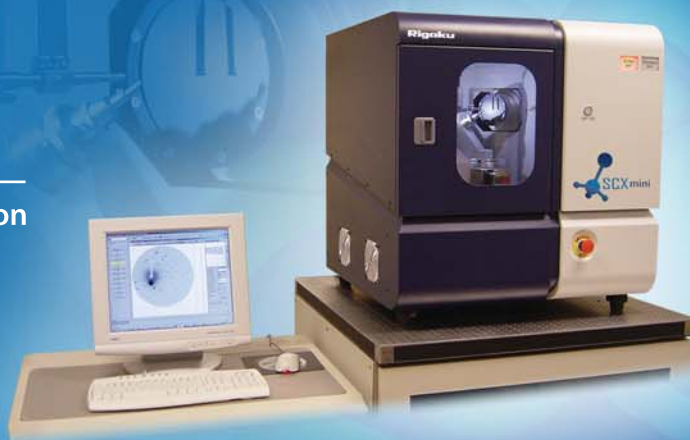


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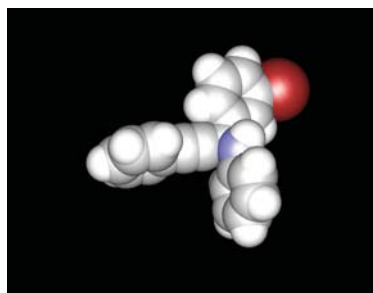
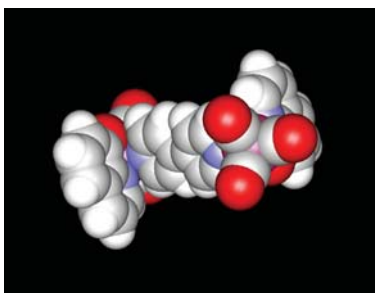
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Table of Contents

2-3	President's Column
3	2007 ACA Awards - Trueblood to Gavezotti - Fankuchen to Herbstein
4	Awards to ACA Members
6	ACA Balance Sheet
6-12	News from Canada
12-13	USNCCr Education Summit
13	Crystallography Web Watch / Robinson Burbank (1921-2006)
14	Update on Bridging the Sciences Activities
14-16	AIP Update
16-18	News from the Evolution/Creationism Front
18	Online Dictionary of Crystallography / Beamline Time for Sale
18	What's on the Cover
19-20	Elizabeth Armstrong Wood (1912-2006)
20	Rueben Rudman (1937-2006)
22	Reminder: Crystallography in Art contest
22	Index of Advertisers
23	ACA Corporate Members
26	New RCSB PDB Website / BioSync
28-36	Candidates for ACA Offices in 2007
38	2005 ACA Macromolecular Summer School
40	SAD Workshop / IUCr Travel Funds Available
42-44	SER-CAT Symposium
45-46	36th Mid-Atlantic Macromolecular Symposium
47	ACA 2006 - Travel Grantees - Sponsors - Exhibitors
48	Contributors to this Issue
48	Calendar of Meetings



Contributions to *ACA RefleXions* may be sent to either of the Editors:

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President's Column: *Neutron Diffraction Comes of Age*

On April 28, 2006 the first neutrons were produced at the new Spallation Neutron Source (SNS) in Oak Ridge, Tennessee, which inaugurates the operation of the next generation neutron sources, the SNS and J-PARC in Japan. This is just a few months short of the 25th anniversary of the start-up of the pioneering Intense Pulsed Neutron Source (IPNS) at Argonne, Illinois.

Neutron diffraction is not a new technique... it has been around for over half a century, but among the single-crystal community it has languished far behind x-ray diffraction as far as its utility and the size of its user community are concerned. The reason for this state of affairs is not difficult to understand: having a neutron source with an intensity high enough to carry out diffraction experiments requires either access to a nuclear reactor or, more recently, a spallation neutron source, coupled with the nontrivial requirement of large samples (typically a hundred times the volume of crystals used in x-ray diffraction). Thus single-crystal neutron diffraction will probably never catch up to x-ray diffraction as a routine technique for investigations in structural chemistry or biology, but the gap is rapidly becoming narrower, and will change even more dramatically in the future, as

powerful new high-intensity spallation neutron sources become operational. That will be the theme of the one-day *Transactions Symposium*, scheduled for the ACA Annual Meeting in Hawaii, organized by Tom Koetzle, Paul Langan, and Alberto Podjarny.

This unique symposium, jointly sponsored by the Neutron, Small Molecule and Macromolecular SIG's, will be divided into two parts. The morning session will focus on the basics: a survey of current facilities; types of small-molecule problems that can be handled; and future developments. The afternoon session will be devoted to applications in macromolecular crystallography: challenging problems that can be solved today with existing facilities; future developments involving smaller crystals; larger proteins; complete deuteration; and shorter data collection times that will be possible with the more powerful neutron sources that will soon become available. Immediately following the afternoon session, an informal meeting will be held in which interested parties can get more information about the user program at the SNS.

Neutron macromolecular crystallography has expanded tremendously in the past five or six years: over a dozen small-to-medium sized proteins have been studied up to resolutions as high as 1.5 Å, and even single crystals of several oligonucleotides (hexameric and decameric DNA duplexes) have been successfully analyzed. In fact, a new data base, the HHDB (Hydrogen-and-Hydration Data Base; hhdb01.tokai-sc.jaea.go.jp/HHDB) is now available that lists the H positions in macromolecules derived thus far from neutron crystallography. Currently there are three facilities in the world capable of studying the neutron structures of macromolecules: the BIX-3 and BIX-4 diffractometers in Ibaraki, Japan; the LADI diffractometer in Grenoble, France; and the PCS (Protein Crystallographic Station) in Los Alamos, New Mexico. *Each of these three instruments, and the results generated from them, will be featured prominently in the Hawaii Transactions Symposium.* Future instruments will largely be based on new, high-intensity Spallation Neutron Sources: the MaNDi diffractometer planned for the SNS in Oak Ridge, Tennessee (details of which were featured on page 30 of the Spring, 2006 *ACA RefleXions*), and the BIX-P1 instrument to be built for the J-PARC Spallation Source in Japan. Also planned is an instrument designed for molecules with large unit cells (called LMX), to be built at ISIS in Didcot, England.

For small molecules, instrumentation has been available for quite some time, and some of the more commonly-used diffractometers today are the SCD instrument at Argonne in Illinois, the SXD diffractometer at ISIS in England, and numerous instruments at ILL in Grenoble, France, including a new, highly successful diffractometer, VIVALDI, that has enabled crystal sizes (and data collection times) to be cut by a factor of ten over older instruments. New and/or upgraded reactors are also coming on line in Munich, Germany and at Lucas Heights, Australia. Space limitations of this column prevent me from giving a complete list of currently-used instruments for small-molecule crystallography. Important applications of neutron diffraction in this area have included (a) the determination of light-atom positions such as those of H atoms, (b) isotopic studies such as the distinguishing of H from D, and (c) studies of magnetic structures. Needless to say, the small-molecule community has been quick to recognize the potential of the new, high-intensity neutron sources referred to earlier, and I have been personally involved in the development of an instrument (called "TOPAZ") at the SNS in Oak Ridge that hopefully will allow investigators to carry out a neutron study on what might be called "x-ray sized" crystals, with volumes as low as 0.1 mm³ and unit cell lattice constants ranging up to 50 Å. *Incidentally, the site of the 2008 ACA Meeting was selected as Knoxville, Tennessee, partly to allow attendees to tour this brand-new 1.4-billion-dollar SNS facility.*

Returning the discussion to macromolecular neutron crystallography, the challenges there are similar: how does one reduce crystal size and data collection time to the point where the technique becomes reasonably accessible to an investigator having "average-sized" crystals who wishes to know the positions of critical H atoms near, say, the active site of an enzyme? We have already touched upon the most important requirement of increasing beam intensity, and have pointed out that two of these new, high-intensity spallation sources, SNS in Tennessee and J-PARC in Japan, are currently beginning operation or are under construction. But that's not enough. Further advances can be made by fully deutrating the sample crystal (because D produces a lower

background in neutron scattering than H). Thus, deuteration labs have been set up in order to express and produce proteins under completely deuterated conditions. Several such labs are already fully functional: at the EMBL in Grenoble, France; at LANSCE in Los Alamos; and at ORNL in Tennessee. Another is being planned at J-PARC in Japan. Cryo-crystallography also helps. Large crystals are notoriously prone to crack on cooling (much more easily than conventional "x-ray sized" crystals), but techniques have been developed to overcome that, as will also be discussed at the *Transactions* Symposium.

In this column I have deliberately focused on the single-crystal aspects of neutron diffraction, and I have not had the chance to discuss the many other facets of this technique, such as the study of magnetic properties, powder neutron scattering, inelastic neutron scattering, diffuse scattering, small-angle neutron scattering, neutron reflectivity, and experiments with polarized neutrons. There simply isn't enough space to cover all those topics in this article - stay tuned for more in upcoming *Reflexions*.

I would be remiss not to mention the many other important events scheduled for the Hawaii Meeting: the Buerger Award Symposium honoring Helen Berman's pioneering developments of information services in crystallography; the Warren Award Symposium honoring Charles Majkrzak's seminal contributions to the development of neutron reflectivity; and the Etter Early Career Award Symposium honoring Carrie Wilmot for her ground-breaking work in previously unrecognized post-translational modifications of amino acids. In addition there will be more than 35 micro-symposia and workshops showing the wide range of research interests represented in the close to 700 submitted abstracts. This is a meeting not to be missed and I hope to see you all in sunny Hawaii!

Bob Bau

2007 Trueblood Award to Angelo Gavezzotti

Angelo Gavezzotti is one of the foremost chemical crystallographers in the world. Over a period of more than thirty years



he has deeply influenced the way we think about molecular packing in crystals. He is the author of the UNI force field (with G. Filippini), of several crystallographic computer programs, such as OPEC (Organic Packing Energy Calculations), Zip-Promet (a program for the generation of possible

crystal structures) and, most recently, the Semiclassical Density Sum Method (Pixel Method) for estimating intermolecular energies, all highly innovative, widely used and successful. He is an outstanding candidate for the ACA Kenneth N. Trueblood Award, which is to recognize exceptional achievement in computational or chemical crystallography.

Philip Coppens (Chair), Larry Dahl, Doug Rees, and Jim Richardson

2007 Fankuchen Award to Frank Herbstein



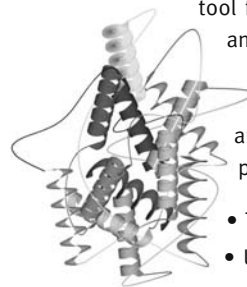
Frank Herbstein's work has illuminated chemical crystallographic perceptions for over half a century and has now culminated in the recent publication of his two-volume encyclopedic work on *Crystalline Molecular Complexes and Compounds*. For the emerging generation

of crystallographers this achievement should set an example of true scholarship combined with critical (and self-critical) attitudes towards a vast and complex body of information. Herbstein's book will be a guide to the perplexed for many years. His lifetime achievements in research, teaching and scholarship eminently qualify him as a most suitable candidate for the 2007 Fankuchen Memorial Award.

Tom Koetzle (Chair), Lachlan Cranswick, Kathy Kantardijeff, Bob Sweet

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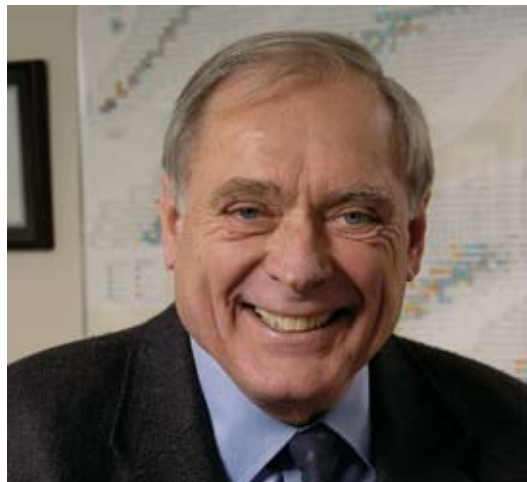
FEBS Journal award to Nicole LaRonde-LeBlanc

Nicole LaRonde-LeBlanc, a postdoctoral fellow in the Macromolecular Crystallography Laboratory, National Cancer Institute, Frederick, MD, was awarded the 2005 **FEBS Journal Prize for Young Scientists**. She was the first author of a paper entitled "Structure and activity of the atypical serine kinase Rio1" (N. LaRonde-LeBlanc, T. Guszczynski, T. Copeland, A. Wlodawer, *FEBS Journal* 272, 3698-3713, 2005), judged by the editors of the FEBS Journal to be "the best published in the journal in 2005 that falls within the rules for our

FEBS Journal Prize for Young Scientists." The prize includes a check for 10,000 euros, as well as an all-expenses-paid trip to the 31st Congress of the Federation of European Biochemical Societies, held in Istanbul, Turkey, at the end of June 2006. She presented her work on determining the crystal structure and autophosphorylation sites of Rio1, a novel kinase involved in ribosome biogenesis and cell cycle progression. Rio1 and related kinases may become important new targets for designing anticancer drugs. (Editors note: Nicole also received the 1005 SER-CAT Award - see *ACA Newsletter*, spring 2005.)

Nicole received her doctoral degree at Johns Hopkins University as a student of Cynthia Wolberger. Having spent almost four years at NCI in Alex Wlodawer's laboratory, she has recently accepted a position as an Assistant Professor at the College Park campus of the University of Maryland and will be moving there in the Fall of 2006.

Alex Wlodawer

2006 Clifford G. Shull Prize to J. M. Carpenter

The Neutron Scattering Society of America (NSSA) established the **Clifford G. Shull Prize in Neutron Science** to recognize 'outstanding research in neutron science and leadership promoting the North American neutron scattering community.' The prize is named in honor of Clifford G. Shull, who received the Nobel Prize in 1994 with Bertram Brockhouse for seminal developments in the field of neutron science.

The 2006 Shull Prize was awarded to **Jack Carpenter**,

Intense Pulsed Neutron Source Division of the Argonne National Laboratory, "For seminal contributions to the development of neutron sources and instrumentation

that have had world-wide impact on neutron scattering across a broad range of scientific disciplines, culminating in the optimized design of the Spallation Neutron Source at Oak Ridge." His work pioneered exploitation of the inherent efficiency of the spallation process for the production of neutrons together with the advantages of pulsed operation and time-of-flight measurements for the study of structure and dynamics of materials. His patented design for the moderator-reflector combination is at the heart of modern neutron source design and his creativity in matching the characteristics of neutron sources to the demands of the instrumentation that continues to serve as an example to the international community.

The prize, with a 5,000 dollar honorarium, was awarded at the NSSA meeting in June, 2006.

ACS Midwest Regional Award to Jerry Atwood

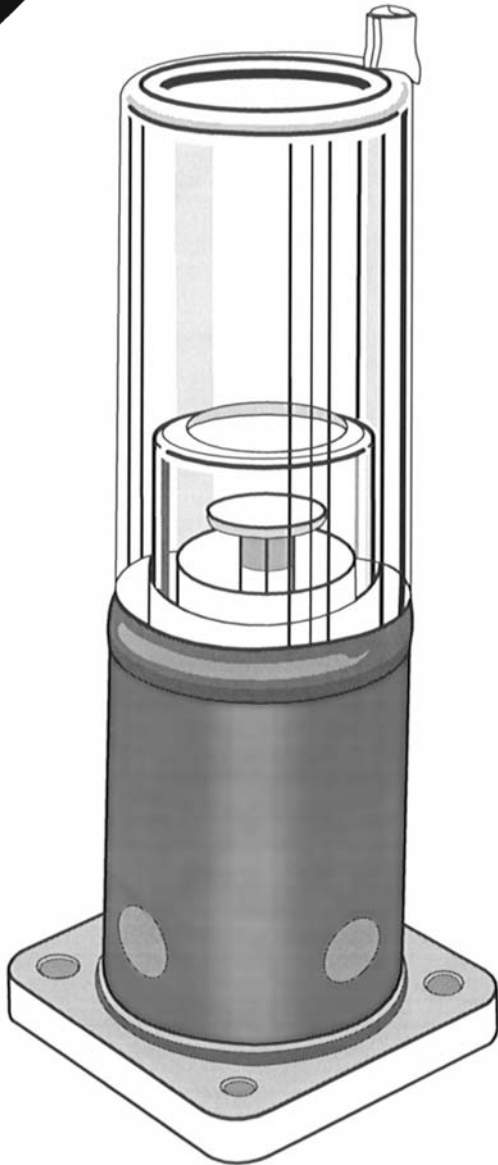
Jerry Atwood, Curators' Professor and Chair of the Department of Chemistry at the University of Missouri was the recipient of the **2005 ACS Midwest Regional Award** for "fundamental contributions to understanding intermolecular, intramolecular, and supramolecular interactions."

During the past two decades, Atwood has become a leader in the area of macrocycles, where he has worked particularly with calixarenes and resorcinarenes. As he did in earlier studies with crown ethers, he strives to identify and understand difficult or improbable complexation cases. He identified aromatic and hydrogen bonded interactions between calixarenes and various chlorocarbon solvents and demonstrated that they could form sandwich complexes with a variety of metals. These compounds led to imaginative and complex self-assembled, hydrogen-bonded capsules that exhibit properties and chemistry that are remarkable. In exploring this, Atwood and coworkers proposed using the principles of Platonic and Archimedean solids to understand supramolecular assemblies.

*Excerpted from C&E News -
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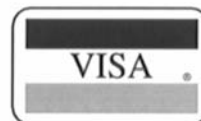


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BALANCE SHEET - December 31, 2004 and 2005**

	CURRENT FUNDS (2005)		TOTAL	
	Unrestricted	Restricted*	All Funds	
			2005	2004
ASSETS				
Current Assets:				
Cash	175,550		175,550	140,957
Investments	437,563	352,915	790,478	778,870
Inventory	5,600		5,600	5,600
Total Current Assets	618,713	352,915	971,628	925,427
Fixed Assets:				
Computers and Printers	4,598		4,598	4,598
Office Equipment	1,300		1,300	1,300
Accumulated Depreciation	0		0	0
Total Fixed Assets	5,898		5,898	5,898
TOTAL ASSETS	624,611	352,915	977,526	931,325
Liabilities:				
Deferred Dues Income			0	0
Total Liabilities	0		0	0
Fund Balance:				
Unrestricted	624,611		594,723	594,723
Restricted		352,915	352,915	336,602
Total Fund Balance	624,611	352,915	977,526	931,325
TOTAL LIABILITIES & FUND BALANCE	624,611	352,915	977,526	931,325

* Current Balances in individual restricted funds - as of December 31, 2005

Buerger Award	35,111
Etter Award	63,141
Fankuchen Award	66,434
Patterson Award	38,582
Pauling Award	30,719
Supper Award	10,225
Trueblood Award	31,153
Warren Award	28,212
Wood Science Writing Award	49,338

A more detailed report on the ACA finances may be obtained by sending a written request to the ACA office in Buffalo, PO Box 96, Ellicott Station, Buffalo, NY 14205-4846.

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Canadian Light Source News (from the CLS E-News, www.lightsource.ca)

Message from **Bill Thomlinson**, the Executive Director: “2005 was an extremely fruitful and exciting year for the CLS. The machine has met or exceeded our design goals, and we have had light in all seven Phase I beamlines. We began hosting friendly users who provided valuable assistance and expertise with beamline commissioning, and with marquee experiments. The first published scientific papers are expected soon.

