

# BCA INDUSTRIAL GROUP AUTUMN MEETINGS

## Pharmaceutical SIG - 7<sup>th</sup> Nov 2007

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:**

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## Autumn Meeting - 8<sup>th</sup> November 2007

**Morning Session - Rietveld applications.**

09:15 REGISTRATION, COFFEE & PASTRIES.

Chair: *Steve Norval*.

09:45 WELCOME.

09:50 **Jeremy K. Cockcroft**, University College London

Rietveld: Pitfalls for the non-Expert.

10:30 **Tony Bell**, Daresbury Laboratory

Time Resolved Synchrotron X-ray Powder Diffraction Study of Biogenic Nano-Magnetite.

11:00 COFFEE

Chair: *Jeremy K. Cockcroft*.

11:30 **Steve Norval**, Intertek MSG.

Versatile Rietveld - Applications to Real Materials.

12:00 **Michela Brunelli**, ESRF, Grenoble.

Rietveld Refinement of organic molecules: investigation of hydrogen-bond patterns

12:30 **Stuart Turner**, Crystallography, Birkbeck College.

Rietveld Fitting of High-throughput Data.

13:00 LUNCH

**Afternoon Session - Crystallography in Industry**

Chair: *Judith Shackleton*.

13:50 **Moataz Attallah**, Materials Science Centre, Univ of Manchester

Utilising energy dispersive synchrotron X-ray diffraction for characterising stresses in two-phase titanium linear friction welds.

14:20 **Ian F. Ferguson**, UKAEA, retired.

Inverse pole figures, their application to a detailed understanding of XRPD measurements.

14:50 **Andrew Winn**, Manchester Materials Science Centre.

Industrial Applications of Residual Stress Measurement using XRD.

15:20 COFFEE

15:40 **Robert Hammond**, University of Leeds.

Application of X-Ray Diffraction In-line to Monitor Solution Mediated Phase Transformations between Polymorphs During Batch Crystallization Processes.

16:10 **James Chisholm**, Cambridge Crystallographic Data Centre.

Analysis of Polymorphic Forms - Understanding and Quantifying Packing Similarity.

16:40 CLOSE.