

## Howard F. McMurdie (1905–2004)—An Appreciation

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Howard F. McMurdie (1905–2004)

Howard F. McMurdie—known as Mac to his friends and colleagues—was an exemplar of good living. Blessed with excellent health, a loving family, and many close colleagues, Mac was active and productive to the very end. It is therefore with the deepest regret that we report the death of Howard F. McMurdie at age 99 of pneumonia only a few months before an anticipated 100 year birthday celebration (although according to several oriental calendars he was indeed 100). Mac's death marks the end of an era—his life spanned almost the entire 20th century and, seen in reverse, it would go back almost to the time of George Washington. His fruitful scientific career of 75 years began in 1928 and spans 3/4 of the history of NIST/NBS (National Institute of Standards and Technology/National Bureau of Standards) and the entire history of the JCPDS (Joint Committee on Powder Diffraction Standards/International Centre for Diffraction Data). This time period included the entire history to date of two important widely used scientific databases in which he played a critical role—the *Powder Diffraction File* and the

*Phase Diagrams for Ceramists*. Although Mac officially retired from NBS in 1966, he continued to work as a consultant in crystallography until 2003. During his “real retirement” party at NIST in April 2003, he was awarded a special certificate of appreciation “for his significant contributions to the Materials Science and Engineering Laboratory of NIST during the past 75 years.” The certificate noted that McMurdie’s “research interests encompassed areas such as measurements of phase equilibria and reference powder X-ray patterns, characterization of solid-state materials, compilation and evaluation of data for Phase Equilibria Diagrams, and for the Powder Diffraction File.” During the final two years of his life, he continued to interact scientifically and socially with his colleagues at NIST and served as an invaluable consultant on a variety of topics.

Howard McMurdie was born on February 5, 1905 in Kalamazoo, Michigan, and graduated from Northwestern University in Evanston, Illinois. He went to work for what was then called the National Bureau of Standards on April 2,

1928. In the early 1930's he was sent to Riverside, California to test the cement that was to be used in the construction of Boulder (now Hoover) Dam. After returning to NBS, he was assigned to the Petrographic Laboratory. His study of Portland cement was the start of what evolved into a lifetime interest in phase diagrams. In those early days, McMurdie also pursued the use of X-ray powder diffraction for phase analysis of solids. These activities paved the way for him to become Chief of the Crystallographic Section. Mac was a beloved chief. He had confidence in his people, encouraged them to pursue their independent research goals, and supported their work. In the role of Section Chief and as a researcher, McMurdie has contributed significantly to many areas of research throughout his 75 years at NIST/NBS. McMurdie considered three areas as especially important, and he has been closely related to two of them for the 38 years following his formal "retirement" in 1966.

His first area of interest centered on the production of powder diffraction patterns and NBS's productive association with the ICDD. In the late 1930's, Mac was one of the founding fathers of the Joint Committee on Powder Diffraction Standards. In 1953, he established an ICDD Research Associateship in the Crystallographic Section. For more than 30 years, this Associateship, under his guidance and leadership, prepared a broad set of important, accurate, and widely used experimental powder diffraction patterns. After his retirement, Mac joined the Associateship and served as an editor for the Powder Diffraction File (PDF). In 1984, he became a Distinguished Scientist of the ICDD. In the 1980's he served as a special consultant to the ICDD Board of Directors. His work with the PDF spanned over 60 years and remarkably he was still deeply interested in the PDF to within a week of his death. In fact, at age 99, he was expressing a strong interest in editing powder patterns again so as to remain mentally sharp. From the very beginning, he loved to attend their periodic meetings in Swarthmore, Newtown Square, and Colorado. Amazingly, his attendance and participation in such meetings continued to age 97. He liked these meetings not only for the scientific discussions, but also to especially socialize with his many friends. In addition to his numerous scientific achievements, he also bestowed funds for a hi-tech video-conference room in the ICDD headquarters. In the late 1990's, ICDD set up a biannual award—the McMurdie Award to honor his tremendous contribution to the organization and to the PDF. This award recognizes distinguished work that improves the Powder Diffraction File in its function of identifying and characterizing inorganic solids.