In March, 2005, Canadian Light Source Inc. (CLSI) welcomed **Tom Ellis** as our new Director of Research. Tom’s vision and leadership have been instrumental in the development of our scientific program.

Spring 2005 was also busy on other fronts. An important milestone was achieved for our industrial science group with the signing of a contract with Synodon Inc. of Edmonton to conduct research on our beamlines. This was the first agreement signed to conduct work solely on CLS facilities. The industrial science group was extremely active in 2005, conducting research on CLS beamlines as well as running analyses at the National Synchrotron Light Source (NSLS), the Advanced Photon Source (APS), and Daresbury.

May 2005 was truly memorable due to the visit of Her Majesty the Queen and His Royal Highness The Duke of Edinburgh. The Royal Couple were impressed with the facility and news of their visit to Saskatoon reached over 2.2 million people across Canada and from as far away as Qatar.

A week after the Royal Visit, CLS history was made once again when **Allen Pratt** from Natural Resources Canada and his team became the first scheduled CLS users. He has since been joined by over 70 other Canadians and other users from as far away as Germany, to conduct research at our facility.

Throughout the summer and fall of 2005, the CLS continued to turn on its programs, as all new synchrotrons do. With the formal completion of the CLS Project in June, CLSI staff and management continued to make advances with an ambitious commissioning schedule, completion of our strategic planning process, enhancing user support and growing the facility with the design and initial construction of Phase II beamlines and support for Phase III proposals.

Thanks to the hard work and dedication of everyone at the CLS and the support of the community, 2005 was indeed a remarkable year. I have no doubt that 2006 will be equally successful.”

CLSI has signed a memorandum of understanding with the Australian Synchrotron in Melbourne intended to promote collaborative opportunities between the two facilities. Australian and Canadian scientists have been working together on a beamline at the CLS targeting minerals industry applications, and plan to transfer the technology to Australia to drive possible development of a similar beamline at the Australian Synchrotron (www.lightsource.ca/media/media_release_20051214.php).

2005 was a record-breaking year for educational outreach. Over 8900 people toured the CLS, including 1338 scientists and academics, 3697 students and educators, 3277 members of the public, and 347 industry representatives.

Pawel Grochulski reports that the first two diffraction images were taken at the Macromolecular Crystallography Facility (CMCF) beamline on March 18 (www.lightsource.ca/media/first_crystallography_results.php).

Machine status is now viewable at www.lightsource.ca/machine/machine_status.php. This display receives real time information from the actual equipment, updating it every minute. More information will be added in the future.

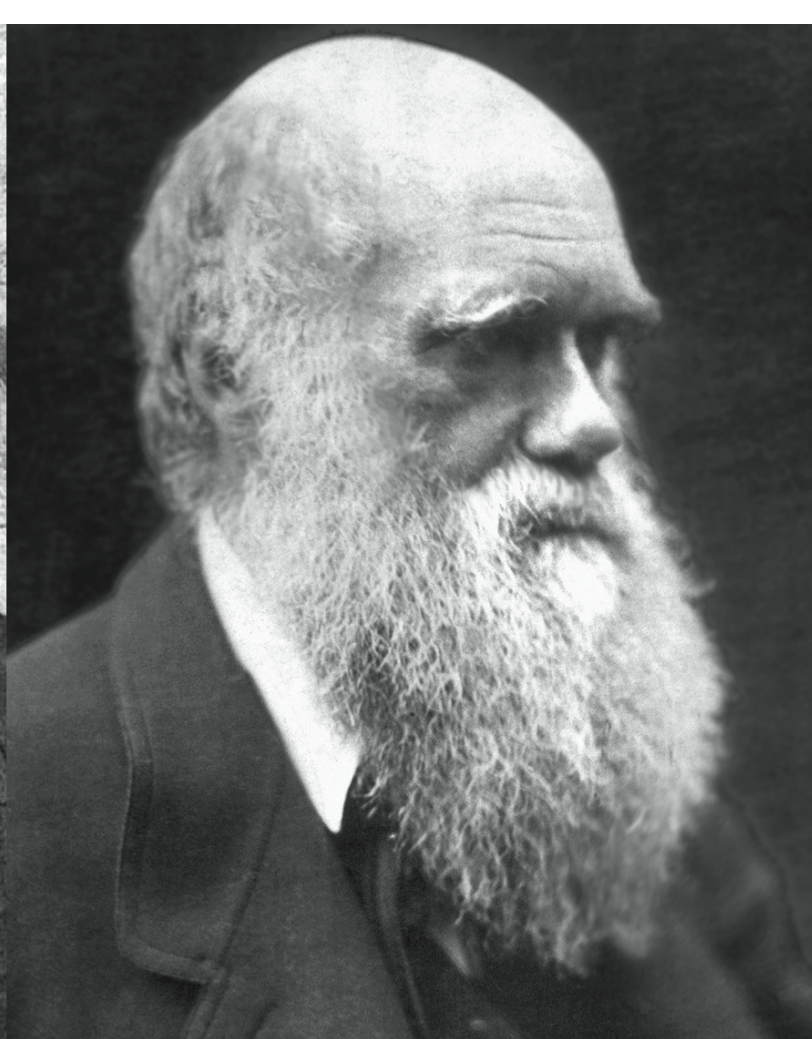
Tom Ellis reports: “The CLS recently marked an important scientific achievement with the publication of the first research papers resulting from experiments performed at Canada’s national synchrotron facility. The research groups, whose papers appeared online the same day, are from the University of Saskatchewan and the University of Western Ontario (for the full news release see www.lightsource.ca/media/media_release_20060417.php.”

The 9th Annual Users Meeting took place June 16-18, 2006. This meeting was held in conjunction with the 3rd Northern Lights Summer Conference of the Canadian Federation of Biological Societies (June 14-16). The theme of the Northern Lights conference is “Shining Light on Biological Processes.” The following workshops were also held in association with the meeting: (1) Molecular Form and Function: Probing Intact Tissues using Synchrotron Light; (2) Synchrotron Protein Crystallography; (3) New Instrumentation for Soft X-ray Photon-In-Photon-Out Spectroscopy; (4) Synchrotron and Advanced Analytical Techniques in the Forensic Sciences; (4) Terahertz (THz) Workshop. There was a prize (\$1,000) for the best poster by a graduate student or postdoctoral fellow.

The main meeting featured talks highlighting CLS-based research activities including presentations by **Helen Nichol** (University of Saskatchewan), **Allen Pratt** (Natural Resources Canada), **Jeanne Percival** (Geological Survey of Canada), **T.K. Sham** (University of Western Ontario), and **Regan Wilks** (University of Saskatchewan). International speakers included **John Bargar** (Stanford Synchrotron Radiation Laboratory), **Giacomo Ghiringhelli** (Politecnico di Milano), and **Ralf-Hendrik Menk** (Sincrotrone ELETTRA). Speakers from Canada’s thriving synchrotron community included **Andrea Damascelli** (University of British Columbia) and **Paul Scott** (University of Alberta). There was also a special presentation on “Research Funding in Canada” by **Isabelle Blain**, Vice-President Research Grants and Scholarships, Natural Sciences and Engineering Research Council of Canada (NSERC) (www.lightsource.ca/uac/meeting2006/).

The inaugural Saskatoon Synchrotron Summer School (SSSI) will take place August 1-4, 2006 at CLS. The school aims to provide postdoctoral, graduate, and senior undergraduate students with synchrotron-specific knowledge and skills applicable to their research. The program will cover topics such as the production and properties of synchrotron radiation, an overview of CLS current and future beamlines, and lectures on synchrotron applications to a number of scientific disciplines (protein crystallography, infra-red, photoemission spectroscopy, and x-ray absorption spectroscopy). Students will also obtain hands-on experience in data collection and data analysis (register at www.lightsource.ca/education/summerschool).

CLSI is currently recruiting for technical support positions in Facility Operations (www.lightsource.ca/careers/).



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lightsources.org, the only web site to comprehensively feature news, information, and educational materials about the world's synchrotron radiation and free electron laser (light source) facilities, celebrated its 1st anniversary on February 17, 2006. Throughout the year, lightsources.org has grown significantly in content and traffic. More than 150 press releases and over 600 synchrotron-related press items have been listed on the web site and distributed to subscribers. Web traffic is continually increasing and is now averaging over 100,000 page views/month. To see the top synchrotron light source news from 2005 based on press coverage visit www.lightsources.org/topnews/.

Canadian Neutron Beam Centre News

The Canadian Neutron Beam Centre (CNBC) of the National Research Council (NRC) at the Chalk River Laboratories in Ontario, recently ran a neutron powder diffraction experiment on radioactive spent uranium-molybdenum-aluminium dispersion nuclear fuel. This work was accomplished using a lead shielded cell developed by Atomic Energy of Canada Limited (AECL) in collaboration with the US Department of Energy, and the NRC C2 multiwire neutron powder diffractometer involving C2 beamline scientists *Lachlan Cranswick* and *Ian Swainson*. The new fuel is being developed as part of an international effort to replace highly enriched research reactor fuel with proliferation resistant low enriched uranium (LEU) fuel.

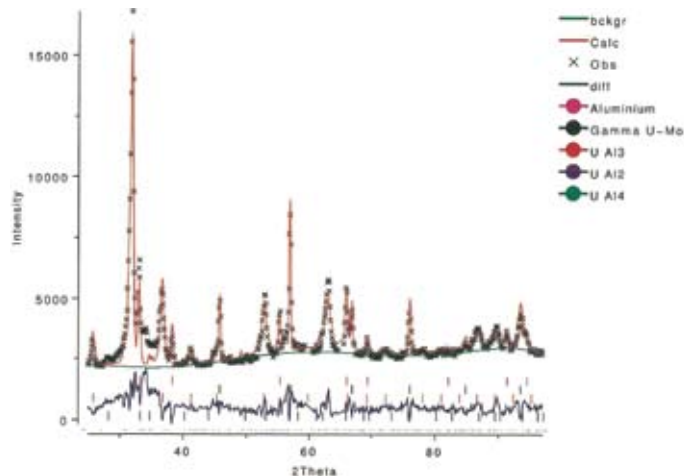
The CNBC group has significant prior experience at performing measurements on radioactive samples, including strain scanning analysis on samples with calculated activities as high as 20,000 REM/hr (200 Sievert/hr) on contact. This was the first powder diffraction based experiment performed at Chalk River with irradiated nuclear fuel (20% burnup); and involved on-contact activities of 80 REM/hr (0.8 Sievert/hr). To ensure safety before and during the experiment, multiple dummy-runs were used to test the experimental procedure in advance and a passive safe-stand-down procedure (by the use of Do-Not-Operate tags placed on the initially unloaded shielded cell) was also included in case any experimentalists or technicians felt the experiment was becoming unsafe in any form during the setup.



(left) bird's-eye and (right) side views of the loaded AECL shielded cell on the NRC C2 neutron powder diffractometer

The aim of the experiment was to help understand the swelling behavior of this potential replacement research reactor fuel with respect to the crystalline and amorphous phases that form within the fuel during irradiation. While some experts expected the spent fuel to be fully amorphized from reactor irradiation,

the fuel samples were found to contain a number of crystalline phases that were analyzed using the GSAS Rietveld refinement software. The results were presented by the two neutron beam users, *Kelly Conlon* and *Dave Sears* of AECL, at the 10th European Nuclear Society Topical Meeting on Research Reactor Fuel Management.



GSAS Rietveld neutron powder diffraction plot (1.33008 Å) of irradiated U-Mo-Al dispersion fuel

6th Canadian Powder Diffraction Workshop

With 21 registrants, the 6th Canadian Powder Diffraction Workshop, chaired by *Bruce Torrie*, was held at the University of Waterloo from May 8-10, 2006. Bursaries for Ph.D. students were provided by the Canadian Institute for Neutron Scattering, and for US based Ph.D. students by the Lujan Neutron Scattering Center of Los Alamos National Laboratory. Lectures were held in the mornings with hands-on computer based tutorials in the afternoon.



The first two days were focused on powder diffraction and the use of the GSAS Rietveld analysis software; with lecturers and tutorial instructors *Bob Von Dreele* (Argonne National Laboratory, and *Allen Larson* of the GSAS software), *Angus Wilkinson* (Georgia Tech), and *Ian Swainson* and *Lachlan Cranswick* (both of the Canadian National Research Council). The third and final day was on Total Scattering/Pair Distribution Function analysis taught by *Thomas Proffen* of Los Alamos National Laboratory.

Bruce Torrie has chaired all the Canadian Powder Workshops, (the first was held in 1991), but indicated this would be his last. The University of Waterloo has proved to be a hospitable, friendly and cost effective venue for this style of workshop. Besides appreciation to Bruce for his work on this and previous workshops, thanks also go to *Pam De Leo* and *Melissa Button* of the Univ. of Waterloo for their help and assistance. The next workshop is expected to be held in May 2007 at the Univ. of Québec at Trois-Rivières, chaired by *Jacques Huot*.

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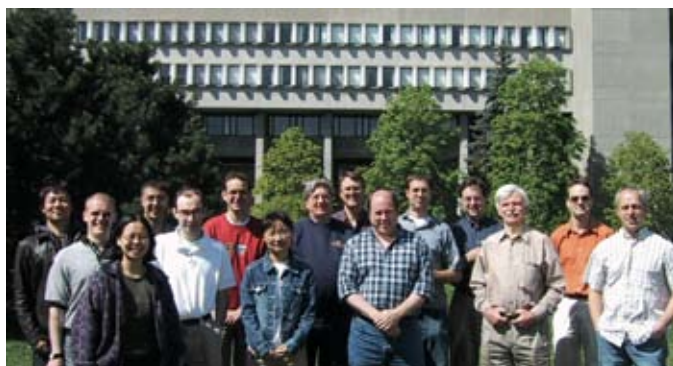


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Workshop group photo; chair Bruce Torrie is in the front row, second from the right.



Facility Profile: The Structural Chemistry Facility and the Centre for Higher-Order Structure Elucidation (C-HORSE) at the University of British Columbia (UBC)

The Structural Chemistry Facility in the Department of Chemistry is managed by **Brian Patrick**, and members include **Anita Lam** and **Jim Trotter** (emeritus). The lab is equipped with two single-crystal x-ray diffractometers (Bruker X8 with Apex II detector and a Rigaku) and two powder x-ray diffractometers (Bruker D8 units). Low-temperature data collection is possible for both types of experiments. The lab has one SGI and five PC workstations for single crystal structure determination and refinement and powder diffraction analysis.

The Facility is part of the Centre for Higher-Order Structure Elucidation (C-HORSE), which was established with funding from the Canada Foundation for Innovation (CFI) in order to integrate the computational and theoretical understanding of the form, function, and fluctuation of complex molecules with the goal of more effective design and synthesis. C-HORSE also includes a state-of-the-art NMR facility featuring a 600 MHz NMR with cryogenic probe (for low gamma nuclei), High Pressure Liquid Chromatographs (HPLCs), and a computer cluster of PCs for visual characterization of molecules (www.chem.ubc.ca/chorse/index.html).

This is the first in what hopefully will become a series profiling crystallographic facilities across Canada.

Member News

Louis Delbaere received the Commemorative Medal for the Centennial of Saskatchewan on February 17, 2006. This medal recognizes individuals who have made a significant contribution to the Province of Saskatchewan.

Gerald Audette will be joining the Chemistry Department at York University, effective July 1st. Gerald did his Ph.D. with Louis Delbaere at the University of Saskatchewan, and was a postdoctoral fellow at the University of Alberta with Bart Hazes.

Lee Groat

Outcome of the Education Summit in June 2005

In 2001 and 2003, the USNCCr Education Subcommittee conducted two surveys to determine the content and extent of coverage of crystallography in university curricula, as well as the views of the broader crystallographic community on the status of crystallographic education and training in the US, in both the physical and the life sciences. These surveys suggested that, perhaps as a result of rapid technological advances in the field of modern crystallography, there appears to be a declining number of master practitioner crystallographers, as well as a lack of sufficient education and training in crystallography for individuals who wish to understand and/or use crystallography as a tool in their hypothesis-driven research.

Recognizing the opportunity to communicate to the broader scientific community the research opportunities afforded by crystallography, as well as the value of crystallographic information, the education committees of the ACA and USNCCr organized an education summit, which took place June 1-2, 2005 at the conclusion of the ACA national meeting in Orlando, FL. Individuals known for their experience and contributions in crystallographic education and training participated in this summit, the outcome of which is a consensus policy statement on crystallographic education and training. The education summit was funded by the USNCCr, the ACA, the California State University Program for Education and research in Biotechnology, and the National Science Foundation.

This document, which will be made available through the National Resource Council of the National Academies (NRC) Press website, summarizes the crystallographic education and training policies endorsed by the ACA and the USNCCr. Organized in a reverse hierarchal fashion, beginning with post-baccalaureate education and working back to the K-12 level, this policy document makes recommendations for a comprehensive re-evaluation of crystallographic education, and suggests ways to develop an appreciation for the value of crystallographic information in the broader scientific community. Moreover, the visual, aesthetic and quantitative nature of crystallography provides an excellent path to introduce science and scientific methods to the general population.



Left to right - Bob Sweet, Simon Billinge, Gloria Borgstahl, Bob Bau, Jim Pflugrath and Bernhard Rupp

The conclusions and recommendations in this document are based on input from the education summit participants comprised of practicing crystallographers in both academia and industry working as biologists, biochemists, chemists, geologists and physicists. The ACA and the USNCCr intend that the document, which stands as the white paper on crystallographic education and training, provides guidelines to professional societies and academic departments for crafting future crystallographic curricula that adequately address the needs of the scientific community. The education committees of the ACA and the USNCCr will provide guidance and support to interested colleagues and policy makers who wish to put these recommendations into practice.

In creating this document, the summit participants have recognized that:

- Crystallography and molecular structure awareness should begin in K-12 education as core components for implementing the established national science standards for all students.
- Many contexts exist in which crystallography could be incorporated in undergraduate education with minimal disruption to current courses, and should be included in the curricula of all undergraduate programs in the physical and life sciences.
- Formal courses and research opportunities in crystallography should be available to senior undergraduates.
- Crystallography-rich courses should be available to all graduate students.
- Professional development beyond the graduate degree, such as provided by crystallographic certificate programs, short courses, summer schools and research opportunities, is a necessary aspect of crystallographic training; this is particularly important in novel subjects such as modulated structures and time-resolved diffraction, where crystallography is increasingly being outsourced.
- The recommendations made and resulting changes effected must benefit the broader scientific community and not just the community of professional crystallographers.



Left to right - Marge Kastner, Cheryl Klein-Stevens, Chuck Campana, Allan Hunter and Jim Kaduk

If the science of crystallography is to remain alive and vibrant, it is critical that crystallography be taught in a way that attracts and retains a broad pool of talented people. Although the United States has played a prominent role in technological and scientific advancement, recently we have observed faltering interest and diminished academic performance in math and science by American students. Crystallography, with its interdisciplinary

nature and diversity of practitioners and users, provides a prime opportunity to re-energize interest in science, and should attract and maintain an important share of scientific talent. Maintaining the vitality of crystallography is important to university departments desiring to advance science. Education and training today will contribute to the production of a successful workforce that will assist the nation to prosper in a world of global economic competition. We hope that the scientific community will embrace this document, and that it will remind scientists of the importance of crystallography in their research endeavors.

