

BCA IG Newsletter

September 2005

EDITORIAL

Welcome to this new look Newsletter! Why the change? Well next year sees the introduction of "payment in proportion" for postal charges. Staying as we were on A4 would see our postal cost increase from 21p to 35p at today's prices. Reducing to A5 avoids the increased postage and the weight we can send goes up from 60g to 100g. We will also use less paper and save money on printing and envelopes. So with no reason to wait and to save money we've made the change now.

We will still compile the Newsletter in our original A4 format (the printer reduces the size to A5). Consequently the download copy (in PDF format) we archive on the web will remain in A4, so you can always print one off if you prefer the larger print of the old format. It is always good to know your views so please let us know what you think about the new format and any other improvements we can make.

Next month we have a 2 day meeting in London with very attractive pricing
Continued on page 2

Forthcoming Events 2005 - 6

Autumn Meeting 2005

Birkbeck College, London, Oct 18th – 19th

18th – Workshop on Patents in Crystallography

19th – Patents and Crystallography in Industry

Please Register online before 14th October

Diary Dates for 2006:

Spring Meeting 4-6th April 2006 Lancaster .

10th May 2006 XRF Meeting, Keyworth.

8th June 2006 Residual Stress Workshop.

9th November 2006 Autumn Meeting

NEW!! XRF Newsletter published

electronically in July. View a copy on the web.



Charity Registration Number: 284718

World Wide Web addresses:

BCA <http://www.crystallography.org.uk>

IG <http://www.crystallography.org.uk/ig/ig.htm>

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THANK YOU



Thanks to **PANalytical** for sponsoring the cost of production and distribution of this edition of the Industrial Group Newsletter.

www.panalytical.com

Editorial Continued:

considering we are bringing you talks from not one but two patent agents! Registration for a single day is £40 and for both just £60 with half price for concessions. The combination of basic crystallography, pharmaceuticals and patents should have a wide appeal and perhaps beyond the scope of our conventional audience. So please let all your friends and colleagues know about this meeting – you would expect to pay ten times the fees for this type of training opportunity elsewhere. We haven't forgotten our traditional Autumn meeting audience and we do have a mix of general interest talks on the 19th October.

Ever wondered if your Rietveld results are correct? We plan to mount two original data sets from our Quantitative Round Robin on the web. The concentrations the data should give will be supplied along with the crystallographic data needed. In fact everything you need to play with to ensure your technique is perfect. So you don't have Rietveld software, well we will cover what is available in the CCP14 talk on 19th October so make sure you are there.

This issue sees the introduction of a dedicated XRF page following on from the success of our first meeting in April. Again we ask your help in making sure your XRF colleagues are aware of our XRF activities and sign up on the web for our specific XRF E-mail list.

We've set you some challenges in this issue. On page 10 there's a very difficult Sudoku grid for you to solve, but the real challenge is to create a working grid with some crystallographical symmetry. I don't think it can be done – can you prove me wrong?

Good at Graphic design? Then have a go at generating a BCA mouse cursor for use in PowerPoint presentations at our meetings!

Web Editor.

Changes to BCA Industrial Group Constitution.

The AGM at Loughborough approved changes to the Constitution.

Following discussion and some minor changes to the wording proposed in the notice of AGM published in the February 2005 Group Newsletter the following revised sections of the constitution were unanimously approved.

11 COMMITTEE.

The affairs of the Group shall be managed by a Committee consisting of the Officers of the Group together with no more than six Ordinary Members of Committee. Not more than three Officers or Members of the Committee shall be from Academic Institutions. The BCA representative to the ICDD shall be a member of the committee ex officio. Additional members may be co-opted from time to time under Rule 13. The Committee shall be broadly based, with no one field or discipline unduly favoured. Only members of the Group shall be eligible for Membership of the committee.

15 NOMINATIONS FOR OFFICERS AND COMMITTEE.

Vacancies for Officers and Ordinary Members of the Committee shall be filled by election at the Annual General Meeting of the Group. Nominations, which shall be proposed by not less than two members of the Group and shall be accompanied by (a) a brief statement demonstrating the nominee's experience in the application of crystallography to industrial research; and (b) the written consent of the nominee, shall be sent to reach the Honorary Secretary of the Group not later than seven days before the Annual General Meeting.

See the Industrial Group Website for a full copy of the Group Constitution.

