

American Crystallographic Association Meeting 17–21 July 2004, Chicago, IL

James A. Kaduk, BP Amoco Chemicals

Once the ~1000 attendees got to Chicago (you can imagine what thunderstorms do to air traffic at O'Hare!), they had a great time experiencing the science, the setting, the weather, and the new Millennium Park. As usual, there was far too much science for one person to cover, so this is a highly-idiosyncratic summary of the meeting.

For "powder people" one of the highlights of the meeting came first, in a symposium on the *Interface Between Powder and Single Crystal Diffraction*, organized by the new Powder Diffraction Special Interest Group (SIG) and partially supported by ICDD. Doug Dorset (ExxonMobil) showed how the full 3-dimensional data sets which can be obtained from microcrystals in the electron microscope can be used for solving structures of polymers and zeolites, with much less ambiguity than when using fiber or powder techniques. Jim Kaduk (BP Amoco) described the solution of the structure of the common pharmaceutical guaifenesin using Monte Carlo simulated annealing techniques applied to synchrotron powder data. Quantum chemical geometry optimizations were key to working his way out of the false minimum into which the simulated annealing structure solutions had identified. Peter Wildfong (Purdue and SSCI) quantified the phase transitions between forms A and C of chlorpropamide as a function of pressure. He solved the structure of form C using high-quality laboratory data. Calculation of attachment energies showed that both forms have a common set of planes, across which intermolecular interactions are weak, and helped understand the mechanism of the phase transition. Peter Zavalij (SUNY Binghamton) described the structures of many *bis*(oxalato)borate salts, which show promise as battery electrolytes. Akhilesh Tripathi (Texas A&M) used cation positions determined from single crystals of pure germanate analogs to develop models for Rietveld refinements of titanosilicates having the pharmacosiderite topology. Bob Grothe (UCLA) showed how the texture can be used to extract better integrated reflection intensities from 2-dimensional diffraction data. Nattamai Bhuvanesh (Texas A&M) showed how to carry out micro powder diffraction studies using specimens mounted in nylon loops and area detectors. Ralph Tissot (Sandia) showed how improvements in sources, optics, and detectors can be used to carry out microdiffraction experiments, and essentially convert powder problems into single crystal ones. Alex Yokochi (Oregon State) presented a number of examples using his new Rigaku/MSR Rapid instrument. Steve Guggenheim (Univ. of Illinois Chicago) showed how simulated Debye-Scherrer and Gandolfi patterns obtained using a Bruker SMART/APEX system could be used for phase identification. Peter Lee (APS) summarized the powder diffraction opportunities available at the Advanced Photon Source, and described the new dedicated powder diffractometer under construction at BM11. Bill Clegg (Univ. of Newcastle) returned to the idea

of microdiffraction, and showed how both synchrotron single-crystal and powder techniques could be used together to solve problems.

A full-day workshop *X-rays, Crystals, Molecules, and You* aimed at high school teachers and students included presentations on the general basics of crystallography and the information that can be gained. The room was overflowing and suggests that a general education/public outreach component to the Denver Conference might be well-received.

The ACA is becoming ever more concerned about the state of crystallographic education, and so held a session on *Teaching Advanced Crystallography*. This included presentations by many of the "usual suspects," including Jenny Glusker, Bernhard Rupp, Michael Sawaya, Bob Gould, Bill Clegg, Larry Falvello, and George Sheldrick. Good ideas are always worth incorporating into one's own teaching materials! There will be an Education Summit immediately after the 2005 ACA meeting in Orlando.

The Young Scientists SIG organized a program of *Topics for Young Scientists*. These included interviewing skills (Joe Ferrara, Rigaku/MSR), the National Postdoctoral Association (Alyson Reed, NPA), academic careers (Frances Jurnak, Univ. California, Irvine), intellectual property and patents (Nabela McMillan, Marshall Gerstein and Borun LLP), and industrial careers (Jim Kaduk, BP Amoco).

