

pretation of such structures is complicated by the fact that we don't know if they are metastable. Hydrogen bonds are only part of the picture; van der Waals interactions are important, too. Hydroxyl groups (especially single OHs) seem to promote $Z = > 1$; perhaps the molecules become frustrated when packing, and just do the best they can. Ton Spek (Utrecht Univ.) described the ADDSYM and NEWSYM tools in PLATON, tools which are useful in the analysis of $Z = > 1$ structures. It's often necessary to examine the Fs to decide what is wrong with a structure; it is therefore important to archive the structure factors in the crystallographic databases. Richard Cooper (Univ. of Oxford) confirmed the tendency of monohydroxyl compounds to crystallize with $Z = > 1$, and described the MATCH software in the CRYSTALS system.

In the session on *Synchrotron Radiation* Simon Teat (Daresbury) summarized the factors which affect diffraction at synchrotrons. New instruments have resulted in increasing numbers of Asupercells; getting the right cell is crucial to getting the right structure! Tony Bell (Univ. of Manchester) described energy-dispersive powder diffraction studies of phase transitions in mercury sulfides. Paul Raithby (Univ. of Bath) showed that, although single-crystal crystallography is usually considered a ground state technique, it can be used to carry out time-resolved studies of coumarin-3-carboxylic acid 2+2 photocycloaddition reactions, even though only ~20% of the crystal volume is excited. He also described several *Awalk before you run* studies of simpler systems, and discussed the prospects for further time-resolved structural studies.

At the DIAMOND SIG meeting, Jeremy Cockroft (Birkbeck College) lamented the fact that a dedicated powder beamline will not be part of the initial instrumentation of this new synchrotron. Paul Raithby described the status of the small molecule single crystal proposal. Chick Wilson (new BCA President) described the new and upgraded instruments included in the ILL Millennium Program and at ISIS.

At the session on *Structure Solution from Powders* Yuri Andreev (Univ. of St. Andrews) showed that maintaining the chain continuity of poly(ethylene oxide) across unit cells was helpful in solving the structures of such polymer electrolytes. Harriot Nowell (Univ. of Cambridge) discussed the importance of the weighting of the restraints in a Rietveld refinement.

During the meeting, ICDD ran an Introduction to Powder Diffraction Workshop, organized by David Taylor and Judith Shackleton, and taught by John Faber and David Taylor with support from Judith Shackleton and Jim Kaduk. The well-received workshop covered introductory XRD and qualitative analysis, with a 2.5-hour hands on session on phase identification.

There were many posters, and I had a great time discussing science with the graduate students during the poster sessions.

James A. Kaduk
BP Chemicals

Calendar of Meetings

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7–12 September 2003

13th Goldschmidt Conference. Kurashiki, Japan. The premier annual meeting for geochemistry and geochemical processes. [Contact: Goldschmidt 2003 Secretariat, International Communications Specialists, Inc., Sabo Kaikan Bekkan 2-7-4 Hirakawa-cho Chiyoda-ku, Tokyo 102-8646, Japan; Tel: 81 (3) 3263 6474; Fax: 81 (3) 3263 7537; E-mail: gold2003@ics-inc.co.jp; Info: <http://www.ics-inc.co.jp/gold2003>].

8–13 September 2003

Aperiodic 2003. Belo Horizonte, Minas Gerais, Brazil. [Contact: Secretaria do Aperiodic 2003, Departamento de Física, Universidade Federal de Minas Gerais, CP 702, Belo Horizonte 30123-970, Minas Gerais, Brazil. Tel: 55 (31) 3499 5672; Fax: 55 (31) 3499 5600; E-mail: ap2003@fisica.ufmg.br; Info: <http://agora.grude.ufmg.br/aperiodic2003>].

14–19 September 2003

SSPD'03 Structure Solution from Powder Diffraction Data. Stara Lesna, Slovakia. [Contact: Dr. Lubomir Smrcok, Institute of Inorganic Chemistry, Slovak Academy of Sciences, Dubravska cesta, SK-842 36 Bratislava, Slovak Republic. Fax: 421 (2) 5941 0444; E-mail: Lubomir.Smrcok@savba.sk; Info: <http://www.sspd-03.sav.sk>].

15–19 September 2003

XV International Conference on X-ray Diffraction and Crystal Chemistry of Minerals. St. Petersburg, Russia. [Contact: Dr. M. G. Krzhizhanovskaya, Department of Crystallography, St. Petersburg State University, University Emb. 7/9, St. Petersburg 199034, Russia. E-mail: xrd2003@crystal.pu.ru; Info: <http://www.lcm3b.u-nancy.fr/cims/forthcoming.htm>].

22–25 September 2003

81. Jahrestagung der Deutschen Mineralogischen Gesellschaft. Bochum, Germany.

22–26 September 2003

17th International Congress on X-ray Optics and Microanalysis. Chamonix Mont-Blanc, France. [Contact: ICXOM XVII, ESRF, Post Office Box 220, F-38043 Grenoble, France. Tel: 33 (476) 882 438; Fax: 33 (476) 882 542; E-mail: icxom@esrf.fr; Info: <http://www.esrf.fr/conferences/icxom.html>].