2005 Autumn Meetings Birkbeck College, London.

18th October 2005 Workshop on Patents in Crystallography.

Organisers: Jeremy Karl Cockcroft & Anne Kavanagh.

Target audience - Non crystallographers with a pharmaceutical interest.

This session will include tutorials on VERY BASIC PXRD, with lots of examples and the absolute minimum of theory. It is aimed at people who need to be able to understand about diffraction experiments but do not necessarily make diffraction measurements. The morning will provide many examples from a wide variety of research areas including industrial applications such as with polymorphs, amorphous versus crystalline components, impurity and mixed phases. The afternoon will provide a VERY BASIC introduction to the use of PXRD in patents with examples from both ceramic/mineral and pharmaceutical industries.

Provisional Programme:

10:30 Coffee

11:00 Introduction to patents.

Sam(antha) J Towlson, Pilkington plc.

11:45 Introduction to crystallography.

Jeremy Karl Cockcroft, UCL/Birkbeck College.

12:30 Lunch

14:00 XRPD & Pharmaceuticals.

Gareth Lewis, AstraZeneca.

14:45 Quantitative PXRD Case Study.

Jeremy Cockcroft, UCL/Birkbeck College.

15:30 Tea

16:00 Pharmaceutical Examples.

Martin Vickers, UCL/Birkbeck College.

16:30 Crystallographic Patents & Seeding,

Mike Glazer, University of Oxford.

17:30 Close.

See the meeting web page for local hotels and venue map.

19th October 2005 Patents & Crystallography in Industry

Morning Session - Patents.

The morning theme will be "Patents" organised by Anne Kavanagh and Richard Morris.

10:00 How to be an expert witness.

Chris Frampton, Pharmorphix.

11:00 Coffee

11:30 Patents legal aspects.

Roger Savidge, consultant.

12:30 Lunch

Afternoon Session - Crystallography in Industry.

The afternoon devoted to "Crystallography in Industry" - a diverse mix of presentations to cover a wide range of interests organised by Judith Shackleton and Steve Norval.

13:30 Low angle Round Robin preliminary results.

Dave Taylor, consultant.

14:00 Standards.

Steve Norval, ICI plc.

14:30 Neutron Diffraction Introduction.

Peter Laggner, Institute of Biophysics and X-Ray Structure Research, Austrian Academy of Sciences

15:15 Tea

15:45 Quantitative Rietveld - *To be advised.*

16:30 CCP14.

Richard Stephenson, UCL/Birkbeck College.

17:00 Close.

See the meeting web page for the latest programme information.

BCA Spring Meeting 2006.

Lancaster University, 4-6 April 2006

Provisional Industrial Sessions and CALL FOR PAPERS.

Tuesday 4th April

A full day XRPD workshop on Phase Identification.

This session will follow the format of previous Phase Identification workshops with the emphasis on understanding and using the Powder Diffraction File (PDF). It will include a mixture of presentations and hands on computer sessions. With a section devoted to extending Phase ID into semi-quantitative and quantitative analysis. Tutors will include David Rendle and Dave Taylor.

Wednesday 5th April

10:30 - 12:00 10:30 - 12:00 Neutron & Synchrotron Opportunities for Industrial Users Session Chair: Jeremy Cockcroft.

Examples of a wide spectrum of industrial uses of neutron and synchrotron facilities.

Speakers include Alan Hewat, ILL.

More details soon.

13:00 – 16:30 Crystallisation and Polymorphism of Pharmaceuticals.

Session Chairs: Roy Copley & Anne Kavanagh

This session will commence with the 2006 **Alun Bowen Lecture** by Ulrich Griesser, University of Innsbruck. (Chair J K Cockcroft)

Other speakers include Roger Davey.

More details soon.

Thursday 6th April

11:00 -12:30 Nanocrystallography.

A joint session with British Association for Crystal Growth.

Session Chairs: Kevin Roberts (BACG) and Richard Morris (BCA)

More details soon.

Thursday 6th April cont.

13:30 - 16:00 Powder Diffraction in Industry.

Session Chairs: David Beveridge & Judith Shackleton

A diverse selection of industrial applications.

More details soon.

Offers of presentations (preferably before 15th October 2005) in any of the above sessions should be made to the appropriate session chairs.

Contact details are on the back page. Keep an eye on the web for updates!

Industrial Group E-mail Mailing lists – Online registration.