The Transactions Symposium was *Crystals in Supramolecular Chemistry*. Sally Price (Univ. College London) showed that most methods for crystal structure prediction search for the structure that corresponds to the global minimum in lattice energy, and generate sets of energetically-favorable crystal structures. She discussed several example molecules, which display a range of distributions of known and hypothetical structures, and attempted a correlation to their crystallization behavior. Joel Bernstein (Ben Gurion, Univ. of Negev) gave an overview of historical and current attempts at polymorph prediction, and made suggestions for future work. Elna Pidcock (CCDC) proposed a new model that describes crystals in terms of packing patterns. The patterns are derived by considering the ways in which boxes of unequal dimensions can closely pack. Packing patterns characterized by low surface area and nearly-equal dimensions are preferred. Qi Gao (Bristol-Meyers Squibb) discussed attempts to find a suitable polymorph of a drug candidate. Ray Davis (Univ. of Texas) showed how useful video-assisted thermomicroscopy can be in understanding phase diagrams.

Scheduling conflicts caused me to miss a lot of the symposium on *Materials for the 21st Century*, but I did get to hear exciting talks by Omar Yaghi (Univ. of Michigan) on rational synthesis of porous frameworks using building blocks, the pair distribution function (PDF) approach by

Thomas Proffen (LANL), and the new upgraded General Purpose Powder Diffractometer (GPPD) by Jim Richardson (IPNS).

Among the several awards symposia was one honoring Dick Marsh (Trueblood Award). Dick himself gave the expected historical discussion of how some crystallographers come to be “Marshed” (for errors in a published crystal structure, mainly incorrect symmetry and/or unreasonable chemistry). Frank Herbstein (Technion) discussed some virtually forgotten ideas of Mnyukh and Ubbelohde, and their application to understanding first-order phase transitions. Hans-Beat Bürgi (Univ. Berne) measured the thermal evolution of anisotropic displacement parameters, and interpreted the dependence in terms of low-frequency normal modes. This procedure leads to better distance corrections for thermal motion, and improved interpretation of crystal structures. Joel Bernstein (Ben Gurion Univ. of the Negev) reviewed the use of graph sets in characterizing hydrogen bond patterns and their utilization in the design of co-crystals with at least two components. Larry Dahl (Univ. Wisconsin Madison) showed how CCD detectors were crucial to the single-crystal characterization of a series of giant polynuclear metal clusters.

As always, most of the science was presented in poster sessions. I particularly enjoyed posters on “Protein Model Validation in Structural Genomics” (Wolfram Tempel, Univ. of Georgia), “FiberNet: Developments in the Research Coordination Network for Biological Fiber Diffraction” (Tom Irving, IIT), “Crystal Structures of Two 4-OT Homologues from *Heliobacter pylori* and *Archaeoglobus fulgidus*” (Rakhi Dasgupta, Univ. of Texas), “Crystal Structure of $\text{Cd}_3(\text{O}_3\text{PC}_2\text{H}_4\text{CO}_2)(\text{H}_2\text{O})_2$: Influence of the Solid State NMR in the Structure Determination” (Abe Clearfield, Texas A&M), “Charge Density Studies of Urotropine-N-oxide-formic acid”, Cara Nygren (Univ. Tennessee), “Diffraction Studies of NaAlH_4 Doped with Ti” (Claudia Rawn, ORNL), “Low Temperature Investigation of Gas Molecules in a Porous Metal-Organic Framework” (Jesse Rowsell, Univ. of Michigan), and “High Energy Resonant Scattering Studies of the Pb/Bi Distribution in the Thermoelectric Material $\text{Pb}_5\text{Bi}_6\text{Se}_{14}$ ” (Yuegang Zhang, ANL). Even though the science at the ACA meeting is dominated by structural biology, there is more than enough to keep a “materials person” more than fully-occupied.