We sincerely thank **Elaine McClanahan**, who facilitated the summit, **Jerry Bell** of the ACS for his keynote address, the ACA Continuing Education Committee, the USNCCr Education Subcommittee, and the summit participants: **Robert Bau(USC)**, **Simon Billinge(Michigan State U)**, **Gloria Borgsdahl(Eppley Institute, U Nebraska)**, **Charles Campana(Bruker-Nonius)**, **Jon Clardy(Harvard Medical School)**, **Frank Fronczek(LSU)**, **Andy Howard(IIT)**, **Allen Hunter(Youngstown State U)**, **Francis Jurnak(UC Irvine)**, **James Kaduk(Innovene)**, **Katherine Kantardjieff(CSU Fullerton)**, **Margaret Kastner(Bucknell U)**, **Cheryl Klein Stevens(Xavier U)**, **Marilyn Olmstead(UC Davis)**, **James Pflugrath(Rigaku MSC)**, **Kent Ratajeski(U West Georgia)**, **Miriam Rossi(Vassar College)**, **Bernhard Rupp(LLNL)**, **Robert Sweet(NSLS)**, **Iris Torriani(U Campinas Brazil)**, and **Victor Young(U Minnesota)**.

*Kathy Kantardjieff, Cheryl Klein-Stevens and
Miriam Rossi*

Education Subcommittee, USNCCr

Crystallography Web Watch

Members of the Communications Committee of the ACA encourage everyone to participate in the Crystallography Web Watch Column. The web address of web sites of interest to crystallographers and a brief description should be sent to Louis Delbaere at louis.delbaere@usask.ca. Thank you in advance for any suggestions.

This issue features sites that may be helpful for teaching crystallography :

IUCr Crystallographic Educational Resources: www.iucr.org/cww-top/edu.index.html

Teaching concepts of unit cell and symmetry for all 17 2D space groups: marie.epfl.ch/escher/

How the structure of space determines the shape of things, e.g. lattice structure, polyhedral framework and crystal habit: www.polymorf.net/knowhere.html

Transition metal coordination and oxidation states (compiled by Jeffrey S. Moore *et al.*): sulfur.scs.uiuc.edu/Intro%20Page/periodictable/pte.html

Robinson Burbank (1921-2006)

Correction: In the obituary for Robinson Burbank (Spring 2006 ACA RefleXions) the last line was truncated due to a printer error. It should have included "to the Metropolitan Opera Company of NY." The authors were Claudia Robinson and Sidney Abrahams.

Bridging the Sciences Activities: Winter 2006

Hill Meetings: At the beginning of March **Ken Dill** and **Mary Barkley** visited Washington, D.C. for meetings in several congressional offices. Along with **John Porter**, **Monique Nolan**, and **Ellen Weiss**, they had meetings in the offices of Senator Frist, Alexander, Bingaman, and Lieberman on the Senate side and with Chairman Boehlert and Representative Ehlers, as well as their staff, on the House side. The discussion focused on the inclusion of a Bridging the Sciences provision in the Innovation and Competitive Legislation moving through the Senate and soon-to-be introduced in the House.

Following up on the meeting, David Goldston, Chief of Staff to Chairman Boehlert, agreed to share a draft of the Competitiveness Legislation Boehlert is working on. That will include a Bridging the Sciences provision. The draft was expected to be available for review in early May.

Grassroots Advocacy: In March members of the Coalition societies were asked to send letters to the directors/secretary of NIH, NSF, and the Department of Energy. Draft letters were provided for the coalition societies to share with their grassroots networks. At least one member received a response from NSF Director Arden Bement. Bement responded that he was an advocate of the goals of a Bridging the Sciences Program.

High Risk/High Reward Research at NIH: At the Biophysical Society Annual Meeting in February, the public affairs committee held a session on peer review at the NIH. Director Toni Scarpa spoke about the changes being made at the Center for Scientific Review—particularly related to process. Ken Dill spoke about the Bridging Coalition and the conclusions of the Coalition regarding how to fund high-risk/high-reward research. Dill relied on the summary document from the June 2004 Coalition meeting in Half Moon Bay as well as the Summary of the NIH-NSF Interagency Meeting on Research at the Interface. Many NIGMS program officers were in attendance and were very interested in Dill's presentation, and invited him and Mary Barkley to come to NIGMS to discuss how to fund innovative research. NIGMS is working on a new mechanism to replace the R21 grants that have been discontinued.

This meeting took place on March 9th. NIGMS was well-represented; Director Jeremy Berg even stopped by for a short period of time. It appears that NIGMS is serious about finding a mechanism to fund innovative and upstream basic research.

Pittcon: The Coalition sponsored a session devoted to Bridging in the Context of Innovation and Competitiveness at the March 2006 Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (Pittcon) in Orlando, Florida. The panel included **John Porter**, **Ken Dill**, **Art Ellis** (head of Chemistry at the NSF), **Belinda Seto** (Deputy Director of the NIBIB at NIH), and **Mik Lubell** (public affairs director of the American Physical Society). The Pittcon meeting attracts over 25,000 attendees

Ellen Weiss (Biophysical Society)

AIP Update - May 2006

The AIP celebrated its 75th birthday at the prestigious Cosmos Club on Embassy Row in Washington, DC in early May with a splendid symposium. In opening remarks, AIP historian **Spencer Weart**, discussed the sobering question: "How do exponential growth curves end?" He concluded that the digital revolution brought seeds of rebirth as information can propagate essentially by itself. **Martin Rees** from Cambridge, UK, summarized where cosmology has been and may be headed. Completion of new accelerators accessing new energies should help us penetrate mysteries such as the strange composition of the universe in which conventional atoms account only for about 4% of the total mass-energy and the extreme fine tuning of physical constants. These and controversies arising from the anthropic principle will be major driving concepts for some time yet. The plenary session was completed with talks by **Marvin Cohen** on condensed matter physics and **Steven Chu** on optics and biophysics.

Shirley Malcom from the AAAS discussed how demographics have changed profoundly with increasing penetration by women into science in general, but noted that entry into physics was lagging significantly behind chemistry and biology. She told the moving story of the first PhD awarded to a black in the US, a degree in physics to Edmund Boucher, a contemporary of J. W. Gibbs at both secondary school and at Yale University, and by some accounts a higher performer at both institutions. Boucher's talent was lost because there simply were no jobs at that time for blacks.

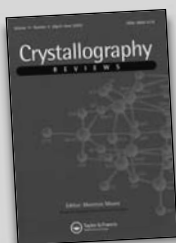
Biology is assuming an increasingly major role in physics. A round table of gifted young physicists comprised the second part of the afternoon program. **Angela Belcher** stole the show from string theorist **Jim Gates** by describing her work at MIT, where she has engineered microorganisms to fabricate lithium ion batteries! Parenthetically, the president elect of the American Physical Society is **John Hopfield** from Princeton, whose research effort is focused on the central nervous system of *C. elegans*. The AIP is well aware of the growing importance of biology. This is reflected in initiatives such as bundling of biophysical papers from *J. Chem. Phys.* for separate electronic subscription.

The final event of the symposium was by **Jack Marburger** on science policy. I had rehearsed several questions I wanted to ask this man, who has been complicit in the contempt for science shown by Bush. The talk, however, was pretty plain, and in the end, Bill Duax convinced me to keep mum. The mood was indeed edgy, nonetheless, and the questions were implicitly skeptical. Marburger had given a talk at the 50th anniversary 25 years ago, and he promised to return for the 100th. I sat next to a European visitor with a surprising amount of science policy experience. His metaphor for Marburger's talk was novocaine. "He engineered it so you felt no pain."

AIP 75th Anniversary events, including videos of the presentations, can be found at www.aip.org/anniversary.

A symposium the following day was devoted to the evolution of publishing. Among the highlights were these: 75% of papers submitted to society journals now come from outside the US, consistent with trends noted by a number of organizations, including the NSF. I was surprised to learn that scientific society publica-

Crystallography Journals from Taylor & Francis



Crystallography Reviews

Volume 12, 2006, 4 issues per year
Print ISSN: 0889-311X Online ISSN: 1476-3508

New joint editor in 2006

Editors: **Professor Moreton Moore**, Royal Holloway, University of London, UK and **Professor John Helliwell**, University of Manchester, UK

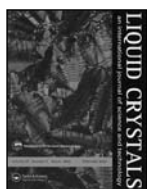
Crystallography Reviews publishes English language reviews on topics in crystallography and crystal growth, covering all theoretical and applied aspects of biological, chemical, industrial, mineralogical and physical crystallography. The intended readership is the crystallographic community at large, as well as scientists working in related fields of interest.

Liquid Crystals

2004 Impact Factor: 1.056
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Volume 33, 2006, 12 issues per year
Print ISSN: 0267-8292 Online ISSN: 1366-5855

Editors: **Corrie T. Imrie**, Aberdeen University, UK and **Noel Clark**, University of Colorado, USA



Liquid Crystals publishes accounts of original research concerned with all aspects of liquid crystal science and technology, including experimental and theoretical studies ranging from molecular design and synthesis to applications engineering.

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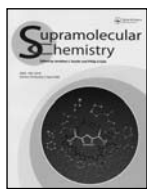
Subscription to **Liquid Crystals** includes online access to **Liquid Crystals Today**, the newsletter of the International Liquid Crystal Society published by Taylor & Francis. Since 1990, **Liquid Crystals Today** has been welcomed by the liquid crystal community as a unique forum for feature articles, book reviews, conference reports and various news items relating to liquid crystal scientists, events and developments

Supramolecular Chemistry

2004 Impact Factor: 1.577
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Volume 18, 2006, 8 issues per year
Print ISSN: 1061-0278 Online ISSN: 1029-0478

Editors: **Jonathan L. Sessler**, University of Texas at Austin, USA and **Philip Gale**, Southampton University, UK



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Phase Transitions

2004 Impact Factor: 0.581
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Volume 79, 2006, 12 issues per year
Print ISSN: 0141-1594 Online ISSN: 1029-0338

Editor: **Jens Kreisel**, Grenoble, France



Phase Transitions is the only journal devoted exclusively to this fast growing subject. It provides a focus for papers on most aspects of phase transitions in condensed matter. Although emphasis is placed primarily on experimental work, theoretical papers are welcome if they have some bearing on experimental results.

Journal of Macromolecular Science, Part B: Physics

Volume 45, 2006, 6 issues per year
Print ISSN: 0022-2348 Online ISSN: 1525-609X

Executive Editors: **Phillip H. Geil**, University of Illinois, USA and **Anthony J. Ryan**, University of Sheffield, United Kingdom

The **Journal of Macromolecular Science, Part B: Physics** is an international journal that contains papers reporting research in transition mechanisms and structure, especially property relationships, the physics of polymer solutions and melts, of glassy and rubbery amorphous solids, and the physics of individual polymer molecules and natural polymers.

Polymer Reviews

Volume 46, 2006, 3 issues per year
Print ISSN: 1558-3724 Online ISSN: 1558-3716

Editor-in-Chief: **Elliot P. Douglas**, University of Florida, USA

Polymer Reviews publishes invited high quality reviews on topics such as: biomedical applications, organic electronics and photonics, nanostructures, micro- and nano-fabrication, biological molecules (DNA, proteins, carbohydrates), polymers for renewable energy and the environment, polymers at the interfaces, and more.

Soft Materials (LSFM)

Volume 4, 2006, 4 online issues per annum
– 1 print issue of all online articles
Print ISSN: 1539-445X Online ISSN: 1539-4468

Editor: **Florian Müller-Plathe**, Technische Universität Darmstadt, Germany

Soft Materials is the first interdisciplinary journal to incorporate all areas of soft matter: chemistry, physics, materials science, and biology. Featured systems and applications include: polymers, biomacromolecules, colloids, membranes, Langmuir-Blodgett films, liquid crystals, granular matter, soft interfaces, complex fluids, surfactants, gels, nanomaterials, self-organization, supramolecular science, molecular recognition, soft glasses, amphiphiles, and foams.

Molecular Crystals and Liquid Crystals

Volumes 444-461, 2006, 18 issues per year
Print ISSN: 1542-1406 Online ISSN: 1563-5287

Editor-in-Chief: **Mortimer M. Labes**, Temple University, USA

Primarily fundamental in tenor, **Molecular Crystals and Liquid Crystals** publishes original research papers of both an experimental and theoretical nature in three areas of specialization: molecular crystals, low-dimensional solids, and liquid crystals. Experimental manuscripts describing both preparation and properties are presented in all three areas.

Ferroelectrics

Volumes 330-344, 2006, 16 issues per year
Print ISSN: 0015-0193 Online ISSN: 1563-5112

Editor-in-Chief: **George W. Taylor**, Princeton Resources, USA

Ferroelectrics provides a forum for people working in ferroelectrics and related materials such as ferroelastics, ferroelectric-ferromagnetics, electrooptics, piezoelectrics, pyroelectrics, nonlinear dielectrics, and liquid crystals. **Ferroelectrics** publishes experimental and theoretical papers aimed at the understanding of ferroelectricity and associated phenomena, along with applied papers dealing with the utilization of these materials in devices and systems.

Ferroelectrics Letters Section

Volume 33, 2006, 6 issues per year
Print ISSN: 0731-5171 Online ISSN: 1563-5228

Editor-in-Chief: **George W. Taylor**, Princeton Resources, USA

Ferroelectrics Letters is a separately published section of the international journal **Ferroelectrics**. Both sections publish theoretical, experimental and applied papers on ferroelectrics and related materials, including ferroelastics, ferroelectric ferromagnetics, electrooptics, piezoelectrics, pyroelectrics, nonlinear dielectrics, polymers and liquid crystals. **Ferroelectrics Letters** permits the rapid publication of quality, short original papers on the theory, synthesis, properties and applications of ferroelectrics and related materials.

Integrated Ferroelectrics

Volumes 70, 2006, 9 issues per year
Print ISSN: 1058-4587 Online ISSN: 1607-8489

Editor-in-Chief: **George W. Taylor**, Princeton Resources, USA

Integrated Ferroelectrics provides an international, interdisciplinary forum for electronic engineers and physicists as well as process and systems engineers, ceramicists, and chemists who are involved in research, design, development, manufacturing and utilization of integrated ferroelectric devices. Such devices unite ferroelectric films and semiconductor integrated circuit chips. The result is a new family of electronic devices, which combine the unique nonvolatile memory, pyroelectric, piezoelectric, photorefractive, radiation-hard, acoustic and/or dielectric properties of ferroelectric materials with the dynamic memory, logic and/or amplification properties and miniaturization and low-cost advantages of semiconductor i.c. technology.

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tions in general (ACS, AIP, APS, IUCr, etc.) have significantly higher impact factors AND are an order of magnitude cheaper per article than commercial publications! Societies provide essential peer review and validation for readership, which likely accounts for their higher impact factor and is the basis of their intellectual property rights. Society publications, however, are under pressure from two sides. Corporate publishers are growing more powerful, in keeping with widespread trends in industry. From the other side, they are subject to important threats from legislated Open Access. Here, society and corporate publishing interests are aligned. Society journals, however, because of their much tighter profit margins, are more vulnerable than the publishing giants, like Elsevier. Recent introduction of a bill by John Cornyn and Joe Lieberman mandating Open Access on publicly-funded research represents a very significant threat to the health of peer review and the scientific enterprise: see www.omidyar.net/group/community-general/news/1282.

The spring Governing Board Meeting is devoted primarily to assessing budget assumptions, which are only of peripheral interest to the ACA membership. Basically, the AIP is an organization that uses publishing revenues to fund substantial public policy activities. As with any such organization, the annual budget is to be neutral, which sets limits on what the AIP can do in the public policy arena. Among the AIP's policy initiatives of interest to the ACA is their work on the confrontation between The Discovery Institute and Intelligent Design. Together with other societies, they recently completed four different focus groups on science teaching, two (one for men, the other for women) in South Carolina and two in Michigan. **Marc Brodsky** likened the results to a Dennis the Menace cartoon in which Dennis is sitting with a dunce cap in the corner saying: "If you didn't want that answer, you shouldn't have asked that question." The transcripts produced few hopeful signs. Most of those interviewed were unaware of how science works, and felt that the teaching of Intelligent Design was basically a matter of "fairness" and maximizing opportunity for their children.

Elsewhere on this front, **Holden Thorp**, Chair of the UNC Chemistry department, wrote a significant op-ed piece for the New York Times, called "Evolution's Bottom Line" (12 May) arguing that teaching intelligent design simply did not contribute to economic competitiveness. Judge Jones's 128 page opinion on the Dover PA lawsuit was a welcome masterpiece. Well-crafted and surprisingly well informed, it states the scientific case almost perfectly. Although there is some modest rejoicing over this opinion, it is but a momentary victory in a small battle. Only time will tell win hearts and minds in the war, which, the focus groups show without doubt, is a far thornier American cultural phenomenon.

One final note of business that may eventually involve ACA membership concerns the National Societies for Black and Hispanic Physicists (NSBP, NSHP), who have requested consideration for full AIP membership. As their combined membership falls well short of the 800 minimum for regular membership, such membership would require a change in the AIP Constitution, as well as approval of a super majority of member societies.

Charlie Carter

Evolution/Creationism News – April – May 2006

Oklahoma: House Bill 2107 (*anti-evolution*) was passed by a vote of 77-10 on March 2, 2006. On March 15, it was referred to the Senate Committee on Appropriations, and then on March 21 to the Appropriations Subcommittee on Education, where it remains.

Antievolution bill in Missouri deemed dead: "A new tack for trying to introduce supernatural explanations for the origin of life into Missouri's public school science classes appears dead this year". The bill, if enacted, would have provided that, "If a theory or hypothesis of biological origins is taught, a critical analysis of such theory or hypothesis shall be taught in a substantive amount."

A new antievolution maneuver in South Carolina: A subcommittee of the South Carolina House voted to approve a Senate bill amended to direct the state board of education to approve only textbooks that "emphasize critical thinking and analysis in each academic content,"

Both antievolution bills in Maryland dead: The General Assembly adjourned on April 10, 2006, meaning that both antievolution bills introduced during the legislative session are dead.

Mississippi "Origin of life" bill revived as amendment: A bill was signed into law that, originally unrelated to evolution education, was amended to include the following: *No local school board, school superintendent or school principal shall prohibit a public school classroom teacher from discussing and answering questions from individual students on the origin of life.*

Antievolution language removed from Michigan bill: Antievolution language was removed before the bill was passed.

Antievolution amendment defeated in South Carolina: A proposal to approve only textbooks that "emphasize critical thinking and analysis in each academic content" was rejected by the House Committee on Education and Public Works.

Minnesota bill would ban teaching "intelligent design": Just before the education bill was approved by the state senate it was amended to ban teaching intelligent design. The House bill does not have the same provision so it could "come back" This is the second bill that would ban the teaching of "intelligent design" to be introduced in a state legislature during 2006; the other, in Wisconsin died in committee on May 4, 2006.

Canadian controversy over funding for research on anti-evolutionism: While delivering a talk on "Intelligent Design, God & Evolution" McGill University's Brian Alters dropped a bombshell. Throughout his talk he had contrasted the contentious state of evolution education in the United States with its relatively sedate counterpart in Canada. But toward the end of his talk, he mentioned a research project to study the effects of the popularization of "intelligent design" on Canadian students, teachers, parents, administrators, and policymakers, for which he had requested funding from the Social Sciences and Humanities Research Council of Canada. He revealed that his proposal was rejected, in part because (the SSHRC wrote) of inadequate "justification for the assumption in the proposal that the theory of evolution, and not intelligent-design theory, was correct."