We now maintain separate lists for XRF and XRD mailings so please register for BOTH if you want to be kept totally in the picture.

The IG sends about six E-mail notices each year to anyone interested (You don't even need to be a BCA member!). These inform of Newsletter postings and the various meetings we organise each year. You can now register for our E-mail lists online - follow the link from the IG home page. There is an opportunity to be removed from the list with each mailing.

****SPONSORS WANTED****

You can sponsor this newsletter!

Sponsors, whether individuals or companies are needed for future editions of this Newsletter. You will be acknowledged on the front page of both the paper and web newsletters and if relevant, your company logo and web address will be included.

Contact the Web Editor to discuss.

Reports from the BCA Spring Meeting - April 2005, Loughborough.

Crystallography in Industry 1 & 2



Pictured: Left to Right: Preuss, Morris, Gill and Cope

Wednesday's afternoon session "Crystallography in industry" was chaired by **Judith Shackleton** and opened with:

Michael Preuss (University of Manchester) lecturing on '**Residual stresses in friction welded aeroengine components**'. He talked about the types of friction welding: friction welding has the advantage over fusion processes which cannot reliably weld many of the high temperature alloys now found in aero engine components: the inertia friction method is used to join discs/shafts and the linear friction method for joining blades onto discs. A consideration during friction welding however is the generation of residual stress, during joining, and stress relief during post weld heat treatment. Industry has turned to synchrotron high energy dispersive X-ray scattering to enable researchers to undertake systematic studies of the residual stress profiles in welds and improve the understanding of how welding parameters and post weld heat treatments affect the residual stress fields and the performance of the welded component. The talk was concluded with the fact that higher temperatures for annealing

brings down stresses to acceptable levels.

Tony Fry (National Physical Laboratory) followed with his lecture on: '**Residual stress measurements at NPL. Increasing confidence and development best practice**' in which he talked about the parameter study to find how robust the x-ray diffraction method is. He went through two projects undertaken at the NPL and ended with mention of the Good Practice Guide authored with the Projects Industrial Advisory Group. The talk ended with a good discussion from delegates in the room.

Martijn Fransen (PANalytical) ended this first session with an enthusiastic lecture on '**The problem of sample fluorescence when dealing with transition metals in industrial samples**'. The talk covered 1-D and 2-D detection systems and posed the question "Can you get good peak/ background ratio?" He went through the best choices of the practical aspects from the monochromator to the detector as a function of the elemental composition of the sample.

The second part of the session, chaired by **Richard Morris**, opened with: **Peter Laggner** (Graz, Austria) on '**Bridging the nano-gap: simultaneous SAXS and XPD on nanomaterials**'. He covered a lot in his talk giving a range of examples such as synthesis of mesoporous materials and dissolution of drug-delivery C/R microspheres. He focused on the design of the HECUS-System3 SWAXS (small and wide angle x-ray scattering) and its use in different applications. The need for SAX for determining domain size and surface roughness and XPD for crystal structure and amorphous content was explained. The session was brought to an end with a interesting lecture from:

(continued on page 6)

Reports from the BCA Spring Meeting - April 2005, Loughborough (cont.)

Ian Cope (Imperial College), Ian explained his PhD research: ***Using XRD to support the study of an iron oxide deposit***, called the Pic de Fon deposit. This deposit is a potential new source of iron ore located in the Eastern Republic of Guinea, West Africa. The aim is to combine XRD and geochemical analysis to constrain the process by which banded iron formation is converted to iron ore.

It was good because as a field geologist he knew little about XRD, but was interested in how it could help in his research. XRD results indicate that distinct crystallographic signature may exist for the different ore grade material types. Each ore-grade material type exhibits different physical properties, hard, biscuit and powder, which in turn will control the metallurgical performance of the final delivered product. All the presentations gave a useful insight into where and how crystallography is used in industry and the different type of demands industry places on crystallographic hardware compared to academia.

Robert Davies (University of Oxford)

Nicola Turvey (Aston University).

Reprinted from June 2005 Crystallography News.

Non-ambient Pharmaceutical Studies.

Jonathan Burley opened this session, chaired by **Anne Kavanagh** with ***Crystal structure and intermolecular forces from variable temperature PXRD***.