His second area of interest focused on refractory oxides. It was through research in this area that he established a relationship with the American Ceramic Society (ACerS) and started the publication of the series, *Phase Diagrams for Ceramists*. After his retirement, Mac continued to be an editor for the phase diagrams until age 98. The evolution and ap-

plication of the *Powder Diffraction File* and *Phase Diagrams for Ceramists* are synergistically entwined. Over the years, the two files have served as indispensable research tools for the academic and industrial communities. In materials science, they have long been used in the development of new materials. Today, materials design is becoming ever more sophisticated especially with the rapid evolution of powerful computer oriented methods in which these databases are indispensable.

The third area, in which he had a keen interest, was initiated in the Crystallography Section and involves the study of materials at high pressure. His vision together with the ingenious work of a group of world-class scientists at NIST/NBS led to the development of the diamond anvil cell (DAC), of the high pressure single-crystal diffraction technique utilizing the DAC, and of an optical ruby fluorescence method to measure very high pressure in the DAC. This work earned NBS/NIST a stellar and international reputation in the field of high-pressure science and technology. Several key papers resulting from this long-term research effort are now widely regarded as key milestones in the evolution of high-pressure science.

Over the years Mac has served as a paradigm of how to live with his emphasis on balance, diversity, and moderation in all things. He began each day with enthusiasm and ended it with a check of the stock market, a search on the Internet, and finally a glass of brandy or bourbon usually with his wife, Mary, before she passed away in 1996. Not only was he a dedicated and hard-working scientist, he was also a thoughtful and generous person who was well-liked. His never-too-old-to-learn attitude has set an excellent example for the younger generations to follow. To balance his scientific work, he developed a broad spectrum of interests including cooking, reading, travel, photography, computing, opera and Gothic architecture. He enjoyed international travels with Mary, with whom he was married for 62 years. Later he took long summer excursions each year with his son, Arthur. He loved attending concerts and the opera at the Kennedy Center with family and friends. He was an active sports fan and referred to the Redskins as "we" especially during the season and after the games. A longtime fan of the old Washington Senators, he was delighted that baseball was returning to Washington. He was a gourmet cook and prepared dinner at his home every Wednesday evening for his extended family (3 children, 6 grandchildren and 5 great grandchildren). Often, he would invite friends to his home for wine and cheese or even a meal and conclude the evening with a glass of fine wine or Rebel Yell, his favorite bourbon-style whiskey. He derived great pleasure from the social interaction with us in our periodic luncheons sometimes held in one of his favorite local restaurants. Clearly Mac will be missed enormously, but he will not be forgotten. He will live on in his work and in our collective fond memories!

# The 53rd Annual Denver X-ray Conference (DXC)

Denise Flaherty, ICDD

The 53rd Annual Denver X-ray Conference (DXC) was held in Steamboat Springs, Colorado at the Sheraton Steamboat Resort. The conference ran from 2–6 August 2004, attracting nearly 300 registered attendees and over 200 exhibit personnel.

Conference week began with 16 tutorial workshops, held on Monday and Tuesday. Topics included: How to do Synchrotron Experiments; Rietveld Applications; Specimen Preparation XRF; Thin Film XRF Analysis; X-ray Physics; Optics; Microbeam X-ray Stress Analysis; Total Pattern Analysis; Quantitative XRF; Fundamentals of XRF; Principles & Use of Micro XRD & XRF; Specimen Preparation XRD; and Small Angle Scattering.

Sixteen special sessions filled the remaining two and a half days of the conference. Topics included: New Developments in XRD & XRF Instrumentation; Thin Films; Small Angle Scattering; Quantitative XRF; Detectors & Sources; Synchrotron Applications; Stress Analysis; Problem Solving/Industrial Applications of XRF; X-ray Optics; Industrial Applications of XRD; Trace Analysis; Microbeam Analysis; Parallel Beam Diffraction; Rietveld Applications; and Polymers.

