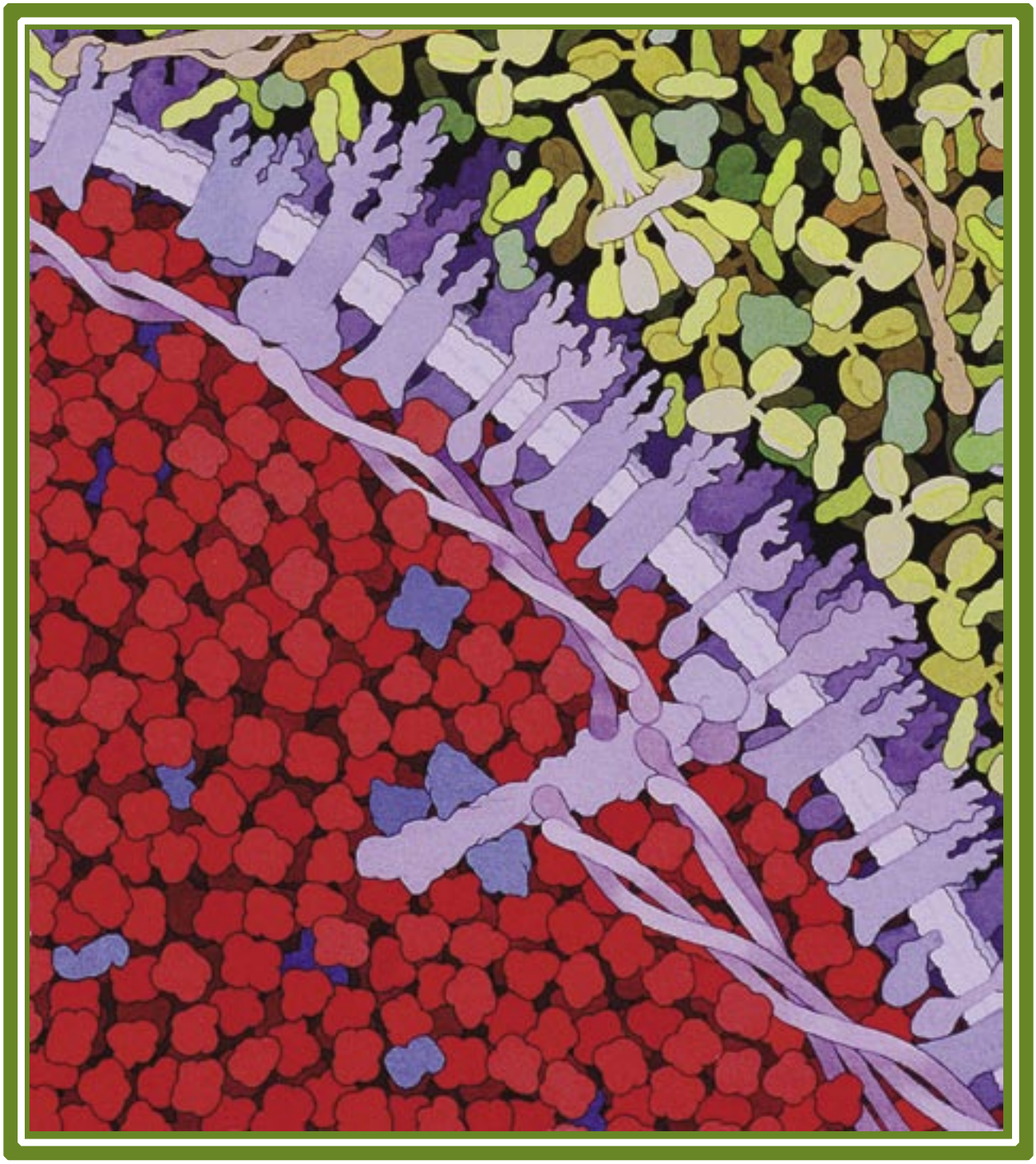
AMERICAN CRYSTALLOGRAPHIC ASSOCIATION

NEWSLETTER

Number 2 *Summer 2005*



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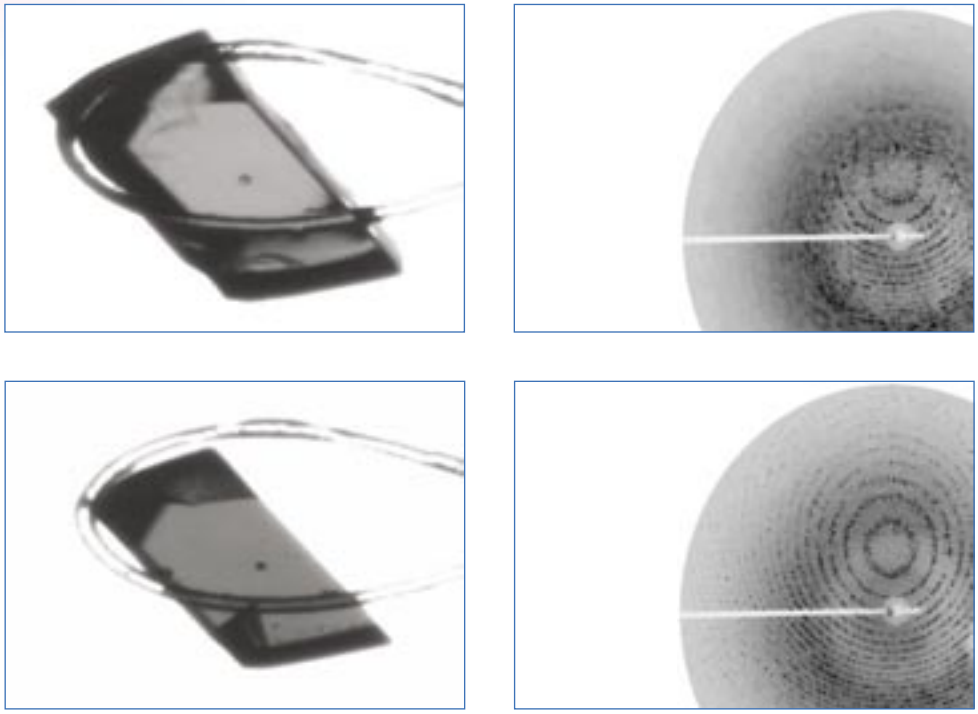

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President's Column

I would like to thank all of the volunteers who do so much for the ACA, especially those involved in our annual meetings. We had a very successful meeting in Orlando, FL thanks in large part to our Program Chair, Edward Collins, Local Chairs, Khalil Abboud and Thomas Selby and their hard working committees. All of our initial reserved hotel space at the Swan hotel was completely booked by our registrants and we were fortunate to be able to expand our reserved hotel accommodation to the Walt Disney World Yacht Club. Thanks also to the ACA staff for all that they do to make our organization successful throughout the year, especially at the annual meeting.

The A. L. Patterson Award recognizes outstanding achievement in the structure of matter by diffraction methods. In particular, significant contributions to the methodology of structure determination are recognized. In Orlando, the 2005 ACA Patterson Award was given to T. Alwyn Jones for his pioneering work on computer graphics software, starting with FRODO and progressing to O.

The Margaret C. Etter Early Career Award recognizes outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career. In Orlando, the 2005 ACA Etter Early Career Award was given to Jennifer Swift for her novel studies on crystal growth mechanisms, particularly in biologically relevant crystals.

Two awards to be presented at the 2006 ACA meeting in Honolulu, Hawaii, are the Warren Award and the Buerger Award. The Bertram Eugene Warren Diffraction Physics Award recognizes an important recent contribution to the physics of solids or liquids using X-ray, neutron, or electron diffraction. Charles F. Majkrzak from the National Institute of Standards and Technology is the 2006 Bertram E. Warren Diffraction Physics Award recipient for his contributions to the development of neutron reflectivity and its use in interface science.

The M. J. Buerger Award recognizes mature scientists who have made contributions of exceptional distinction in areas of interest to the ACA. Helen M. Berman from Rutgers University is the recipient of the 2006 M. J. Buerger award for her pioneering development of information services all the producers and users of macromolecular structural data.

The Latin America Country membership has been developed by the ACA. There must be a national group or organization that represents the crystallographic community of the country. The group must designate an official representative who will

submit the annual country membership dues, and at least two members to act as the liaison with the ACA. Travel support is available for the leader and three students to attend the annual ACA meeting. Brazil has applied for this membership and Iris L. Torriani is the designated representative. Argentina has also applied for this membership and Ricardo Baggio is the current president of the Asociacion Argentina de Cristalografía. We wish these countries success in their membership and look forward their contributions to the ACA.

Louis Delbaere

Guest Editorial: Chuck Kissinger on The ACA Industrial Special Interest Group

A growing number of ACA members are employed in the commercial sector. These crystallographers work in a variety of fields, from pharmaceuticals to electronics. Although they share the tools and techniques of their academic colleagues, many other aspects of their professional existence are quite different. Supporting and involving these industrial scientists is important to the continuing growth and vitality of the ACA.