The structure was that of Glipizide, a major drug for treating diabetes. Variable temperature data were used to confirm the index of the cell, and Jonathan recommended this as a facile method of ensuring crystals are correctly indexed when using powder diffraction. Since structure-

property relationships are of interest, he investigated intermolecular forces quantitatively by working out the Debye temperatures along the cell axes. This temperature is a measure of the lattice stiffness, i.e. bond strength. The anisotropic lattice expansion was fitted to the sum of phonon modes. Jonathan showed that glipizide has single phonon modes along the *a* and *c* axes, which he attributed to π - π interactions and hydrogen bonding respectively, and the *b* axis is characterised by two phonon modes, which correspond to van der Waals interactions and steric interlock.

For a patent, every pharmaceutical requires characterization; this is often achieved, at least in part, by powder diffraction. One of the questions **Jeremy Cockcroft** considered in his talk ***Obtaining accurate non-ambient laboratory PXRD data for pharmaceutical studies*** was whether the powder diffraction patterns always represent a polymorph of the material. In order to answer this, accurate data are required, ideally without preferred orientation. To get good data, the diffractometer configuration has to be considered and the calibration of the equipment checked. Low temperature diffraction is often a useful tool, providing turbulence, draughts and icing problems can be dealt with. LT work requires capillary geometry, which has the advantage of reducing or removing preferred orientation. Several case studies were presented.

Steve Cosgrove finished the first session with ***Probing (De)Hydration Behaviour by High Resolution X-ray Powder Diffraction***. He described studies of a candidate drug, as its sodium salt, which was known to

(continued on page 7)

2005 Spring Meeting Reports continued

Non-ambient Pharmaceutical Studies. (continued)

crystallise as four polymorphs, three hydrates and a number of other solvates. Steve discussed DSC and derivative TGA for probing dehydration and hydration of the compound. Mass spectrometry is also used, with monitoring of the $m/z = 18$ peak indicating the loss of water from the compound. Dynamic vapour sorption is also used to cycle the compound within various humidity environments to monitor moisture sorption and dehydration. This method can highlight stable higher hydrates, which would be more appropriate for manufacture as the risk of water sorption by a lower hydrate would cause problems during weighing stages.

After the coffee break, **Roy Copley** took the chair, and **Francesca Fabbiani** spoke on **Probing Polymorphism with High Pressure** based on a search for high pressure polymorphs of piracetam. Varying of pressure adds an additional dimension to the search for polymorphs of pharmaceuticals. Three approaches are available - direct compression (best for very small molecules), growth of crystals from the melt and recrystallisation from solution under pressure. Three new polymorphs of piracetam have been structurally characterised.

Francesca used graph set analysis to demonstrate the differences in the hydrogen bonding patterns within the polymorphs, and also introduced the concept of Hirschfeld surfaces to differentiate between the polymorphs.

Emphasising the importance, and often difficulty, of understanding polymorphs and

hydrates of pharmaceuticals, **Angus Foster** discussed ***The Use of X-ray Diffraction in the Pharmaceutical Development of a Dihydrate API***, a compound with complex hydration behaviour, which readily loses water under typical manufacturing conditions. Many techniques, including single crystal and VT powder XRD, VT-FTIR and isothermal-TGA to investigate under which conditions the compound could be dried and still remain crystalline.

Peter Laggner finished the session by discussing ***Monitoring non-ambient nanophase processes by TR-SWAXS***.

He gave a description of the equipment used, and then went on to discuss lipid polymorphism. By using temperature jump and pressure studies on membranes he could show that cholesterol induces softening when present in low concentration, but at high concentrations caused hardening of the membrane.

*Sophie Dale (University of Newcastle)
Katharine Bowes (University of Cambridge).*

Reprinted from June 2005 Crystallography News.

Session Speakers and Chairs:



Pictured Left to right: Kavanagh, Burley, Fabbiani, Forster, Cockcroft, Copley

2005 Spring Meeting Reports (continued)

In Situ: Processing in Industry.

In-Situ Processing in Industry

This session aimed to present some applications of diffraction to the study of real industrial processing systems where the *in-situ* approach has given an essential insight for understanding and development.

"Surfactant Formulation"

Gordon Tiddy (University of Manchester) gave an amusing talk based on many years of experience at Unilever. He covered chemical details of detergents and fabric conditioners and their complex phase transitions. The trend to washing clothes at lower temperatures gives interesting scientific challenges. There were tips on differentiating between 'money well spent' and 'PR hype'.