The Plenary Session, “Red Hot X-rays”, was organized by Charles Prewitt, University of Arizona, Tucson, AZ and Robert Snyder, Georgia Institute of Technology, Atlanta, GA. Four invited talks were presented during the Plenary: “GETTING THE HOT STRUCTURES”, K.F. Kelton, Department of Physics, Washington University, St. Louis, MO; “THE STRUCTURE OF LIQUID AL ALLOYS AT HIGH SUPERHEATS USING HIGH ENERGY X-RAYS”, M.J. Kramer, Ames Laboratory, Iowa State University, Ames, IA; “DIFFRACTION STUDIES OF ORDER-DISORDER AT HIGH PRESSURES AND TEMPERATURES: TRANSITIONS IN DOLOMITE AND ANHYDRITE”, J.B. Parise, Geosciences, State University of NY, Stony Brook, NY; “LAUE MICRODIFFRACTION FOR STRUCTURE ANALYSIS AT ULTRA HIGH PRESSURE (LAMSA UHP)—AN OLD SOLUTION TO A NEW PROBLEM”, P. Dera, Carnegie Institution of Washington, Geophysical Lab, Washington, DC.

An awards presentation also took place during the Plenary Session to honor a variety of important contributions to the field of materials analysis. The 2004 Birks Award was presented to Tomoya Arai, Rigaku Industrial Corporation, Osaka, Japan, presented by Michael Mantler, Vienna University of Technology, Vienna, Austria. The 2004 McMurdie Award was presented to Winnie Wong-Ng, National Institute of Standards & Technology, Gaithersburg, MD, presented by Camden R. Hubbard, Oak Ridge National Laboratory, Oak Ridge, TN. The 2004 Hanawalt Award was presented to Robert L. Snyder, Georgia Institute of Technology, Atlanta, GA, presented by James A. Kaduk, BP Chemicals, Naperville, IL. Dr. Snyder also gave a brief lecture after receiving the Hanawalt Award, “THE EVOLUTION OF TOTAL PATTERN ANALYSIS”.

Poster sessions were held on Monday, Tuesday, and Wednesday evening of conference week. Judges were ap-



Tomoya Arai, Rigaku Industrial Corporation, Osaka, Japan, addresses the audience after receiving the 2004 Birks Award.

pointed each night to select the best posters. The following posters were selected: “ON THE FORMATION OF BROWNMILLERITE AND THE CHOICE OF STRUCTURE ON THE ACCURACY OF THE RIETVELD METHOD”, S.Y. Nelson, C. Mattern, R.S. Winburn, Minot State University, Minot, ND; “PHASE EQUILIBRIA DETERMINATION OF  $\text{NH}_4\text{NO}_3$ - $\text{KNO}_3$  MIXTURES BY USING X-RAY DIFFRACTION METHOD”, W.-M. Chien, D. Chandra, J. Smith, University of Nevada, Reno, Nevada, C.J. Rawn, Oak Ridge National Laboratory, Oak Ridge, TN, A.K. Helmy, Special Devices, Inc., Moorpark, CA; “INVESTIGATION OF THE MICRO STRUCTURE OF ENERGETIC CRYSTALS BY MEANS OF X-RAY POWDER DIFFRACTION”, M. Herrmann, Fraunhofer Institut für Chemische Technologie, Pfünz, Germany; “THE COMPARISON OF QUANTITATIVE XRD, OPTICAL MICROSCOPY AND CATHODOLUMINESCENCE TECHNIQUE ON ORDINARY PORTLAND CEMENT CLINKERS”, N. Winkler, H. Pöllmann, University of Halle, Germany, J. Göske, Center for Materials Analysis, Lauf a. d. Pegnitz, Germany; “EVALUATION OF LOCAL SHORT-RANGE ORDER AROUND Fe ATOMS IN FePt FILMS BY X-RAY FLUORESCENCE HOLOGRAPHY”, Y. Takahashi, K. Hayashi, E. Matsubara, T. Shima, K. Takanashi, Tohoku University, Sendai, Japan; “ELEMENTAL MAPPING OF HUMAN BRAIN BY SR- $\mu$  XRF”, N. Zoeger, C. Strelt, P. Wobrauschek, C. Jokubonis, Atomintstitut, Vienna University of Technology, Vienna, Austria, G. Pepponi, ITC-irst, Trento, Italy, P. Roschger, Ludwig Boltzmann-Institut für Osteologie, Vienna, Austria, S. Bohic,