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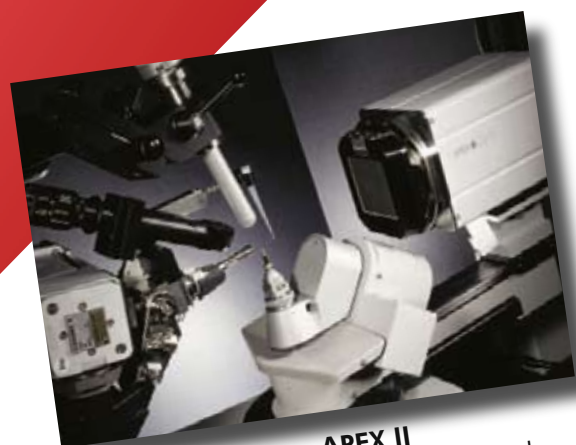
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Royal Society stand on evolution: A statement opposing the misrepresentation of evolution in schools to promote particular religious beliefs was published in April. Describing evolution as “the best explanation for the development of life on Earth from its beginnings and for the diversity of species” and as “rightly taught as an essential part of biology and science courses in schools, colleges and universities across the world,” it also emphasized the importance of evolution in understanding and solving problems of practical importance in medicine and agriculture.

Scientific Illiteracy and the Partisan Takeover of Biology: A new article in *PLoS Biology* (April 18, 2006) discusses the state of scientific literacy in the United States, with special attention to the survey research of Jon D. Miller, who directs the Center for Biomedical Communications at Northwestern University Medical School. To measure public acceptance of the concept of evolution, Miller has been asking adults if “human beings, as we know them, developed from earlier species of animals” since 1985. He and his colleagues purposefully avoid using the now politically charged word “evolution” in order to determine whether people accept the basics of evolutionary theory. Over the past 20 years, the proportion of Americans who reject this concept has declined (from 48% to 39%), as has the proportion who accept it (45% to 40%). Confusion, on the other hand, has increased considerably, with those expressing uncertainty increasing from 7% in 1985 to 21% in 2005.

Kitzmiller judge among Time's 100: Judge John E. Jones III, who presided over the *Kitzmiller v. Dover* trial in which teaching “intelligent design” in the public schools was ruled to be unconstitutional, was named one of *Time* magazine’s “Time 100: The People Who Shape Our World.”

Excerpted from the National Center for Science Education Website (www.natcensci.ed.org)

Online Dictionary of Crystallography

The Dictionary Working Group of the Commission on Crystallographic Nomenclature (CCN) was set up during the IUCr Congress in Florence to provide guidance on the establishment and conduct of a project to develop an “online dictionary of crystallography”. The project is primarily confined to the subject of crystallography, but will include key definitions where crystallography interfaces with chemistry, physics, biology, materials science etc.. A pilot dictionary providing definitions for about 50 crystallographic terms has been set up by **Andre Authier**, the Chair of the Working Group, and **Brian McMahon**, the Research and Development Officer at the IUCr, with entries provided by members of the Working Group. It is now available to the community on the website reference.iucr.org/dictionary. It is envisaged that many additional definitions will be added over the coming months and readers are encouraged to send additional definitions, following the format guidelines described on the website, to **Paul Raithby** at the University of Bath, UK (p.r.raithby@bath.ac.uk), who is coordinating the inclusion of entries on behalf of the IUCr Commission for Structural Chemistry.

Paul Raithby

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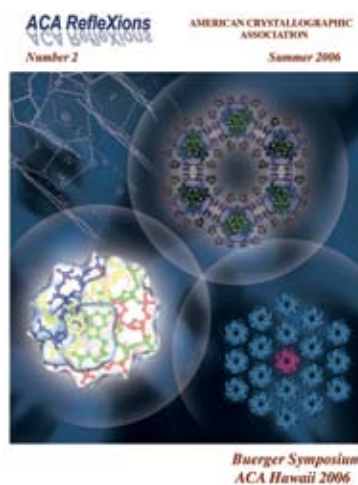
The Molecular Biology Consortium (MBC) is an organization of 10 academic institutions that operates the synchrotron beam line 4.2.2 at the Advanced Light Source (Berkeley) for macromolecular crystallography. The Cleveland Center for Structural Biology is interested in selling its share in this consortium. Shareholders have guaranteed access to beam time, approximately 16-20 days each year, and beam time is available in 2-day slots.

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Menachem Shoham

What's on the Cover and Behind the Scenes



Some representative images of structures done in the course of Helen Berman’s research career: hydration pattern around a dinucleotide phosphate-drug complex (1), crystal packing in a structure of a ternary complex among CAP, DNA and α CTD (2), crystal packing of a collagen peptide showing the extensive hydration (3), and a view down the helix axis of a

B-DNA helix (4). References are in order for the images starting at the upper left and moving clockwise.

1. Neidle, S., Berman, H. and Shieh, H.S. (1980) Highly structured water network in crystals of a deoxydinucleotide-drug complex. *Nature*, 288, 129-133.
2. Benoff, B., Yang, H., Lawson, C., Parkinson, G., Liu, J., Blatter, E., Ebright, Y.W., Berman, H.M. and Ebright, R.H. (2002) Structural basis of transcription activation: The CAP- α CTD-DNA complex. *Science*, 297, 1562-1566.
3. Bella, J., Brodsky, B. and Berman, H.M. (1995) Hydration structure of a collagen peptide. *Structure*, 3, 893-906.
4. Berman, H.M. (1997) Crystal studies of B-DNA: the answers and the questions. *Biopolymers*, 44, 23-44.

Background image for pages 6, 22, and 23 is from the cover of Acta D: The figure illustrates conservation of amino-acid residues in the active site of hyaluronidases from glycoside hydrolase family 56. L. K. Skov, U. Seppälä, J. J. F. Coen, N. Crickmore, T. P. King, R. Monsalve, J. S. Kastrup, M. D. Spangfort and M. Gajhed, Acta Cryst. (2006) D62, 595-604.

Elizabeth Armstrong Wood (1912-2006)



Following a very active life filled with many interests, Elizabeth A. Wood died March 23, 2006 of a stroke about a month after a pacemaker was installed. Born October 19, 1912 in New York City, she earned her BA at Barnard College and her MA and PhD in geology at Bryn Mawr College. Her

growing enthusiasm for crystallography was encouraged by A. Lindo Patterson who was then in the Bryn Mawr Physics Department. Betty became an instructor in geology at Bryn Mawr from 1934 to 1935 and again from 1937 to 1938. She was also an instructor in geology and mineralogy at Barnard from 1935 to 1937 and from 1938 to 1941, becoming a research assistant at Columbia University before joining the Physical Research Department at Bell Telephone Laboratories (BTL) in 1942 where she was the first woman scientist. She maintained an active crystallographic research program for the next 24 years at BTL.

Her interests ranged from the growth of single crystals with useful semiconducting, lasing, magnetic or superconducting properties to the crystallographic investigation of new materials with unusual properties such as the exhibition of both ferromagnetism and piezoelectricity. She also worked on material phases that could be changed by the application of appropriately oriented electric fields and on the formation of new superconductors. The ability to walk down the corridor and be able to consult with a world authority on almost any aspect of physics was a BTL hallmark; Betty was one whose advice was regularly sought by many of the most inventive minds at BTL including B. T. Matthias, W. L. Bond, R. M. Bozorth and L. H. Germer among others who are less well known to crystallographers.

BTL management greatly appreciated Betty, often asking her to undertake ceremonial duties. Among these was the opening of Picturephone service between three major cities in 1964, inaugurated with a call from Mrs. Lyndon B. Johnson in the White House to Dr. Wood at the Picturephone center in Grand Central Terminal, New York where she was graced by the presence of



Robert F. Wagner, the mayor of New York as seen in the Bell System photograph to the right.

As secretary of the American Society for X-Ray and Electron Diffraction

(ASXRED) in 1947 Betty, together with William Parrish who was secretary of the Crystallographic Society of America (CSA), issued an invitation on behalf of the two societies to the newly formed International Union of Crystallography (IUCr) to hold their first Congress and General Assembly in the United States at Harvard University. She met with other officers of ASXRED and CSA during the Congress to explore the possibilities of a merged society. Their resulting proposals were accepted by both societies, but not without vigorous discussion as feelings on the plan ran surprisingly high. The following year she, Isadore Fankuchen, Bill Parrish and Lindo Patterson drafted a Constitution for the proposed American Crystallographic Association that also met with formal acceptance. In 1957, she became the first woman president of the ACA; the second, Isabella Karle, was not elected until 1976.

She chaired the US delegation to the second IUCr General Assembly in 1957 and was a delegate to the tenth. She served on the Governing Board of AIP from 1963 to 1969, was on AIP's Visiting Scientist in Physics program 1961-1972 and the Commission on College Physics 1967-1971, and was Associate Director of the National Science Foundation project Physical Science for Nonscience Students 1965-1971. She was also an Advisory Board member of the School of Mathematics Study Group 1966-1969 and a member of the IUCr Commission on Crystallographic Teaching 1969-1972. A Fellow of the American Physical Society, she was also a member of AAPT, AAAS, Sigma Xi and the NJ Science Teachers Association among other societies. She was awarded a D.Sc. (*honoris causa*) by Wheaton College in 1963, Western College, Ohio in 1965 and Worcester Polytechnic in 1970.

Her reputation for clearly written texts spread as a result of her *Rewarding Careers for Women in Physics* (1962) and *Pressing Needs in School Sciences* (1969) published by the American Institute of Physics (AIP) in 1962. It became wider still with the publication of her *Crystal Orientation Manual* in 1963, which expounded the art and science of preparing shaped pieces of large accurately oriented single crystals for technicians and her 1964 *Crystals and Light: An Introduction to Optical Crystallography* under the auspices of the Commission on College Physics, written for students with no previous knowledge of crystals or light. That same year, *Experiments with Crystals and Light* came out in the Bell System High School Series as both a booklet and a kit. Five years later, her *Science for the Airplane Passenger* was published and proved very successful, appearing for many years in airport bookstores throughout the US and other countries. Her deep interest in improving the scientific understanding of the general public was recognized by the ACA's establishment of an Elizabeth A. Wood Science Writing Award. Its purpose is to honor the authors of outstanding publications that bring science to the attention of the general public. The first award was presented in 1997 to Nobel laureate Roald Hoffmann.

Betty's interests were not confined to science. For many years, she and her husband Sandy hybridized and raised the most beautiful irises in their large Murray Hill garden. She was elected president of the Garden State Iris Society and the Median Iris Society. She loved ocean sailing, putting her sailboat to regular use until a year or so ago. She was also a skilful thespian both

as actor and playwright. Her other interests included recording numerous textbooks for the blind over many decades. Her warmth and outstanding presence will be sorely missed by her many friends.

Sidney Abrahams

Editors note: Thanks are due to Betsy Booth and Ann Cooper for photos and background material. Following is a short note from ACA RefleXions co-editor Connie Chidester on her interactions with Elizabeth Wood.

I met Betty Wood at the 2000 ACA meeting in St. Paul, MN. The ACA Council had decided that it would be appropriate to celebrate the 50th anniversary of the ACA by honoring former ACA Presidents so, knowing that Betty Wood had given a charming talk on the occasion of the 25th anniversary of the ACA, I invited her to give the response on behalf of former presidents at the banquet. Betty's 25th anniversary address was included in *Crystallography in North America*, and it was reported that she received a standing ovation. I only wish that we had a transcription of her 50th anniversary talk! I do remember clearly that it was elegant, funny, and concise; that Betty's sense of timing was impeccable, and that once again she received a standing ovation. It was obvious that Betty had not yet made any major concessions to advancing age, although she did admit that she had reluctantly given up her sailboat the preceding summer. Her constant companion during the St. Paul meeting was her long time friend and colleague in crystallography, Robinson Burbank, also a former ACA President. Sadly, Robinson Burbank died in February. (*Spring 2006 ACA RefleXions*, p.22.)

Betty Wood and Lindo Patterson together formulated the constitution and by-laws for the ACA when the decision was made to join ASXRED and the Crystallographic Society of America. Betty was the first woman to serve as President of the ACA (in 1957). Betty wrote *Crystals and Light* a small monograph re-

cently reprinted, and *Science from your Airplane Window* (first published as *Science for the Airplane Passenger*), among other things. In 1997 the Elizabeth A. Wood Award was established in her honor. The guidelines state that the award should be given for "exceptional writing or commentary that brings science to the attention of a wider community." Recipients of this award so far have been: Nobelist Roald Hoffman in 1997, Robert Hazen in 1998, and Robert A. Weinberg in 1999. In 2001 the award was given to K.C. Cole, a science writer for the L.A. Times who wrote *The Universe and the Teacup* and *First You Build a Cloud*; in 2002 Ira Flatow, host of NPR's *Science Friday* received the award; and in 2004 the award went to Oliver Sacks, a physician and professor of neurology who wrote *Awakenings*, *The Man Who Mistook His Wife for a Hat*, and *Uncle Tungsten*.

Since 2000, I have corresponded with Betty once or twice a year, always concerning the Wood Award. The fund for the Wood Award is one of ACA's best endowed; it receives widespread support from ACA members, but I suspect that another reason for it's financial health is that Betty herself was a major donor. I regret that Betty did not approve of the choices made while I was on the Council – she felt strongly that the award should go to someone who had scientific credentials of the highest order, as well as outstanding ability to write for the layman. The Award is to be given again in 2007.. I wrote Betty to let her know that someone she had suggested in 2005, David Goodstein, professor of physics and vice-provost at Caltech and the author of *Out of Gas* was one of the final nominees, and that the other finalists also were distinguished scientists. (*Out of Gas* was reviewed in the Spring *ACA RefleXions*.)

Betty's niece Betsy Booth told me that about two weeks before her death, when Betty was still in the rehab center because of her car accident, she prepared and taped a marvelous talk which was then transcribed and read by a stand-in speaker before the Unitarian Church congregation. It would not surprise me in the least if that talk got (*in absentia*), a standing ovation.

Connie Chidester

Reuben Rudman (1937 – 2006)



Reuben Rudman died suddenly on February 15 in Jerusalem, Israel. He was born in New York and received an M.A. from Columbia (1957) and rabbinic ordination as well as M.H.L. from Yeshiva University (1959). He was awarded a Ph.D. in 1966 from Brooklyn Poly under the guidance of Ben Post. Reuben devoted his scientific career to crystallography: research; teaching; and serving the crystallographic community. His research interests included the systematic study of phase transitions exhibited by pseudo-spherical molecules supplemented by differential calorimetric investigations; instrumentation for low temperature x-ray diffraction both for single crystal and powder methods. He published more than 70 scientific papers in these fields. He served as chair and member of a number of committees of IUCr, ACA and Gordfon Research Conferences. He was professor of chemistry at Adelphi University for 35 years, where he taught general, inorganic and solid chemistry, and crystallography until his retirement in 2003.

His book: *Low-temperature X-ray diffraction. Apparatus and Techniques* published by Plenum Press, N.Y, was written during his sabbatical in Israel 1973-74, where he served as a visiting professor at the Institute of Chemistry of the Hebrew University Jerusalem. He returned to the Hebrew

University again after his retirement and volunteered to teach x-ray crystallography to graduate students until his sudden death.

Reuben was beloved by his many friends and colleagues, he was an excellent teacher highly appreciated by his students. He is survived by his wife Idelle, five children, grandchildren and a great-granddaughter.

Mayer Itzhak and Shmuel Cohen

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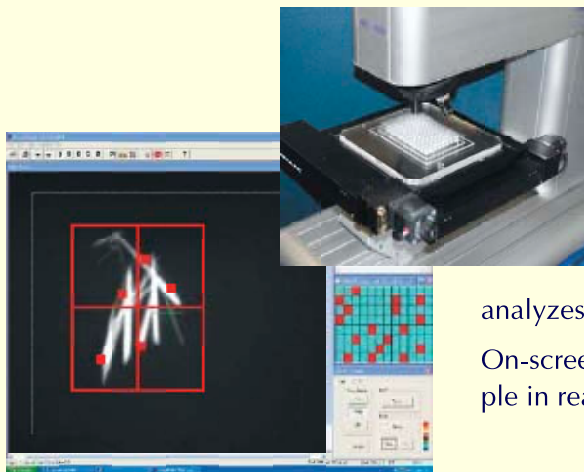
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Reminder: Art in Crystallography Prize

In 2005 the Editors announced a new competition open to all ACA members: **Art in Crystallography**, sponsored by ACA *Reflexions*, together with the ACA Council. Entries are accepted in the form of images emailed to either of the Editors (conniechidester@earthlink.net or flippen@rcsb.rutgers.edu). Each entry should be accompanied by a paragraph explaining the science and the method of producing the image. We would appreciate receiving a photo of the artist as well, but this is not required. The winning entries will be posted on the web, and there will also be a display of printed images at an ACA Meeting. We will also feature some of the images in *Reflexions* from time to time. Judging will be by a panel appointed by the Editors; please let us know if you are interested in being a judge.

The first winners were announced in 2005 and were featured at the ACA meeting in Orlando. A silent auction for the framed photos of the entries raised money for the ACA Student Travel Fund. Because of the costs involved with setting up the exhibit at the meeting we decided not to do it in Hawaii but the exhibit will be back at the ACA meeting in Salt Lake City in 2007.

You can also enter the photo contest for photos to appear on the cover of *Crystal Growth and Design* which began monthly publication in January 2006 (see ACS ad on page 31). The same photo can be entered in both competitions

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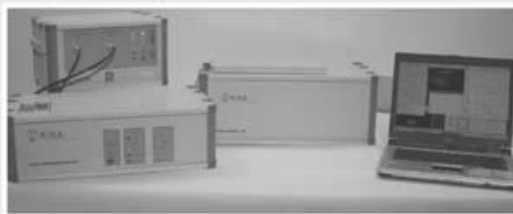
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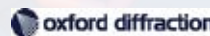
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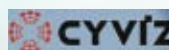
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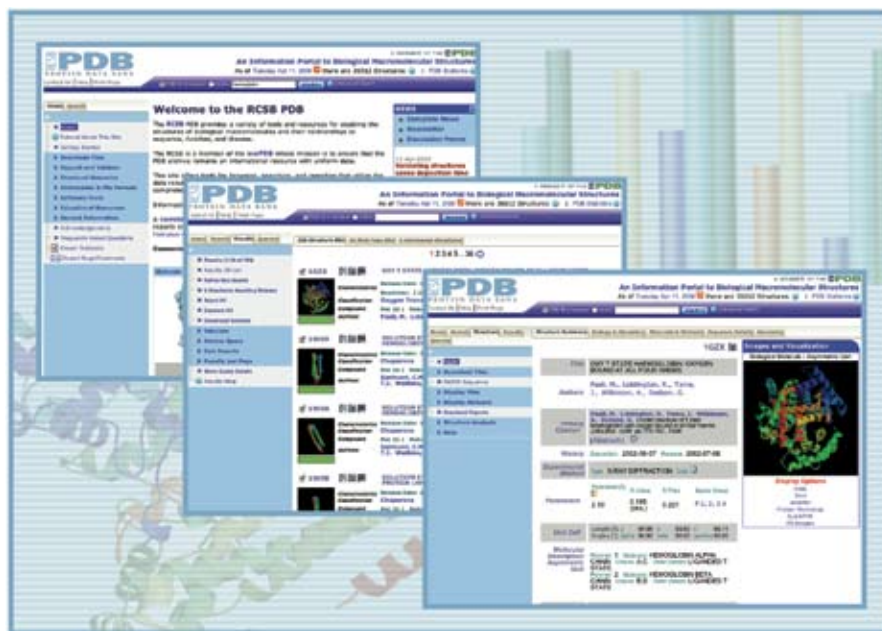
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New RCSB PDB Website

On January 1st the RCSB PDB released its revised website and launched an extensive suite of new tools for data access and visualization. New features include a redesigned advanced search interface, improved ligand searching, integration of SCOP and CATH, and a new sequence visualization tool. In addition to the traditional search mechanisms, users may now browse the database using hierarchical navigation schemes such as Gene Ontology, enzyme classification, disease, genome location, and structural classifications. Histograms highlighting select features of PDB content provide an up-to-date qualitative snapshot of the entire repository. These histograms include experimental parameters, such as resolution, R-free, as well as structural features such as residue count, atom count and formula weight.