Third Japan-US Workshop on Combinatorial Material Science and Technology

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In recent years, combinatorial research has been developed into a major research discipline. It finds its way into almost every major material area, including ferroelectrics, hydrogen storage, superconductors, semiconductors, thermoelectrics, microwave materials, and optoelectronic materials, etc. New scientific journals are being created to capture important results of state-of-the-art combinatorial material research and technology developments. In order to follow the latest advancements of this important field, to provide a forum for discussion, and to identify the latest research/engineering issues, international conferences and workshops are of primary importance for all players in the field. To fulfill this purpose, the *Third Japan-US Workshop on Combinatorial Material Science and Technology* was planned and carried out with great success.

The workshop took place at the Loisir Hotel in Naha City on the historical island of Okinawa, Japan, from 7–10 December 2004. The Loisir Hotel provides a friendly and relaxed atmosphere, as well as an excellent meeting facility (including several international dining facilities). Naha is the capital and economic hub of Okinawa Island, which lies in the southern tip of the Japanese Ryukyu Islands. Okinawa, also known as the “Japanese Hawaii,” is a beautiful island setting for holding conferences. One can find stretches of gorgeous beaches, ample tropical trees and plants, and beautiful flowers everywhere in the island. This small island is full of unique history and has a marvelous cultural heritage. It was formerly an independent kingdom, known as the Kingdom of the Ryukyus, which existed for about 450 years, from the 13th century to the Meiji era. Many foreign influences are evident on the island as a result of commercial and

cultural interactions with China, Japan, Korea and other neighboring countries. Tourists can find various native arts and crafts throughout the island. Taking a stroll around Naha, one will witness the intermingling of rich history with modern life. For example, not too distant from modern buildings, shopping malls and monorail trains, tourists will be delighted to find an enchanting Fuchow Garden (Fukusyu-En) which features a beautiful pond, exotic koi (gold fish), attractive plants and buildings of ancient oriental style.

The 2004 workshop was the third of a series of Japan-US Combinatorial Materials Exploration and Technology (COMET) workshops. The first of the series took place in Maui, Hawaii in October 2000, followed by the second workshop in Winter Park, Colorado on December 2002. The 2004 workshop, which was very much of the “Gordon Conference Style,” was organized by members of COMET, and was supported by the National Institute for Materials Science (NIMS), Japan Society for the Promotion of Sciences (JSPS), Nanotechnology Researchers Network Center of Japan (Nanonet), and Combinatorial Sciences & Materials Informatics Collaboratory (COSMIC). NIMS has a close collaboration with the Materials Science and Engineering Laboratory (MSEL) of the National Institute of Standards and Technology (NIST). A number of officials and scientists from NIST were invited as participants and speakers at this workshop.

This successful scientific workshop was well planned—with a very rich scientific and social program. The general chairs of the workshop (H. Koinuma, X.D. Xiang, T. Chikyow, and M. Fasolka), the program chair (S. Inoue)

and the organizers from both Japan and the US sides performed an admirable job of organizing this workshop.

The program featured a total of 64 presentations which included plenary, invited, and contributed talks, and a poster session. There were two keynote speeches (Combinatorial Material Approaches to Energy and Environmental Problems by H. Koinuma of Tokyo Institute of Technology, and Polymer Research at the NIST Combinatorial Methods Center by M.J. Fasolka of NIST), one special lecture (Combinatorial Research at Dutch Polymer Institute by U. S. Schubert of Eindhoven University of Technology), 21 invited lectures, and 27 poster presentations. A total of approximately 80 attendees from Europe, Asia, and North America participated in this three-day workshop. Participants included managers and leading researchers from government, industrial and university laboratories.