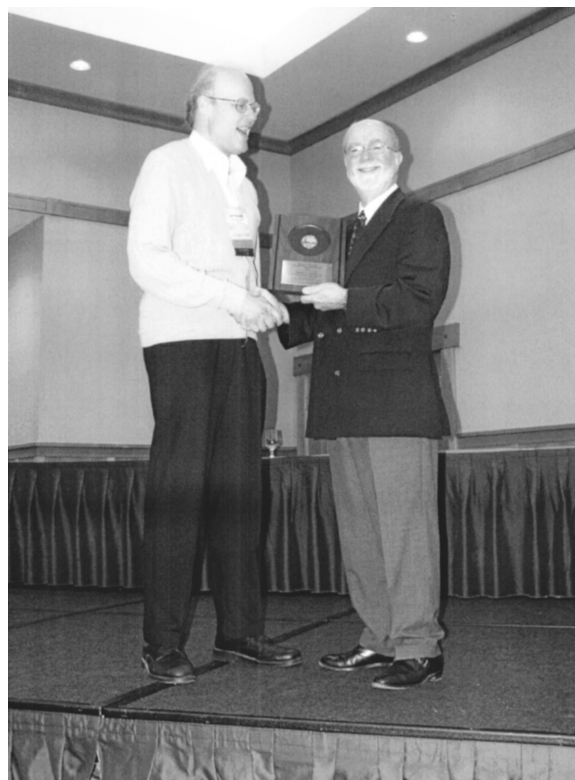




Winnie Wong-Ng, National Institute of Standards & Technology, Gaithersburg, MD receives the 2004 McMurdie Award, presented by Camden R. Hubbard, Oak Ridge National Laboratory, Oak Ridge, TN.

ESRF, Grenoble, France, W. Osterode, Universitätsklinik für Innere Medizin IV, Vienna, Austria; "CHEMICAL-PHYSICAL CHARACTERISATION OF POLLEN WITH TXRF AND TOF-SIMS", G. Peponi, P. Lazzeri, ITC-irst, Trento, Italy, E. Gottardini, F. Cristofolini, F. Corradini, IASMA, Trento, Italy, G. Clauser, APPA, Trento, Italy, A. Torboli, Ital Structures, Riva del Garda, Italy.

Exhibits at the conference ran from Monday to Thursday where 41 companies displayed their various products and services for X-ray powder diffraction and X-ray fluorescence spectrometry. The following companies participated at the exhibits: AMPTEK, Inc.; ATPS, Inc.; Australian X-ray Tubes Pty Limited; Blake Industries, Inc.; Bruker AXS, Inc.; Brushwellman Electrofusion Products; Chemplex Industries, Inc.; Corporation Scientifique Claisse, Inc.; EDAX, Inc.; Engelhard Corporation; GBC Scientific Equipment Pty Ltd.; Gresham Scientific Instruments; Handley Analytical Services; Hecus X-ray Systems GmbH; Inel, Inc.; Initiative Scientific Products; International Centre for Diffraction Data; Kitco, Inc.; Kratos Analytical; Laval Lab, Inc.; LND, Inc.;



Robert L. Snyder (right), Georgia Institute of Technology, Atlanta, GA, receives the 2004 Hanawalt Award, presented by James A. Kaduk (left), BP Chemicals, Naperville, IL.