The new website also includes several structure visualization tools such as KiNG, QuickPDB, Jmol and a new high-end graphics molecular viewer called Protein Workshop. These tools are fully integrated with the website and require no installation beyond the current release of Java™. Protein Workshop, built by the RCSB PDB group, includes a mechanism for saving high-resolution structure images for posters and publications. Included in the suite of visualization programs is a 3-D Ligand Interaction Viewer that highlights user-selected ligands with respect to interactions with neighboring protein chains and other ligands. The chemical structure of ligands as a canonical 2-D representation can also be studied using the Ligand Structure viewer. This viewer also presents chemical formula and SMILES string representation.



The PDB team has initiated several enhancements, based on user requests. These will deploy iteratively over the next few months.

Enhancements include:

1. Additions to the ligand viewer
2. New features to sequence visualization
3. An overlay feature for Protein Workshop
4. More tutorials
5. A better sequence alignment tool for FASTA and BLAST searches on the PDB database.

Jeff Milton

BioSync is Alive and Growing



BioSync (Structural Biology Synchrotron Users Organization) was formed in 1990 as a grassroots organization intended to promote access to synchrotron radiation. One of their goals was to organize a web-based clearing house of beamline information. BioSync (BioSync.rcsb.org): A structural Biologist's Guide to Synchrotron Facilities was the result. The site, originally designed and hosted by USCD/SDSC, is now being maintained by the RCSB PDB.

The site, with a new look, currently contains updated beamline descriptions for operational US synchrotron beamlines used for single crystal macromolecular crystallography. International sites and beamlines are listed and will go 'live' as data are added for each one. PDB deposition statistics, cross-linked to the structure summary pages in the RCSB PDB, grouped by site and beamline, are also available.

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Marv Hackert, Vice-President

Professor of Chemistry and Biochemistry, Associate Dean of the Graduate School, University of Texas, Austin, TX 78712.

Education: B.S. Chemistry, Central College, 1966; Ph.D. Physical Chemistry/Crystallography, Iowa State, 1970 with Bob Jacobson; Postdoc, Purdue University (1970-1974) with Michael Rossmann.

Professional Activities: USNCCr (1993-2002), Chair Elect / Chair (1996-2002); IUCr—Commission on Macromolecules (2002-2005); ACA—Co-Chair (with Ray Davis) of Local Committee for ACA meeting in San Antonio (2002), Member Local Committee, ACA meeting in Austin (1987); ACA Publications Comm. (1988-91, Chair 1991); ACA Service Award (1992); Member BioMac SIG (Sec-Treas. 1986-89, Chair 1991-92); Advisory Council UCSD Multiwire Area Detector Facility (1986-1995). **Other Administrative Experience:** Chair - Dept of Chem. and Biochem. (1995-2000); Faculty Council (2000-2005, Chair 2003-04); Graduate Assembly (1989-1995; Chair 1991-92); Director – Biochemical Institute (1995-present); Assoc. Dean of the Graduate School and Director of Faculty Development Programs (2005-present).

Research Interests: Structural biology of macromolecules with particular interests in PLP- and pyruvoyl- dependent enzymes in polyamine metabolism, and the structures, function and evolutionary relationships among members of the 4-OT superfamily of proteins.

Candidates for ACA offices in 2007

The Nominating Committee has selected the following candidates for the 2006 elections for ACA offices in 2007

Vice-President: Marvin Hackert and Bernard Wuensch

Treasurer: Charlotte Lowe-Ma and Bernie Santasiero

Standing Committees:

Communications: Qun Shen and Alice Vrielink

Data, Standards & Computing: John Rose and Winnie Wong-Ng

Continuing Education: Bill Furey and Jeanne Stuckey

2006 Nominating Committee:

Wayne Anderson (Chair), Fran Jurnak and Brian Toby

To nominate write-in candidates for any of these offices, write to the ACA Secretary: Lisa J. Keefe, IMCA-CAT, Sector 17, Bldg. #435A, Advanced Photon Source, Argonne National Laboratory, 9700 South Cass Ave., Argonne, IL 60439. (Fax: (630) 252 0521) Letters must be received by September 15, 2006 and must be signed by 5 supporting ACA members and include a signed statement by the candidate describing his or her qualifications. Statements from all candidates will be included with the ballots which will be sent to all members in October 2006.

Statement: I am honored to stand for election as your next Vice-President. The ACA means a lot to me – it is both an important scientific organization and a fraternity of scientific friends and colleagues. In the nearly forty years that I have been part of the ACA, I have seen it grow from a relatively small, low-budget operation that met on university campuses where attendees were housed in dorms, to a larger, more professional organization with over two thousand members and annual meetings attended by nearly 1000. Our larger size has enabled us to hire staff responsible for taking care of many of the day-to-day business matters of the organization, thereby enabling the Vice-President and President to concentrate on administrative and policy decisions.

The Vice-President's duties are to serve as a member of the ACA Council, serve as an ACA representative on the USNCCr, assist the President in making policy decisions for the organization, provide input for the site selection for our annual meetings, and assist in the staffing of various committees.

As your Vice-President, I would seek to use my breadth of research and administrative experience to assist the ACA in meeting its goals while at the same time working to ensure that the ACA serves

the needs of all its members. The ACA has always been an inclusive organization – recognizing the central role that structure determination plays in a wide variety of fields and appreciating the benefits that we all gain from our interactions with each other at our annual meetings.

Much of the growth in the ACA occurred with the growth of macromolecular crystallography, but numerous other areas have emerged as well. It is exciting to see that new applications and new imaging methods continue to be active areas of research. The SIGs emerged in the 1980's. They have provided not only a voice for the many special interest groups within the ACA, but have also become a tremendous asset to the officers of the ACA in running the organization and planning our annual meetings. As Vice-President of the ACA, I will work to make sure that SIGs remain a strong voice in the affairs of the ACA.

Our annual meetings need to remain the centerpiece of our efforts. Their success has always been due to the dedication of our members who readily step up to the plate when asked to help organize sessions, serve on committees, and volunteer their time and expertise in a variety of ways. My experience on the local committees of two ACA meetings will serve me well when making future decisions to ensure that our

annual meetings are intellectually stimulating, a good value for our members, and a means to attract new members. I would work to promote joint meetings involving other organizations as appropriate.

The ACA needs effective means of communicating to ensure that its members can voice their concerns so that their needs can be met. Expanded use of the internet and our web site for disseminating information will provide better access to resources and data that our members need.

The ACA also plays a role in representing the interests of US crystallographers in the world community by working with the USNCCr. The experience gained from nine years service on the USNCCr and efforts at three General Assembly meetings of the IUCr will help me to represent your interests in the international community as well as build on our past efforts to reach out to fellow crystallographers in Latin America.

Finally, the ACA should place a high priority not only on training and educating future generations of crystallographers, but also on providing professional development services to help promote the training and careers of our young scientists. This can be in the form of training sessions at our annual meetings, workshops or summer courses, or by expanding our web site services for such purposes. I also believe that there is much to be gained by exploring new ways to utilize the experience of our senior members to help mentor our younger members.

I close by repeating that it is an honor to stand for election as your next Vice-President and that, if elected, I will do my best to represent all ACA members and be a strong advocate for their interests.

Bernard Wuensch, Vice-President

Professor of Ceramics, Dept of Materials Science and Eng, MIT, Cambridge, MA 02139

Education: S.B., Physics, MIT (1955); S.M., Physics, MIT (1957); Ph.D., Crystallography, MIT (1963).

Professional Activities: Asst. Prof. of Ceramics, Dept of Mat. Sci. and Eng., MIT (1964-69), Assoc. Prof. (1969-74), Prof. (1974 -); TDK Mat. Sci. and Eng. (1985-90). Director, Center for Mat. Sci. and Eng. MIT (1988-93); Acting Head,



Dept of Mat. Sci. and Eng. MIT (1980). Saabbaticals: Visiting Prof., Universität Saarland, Saarbrücken (1973); Physicist, Max Planck Institut für Festkörperforschung, Stuttgart (1981).

Member, USNCCr (1980-82, 1989-94); Alternate Delegate to IUCr XII Ottawa (1981), Delegate to IUCr XVI Beijing (1992). **Editorial Activities:** Co-Editor (with J.M. Cowley, J.B. Cohen and M.B. Salamon) "Modulated Structures – 1979" *AIP Conference Proc.* 53 (1979); Co-Editor (with D.A. Neumann and Thomas P. Russell) "Neutron Scattering in Materials Science" *Mat. Res. Soc. Symp. Proc.* 376 (1995). Advisory Editor, *Physics and Chemistry of Minerals* (1976-85); Associate Editor, *Canadian Mineralogist* (1978-80); Editor, *Zeitschrift für Kristallographie* (1981-88); Editor, *Journal of Ceramic Processing Research* (2000-). **Honors and Awards:** Ford Foundation Postdoc (1964-66); Fellow, Mineralogical Soc. of America and American Ceramic Soc. (Outstanding Educator Award 1987); Honorary Doctorate of Engineering, Hanyang University, Seoul, Korea (2003).

Research Interests: Crystal chemistry of sulfide and sulfosalts minerals, materials synthesis and crystal growth of inorganic materials: chalcogenides, silicates and oxides. Structure-property relations in materials such as measurement of self-diffusion, impurity diffusion and grain-boundary diffusion in high-purity single crystals of oxides. Connection between disorder, composition and temperature and the transport properties of fast-ion conducting chalcogenides, and of oxides of interest in solid-oxide fuel cells and

oxygen sensors. The measurement of site occupancies, anisotropic and anharmonic temperature factors as a function of temperature and composition in our recent studies has provided remarkable insight into the mechanism and magnitude of ionic conduction.

Statement: I am one of the few graduates of an American academic institution (other than the U of Pittsburgh!) to have received a doctoral degree specifically in crystallography. My interests in our field began with study of solid state physics and research that introduced me to the growth of ionic crystals from melts and characterization of the products through use of optical properties and x-ray diffraction. I was hooked! I knew what I wanted to do! In a day when the boundaries between disciplines were not nearly as permeable as they are today, one could petition a Dean to establish a special interdepartment committee to supervise study in an interstitial (so to speak) discipline. And so it was that I came to work for a doctorate in crystallography in the laboratory of Martin Buerger. My committee members constituted a daunting collection of crystallographers in a broad range of departments: B.E. Warren of Physics, Dave Shoemaker from Chemistry and F.H. Norton in Metallurgy. They taught me crystallography from an amazingly broad perspective and, given their stature within our field, instilled a strong dose of humility as well. This was an exciting period as "modern" crystallography was emerging. The first counter diffractometers were just coming into use, and IBM had donated a 704 computer to MIT that batch-processed punched cards. Such progress has continued and is reported, as it should be, in the meetings and publications of the ACA.

I am both flattered and humbled by the invitation to be considered as a candidate for Vice-President. Our society is extremely well administered. Small-molecule crystallography is a strong component of our programs, as is the exciting progress in protein analysis – study of the very fabric of life itself. Other sessions are devoted to instrumentation and reports on the capabilities and status of new instruments and radiation sources under development in our national laboratories. All of this is essential and must continue. It would be presumptuous to suggest or identify matters that are not handled well or that

should be done differently.

From the perspective of one with crystallographic interests that are unabashedly inorganic and non-metallic, I would, however, make a few observations that have given me pause for thought. At the Beijing IUCr Meeting (admittedly, a meeting to which travel was expensive) the session on mineralogical crystallography was the largest and the one most heavily attended. As I recall, however, there were only two contributions from the US (one of which was mine). Where are the mineralogists and earth scientists at ACA Meetings? In 1994, Tom Russell, Dan Neumann and I organized a session entitled "Neutron Scattering in Materials Science" for the meeting of the Materials Research Society in Boston. It attracted 146 contributions that filled thirteen sessions and led to an 800-page volume as the symposium proceedings. Why are these colleagues not more strongly represented in the ACA and, in particular, the Materials Science SIG.

My final observation is also anecdotal. I attended my first ACA meeting with Charlie Prewitt and Charlie Burnhan. Cruising the hospitality suites shortly after they had opened (as graduate students continue to do) we spotted a gentleman sitting by himself on a sofa. "Isn't that Patterson?!" one of the Charlies exclaimed. "Let's ask him how the Patterson function was *really* discovered." (We had heard two very different stories – one from Bert Warren and one from Martin Buerger.) We drew straws. I lost. With a lump in my throat and heart pounding, I approached the sofa, introduced myself and inquired whether we could presume to ask how he had arrived at this discovery. Patterson responded warmly and invited us to join him. He spent over half an hour with us despite our lowly stature in the ACA. (Unfortunately, space does not permit me to share his response.) My point is that the ACA has always been a warm and welcoming organization, making newcomers and especially graduate students feel at home and permitting them to meet even the most prominent crystallographers. This has become more difficult as the Association has grown larger, but I feel that it is important that we work to retain and improve this ambience, especially if we are to attract bonafide crystallographers who do not regularly participate in our meetings.

Charlotte Lowe-Ma, Treasurer



Currently undergoing a career transition. Formerly employed at Ford Motor Company Research & Advanced Engineering, Dearborn, MI, and Naval Air Warfare Center, Chemistry, China Lake, CA.

Education: Ph.D. in Chemistry, California Institute of Technology, Pasadena, CA. B.S. in Chemistry with Academic and Departmental Honors, California State University, Los Angeles, CA. Fellow of the International Centre for Diffraction Data (2000). Naval Air Warfare Center-Weapons Division Fellow (1993).

Professional activities: USNRC Board of Assessment sub-panel for NIST's Center for Neutron Research (2001-2003), Chair of the Governance Committee of the AIP (2002-2003), Governing Board of the AIP (1995-2004), Executive Committee of the AIP (1999-2000), Board of Directors of the ICDD (1994-1998), Secretary of the ACA (1994-1996), AIP Advisory Committee for the *Industrial Physicist Magazine* (1996-1999), appointed by Commander Naval Weapons Center as Chair of the Naval Weapons Center Ionizing Radiation Control Committee (1990-1994), ICDD Scholarship Evaluation Committee (inception to present), Volunteer for the Ford High School Science & Technology Program (1998-1999), Volunteer editor of the ICDD Explosives and Related Materials Index of the Powder Diffraction File, Chair of the ICDD Task Group on Calculated Pattern Intensities (1992-1997), USNCCr (1995), Chair of the ACA Applied Crystallography (Materials) SIG (1994, 2000-2003), Chair of the ICDD Organic and Forensics Subcommittee (1992-1994), Chair of ICDD

Target Systems Task Group to improve the quality of powder diffraction data available for propellants and explosives (1988-1992).

Statement: I am honored to be selected as a candidate for Treasurer of the ACA. The ACA is a warm and welcoming scientific society providing very interesting and informative scientific programs at its annual meeting. By serving the ACA as Treasurer I would hope to return to the ACA some of the value that I have derived over the years as a member. I view the position of Treasurer as having a serious responsibility for insuring that the ACA can continue to provide good value to its members while also continuing to provide forums for effective scientific interchange.

My background is as a small-molecule crystallographer who broadened out to include materials characterization. In my most recent position at Ford as a technical leader, I led a series of cross-functional research projects involving materials characterization in the area of catalysis in addition to initiating a project in high-throughput materials discovery in heterogeneous catalysis. My research interests were in applying data mining techniques to complex scientific and powder diffraction data. Besides automotive catalysts, my career has included examining a variety of materials important to the military and the automotive industry. These materials included automotive components, high-temperature superconducting materials, long-wavelength infrared-transmitting optical sulfides, organic propellants and explosives, non-linear optical materials, and quasi-one-dimensional conductors. I have benefited from discussions at ACA meetings on a range of topics related to these various materials.

One of the strengths of the ACA is the member involvement through SIGs that enables ACA meetings to support a broad range of topics in crystallographic techniques and different materials – breadth that facilitates lively interchanges and cross-fertilization of ideas. As treasurer I would work to help the ACA continue to financially support SIG suggestions for discussions of crystallographically-relevant topics. I enthusiastically welcome the opportunity to serve the ACA in remaining a strong, inclusive, and scientifically effective organization.

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Bernard D. Santarsiero, Treasurer



Research Professor, Center for Pharmaceutical Biotechnology, University of Illinois at Chicago, Chicago, IL 60607.

Education: B.S., Chemistry, Harvey Mudd College (1975). Ph.D., Physical Chemistry, University of Washington (1980).

Professional Activities: Member ACA, ACS, Protein Society; ACA Apparatus and Standards Committee (1997-1999); Structural Biology Review Board, NASA (1998-2002); SER-CATAutomation Committee (2002-present); Co-founder and Consultant, Syrrx (1996-2002); Local co-chair, ACA Annual Meeting Chicago 2004; Instructor, ACA Crystallography Summer Course (2002-2004); Manager, Information Technology (2003-present); Director, Small Molecule X-ray Diffraction Facility (2003-present); Co-director, Macromolecular Structure Facility (2004-present); Science Advisory Board, Shamrock Structures (2003-present); Secretary, Gerber-Hart Library (2005-present); U.S. National Committee for Crystallography (2006-2009).

Research Interests: My research spans four major themes: structure-based drug design of therapeutics against disease, identification of natural products as chemopreventative and anti-cancer agents, manipulating of enzymes to modify

specificity, stability, and reactivity, and the development of enabling technologies in biological and chemical crystallography for high-throughput structural genomics.

Statement: The ACA Treasurer serves the membership by overseeing the financial commitments of the organization and as a representative on the council. The ACA is in excellent financial shape after a decade of strong leadership. We continue to keep membership dues and conference costs low while still providing the resources necessary to host interesting annual meetings by choosing meeting sites wisely and organizing excellent scientific programs. The council continues to do a good job in broadening the appeal of membership in the ACA, and in fostering the education of physical, chemical, and biological crystallography on a national and international scale. I am a strong advocate for education, sustained government support of our research, and the continuing vision of molecular structure as a unique portal towards the understanding of function, reactivity, and energetics in physical, chemical, and biological systems. On a personal level, I have been a member of the ACA for over twenty years, and thoroughly enjoy attending the annual meetings with old colleagues and new acquaintances. It is an honor to be nominated, and, if elected, I look forward to “giving back” something to the organization.