The workshop highlighted various aspects of the combinatorial investigations, including applications to a wide spectrum of materials science and engineering research, and the need for informatics for organizing and retrieving vast amounts of data. Examples of materials categories covered included polymers, sensor materials, materials for energy applications (superconductors, thermoelectric materials, hydrogen storage materials, and fuel cell materials), ferroelectric materials, catalysts, biodegradable packaging materials, Si CMOS, new glasses, conducting and magnetic materials, and materials with low friction properties. Novel film characterization techniques applicable to the combinatorial approach included the electrostatic atomization system, thermal probe method, and x-ray microscopes. Diffraction and fluorescence methods once again have been demonstrated to be an indispensable technique in obtaining important structural, textural, and chemical information of the combinatorial films. Other talks were devoted to the improvement of the combinatorial technology. A number of talks discussed the importance of materials informatics. On the last day, before the conclusion of the meeting, a summary discussion session

about the future needs for combinatorial research was led by M. Kawasaki, I. Takeuchi, T. Chikyow and M. J. Fasolka.

An enjoyable social program was another unforgettable part of the meeting. This social program highlighted a welcoming reception on Tuesday evening, an afternoon tour on Wednesday, and a large-scale banquet on Wednesday evening. Japanese cuisine is well known for its flavor and artistic arrangement. The cuisine at the meeting was simply elegant, appealing, and delicious. The attendees all enjoyed the traditional Japanese banquet in which a large display of mouth-watering sushi was featured. On Wednesday afternoon, a tour was organized for the attendees to visit two of the main attractions of the island, namely, the Shuri Castle, and the Manza-mo. The Shuri Castle is a unique historical site that was the ancient palace of the King of the Ryukyus. Manza-mo is one of Okinawa's famous scenic spots. There one can admire the fabulous scenery of the emerald-blue ocean by standing on the uplifted coral reef cliff. At the conclusion of the meeting, some attendees had an opportunity to visit other interesting sites of Okinawa. Examples of sites with historical importance include the navy underground park that was the Okinawa district headquarters of Japanese Navy during the second world war, and the Peace Prayer and Memorial Museum which featured the famous battle during the war. The graphic images depicted in a special photo-gallery convey the heartrending consequence of wars. As part of the education program of the Japanese schools, many students have an opportunity to visit Okinawa to learn about the war and the importance of world peace.

The weather during the meeting was very cooperative—mostly sunshine and mild temperature, which added much enjoyment to the entire experience for the attendees. At the conclusion of this enjoyable and informative workshop, attendees all look forward to the next reunion (the Fourth Japan-US Workshop) that will take place in 2006 in Puerto Rico. Professor Smotkin of University of Puerto Rico has agreed to be the local organizer for this meeting.



Participants of The Third Japan-US Workshop on Combinatorial Material Science and Technology.

Calendar of Meetings

Donald R. Petersen
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14–18 March 2005

International Centre for Diffraction Data, Spring Meeting. Newtown Square, Pennsylvania, USA. [Contact: Linda Shertz, International Centre for Diffraction Data, 12 Campus Boulevard, Newtown Square, PA 19073-3273, USA. Tel: 1 (610) 325 9814; Fax: 1 (610) 325 9823; E-mail: shertz@icdd.com; Info: <http://www.icdd.com>].

28 March–1 April 2005

Materials Research Society Spring Meeting. San Francisco, California, 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>].

29 March–1 April 2005

Crystal 24. The 24th Biennial Conference of the Society of Crystallographers in Australia and New Zealand. Marysville, Australia. [Contact: E-mail: crystal24@csiro.au; Info: <http://xrsci.cmit.csiro.au/Crystal24>].

10–13 April 2005

107th Annual Meeting and Exposition of The American Ceramic Society. Baltimore, Maryland, USA. [Contact: The American Ceramic Society, 735 Ceramic Place, Westerville, OH 43081, USA. Tel: 1 (614) 794 5890; Fax: 1 (614) 794 5892; E-mail: info@ceramics.org; Info: <http://www.ceramics.org/meetings>].

12–14 April 2005

British Crystallographic Association Annual Spring Meeting. Loughborough, England, United Kingdom. [Contact: Info: <http://crystallography.org.uk>].