Materials Data, Inc.; MOXTEK, Inc.; Omega Data Systems BV; Osmic, Inc.; Oxford Instruments; PANalytical; Premier Lab Supply; Rigaku/MSC, Inc.; Rocklabs Ltd.; Sietronics Pty Limited; Sigma Chemicals; Spectro Analytical Instruments; Spectrum Plus; SPEX CertiPrep, Inc.; Thales Components Corporation; Thermo Electron; Wiley; Xenocs SA; X-ray Instrumentation Associates; and X-ray Optical Systems, Inc.

A special thank you to the vendors who sponsored evening receptions: Australian X-ray Tubes Pty Limited; Blake Industries, Inc.; Bruker AXS, Inc.; Corporation Scientifique Claisse, Inc.; Englehard Corporation; Handley Analytical Services; Kitco, Inc.; Kratos Analytical; Laval Lab, Inc.; Materials Data, Inc.; MOXTEK, Inc.; Osmic, Inc.; PANalytical; Rigaku/MSC, Inc.; Rocklabs Ltd.; Spectrum Plus; SPEX CertiPrep, Inc.; Thales Electron Devices; Thermo Electron; and Wiley.

For a preview of the 2005 Program, please visit our web site at [www.dxcicdd.com](http://www.dxcicdd.com).



# Review of Molecular Modeling of Clays and Mineral Surfaces

(CMS workshop lectures, Volume 12), edited by J.D. Kubicki and W.F. Bleam  
(The Clays Minerals Society, Aurora, CO) 2003.

by Eric Cockayne

Ceramics Division, NIST, Gaithersburg, MD 20899

Many issues in environmental science require understanding the interaction between soils, water, and sediments. For example, the containment of radioactive or chemical wastes is related to the ability of the constituent soil materials to chemically bind these materials. As available computational power has grown in recent years, molecular modeling has become an important tool in the field. This book gives an overview of state-of-the-art methods and results in using molecular modeling to investigate the interaction of clay and mineral surfaces with water and with water containing solvents.

Chapter 1 gives an overview of molecular modeling methods. Different methods are preferred for different length scales. For systems containing tens of atoms, fully quantum mechanical solution of the electronic structure problem is preferred. For larger systems (generally including systems large enough to model the interaction of water and solutes with surfaces), empirical "force field" methods are preferred. The advantages and disadvantages of each method are discussed, as well as how hardware considerations affect the size of the system that can be practically simulated. The description of various packages available for molecular simulations will be useful to those wishing to incorporate molecular modeling into their research.

The subsequent chapters are devoted to the use of molecular modeling to investigate specific problems involving mineral surfaces and sorption. Chapter 2 discusses electronic structure methods for treating the interfaces between mineral surfaces and water. In chapters 3 and 4, force-field models

are used to study the interaction of water and aqueous ions with clay surfaces. Chapter 5 presents a more abstract model, designed for the larger-length scale problem of how metal ions bind with chemically heterogeneous soil materials. These chapters discuss the power of molecular modeling to predict structure, thermodynamics, preferred binding sites, the dynamics of ion diffusion and binding, and the effects of pH on sorption.

Several common themes run through this volume. The importance of first understanding existing experimental results before making predictions is emphasized. Furthermore, modeling should not be done independently of, or thought of as a replacement for experiments, but, in fact, even more experiments are necessary, not only to confirm the modeling predictions, but also to provide necessary inputs for better models. Technical difficulties involved in modeling surfaces realistically are discussed. Finally, it is pointed out that it is still computationally expensive to get good agreement with experiments in many cases.

The faults of this book are some minor errors, oversimplification in the discussion of statistical mechanics and electronic structure methods in places, and the use of jargon and symbols that are not familiar except to specialists. Still, it provides a good overview for those who may wish to become more familiar with modeling the interactions of aqueous solutions with mineral surfaces, and leaves one with the hope that a combination of experimental and modeling methods will provide new solutions to related environmental and industrial problems.