"Processing block co-polymers for nanopores"

Geoff Moggridge (University of Cambridge) spoke about work to try and make polymer membranes for separation. The aim is high volume fraction monodisperse pores ~1-10nm. The route is phase separation in block copolymers to give aligned cylinders which can then be etched away to leave the filter. Techniques for study include X-ray diffraction under shear.

"In Situ Crystallisation Studies of Pharmaceutical Materials"

Simon Jacques (University College London) described the use of TEDDI (Tomographic Energy Dispersive Diffraction Imaging) at Daresbury to follow in-situ crystallisation of pharmaceutical materials. A white beam is collimated to illuminate a relatively small volume (~50µm), the sample is then scanned in x, y and z to build up a 3-D image and the scattered radiation can be analysed with respect to diffraction,

fluorescence and/or absorption. The technique is still being developed. Other related applications include maps of different crystalline phases in tablets.

*Mary Vickers,
University of Cambridge.*

On The Web:

2005 Exhibition Stand Photographs.

There are photographs of all the 2005 Spring Meeting exhibition stands posted on the web. To find them follow the link from the top of the IG homepage:

Latest News: >>>>News archive<<<<
Then *Spring Meeting Exhibition photographs*

Meeting Diary.

Our two year UK meeting Diary is a useful web page, find its link "2 year UK Meeting diary", under **Meeting Programmes & Reports**. Hover over any of the icons and a pop up appears with the name of the meeting. Click on the icon and you are taken to the appropriate web page if available. We also list important overseas meetings to try to avoid clashes. Their icon is a no entry symbol and links are implemented. At the top of the diary page is a link to future BCA Spring Meeting planning dates through to 2011! Contact the web editor to have your meeting featured on the diary page.

What would you like to see?

We will always consider your suggestions for improving the Industrial Groups web pages, this Newsletter or the meetings we arrange. Feel free to contact any of our committee members to discuss your ideas or suggestions.

Contact details on back page.

X-RAY FLUORESCENCE (XRF) PAGE

Welcome to the first page of our newsletter dedicated to the XRF community. Our aim is to keep you informed about BCA XRF activities. We also send out an Electronic Newsletter with the first edition sent out in July. Our target is to mail at least two editions per year. If you did not get an E-mail notice of it's posting you need to register on-line for our specific XRF mailing list.

Our goal is to provide a UK forum for XRF users with regular meetings, workshops and a major meeting with a commercial exhibition every two years. Help us promote this XRF initiative by spreading the word to your friends and colleagues and help us expand our mailing list. Our goal is to reach out to all UK XRF users.

Success Story - our first XRF meeting.



Please view the larger group photo on the web!

The inaugural meeting at Loughborough in April 2005 was a great success. By working closely with XRF vendors we were able to put together a diverse programme and treat delegates to a commercial exhibition which exceeded all expectations.

Both Exhibitors and delegates were pleased with the meeting and we will build on this success for our next 3 day meeting in 2007. We thank all the speakers, session chairs, exhibitors and delegates (especially Xiaoming Lu who made the trip from China to present his poster) for their contribution to this success.

More details, photographs and meeting reports can be viewed on our dedicated XRF web pages.

<http://bca.cryst.bbk.ac.uk/bca/ig/XRF/xrf.htm>

Forthcoming XRF Events:

10th May 2006 - one day XRF meeting of general interest at the British Geological Survey, Keyworth, Nottingham.

More details on the web and offers of presentations are now sought.

4-6th April 2007 - XRF at the BCA Spring Meeting.

A full three day programme with commercial exhibition.

Let us have your ideas now for things you would like to see in the programme!

OUR XRF TEAM.

The Industrial Group Committee has set up an Ad-hoc committee with responsibility for developing XRF as a special interest group. The existing team of Dave Taylor and David Beveridge has been strengthened by the addition of Margaret West and Mark Ingham to form this new committee.

Contact details are on the web pages.

XRF WEB PAGES.

We need your help to build our XRF web pages.

What would you like to see added to the content?

Send in your **links** to other useful XRF sites and web pages.

Your suggestions are needed for our web page of the month.

Take a look at the XRF web pages now. Don't forget to register on line to be kept informed of any XRF specific information we send out and remember we give you the option of being removed from the list with every mailing.

NEWS AND COMPETITIONS

Situations Vacant:

We plan to start a web page offering links to situations vacant in the XRF and XRD fields. We will not host any advertisements on our own pages but will provide links to other sites advertising suitable jobs.