22–26 May 2005

3rd Meeting of the International Union of Microbeam Analysis Societies, held together with the **9th EMAS Workshop on Modern Developments and Applications in Microbeam Analysis,** Florence, Italy. [Contact: European Microbeam Analysis Society Secretariat, University of Antwerp, Department of Chemistry, Attn: Mr. Luc Van't dack, Universiteitsplein 1, BE-2610 Antwerp-Wilrijk, Belgium. Tel: 32 (3) 820 23 43; Fax: 32 (3) 820 23 43; E-mail: Luc.Vantdack@ua.ac.be; Info: <http://www.emas-web.net/Content/EMAS2005.htm>].

28 May–2 June 2005

American Crystallographic Association Annual Meeting. Orlando, Florida, USA. [Contact: Khalil Abboud at abboud@chem.ufl.edu; Ed Collins at edward_collins@med.unc.edu; Info: <http://www.hwi.buffalo.edu/ACA>].

27 June–1 July 2005

Joint 20th AIRAPT-43rd EHPRG International Conference on High Pressure Science and Technology. Karlsruhe, Germany. Associated with the **7th EMU School in Mineral Behaviour at Extreme Conditions** in Heidelberg, 19–28 June. [Contact: Prof. Dr. Eckhard Dinjus, Forschungszentrum Karlsruhe (ITC-CPV), PO Box 3640, D-76021 Karlsruhe, Germany. Tel: 49 (7247) 82 24 00; Fax: 49 (7247) 82 24 44; Info: <http://hikwww2.fzk.de/ehprg>].

1–5 August 2005

54th Annual Denver X-ray Conference. Colorado Springs, Colorado, USA. Workshops on XRD and XRF (August 1–2). Invited talks (August 3–5). [Contact: Denise Flaherty, International Centre for Diffraction Data, 12 Campus Boulevard, Newtown Square, PA 19073-3273, USA. Tel: 1 (610) 325 9814; Fax: 1 (610) 325 9823; E-mail: flaherty@icdd.com; Info: <http://www.dxcicdd.com>].

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 6240; Fax: 39 (055) 479 6342; E-mail: iucr@iucr2005.it; Info: <http://www.iucr2005.it>].

9–13 October 2005

32nd Annual Conference of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS). Quebec, Canada. [Contact: FACSS, 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://www.facss.org>].

28 November–2 December 2005

International Conference on Neutron Scattering. Sydney, Australia. [Contact: Brendan Kennedy, School of Chemistry, Building F11, University of Sydney, Sydney, NSW 2006, Australia. E-mail: b.kennedy@chem.usyd.edu.au; Info: <http://www.icns2005.org/>].

Summer 2006

23rd European Crystallographic Meeting. Leuven, Belgium.

16–23 July 2006

7th International Conference on the Occurrence, Properties, and Utilization of Natural Zeolites. Socorro, New

Mexico, USA. [Contact: Robert Bowman, New Mexico Institute of Technology, Socorro, New Mexico, USA. E-mail: bowman@nmt.edu].

Summer 2008

21st IUCr General Assembly and International Congress of Crystallography. Osaka, Japan.

Short Courses & Workshops

14–17 March 2005

ZEKAM Workshop 2005 Rietveld-Analytik. Bremen, Germany. Grundlagen und Anwendung. Ein Einführungskurs für Praktiker. Unterrichtssprache ist deutsche. [Contact: Dr. Michael Wendschuh, Zentrallabor für Kristallographie und Angewandte Materialwissenschaften im Fachbereich Geowissenschaften der Universität Bremen, Klagenfurter Strasse, 28359 Bremen, Germany; Tel: 49 (421) 218 39 68; Fax: 49 (421) 218 71 23; E-mail: zekam@uni-bremen.de; Info: <http://www.brass.uni-bremen.de/RW2005/RW2005>].

28–29 March 2005

Remote Access and Automation Workshop. Marysville, Australia. Part of **Crystal24**, which follows immediately at the same venue. Discussion centered on various large-scale data collection projects, typically involving synchrotron sources. [Contact: Info: http://xrsi.cmit.csiro.au/Crystal24/mmsn_ws05_programme.html].