19–23 October 2003

30th Annual Meeting, Federation of Analytical Chemistry and Spectroscopy Societies. Ft. Lauderdale, Florida, USA. [Contact: FACSS National Office, Post Office Box 24379, Santa Fe, NM 87502, USA. Tel: 1 (505) 820 1648; Fax: 1 (505) 989 1073; E-mail: facss@facss.org; Info: <http://facss.org/facss>].

27–31 October 2003

ISRP-9 9th International Symposium on Radiation Physics. Cape Town, South Africa. This triennial event is sponsored jointly by the International Radiation Physics Society, the iThemba Laboratory for Accelerator Based Sciences (formerly the National Accelerator Centre.), the South African Nuclear Energy Corporation, and the International Centre for Diffraction Data. A two-and-one-half day **Workshop on Radiation-based Analytical Techniques** will be held immediately prior to this meeting (24–26 October 2003) with emphasis on XRD, XRF, and PIXE (particle-induced X-ray emission.) [Contact: Dr. D. T. L. Jones, iThemba Laboratory, Post Office Box 722, Somerset West 7129, South Africa. Tel: 27 (21) 843 1336; Fax: 27 (21) 843 3382; E-mail: isrp9@tlabs.ac.za; Info: <http://www.isrp9.tlabs.ac.za/conferences/isrp9>].

1–5 December 2003

Fall Meeting of the Materials Research Society. Boston, Massachusetts, USA. [Contact: Materials Research Society,

506 Keystone Drive, Warrendale, PA 15086-7573, USA. Tel: 1 (724) 779 3003; Fax: 1 (724) 779 8313; E-mail: info@mrs.org; Info: <http://www.mrs.org>].

14–18 March 2004

133rd Annual Meeting of the Minerals, Metals & Materials Society. Charlotte, North Carolina, USA. [Contact: TMS, 184 Thorn Hill Drive, Warrendale, PA 15086, USA. Tel: 1 (724) 776 9000; Fax: 1 (724) 776 3770; E-mail: ckobert@tms.org; Info: <http://www.tms.org/Meetings/Annual-04/AnnMtg04Home.html>].

17–22 July 2004

ACA'04 American Crystallographic Association Annual Meeting. Chicago, Illinois, USA. [Contact: Bernie Santarsiero, bds@uic.edu; Karl Volz, kvolz@uic.edu; Info: <http://www.hwi.buffalo.edu>].

2–5 September 2004

EPDIC 9 Ninth European Powder Diffraction Conference. Prague, Czech Republic. Held at Charles University. [Contact: E-mail: kuzel@karlov.xray.cz/epdic; Info: <http://www.xray.cz/epdic>].

7–10 September 2004

X-TOP 2004 7th Biennial Conference on High Resolution X-ray Diffraction and Imaging. Prague, Czech Republic. Held at Pruhonice Castle (near Prague.) [Contact: Info: <http://www.physics.muni.cz/kfpf/xtop>].

23–31 August 2005

20th IUCr General Assembly and International Congress of Crystallography. Florence, Italy. [Contact: Congress Secretariat, XX Congress IUCr, Dipartimento di Energetica, Università di Firenze, via S. Marta 3, 50139 Firenze, Italy. Tel: 39 (055) 479 6209; Fax: 39 (055) 479 6342; E-mail: iucr@iucr2005.it; Info: <http://www.iucr2005.it>].

28 November–2 December 2005

International Conference on Neutron Scattering. Sydney, Australia.

Short Courses & Workshops

4–7 September 2003

Summer School on Polycrystalline Structure Determination by Direct Methods. Krakow, Poland. Under Prof. Carmelo Giacobozzo of CNR, Bari, Italy. Directly follows the **19th Conference on Applied Crystallography.** [Contact: Dr. Danuta Stró, University of Silesia, Institute of Physics and Chemistry of Metals, ul. Bankowa 12, 40-007 Katowice, Poland. Tel/Fax: 48 (32) 59 69 29; E-mail: dana@us.edu.pl; Info: www.us.edu.pl/universytet/konferencje/2003/cac/tekst/index.shtml].

8–18 September 2003

8th Oxford School on Neutron Scattering. Oxford, England, UK. Held in Mansfield College of the University of Oxford. [Contact: Prof. C. C. Wilson, ISIS Facility, CLRC

Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, UK. Fax: 44 (1235) 445 720; E-mail: c.c.wilson@rl.ac.uk; Info: <http://www.isis.rl.ac.uk/conferences/osns2003>].

6–8 October 2003

Basics of X-ray Powder Diffraction in Pharmaceuticals. Stamford, Connecticut, USA. [Contact: Info: <http://www.assainternational.com/seminars/about.htm>].

9–10 October 2003

Advanced X-ray Powder Diffraction in Pharmaceuticals. Stamford, Connecticut, USA. [Contact: Info: <http://www.assainternational.com/seminars/about.htm>].