John P. Rose, Data, Standards and Computing



Associate Professor of Biochemistry and Molecular Biology, University of Georgia, Athens, GA 30602. Assistant Director, Southeast Regional Collaborative Access Team, Advanced Photon Source, Argonne National Laboratory.

Education: Ph.D. (1980) in Physical Chemistry, Rutgers University, Newark NJ with Roger A. Lalancette, B.A. in Chemistry (1974) Benedictine College, Atchison KS.

Professional activities: ACA Member, Local organization ACA Annual Meeting, Pittsburgh (1992), Poster Chairman ACA Annual Meeting, Pittsburgh (1992), Tutor ACA Summer Course for Crystallographers (1992-2001), Lecturer ACA Summer Course for Crystallographers (1997-2001), Consultant Protein Data Bank (1989-1999), Member APS Users Organization Steering Committee (2001-2004), Director Bioinformatics Core, Southeast Collaborative for Structural Genomics (2000-2006), Chairman APS MC Proposal Review Panel (2006-).

Research interests: Methods development in macromolecular crystallography in the areas of soft x-ray data collection and phasing, Sulfur-SAS structure determination, high throughput methods for structural genomics, data validation, archiving, and visualization, remote systems for synchrotron data collection.

Statement: As crystal structure determination becomes a more general tool for the scientific community it is imperative that structures are validated against strict standards and all information describing the experiment is recorded. In addition, the explosion of structural information available via the web also calls for reliable and validatable data standards. My experience as a producer of structures, PDB annotator and consumer of structural information has given me a unique perspective on data validation, archiving, and visualization, which should be of benefit to the ACA. I am also a firm proponent of open-source software and feel that at times science is limited by access to the “best” software due to its cost.

Winnie Wong-Ng, Data, Standards and Computing



Senior Research Scientist, Ceramics Division, NIST, A256 MATLS, 100 Bureau Drive, Mail Stop 8520, Gaithersburg, MD 20899

Education: B.Sc., Chemistry, Chinese University of Hong Kong (1969). Ph.D., Inorganic Chemistry, Louisiana State (1974) with Steve Watkins; Postdoctoral fellow/Research Associate/Lecturer in Chemistry Department, University of Toronto, Canada, with Stan Nyburg.

Professional Activities: Local Chair, 1998 ACA annual meeting, Arlington, VA; Chair/Member, ACA Continuing Education Committee (2001-2003); secretary/treasurer, USNCCr, (2000-2003); Chair, ACA Warren Award Committee (2005); Chair/Member: ACA Nominating Committee (2002-2003); Co-organizer of four ACA scientific sessions (1989, 1992, 1993, 1998); Co-organizer of more than 20 symposia/workshops at various other scientific meetings; Chair, Membership Committee, International Centre for Diffraction Data (ICDD, 2001-2004); Chair, Ceramics Subcommittee, ICDD (1994-2000); Editor, international report section of Powder Diffraction (1999 - present); Chair, McMurdie Award Committee, ICDD (2006); Chair, Electronics Division, American Ceramic Society (2005-present); about 250 publications.

Research Interests: Crystallography, crystal chemistry, phase equilibria, and structure/property relationship of high temperature materials; standard reference materials; reference x-ray powder

patterns/data; single crystal and powder diffraction crystallography; high-temperature x-ray diffraction; superconductors; thermoelectric materials.

Statement: I am delighted to accept the nomination to this important ACA committee. Having worked at NIST for almost 20 years and having been involved in the development of two standard reference materials related to x-ray diffraction, I appreciate the importance of data, standards and computing to every day crystallographic research.

In my view, four particular activities would be important to pursue. Firstly, due to the advent of computer technology, an increasing amount of crystallographic software is available, and it is important for software developers to maintain adequate documentation and to make available the source code so users can make modifications for local needs. Secondly, in addition to the availability of macromolecular information from high throughput techniques, a vast volume of other diffraction data will soon be available due to the increasing importance of the combinatorial approach in materials research, an area that I am also involved in nowadays. To be able to access this large volumes of diffraction data, various computational strategies and standards are critical for data collection, storage, transport and exchange. Thirdly, communication and cooperation between creators/producers of crystallographic databases and those responsible for databases of other properties is important in order to maximize research opportunities for users. Fourthly, user training in utilizing various databases, in recognizing existing standards and in using various crystallographic computing software is critical for crystallographers in today's computerized world.

If elected, I would work with the Committee and the ACA to push forward the above activities, namely: encourage cooperation between various database producers; encourage software developers to maintain good documentation; promote crystallographic informatics as an area of importance; and encourage the ACA to continue organizing workshops/symposia to address applications and issues related to data, standards and computing topics, in both macromolecule and small molecule crystallography.

William Furey, Continuing Education



Professor, Department of Pharmacology, University of Pittsburgh School of Medicine, Pittsburgh PA 15261

Education: B.A. Chemistry (1974) Rutgers University; Ph.D Physical Chemistry/Crystallography (1977) Rutgers University; Postdoctoral Research Associate (1977-1981) University of Pittsburgh Department of Crystallography.

Professional Activities: Research Assistant Professor (1982-83) University of Pittsburgh Dept. of Crystallography; Adjunct Assistant Professor (1983-87) University of Pittsburgh Dept. of Crystallography; Assistant Director Biocrystallography Laboratory (1987-2002) VA Medical Center; Adjunct Associate Professor (1987-93) University of Pittsburgh Dept. of Crystallography; Chairman, ACA Committee on Crystallographic Computing and Data (1987 & 89); Organizer and Instructor for NIH sponsored workshop on "Application of Supercomputers for Refinement of Macromolecular Structures," Pittsburgh Supercomputer Center (1988); "Core" instructor at Cold Spring Harbor Protein Crystallography Course (1990-present); Session Chair or co-chair at ACA meeting sessions on Crystallographic Computing, Difficult Structures, and Protein Phasing (1990, 2001 & 2005, respectively); Adjunct Professor (1993-99) University of Pittsburgh Dept. of Crystallography; Nine-time participant in NIH Study Section Review panels, chairing one session, since 1993. Workshop organizer and instructor for "Isomorphous Replacement Methods in Macromolecular Crystallography", ACA

Workshop, Atlanta, Ga., (1994); Elected Secretary/Treasurer of ACA Biological Macromolecule SIG (1994); Instructor National Research Council sponsored joint US-Mexican course on Protein Crystallography, Mexico City, (1995); Session Chairman, Gordon Research Conference on Diffraction Methods, 1996; Instructor NIH sponsored workshop on Protein Phasing Methods, Pittsburgh Supercomputing Center (1997); Instructor at ACA Summer Schools (1998 & 2005); Visiting Professor of Pharmacology (1999-00) University of Pittsburgh Dept. of Pharmacology; Full Professor of Pharmacology (2000-03) University of Pittsburgh Dept. of Pharmacology; Director Biocrystallography Laboratory (2002-present) VA Medical Center; Instructor European Molecular Biology Crystallography Course, Heidelberg, Germany (2002); Full Professor of Pharmacology with tenure (2004-present) University of Pittsburgh Dept. of Pharmacology; Co-Director X-ray Crystallography Laboratory (2006) University of Pittsburgh Dept. of Structural Biology.

Research Interests: Determination and analysis of structure-function relationships in macromolecules of biological interest, including thiamin diphosphate dependent enzymes, bacterial toxins, and cell cycle regulating enzymes. Development of techniques for the structural analysis of macromolecular crystal structures. Application and development of computing techniques and algorithms for understanding biological function on a molecular level.

Statement: The detailed structural information obtainable by x-ray crystallography is extremely valuable in furthering our understanding of biological processes, and especially in the case of large molecules such as large proteins or assemblies, and is generally unobtainable by other techniques. While there is no doubt that technical, theoretical, and computer speed improvements have simplified and accelerated the structure determination process to the point where in favorable cases novices can often solve protein structures, it is also clear there will always be difficult problems ahead that likely will not yield to "black box" automated approaches. The challenge is to insure that the next generation of crystallographers will know what to do in these situations. This will require

properly educating new crystallographers on the basics, i.e. what's really happening inside the black box, and how to assess the results. In addition, the major journals are now placing less and less emphasis on experimental and processing details, often banishing the crystallographic data and procedures critical in evaluating a paper to an archive, or not making them available at all! This makes the need for a fundamental understanding of crystallographic basics all the more important, since one must be able to assess the accuracy of the analysis and conclusions from very few published values or from a PDB entry alone. I will work to promote and participate in additional workshops/courses dedicated to teaching new crystallographers diffraction basics along with applications, and not just "what buttons to push" on whatever is the current breed of automated software followed by the "pray that it works" approach

Jeanne Stuckey, Continuing Education



Research Assistant Professor, Life Sciences Institute, Department of Biological Chemistry and Biophysics Research Division, University of Michigan, Ann Arbor, MI 49109-2216.

Education: B.A. Science, University of Findlay (1986); Ph.D. Biochemistry, Wayne State University School of Medicine (1992); Post-doctoral Fellow, University of Michigan with Mark Saper and Jack Dixon.

Professional Activities: Member ACA since 1987. Member of ASBMB and of the LS-CAT end station equipment committee.

Also, member of the University of Findlay Board of Governors (1992-1999).

Research Interests: Cancer; Biochemistry; Structure-based drug design, high-throughput crystallization and structure determination; automated visualization methods for protein crystal growth.

Statement: I am both delighted and honored to be nominated for the Continuing Education Committee. Education has always been near and dear to my heart. I have a love for teaching and a desire to explain complex ideas in simplistic terms. In my position as Managing Director of the University of Michigan's Center for Structural Biology, I have been able to teach aspects of x-ray crystallography to local elementary students and community groups as well as undergraduates, graduates and post-doctoral fellows. In addition, this position has afforded me the opportunity to bring x-ray crystallography to non-structural biologists ranging in research interests from toxicology to engineering. I am always going back to the basics and am well aware of how important it is to have reference materials, both on-line and hardcopy, available for teaching crystallography. In the age of plug-and-play, making sure scientists new to the field of crystallography understand and appreciate the details of structure determination and analysis is key to the integrity of the structures in the literature and databases. Having these materials readily available to increase their learning potential is vital. As a member of the Continuing Education Committee, I will bring my knowledge gained from these interactions to aid in the development of readily accessible teaching tools.

Although books and on-line materials are essential for learning, nothing can beat sitting at an ACA meeting and talking to the people that developed the technique, program or overcame that twinning problem. I have fond memories of attending the ACA annual meetings during graduate school and found it to be a vital component of my crystallographic education. The ACA meetings provide a welcoming environment, especially for students and post-docs, to speak with more experienced members and learn the little tricks/tips that can make or break their project. As a member of the Continuing Education Committee, I will work with the committee to foster more

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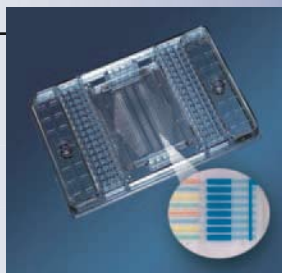
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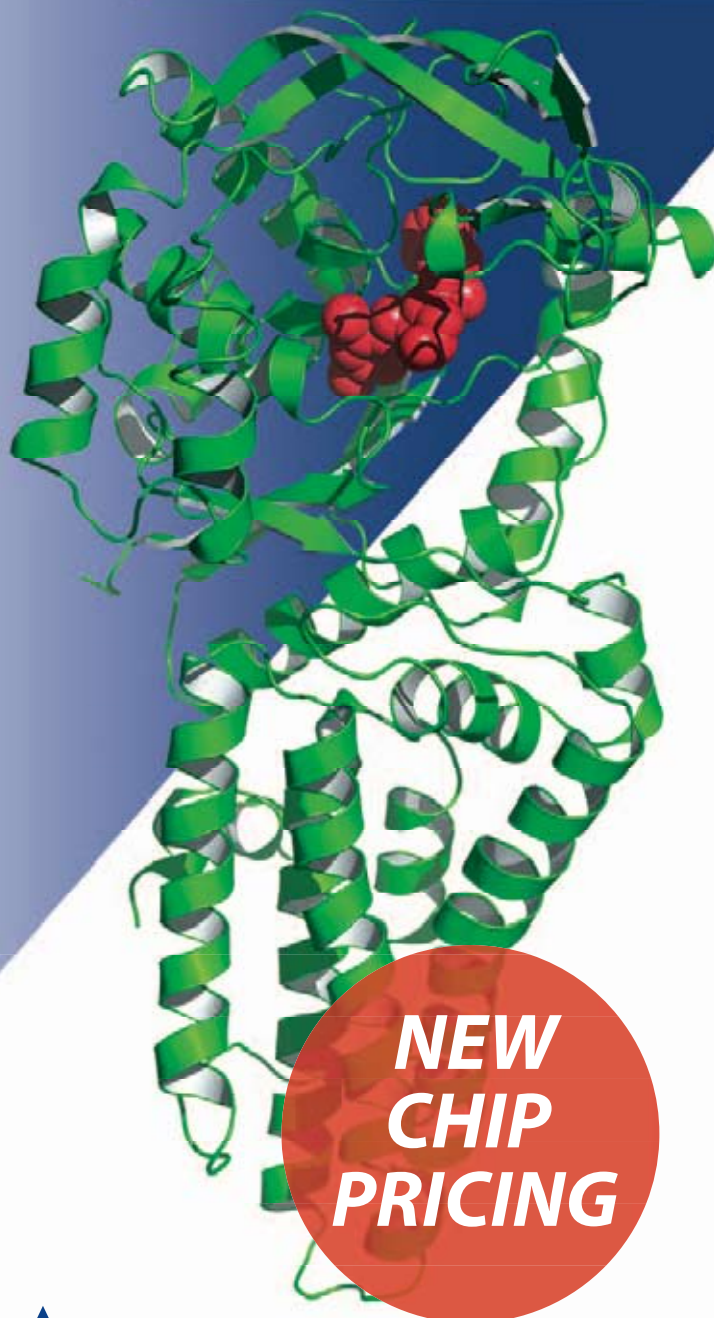
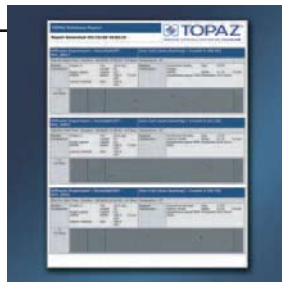
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of these interactions through workshops and special sessions and help find ways to attract more students to the ACA meetings. I thank you for the nomination and look forward to serving you.

Qun Shen, Communications



9700 South Cass Avenue, Bldg.401/B3170, Argonne National Laboratory, Argonne, IL 60439

Education: BS, Physics, Peking University (1981), PhD Physics, Purdue University (1987), 1987-89, Postdoc, Applied Physics, Cornell University (1987-1089)

Professional Activities: Recipient of the 1988 S.S. Sidhu Award of the Pittsburgh Diffraction Society, 2004 Distinguished Alumnus Award from the School of Science, Purdue University, and Fellow of the American Physical Society (2005). Head of microscopy and imaging group at the APS.

Research Interests: X-ray physics of materials, crystallographic phasing methods, and development of advanced synchrotron x-ray techniques. Phase retrieval from x-ray diffraction patterns of both crystals and nonperiodic specimens, and applications of lens-based x-ray microscopy and phase-contrast methods in crystal diffraction for high-resolution imaging of strain-field and defects.

Statement: It is indeed an honor to be nominated to stand for election to the ACA Communications Committee. Communications are vitally important in any society. As a synchrotron x-ray physicist for more than twenty years, I have witnessed and have been personally involved in the explosive growth of biological crystallography. Today's crystallography covers a diverse scientific community ranging from hard and soft materials scientists and engineers to molecular biologists and biochemists, and from synchrotron beamline scientists to applied mathematicians and computer software developers. This diversity is a necessary part of the growing importance of crystallography, but at the same time presents challenges to everyone in the community, in terms of how to best communicate ideas and results and how to communicate with each other and keep society's interests alive. With new technical developments on the horizon in closely related fields such as microscopy and imaging, and with ever expanding crystallographic applications in more non-expert research areas, I would be thrilled to have a chance to work with others on more effective communication approaches to address the challenges we face today and will face in the future.

Education: BSc Chemistry, University of Calgary (1982); MSc Physical Chemistry, University of Calgary (1986); PhD Physics, Imperial College of Science and Technology, University of London (1989); Diploma of Imperial College in Crystallography (1989); Postdoctoral Fellow: (i) Imperial College, London (1989 – 1990) with David Blow, (ii) University of California Los Angeles (1990 – 1992) with David Eisenberg, (iii) Imperial Cancer Research Fund (1992 – 1994) with Paul Fremont.

Professional Activities: Member of the ACS and ACA; Co-editor of Acta Crystallographica Section D (2002 – present); *ad hoc* reviewer for NIH study Sections (2003 – 2005); Secretary/Treasurer, Biological Macromolecules SIG, ACA (2002-2003); Member of the Biochemistry and Molecular Biology Grant Review Committee, Medical Research Council of Canada (1997-2000).

Research Interests: Crystallographic structure determination of flavoenzymes, multifunctional enzymes involved in substrate channeling and protein transcription factors. Technical interests include coordinating atomic resolution crystallography with single crystal microspectrophotometry to monitor different structural states in enzymatic reactions.

Statement: I am honored to have been nominated to the Communications Committee and look forward to having the opportunity to serve the crystallographic community in this context. The ACA is an outstanding professional organization bringing together an ever-growing community of scientists with common interests in the techniques of crystallography as a means of better understanding molecular structure. We are currently facing far-reaching changes within the scientific community, particularly at the funding level. If elected to this position, I will focus on strengthening a dialogue within the ACA community in order to identify steps to resolve these current issues. Furthermore, I will work with the committee to highlight the extensive achievements of researchers in our discipline to the broader scientific community, and to maintain a strong, united voice to better address our needs and concerns.