2–6 May 2005

ICDD X-ray Clinic: Practical X-ray Fluorescence Spectrometry. Newtown Square, Pennsylvania, USA. Sponsored by the International Centre for Diffraction Data. A week-long session directed to both relative newcomers and to more experienced users wishing to broaden their understanding of fundamental concepts and established procedures. Held in the ICDD Headquarters building. The \$1600 fee includes textbooks, laboratory notebook, use of computers, and daily lunch. [Contact: Leah Mooney, Education Coordinator, International Centre for Diffraction Data, 12 Campus Boulevard, Newtown Square, PA 19073-3273, USA. Tel: 1 (610) 325 9814; Fax: 1 (610) 325 9823; E-mail: clinics@icdd.com; Info: <http://www.icdd.com/education/xrf.htm>].

22–26 May 2005

9th EMAS Workshop on Modern Developments and Applications in Microbeam Analysis, held together with the 3rd Meeting of the International Union of Microbeam Analysis Societies. Florence, Italy. [Contact: European Microbeam Analysis Society Secretariat, University of Antwerp, Department of Chemistry, attn Mr. Luc Van't dack, Universiteitsplein 1, BE 2610 Antwerp-Wilrijk, Belgium. Tel: 32 (3) 820 23 43; Fax: 32 (3) 820 23 43; E-mail: Luc.Vantdack@ua.ac.be; Info: <http://www.emas-web.net/Content/EMAS2005.htm>].

28 May 2005

Workshop on Structure Solution and Refinement of Difficult Structures using Powder Diffraction. Orlando, Florida, USA. Sponsored by the Powder Diffraction Special Interest Group of the American Crystallo-

graphic Association, and held immediately prior to the **ACA Annual Meeting**. Supported by the International Centre for Diffraction Data and the Canadian Institute of Neutron Scattering. [Contact: Nattamai Bhuvanesh at nbhuv@mail.chem.tamu.edu; Info: <http://www.chem.tamu.edu/xray/acawork/acaworkshop.html>].

5–10 June 2005

IWPCPS-7 Seventh International Workshop on Physical Characterization of Pharmaceutical Solids. Kona, Hawaii, USA. [Contact: Adair Garis, Assa International, 3B East Lake Road, Danbury, CT 06811, USA. Tel: 1 (203) 312 0682; Fax: 1 (203) 312 0722; E-mail: assa.info@assainternational.com; Info: http://www.assainternational.com/workshops/iwpcps_7/iwpcps_7.cfm].

6–10 June 2005

ICDD X-ray Clinic: I. Fundamentals of X-ray Powder Diffraction. Newtown Square, Pennsylvania, USA. Sponsored by the International Centre for Diffraction Data. A week-long session directed to both relative newcomers and to more experienced users wishing to broaden their understanding of fundamental concepts and established procedures. Held in the ICDD Headquarters building. The \$1600 fee includes textbooks, laboratory notebook, use of computers, and daily lunch. [Contact: Leah Mooney, Education Coordinator, International Centre for Diffraction Data, 12 Campus Boulevard, Newtown Square, PA 19073-3273, USA. Tel: 1 (610) 325 9814; Fax: 1 (610) 325 9823; E-mail: clinics@icdd.com; Info: <http://www.icdd.com/education/xrd.htm>].

13–17 June 2005

ICDD X-ray Clinic: II. Advanced Methods in X-ray Powder Diffraction. Newtown Square, Pennsylvania, USA. Sponsored by the International Centre for Diffraction Data. A week-long session designed for the experienced user and focusing on computer-based methods of qualitative and quantitative phase analysis. Held in the ICDD Headquarters building. The \$1600 fee includes textbook, laboratory notebook, use of computers, and daily lunch. [Contact: Leah Mooney, Education Coordinator, International Centre for Diffraction Data, 12 Campus Boulevard, Newtown Square, PA 19073-3273, USA. Tel: 1 (610) 325 9814; Fax: 1 (610) 325 9823; E-mail: clinics@icdd.com; Info: <http://www.icdd.com/education/xrd.htm>].