## Calendar of Meetings

Donald R. Petersen  
Greenleaf Associates  
6210 Siebert Street  
Midland, MI 48640-2724, USA  
drpetersen@tm.net

### 6–7 December 2004

**Micro- and Mesoporous Mineral Phases.** Rome, Italy. Organized by the IUCr Commission on Inorganic and Mineral Structures and the Accademia Nazionale dei Lincei. To include mineralogical, crystallographic, and technological aspects of these materials. [Contact: Info: <http://lcm3b.uhp-nancy.fr/cims/micromesoporous.htm>].

### 13–17 February 2005

**Neutron Diffraction Characterization of Mechanical Behavior.** San Francisco, California, USA. A symposium to be

held during the **134th TMS Annual Meeting & Exhibition.**

[Contact: TMS Meeting Services, 184 Thorn Hill Road, Warrendale, PA 15086, USA. Tel: 1 (764) 776 9000 ext 243; Fax: 1 (764) 776 3700; E-mail: [mtgserv@tms.org](mailto:mtgserv@tms.org); Info: <http://www.tms.org/Meetings/Annual-05/AnnMtg05Home.html>].

### 14–18 February 2005

**Australian X-ray Analytical Association 2005 Conference and Exhibition.** Perth, Western Australia, Australia. [Contact: Dr. Brian O'Connor, Curtin University, GPO Box U1987, Perth, WA 6001, Australia, [toconnorb@](mailto:toconnorb@)

cc.cutin.edu.au or Tulips Meeting Management, Post Office Box 116, Salamander Bay, NSW 2317, Australia. Tel: 61 (2) 4984 2554; Fax: 61 (2) 4984 2755; E-mail: axaa@pco.com.au; Info: <http://www.pco.com.au/axaa2005>].

#### 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>].

#### 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.

#### 28 May–2 June 2005

**American Crystallographic Association Annual Meeting.** Orlando, Florida, USA. [Contact: Khalil Abboud at [abboud@chem.ufl.edu](mailto:abboud@chem.ufl.edu); Ed Collins at [edward\\_collins@med.unc.edu](mailto: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. [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.sct.gu.edu.au/icns2005>].

#### 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

#### 1–4 December 2004

**Fifth International School of Crystallography and Diffraction.** Havana, Cuba. [Contact: Dr. Ernesto Estevez Rams, Instituto de Materiales y Reactivos, Universidad de La Habana, Zapata y G., CP: 10400, Ciudad de La Habana, Cuba. Tel: 53 (7) 870 7666; Fax: 53 (7) 879 4651; Info: [http://www.cristalografia.net/home\\_en.htm](http://www.cristalografia.net/home_en.htm)].

#### 21–24 February 2005

**PPXRD-4 Pharmaceutical Powder X-ray Diffraction Symposium.** Barcelona, Spain. [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: ppxrd@icdd.com; Info: <http://www.icdd.com/ppxrd>].

**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 \$1,740 fee includes textbooks, 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](mailto:clinics@icdd.com); Info: <http://www.icdd.com/education/xrf.htm>].

**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](mailto:assa.info@assainternational.com); Info: <http://www.assainternational.com>].

**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 \$1,740 or \$3,150 for both XRD I & XRD II 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](mailto: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 \$1,740 or \$3,150 for both XRD I & XRD II 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](mailto: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](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>].

**18–23 August 2005**

**IUCr School of Crystallographic Computing.** Siena, Italy. Held just prior to the **20th IUCr Congress** in Florence. [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](mailto:iucr@iucr2005.it); Info: <http://www.iucr.ac.uk/iucr-top/comm/ccom/siena2005>].

**2–8 September 2005**

**New Frontiers in Electron Crystallography.** Brussels, Belgium. A summer school organized by Stavros Nicolopoulos. [Contact: E-mail: [bright\\_electron@yahoo.es](mailto:bright_electron@yahoo.es); 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.crystallerice.org/2007htm>].