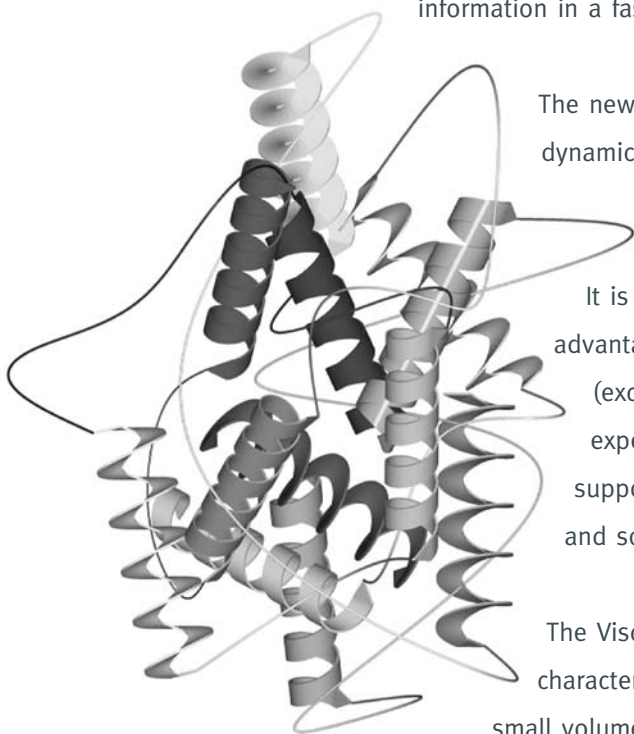
Alice Vrielink, Communications



Research Professor, Department of Chemistry and Biochemistry, University of California Santa Cruz, CA, 95064

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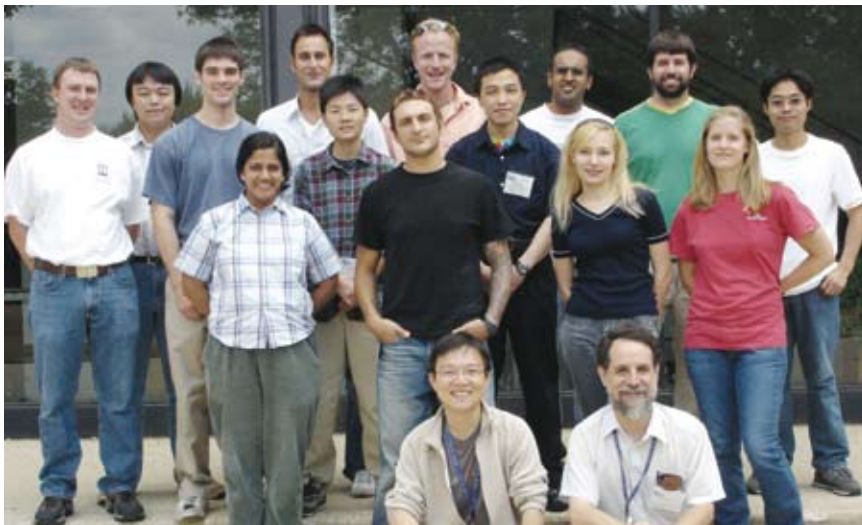


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2005 ACA Summer School in Macromolecular Crystallography



The school was held at Illinois Institute of Technology (Chicago, IL) and the Advanced Photon Source (APS, Argonne, IL) from 18 July through 30 July 2005. The school is designed for upper-level graduate students and postdocs, but lower-level graduate students and industry scientists have also been accepted during the three years that the school has operated at IIT and the APS. The 2005 school included 22 lectures by eminent crystallographers and qualified graduates of our own program, plus extensive chemical and crystallographic lab work and a minimum of four visits per student to macromolecular beamlines at APS. Students worked on crystallizing their own proteins and learned crystallization techniques using commercial proteins; they also collected diffraction data at the APS on their actual research samples and on test crystals.

Most of the first week was spent at IIT, with time divided among lectures and labs. The second week was held partly at IIT and partly at the APS, where students not only collected data but engaged in training experiences shepherded by the beamline staff scientists. The schedule and the content of the lectures, labs, and beamline visits are listed on the school website (acaschool.iit.edu). Social events were included in the school, and the students were allowed free time to visit Chicago's attractions in the evenings and during the weekend between the two work weeks.

The school's location in Chicago made it easy to recruit world-class scientists to lecture and lead lab demonstrations. Only one of our featured academic speakers, Bill Furey, was from outside the Chicago area. Several industry scientists were also on our teaching team.

Almost all of the lecturers provided lecture notes that were made available on the website. In addition, almost all the lectures were digitally video-recorded, and the video record is now on file in Chicago. It will be made available to the ACA and interested participants for free, and to others for a modest fee.

Lecturers: Spencer Anderson (BioCARS / U.Chicago), Grant Bunker (IIT), Chuck Campana (Bruker AXS), Jim Cary (NIU), Chris Dankulich (Fluidigm), Zeeshan Farooq (Nextal), Bill Furey (Pittsburgh VA / U. Pittsburgh), Andy Howard (IIT), Tom Irving (IIT), Jim Kaduk (Innovene), Gocha Khelashvili (IIT), Tim Morrison (IIT), Allan Myerson (Provost, IIT), Jim Pflugrath (Rigaku / MSC), Narayana Sukumar (NE-CAT / Cornell).

Lab Facilitation: Jim Cary (NIU), Shih-Chia Chang (IIT), David Ehle (IIT), Andy Howard (IIT), Anita Patil (Kansas City VA), Sireesha Ratakonda (IIT), P. Reinfelds (IIT), Greg Sahli (IIT)

Administration and Technical Assistance: David Ehle (IIT), Sandra Howard (IIT), Faith Kancauski (IIT)

Beamline Science User Support:

Randy Alkire (SBC-CAT), Norma Duke (SBC-CAT), Stephen Foundling (SER-CAT), Zhongmin Jin (SER-CAT), Lisa Keefe (IMCA-CAT), Jun Wang (NE-CAT), Zdzislaw Wawrzak (DND-CAT)

Students: Olga Antipova (IIT, Russia), Bret Dillard (U.Georgia), Bin Fang, (Georgia State, China), Todd Gangelhoff (U.Colorado Health Sci.), Feng Guo (IIT, China), Jake Herman (U. Colorado Health Sci), Krista Hill (U. Colorado Health Sci), Tengchuan Jin (IIT, China), Christopher Kimberlin (Scripps), Haidong Li (Dana Farber, China), Anna Thode (U. Colorado Health Sci), Navtej Toor (Yale, Canada), Yi Xue (Northwestern, China), and Min Zhao (U. Georgia, China)

Analysis: The participants filled out a survey at the end of the school and provided informal feedback as well. Most were very pleased with the operation and the outcome of the school. Most students were satisfied with the amount of time spent on the lecture, laboratory, and beamline portions of the school. Some concerns over the quality of food at IIT were voiced, and some students received inadequate information about the school in advance. The students were generally pleased with the professionalism and enthusiasm of the beamline support personnel at the APS CATs that participated in the school, particularly at SBC-CAT.

Plans for the Future: For 2006 we hope to improve the food at IIT and add more lectures to make the experience deeper and richer. We will probably reinstate the practice of having application seminars in the evenings that would be distinct from the methods-oriented lectures offered during the day, and would instead illustrate the way that molecular and cell biologists use the results from crystallographic studies. We will provide all students with a comprehensive set of instructions on how to prepare for the School, and will mail the course textbook to the students ahead of time. We will have \$6000 in scholarship and travel funds from the USNCCr for students from Latin America. We hope the school will continue to be an important resource for the crystallographic and biochemical community, and that it can serve to acquaint a wider circle of scientists with the realities of macromolecular crystallography.

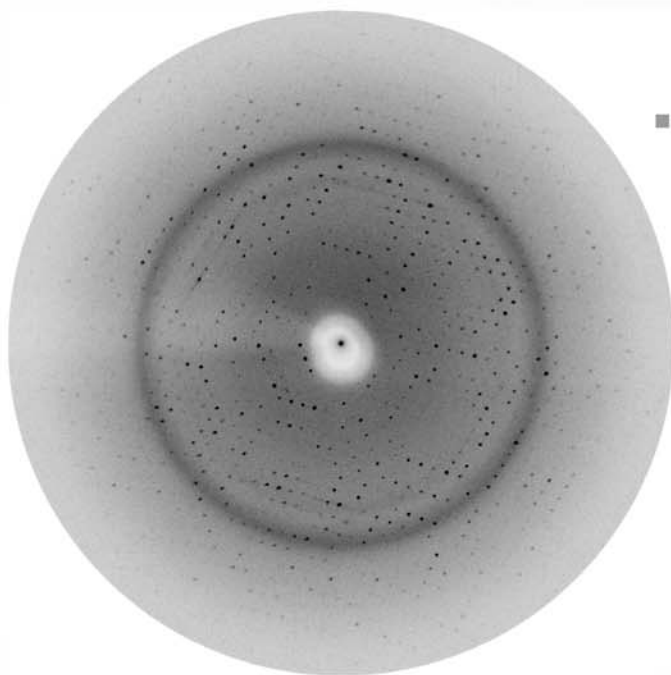
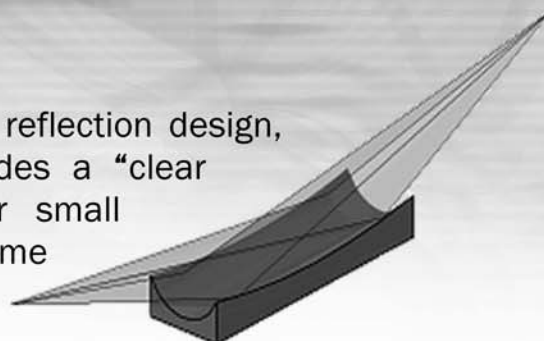
Andy Howard

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Data Courtesy of Dr. Andrew GW Leslie
MRC Laboratory of Molecular Biology, Cambridge.

The crystal belongs to space group C222 with cell dimensions $a=72.1\text{\AA}$, $b=97.4\text{\AA}$, $c=191.0\text{\AA}$. Images were collected with an oscillation angle of 0.4° .

The crystal was a thin plate with approximate dimensions $200 \times 75 \times 50 \mu\text{m}^3$.

The generator was a Rigaku RuH3R running at 50kV, 100mA (300 μm focus) and the data were collected on a Mar345 image plate detector.

	classical confocal multilayer system	Xenocs FOX2D CU 25_25P
Exposure time per frame	4 min	4 min
R_{merge} (22.7.-2.43A)	8.8%	6.4%
R_{merge} (2.57-2.43A)	44.1%	26.2%
$\langle I \rangle / \langle \text{sig} \rangle$ (22.7.-2.43A)	12.1	15
$\langle I \rangle / \langle \text{sig} \rangle$ (2.57-2.43A)	2.5	4.1
Mean multiplicity	3.3	3.3

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First Annual Rigaku SAD Workshop, April 2006



The workshop, hosted by the University of Texas M. D. Anderson Cancer Center, was sponsored by Rigaku Americas Corporation to help users make the jump from MAD to SAD in a routine fashion.

On the first day we heard opening remarks by **Joe Ferrara** (RAC) and **Dick Brennan** (UTMDACC). **Bi-Cheng Wang** (University of Georgia) gave a presentation on the “Theoretical Aspects of Sulfur SAD Phasing and Direct Crystallography”. B.C. gave a brief history of single wavelength anomalous scattering experiments and then described methods for eliminating phase ambiguity. He also explained the effects of signal, noise and handedness on the structure solution pathway. Finally, he gave us a number of examples of successful SAD structures.

Zbigniew (Zbyszek) Dauter (Argonne National Laboratory) presented “SADPhasing” which described the physics of resonance (anomalous) scattering, how it effects diffraction data in MIR, MAD and SAD cases and how that information is extracted. Zbyszek paid his respects to **David Blow**, perhaps the first person to use Cr radiation in macromolecular crystallography (in 1958!) and left us with the adage “SAD is not sad, SAD is jolly.”

Aiping Dong, (SGC-Toronto) presented “Phasing at Home: Sulfur SAD” and reviewed a number of data sets collected with Cr radiation and offered some insight into the successes and failures. Six of eleven data sets were phased successfully. The unsuccessful data sets likely failed as a result of poor data quality or the majority of sulfur atoms were located in highly mobile regions of the protein. Aiping also gave us his strategies for solving more difficult cases.

After lunch we took a tour of the new x-ray facility at UTM-DACC, which includes a FR-EDW SuperBrightT rotating anode x-ray generator with both Cr and Cu optics and an R-AXIS HTC imaging plate detector. After the tour **Jim Pflugrath** (RAC) described the finer points of collecting data in “How to Obtain Accurate Data.” Aiping brought several processed diffraction data sets for the workshop attendees to try various software packages. Everyone solved a Cr SAD structure.

On the second day, **James Liu** (Institute of Biophysics, Chinese Academy of Sciences and University of Georgia) presented “Practical Aspects of Sulfur SAD Phasing” and started a lively discussion on the merits of collecting multiple data sets. James then described the University of Georgia scale-to-structure pipeline and gave a real-time demonstration over the network.

Cheng Yang (RAC) discussed “In-house S and Se Phasing with Cr KE1 Radiation” and described the instrumentation required by the SAD experiment at home. Cheng also gave a number of very interesting success stories and finished by reminding us we should “know before you go.”

John Badger (ActiveSight) described “Automated Scripts for SAD Phasing” with a lecture detailing the methods and demonstrated automated Python scripts he has written for SAD phasing.

The second afternoon was filled with more SAD phasing hands-on training by Aiping Dong, James Liu and Cheng Yang. The workshop closed with a mixer on the 7th floor of the UTMDACC Mitchell Basic Sciences Building overlooking the massive Texas Medical Center, the largest medical complex in the world.

We would like to thank our hosts **Dick Brennan** and **Maria Schumacher** for their support and use of facilities, tutors **Aiping Dong** and **James Liu** for the added effort required to prepare phasing examples in addition to their lectures, **Judy Bryan** and **Deborah Watkins** for organizing the rooms, meals, and travel. Finally, special thanks to **Cheng Yang** and **Angela Criswell** for putting together a very successful workshop on very short notice.

Joe Ferrara



Canadian National Committee for
Crystallography (CNCC)
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Student Travel Fund

Donations are being solicited for the Larry Calvert Trust Fund which offers travel awards for students presenting a poster or talk at the triennial IUCr congresses. Cheques made from Canadian bank accounts are tax deductible and should be made out to “L.D. Calvert CNC/IUCr Trust Fund” and sent directly to:

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Travel awards to the Florence 2005 IUCr Congress were granted to **Sung Yeun Choi** (Department of Chemistry, University of Toronto), **Jason Dwyer** (Departments of Chemistry and Physics, University of Toronto), **Jason Thomas Mayne**, (Department of Biochemistry, University of Alberta, Edmonton) and **Elitza Tocheva** (Department of Microbiology and Immunology, University of British Columbia, Vancouver)

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Third Annual SER-CAT Symposium at Georgia State University, March 2006



The symposium was attended by approximately 70 people. Of special significance was the presentation of the first SER-CAT Service Award to **C. Michael Cassidy** of the Georgia Research Alliance for his initial and ongoing support for SER-CAT. The award was presented by B. C. Wang as seen in the photo on the left.

The program included nine invited speakers: **Theodore Jardetzky** (Northwestern University), **Stephen White** (St. Jude Children's Research Hospital), **Brian Geisbrecht** (University of Missouri-Kansas City), **Karl Volz** (University of Illinois at Chicago), **Patricia Weber** (Consultant to ExSAR, Monmouth Junction, NJ), **Alexander Wlodawer** (National Cancer Institute), **Brian Savory** (Southern Light Rail, Atlanta, GA), **Jim Fait** (SER-CAT) and **John Rose** (University of Georgia). In addition, sixteen posters were provided by various member groups of SER-CAT. A summary of speaker presentations is given below:

Theodore Jardetzky presented structural insights into the paramyxovirus fusion protein folding and function. The paramyxoviridae are enveloped viruses that include mumps, measles and several other pathologic viruses. Crystal structures of the

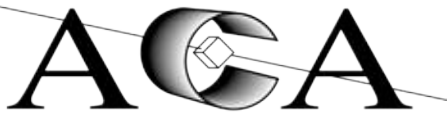
pre- and post-fusion protein have been determined. Comparison of these two structures reveals major conformational changes in both secondary and tertiary structures. The positions and structural rearrangements of key parts of the fusion machinery clarify how a novel metastable protein fold and its conformational transition to a more stable state can trigger membrane fusion.

Stephen White reported on his efforts in structure-based drug design. The focus of his talk was the development of novel antimicrobial therapeutics to treat emerging drug-resistant organisms. The structures of key enzymes in the biosynthesis of fatty acids and folate in bacteria have been extensively studied. His presentation described three enzymes in these pathways and progress towards identification of novel inhibitory small molecules.

Brian Geisbrecht spoke on the structural and mechanistic studies of immunomodulatory virulence factors in *Staphylococcus aureus*. The extracellular fibrinogen-binding protein (Efb) of *Staphylococcus aureus* is a multifunctional virulence factor. A truncated form of Efb (Efb-C) was expressed, crystallized and the x-ray structure determined. The Efb-C structure consists of a closed, left-handed-twisting three helix bundle and belongs to the immunoglobulin/albumin binding domain-like fold class. Additional studies of a complex between Efb-C and C3d show very interesting empirical structural evidence for the importance of electrostatic forces in the formation of protein complexes.

Karl Volz reported results on studies of iron regulatory proteins (IRP1 and IRP2) and iron regulatory elements (IREs). The structures of IRP1 in complex with ferritin mRNA IRE, and the IRP1-IRE-aconitase complex has been determined. These results provided structural rationales for both selectivity in IRP1:IRE binding and regulation of IRP1's functional interconversion.

Patricia Weber discussed the use of high resolution H/D exchange measurements to design recombinant proteins that are more



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likely to crystallize. The H/D exchange rates provide information about the intrinsic flexibility of protein segments. The talk also included information concerning the design of recombinant proteins from the rate information and ligand-dependent alterations in protein conformation.

Alexander Wlodawer discussed the difficulties and challenges encountered in determination of the structure of HTLV-1 protease, a retrovirus associated with diseases such as adult T-cell leukemia. The structure of a truncated HTLV-1 was determined. Crystals of the truncated HTLV-1 were difficult to grow and the structure solution by MR was quite challenging. The structural data do provide an understanding of the resistance of HTLV-1 to HIV drugs and provide clues for the design of new drugs.

Brian Savory explained the operations of the Southern Light Rail, headquartered in Atlanta, which provides ultra-high speed connections to the National Lambda Rail which in turn allows connections to more than 150 universities, research institutions and other organizations nation-wide. He presented a chart of the entire network and went into some detail about the complex pathway that was used to connect Georgia State University to APS at Chicago. Later in the program, we had a successful demonstration of this connection.

Jim Fait described the efforts at SER-CAT to fully automate the x-ray data collection process at SER-CAT. The beamline setup, sample handling, strategy, data collection, data reduction, structure solution and data archiving are either already automated or in the process. Robotics, image processing and multiprocessor computing contribute extensively to the ease of completing the synchrotron experiment. Details of the implementation were presented as well as some case studies.

John Rose detailed his experiences with the SER-CAT remote user participation program. This innovative program is important to SER-CAT users since many of the members are hundreds of miles from the beamline. The system consists of a crystal mounter, the SERGUI user interface and secure Access Grid based communications between the remote user and the beamline. After the alpha testing is completed, the system should be released to users in approximately June 2006.

Two SER-CAT Science Awards were also presented during the meeting. Both awards are designed to recognize important scientific accomplishments at, or of benefit to, SER-CAT.

The SER-CAT Outstanding Science Award was presented to **Bin Zhao** (Vanderbilt University - right photo), recognizing the scientific impact of his work on active site water molecules and substrate hydroxyl groups in oxygen activation. His talk highlighted the structure of CYP158A2, one of the 18 cytochrome P450 genes in the actinomycete *Streptomyces coelicolor*.



The SER-CAT Young Investigator Award was presented to **Jianhua Gan** (National Cancer Institute-Frederick -left photo), recognizing his work on structural insights into the mechanism of double-stranded RNA processing by Ribonuclease III. His presentation provided interesting details of the structure of the first observed RNase-product complex of this family.

At the end of the meeting, another very important development was highlighted. The SER-CAT team from Argonne National Laboratory (Jim Fait and John Chrzas) and John Rose (UGA) successfully demonstrated the use of a direct gigabit internet connection that allowed for a firewall-free point-to-point two-way communication between Georgia State University lecture hall and the SER-CAT bending magnet beamline at APS in Chicago. The demonstration highlighted the use of Southern Light Rail/National Lambda Rail to control the Advanced Photon Source (APS) beamline instrument using remote access and robotics. We are very grateful for the cooperation of the personnel at approximately 20+ connection sites between Georgia State University and Argonne National Lab, which made this two-way communication possible. This development opens the possibility of a new paradigm for synchrotron data collection.