To have a link to your job vacancies on the IG page contact the IG Web Editor
Keep an eye on the web for details!

Sudoku:

There is some debate about whether it is possible to generate a grid that has some symmetry and can be related to crystallography. I've tried and failed, although there is a pattern of sorts in the one given below, it is very difficult to solve. The challenge is can you come up with a crystallographically related grid for the next issue.

The solution and the best of your crystallographic grids will be published in the next issue.

1			2			3		
2		4			5			6
3	7			8			9	
4			5			6		
5		7			8			9
6	1			2			3	
7			8			9		
8		1			2			3
9	4	3	1	5	7	8	6	2

Large Cursors and pointers.

Tony North started a discussion in Crystallography News about using the mouse pointer rather than a laser pointer when giving presentations. This means that you don't turn your back on the audience.

The custom pointer is too small so David Watkin in the last issue gave further details and supplied a couple of more suitable cursors. We have now made these available for download from the IG web pages and also added a couple more that identify with the BCA. You can view these on the web page and we give more information on other sources of cursors and how to install them. Currently this only applies to Windows systems. If you have solved the problem for other operating systems then please let us know.

Can you design a better BCA pointer? If so send them to the IG Web Editor and we will install the best on our web pages.

Struggling with Rietveld?

The IG plan to make data available on the web from the quantitative round robin we ran a couple of years ago.

You will be able to download the inorganic and organic scans along with coordinates and the definitive results. This will give you everything you need to test that your procedures give the right results.

Don't have Rietveld software? Then make sure you attend the Autumn meeting where the CCP14 presentation will include more details on what is available for download. We will also try to fit some discussion on Rietveld problems into the Autumn meeting session.

NOTICES

Articles Wanted:

Why not put pen to paper and write a short article for our next Newsletter. There are lots of examples to give you some ideas in our Hints & Tips section on the WEB. Don't forget, if you attend a conference, please send in an article about it.

We are also looking to expand the range of Industrial Applications of XRD on our WEB Site. All we need are a few well-chosen pictures and a few words. How about something on CEMENTS, MINERALS, MUSEUMS, PHOTOGRAPHY, DETERGENTS, PIGMENTS, POLYMERS

INDUSTRIAL GROUP AWARD

It is the intention of the BCA Industrial group to make an Industrial Crystallography Award to suitable UK crystallographers working in industry or in academic institutions. The Award will be given in recognition of a sustained contribution to industrial crystallography including crystallographic and diffraction work of all kinds.

The Committee of the Industrial group will make the final decision concerning the Industrial crystallography Award. They intend the Award to take a form that fittingly marks the contribution made by the recipient.

Nominations for this Award are invited now and should be sent to the Secretary of the Industrial group. Besides the name and affiliation of the person proposed, nominations should state briefly why she or he merits the Award, giving a brief account (ideally not more than one sheet of A4) of her or his crystallographic work and its industrial significance. If desired, the proposer may suggest the form that the award should take.

Newsletter Mailing

To keep cost down and to ensure that the newsletter gets to the appropriate people it is essential that we know your correct address. Also if there is a more appropriate contact in your organisation or if you no longer require a copy please let us know by contacting any of the committee officers.

The newsletter is also now posted on our WEB site

(<http://bca.cryst.bbk.ac.uk/bca/ig/ig.htm>) If you would like an e-mail notification of the WEB posting rather than a paper copy, then send an e-mail to

djtaylor@lineone.net – with the title
SUBSCRIBE WEB NEWS

The 5th Pharmaceutical Powder X-ray Diffraction Symposium

14-16 February 2006

Somerset, New Jersey, U.S.A

Call for papers - by 15 October 2005

Sessions include:

- X-rays in Drug Research & Discovery
- Formulation, Product Development, Drug Delivery and Polymorph & Salt Screening
- Patent and Regulatory Issues
- Process Analytical Technology
- Complementary Techniques (DSC, TGA, Hot Stage Microscopy, FTIR, Raman, NMR, SEM, AFM, Light Microscopy, XRF, SAXS, SANS)
- XRPD Structural Techniques (Acquisition and Use of XRPD Data, Indexing, Structure Determination, Rietveld Refinement)
- New Frontiers for XRD in Pharmaceutical R&D

www.icdd.com/ppxrd

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