19–28 June 2005

7th European Mineralogical Union School: Mineral Behaviour at Extreme Conditions. Heidelberg, Germany. A

satellite event of the **International Conference on High Pressure Science and Technology** in Karlsruhe, June 27–July 1. The language of the school is English. [Contact: Info: http://www.univie.ac.at/Mineralogie/EMU/emusch_7.htm].

20–24 June 2005

International School on Mathematical and Theoretical Crystallography. Nancy, France. Held at the Université Henri Poincaré Nancy 1. The language of the school is English. [Contact: Info: <http://www.lcm3b.uhp-nancy.fr/mathcryst/nancy2005.htm>].

1–2 August 2005

Workshops at the 54th Annual Denver X-ray Conference. Colorado Springs, Colorado, USA. **X-ray Microtomography** (S. Stock); **X-ray Optics** (G. J. Havrilla); **Rietveld Applications** (A. Kern, J. Faber); **Stress Analysis** (I. C. Noyan); **Line Profile Analysis by Whole Powder Pattern Fitting** (D. Balzer); **Two-dimensional X-ray Diffraction** (T. Blanton, B. He); **XRF Specimen Preparation** (J. Anzelmo, D. Broton); **Energy Dispersive XRF** (M. A. Zaitz); **Quantitative XRF** (M. Mantler); **Basic XRF** (L. Creasy); **Monte Carlo Techniques in X-ray Fluorescence** (R. Gardner). [Contact: Denise Flaherty, International Centre for Diffraction Data, 12 Campus Boulevard, Newtown Square, PA 19073-3273, USA. Tel: 1 (610) 325 9814; Fax: 1 (610) 325 9823; E-mail: flaherty@icdd.com; Info: <http://www.dxcicdd.com>].

18–23 August 2005

Crystallographic Computing School. Siena, Italy. Held just prior to the **20th IUCr Congress** in Florence. [Contact: Con-

gress Secretariat, XX Congress IUCr, Dipartimento di Energetica, Università di Firenze, via S. Marta 3, 50139 Firenze, Italy. Tel: 39 (055) 479 6240; Fax: 39 (055) 479 6342; E-mail: iucr@iucr2005.it; Info: <http://www.iucr.ac.uk/iucr-top/comm/ccom/siena2005>].

23 August 2005

Workshops held in conjunction with the **20th IUCr Congress.** Florence, Italy. Including **Introduction to Small-Angle Scattering** (Jan Skov Pedersen); **Structural Analysis of Aperiodic Crystals** (Sander van Smaalen, Ray L. Withers); **Small Molecule Crystallization** (Roland Boese, Chick Wilson). [Contact: E-mail: Paola Gilli at paola.gilli@unife.it; Martin U. Schmidt at m.schmidt@chemie.uni-frankfurt.de].

2–8 September 2005

New Frontiers in Electron Crystallography. Brussels, Belgium. Held just after the **20th IUCr Congress** in Florence. Organized by Stavros Nicolopoulos. [Contact: Congress Secretariat, XX Congress IUCr, Dipartimento di Energetica, Università di Firenze, via S. Marta 3, 50139 Firenze, Italy. Tel: 39 (055) 479 6240; Fax: 39 (055) 479 6342; E-mail: iucr@iucr2005.it; Info: <http://www.elcryst2005.de>].

7–17 June 2007

Engineering of Crystalline Materials Properties: State-of-the-Art in Modeling, Design, and Applications. Erice, Italy. The 39th Crystallographic Course at the Ettore Majorana Centre. The course directors are D. Braga (Bologna) and J. Novoa (Barcelona). [Info: <http://www.crystalerice.org/2007.htm>].