We gratefully acknowledge **Irene Weber** and her Georgia State team for the excellent organization and program. The Georgia State facilities were spacious and very well suited for this symposium. The Fourth Annual SER-CAT symposium will be hosted by Alexander Wlodawer, (National Cancer Institute) on the Frederick, MD campus in Spring 2007.

Gary Newton

36th Mid-Atlantic Macromolecular Crystallography Meeting

This year's meeting, held on the Reynolda Campus of Wake Forest University in Winston-Salem, North Carolina, took place June 1-3. The meeting was organized by *Al Claiborne - seen on the left with Joshua Warren on the right* (Duke) of the WFU



Center for Structural Biology, with special assistance from *Conn Mallett* (Rigaku), and with help from *Tom Hollis, Todd Lowther,* and *Bernie Brown* of WFU. The keynote session focused on the topic of supramolecular assemblies and included talks by *Tomitake Tsukihara - on the left* (Osaka University) and *Jack Johnson - on the right* (Scripps); Tsuki and Jack were associated



with Michael Rossmann's lab in the late 1970s and coauthored the seminal 1980 publication in *Nature* on the crystal structure of southern bean mosaic virus.



Carla Mattos, Lorena Beese, and Traci Hall pay close attention to the speakers.

Tsuki updated the audience of ~185 participants with new crystallographic implications from his lab for the proton pumping

mechanism of cytochrome c oxidase, while Jack spoke on the combination of crystallography and cryo-electron microscopy approaches to the analysis of virus particle maturation. After the keynote talks, participants enjoyed a lively reception with wine and beer, followed by a buffet dinner.



On June 2, *Matt Redinbo* (UNC-Chapel Hill) - *seen on the right above with Charles Pemble on the left* (Wake Forest) chaired

the first scientific session, which included talks by *Kevin Madauss* (Glaxo-SmithKline) and *Stephen Soisson - to the right* (Merck Research Laboratories) on progesterone receptor complexes with Asoprisnil and corepressor peptides and on novel antibiotics targeting bacterial fatty acid biosynthesis, respectively. *Tom Hollis*



(Wake Forest Univ.) chaired a session on DNA repair enzymes and protein-nucleic acid interactions that featured talks by *Brandt Eichman* (Vanderbilt) and *Clara Kielkopf* (Johns Hopkins) on 3-methyladenine DNA glycosylase I and the pre-mRNA splicing factor U2AF65, respectively.



Zbigniew Dauter and Zygmunt Derewenda looking forward to the next speaker.

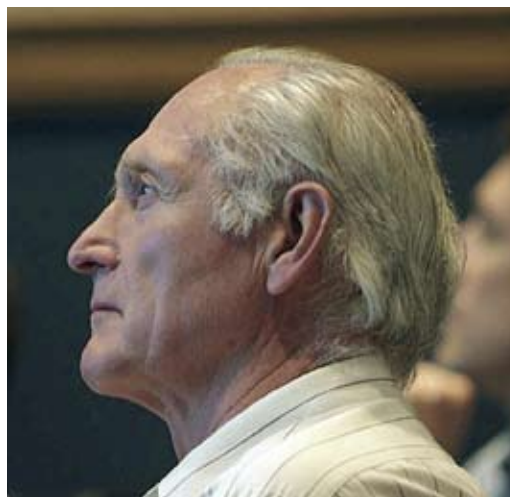
Among the 23 commercial vendors participating in the meeting, Wyatt Technology, Qiagen, and Formulatrix presented their newest technologies related to protein crystallization. The poster session featured ~50 presentations and was well attended. The social highlight of the meeting included a catered dinner in downtown Winston-Salem, with music provided by Cle Thompson, as

well as a visit to the First Friday Gallery Hop in the Downtown Arts District.

On the last half-day of the meeting, WFU graduate student **Jamie Wallen** (Al Claiborne lab) spoke on the structures of NADH and NADPH complexes of the anthrax coenzyme A-disulfide reductase and a novel dual substrate specificity mechanism, while WFU postdocs **Thomas Jönsson** (Todd Lowther lab) and **Nathan Nicely** (Claiborne lab) spoke on the interaction between sulfiredoxin and its target peroxiredoxin sulfenic acid substrate and on the novel anthrax type III pantothenate kinase, CoaX, respectively. **David Shultis**, a graduate student with Michael Wiener at Virginia, gave a great talk on the new structure for the BtuB-TonB complex involved in cobalamin transport across the bacterial outer membrane, and **Michael Purdy** (Virginia) spoke on the application of F_{ab} fragments to structure determinations with integral membrane protein-monoclonal antibody complexes.

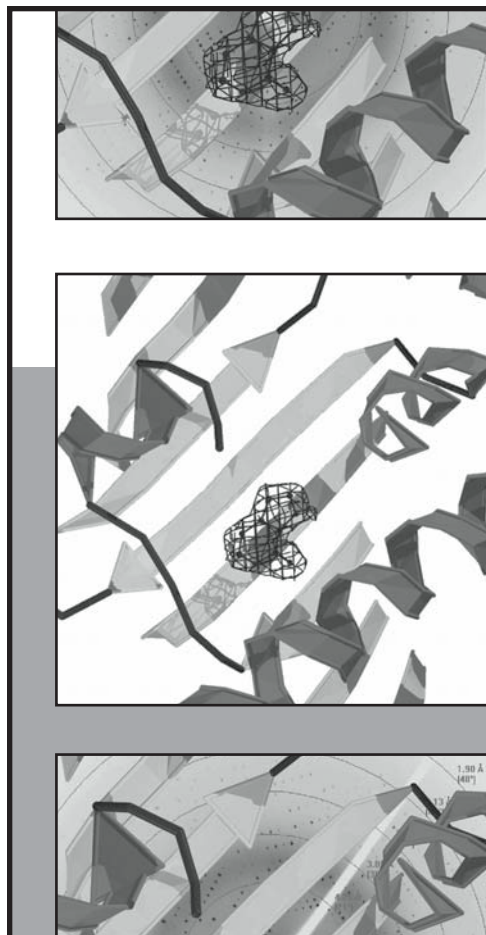
Five years ago there was no protein crystallography facility at Wake Forest Univ., and the 2003 Mid-Atlantic Meeting held at Duke represented the first appearance by WFU structural biologists in this longstanding series of outstanding conferences. The 36th annual Mid-Atlantic Meeting introduced the established "East Coast" crystallography community to the newer Wake Forest University research setting and provided a great venue for a highly interactive and enthusiastic group of both young and

established macromolecular crystallographers. Michael Wiener will organize the next meeting at the University of Virginia in Charlottesville from June 7-9, 2007.



Bob Kretsinger - one of the Mid-Atlantic pioneers remembering when the group was small enough to have the conference dinner in his back yard in Charlottesville and thinking barbecue next year?

Al Claiborne



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Background image from the cover of Acta C: A perspective view of bis(μ_6 -cis-2,4,6,8,10,12,14,16-octamethylcyclooctasiloxane-2,4,6,8,10,12,14,16-octolato)octakis[(dimethylformamide)copper(II)] dimethylformamide pyrazine solvate. L. Zherlitsyna, N Auener and M. Bolte. Acta Cryst. (2006). C62, m199-m200

JULY 2006

22-27 ACA Annual Meeting, Sheraton Waikiki, Honolulu, Hawaii.

AUGUST 2006

6-11 **23rd European Crystallographic Meeting**, Leuven, Belgium. www.ecm23.be

7-11 **Denver X-Ray Conference**, Denver Marriott Tech Center Hotel - www.dxcicdd.com

16-21 **11th ICCBM (International Conference on Crystallization of Biological Macromolecules)** Quebec City, Quebec, Canada www.iccbm11.com

**SEPTEMBER 2006**

1-4 EPDIC-10 **10th European Powder Diffraction Conference**, Uni Mail, Geneva. www.symporg.ch

JANUARY 2007

23-24 **Advances in Protein Crystallography**, South San Francisco, CA, www.ProtCrystConf.com

JUNE 2007

7-17 **Engineering of Crystalline Materials Properties: State-of-the-Art in Modeling, Design, and Applications**, the 39th crystallographic course at the Ettore Majorana Centre, Erice, Italy.

JULY 2007

21-26 **ACA Annual Meeting - Salt Lake City, Utah**. *Local Chair: Chris Hill (U of Utah, chris@biochem.utah.edu) Program Chair: Jill Trehwella (Univ. of Sydney - b2jtrehwella@usyd.edu.au)*

MAY 2008

31-June 5 **ACA Annual Meeting -Knoxville, TN** *Local Chair: Jason Hodges (SNS Division - ORNL, hodges@ornl.gov) Program Chair: Paul Butler (NIST - 2028butler@nist.gov)*

**Second Meeting of the Asociación Argentina de Cristalografía, Puerto Madryn, Argentina, 25-27th October, 2006**

The second meeting of the AACr, Asociación Argentina de Cristalografía (Argentine Crystallographic Association) will be held at Puerto Madryn, Chubut, Argentina from 25 to 27th October 2006.

The aim of the meeting is to gather, in a friendly environment, all the Argentine researchers (interested people from abroad are deeply encouraged to join us) with a strong interest in crystallography and its many branches of application. The first meeting took place in October 2005 in La Plata, Argentina, and there it was agreed to go on with these meetings on an annual basis, rotating the location among interested institutions.

This year the organizers will be the Crystallography Group at the Puerto Madryn site of the Universidad Nacional de la Patagonia "San Juan Bosco" (UNPSB) and the Centro Nacional Patagónico (CENPAT), a CONICET institute. The meeting event will include poster presentations, invited talks, brief courses and round tables, and will close with the Ordinary Assembly of the AACr.

The local committee is working to provide some convenient lodging facilities and reservations. However, given the character of the venue, a world renowned centre with a heavy international tourist demand, we strongly advise making prompt reservations. Once the in-advance booking term is over, it could be difficult to find proper or convenient lodging facilities at reasonable prices.

As further details emerge they will be posted on the meeting website: www.tandar.cnea.gov.ar/~vegal

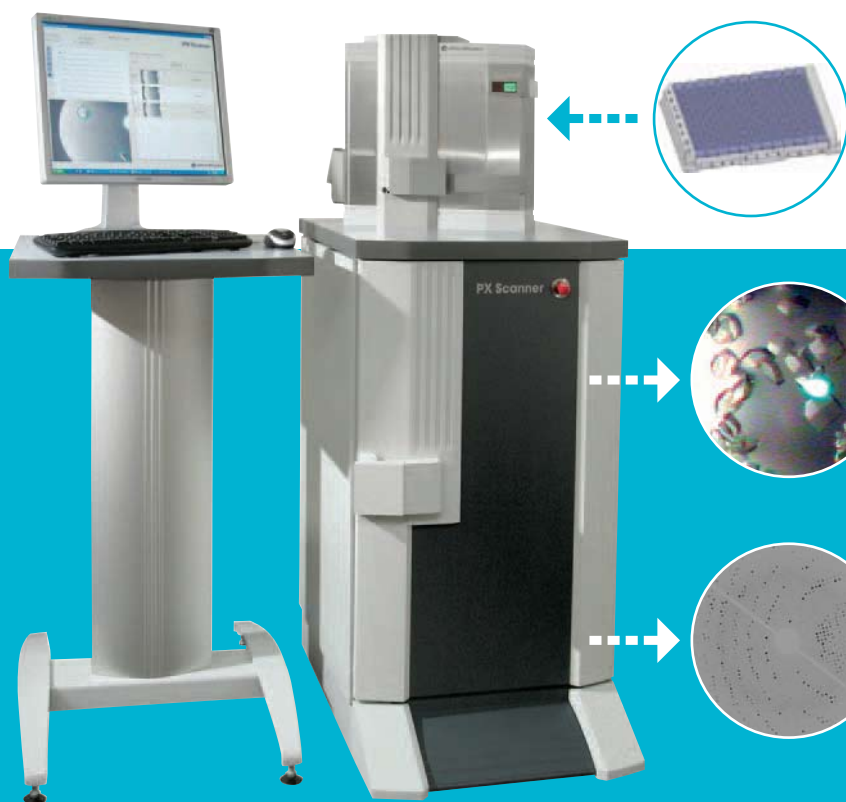
XIVth Ibero-American Congress and IVth School of Crystallography, Caracas, Venezuela, 17-25 January 2007

The Ibero-American crystallography congresses that bring together Latin American, Spanish and Portuguese crystallographers began in the 1960s and have been held regularly every 2 or 3 years. The current name for the congress was adopted in 1990. Topics for the 2007 gathering will include: neutron, electron and powder diffraction, structures of small molecules and proteins, synchrotron radiation, electron microscopy, crystallization techniques and new materials.

For more information: www.idea.gov.ve/iberocris07

Contributors to this issue: Sidney Abrahams, Bob Bau, Helen Berman, Charlie Carter, Connie Chidester, Al Clairborne, Shmuel Cohen, Marcia Colquhoun, Louis Delbaere, Joe Ferraro, Bill Furey, Lee Groat, Marv Hackert, Andy Howard, Mayer Itzhak, Kathy Kantardjieff, Cheryl Klein-Stevens, Charlotte Lowe-Ma, Jeff Milton, Gary Newton, Paul Raithby, N. Rao, John Rose, Miriam Rossi, Bernie Santasiero, Qun Shen, Menachem Shoham, Jeanne Stuckey, Alice Vrielink, Ellen Weiss, Alex Wlodawer, Winnie Wong-Ng, Bernard Wuensch, and Christine Zardecki. Special thanks to Maria Voigt for the cover graphic.

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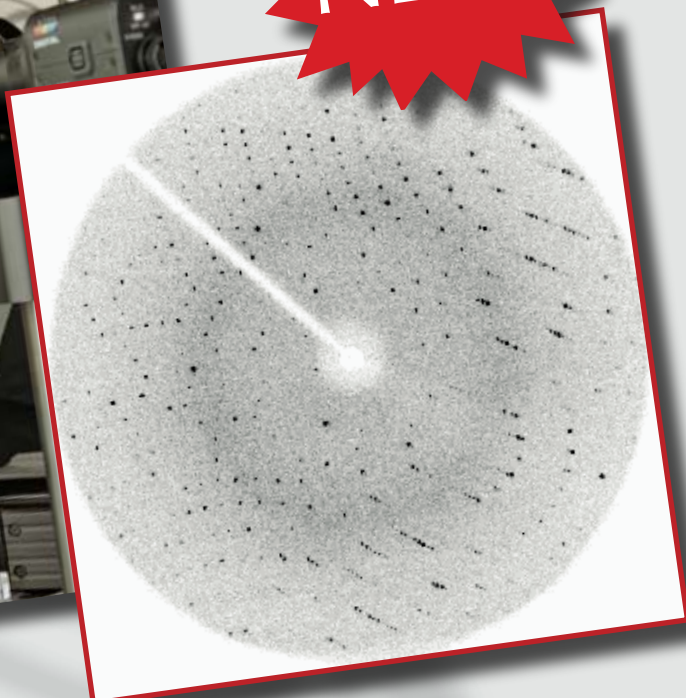
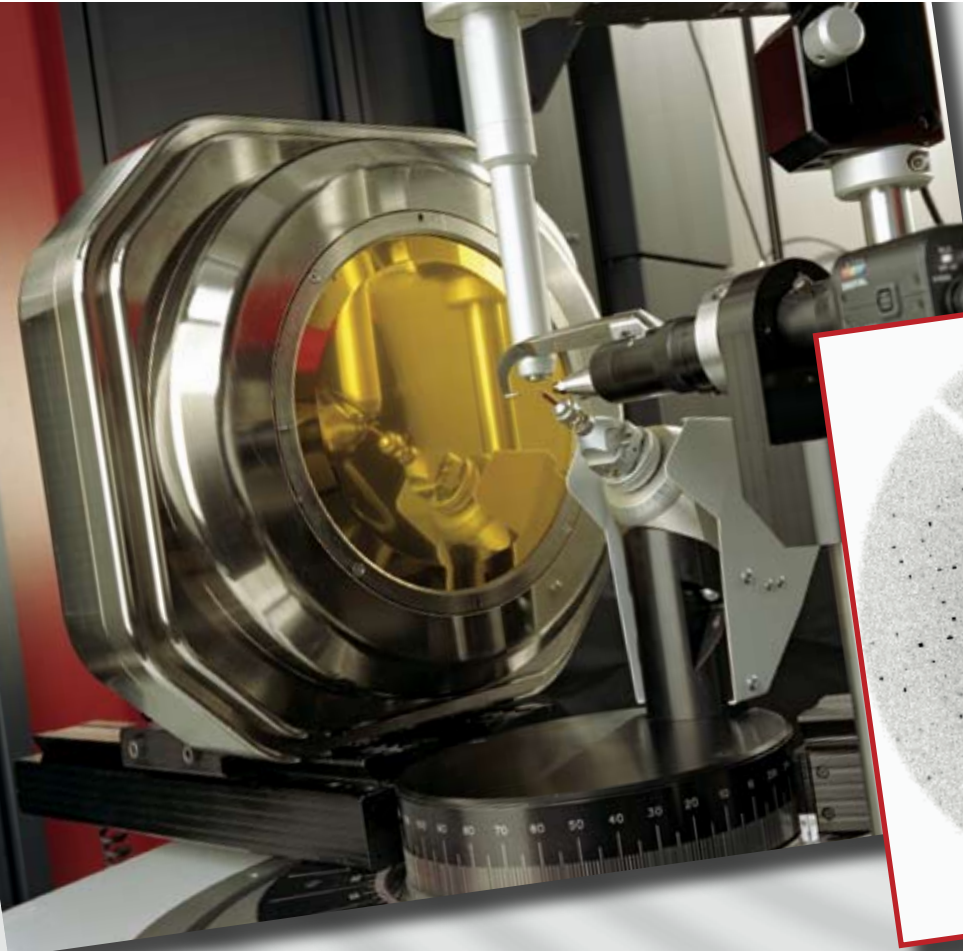
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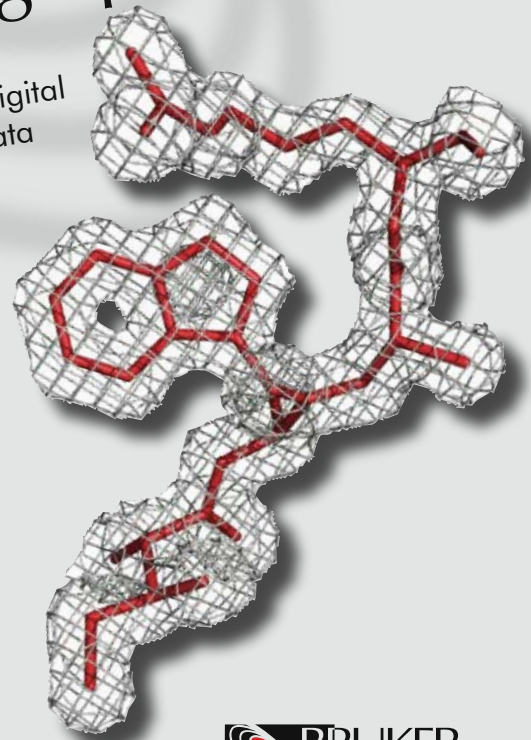
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