Polymorphs During Batch Crystallization Processes.

**14:20 Ian F. Ferguson**, Inverse pole figures, their application to a detailed understanding of XRPD measurements.

**14:50 Andrew Winn,** Industrial Applications of Residual Stress Measurement using XRD.

**15:20 COFFEE** 

**15:40 Moataz Attallah**, Utilising energy dispersive synchrotron X-ray diffraction for characterising stresses in two-phase titanium linear friction welds.

**16:10 James Chisholm**, Analysis of Polymorphic Forms - Understanding and Quantifying Packing Similarity.

16:40 CLOSE.

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More details at: <a href="http://bca.cryst.bbk.ac.uk/bca/ig/meet07AM.htm">http://bca.cryst.bbk.ac.uk/bca/ig/meet07AM.htm</a>