One of the most effective means that we have for engaging different subsets of our members are Special Interest Groups. Somewhat surprisingly up to now there has not been a SIG that represents our members employed in industry. At the 2004 Annual Meeting in Chicago, a meeting was held to discuss the possibility of forming such a SIG. There was considerable enthusiasm for the idea, and the decision was made to move ahead with creation of an Industrial SIG. A petition to officially form the SIG was presented to the ACA Council at the 2005 meeting in Orlando

The time is right for an Industrial SIG. Recent trends have contributed to a rise in the number of commercially employed crystallographers. The tremendous growth in the number of protein crystallographers working in the pharmaceutical industry, and the increase in the number of companies developing and marketing crystallographic hardware, software, supplies and services. Indicative of that latter trend, corporate memberships in the ACA have increased by a third in just the last two years. Although it is impossible to predict what future employment trends will be, it is clear that industrial crystallographers will remain an important constituency within the ACA.

There are a number of ways that the new Industrial SIG can serve the community. One of primary responsibilities of a SIG is to sponsor sessions at ACA meetings. As the first order of business for the nascent Industrial SIG, a session was organized for the 2005 meeting entitled "High-throughput Crystallization and Visualization: Focus on Hardware and Methodology," chosen from topics suggested by those attending the 2004 organizational meeting. By continuing to ensure that the topics of greatest interest to industrial crystallographers are presented at the annual meetings, and that they are appropriately represented among the speakers, the Industrial SIG has the potential to help increase meeting attendance and build our membership.

The Industrial SIG is intended to represent members employed in commercial enterprises, including those working for commercial hardware and software vendors. Many of these vendors are corporate members and are an important source of support for the organization. In addition to representing the scientists employed at these companies, the SIG can provide a new forum for communication between the ACA and its corporate members. The Industrial SIG will be well positioned to help bring new corporate members into the ACA.

The SIG can play an even broader role by helping to ensure that students are well informed about opportunities and options in the industrial sector. One way this can be done is by working with the Young Scientists SIG to maximize the participation of industrial scientists in the events and sessions sponsored by that SIG.

The Industrial SIG will also, of course, provide a forum for discussing issues of common interest to industrial scientists. There are unique challenges in doing research in a commercial environment. For instance, access to software and to shared resources such as synchrotrons is very different for industrial scientists than for our academic colleagues. Most of the software tools that academic crystallographers use routinely are available to them free of charge or at a very low cost. Almost nothing is free to industry scientists. The comparative evaluation of software and other tools is of heightened importance in commercial environments, since it is not financially practical to have every tool on hand. Again, the Industrial SIG can help by ensuring that the information necessary to make informed decisions is presented at annual meetings.

My greatest hope is that the SIG will also play a role in facilitating a greater degree of scientific cooperation between industry crystallographers. There are vast amounts of data and experience that have been gathered in industry. Too little of it is shared with the greater scientific community. For example, consider all the protein-ligand crystal structures that have been determined in the pharmaceutical industry, the great majority of which remain unpublished. The number of such structures has been estimated to be as high as 10,000. Many of these no longer have any proprietary value, but they could have immense collective value if made available in the Protein Data Bank. This can happen, despite the competitive nature of the pharmaceutical industry, but it is unlikely to occur without some organized impetus. This is an area where the ACA can be influential, and where the Industrial SIG can have an important role.

It has been a great pleasure for me to serve as an organizer of the new SIG and to bring it into existence. The Industrial SIG can play a critical role in keeping the ACA growing and thriving. I encourage you to join, to contribute your ideas and to help make this new SIG a success.

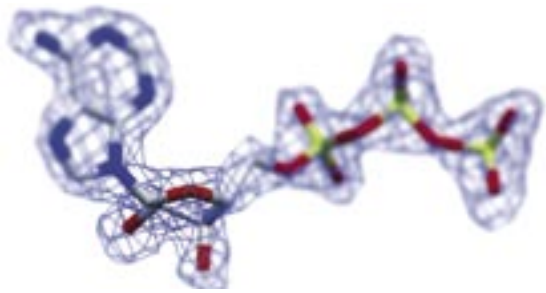
Chuck Kissinger

News from Canada

The new Canadian Representative to the ACA is ***Lee Groat***, of the Department of Earth and Ocean Sciences at the University of British Columbia (lgroat@eos.ubc.ca). Lee grew up in Kingston, Ontario, and attended Queen's University for his B.Sc. He obtained his Ph.D. (in Geological Sciences) from the University of Manitoba in 1988, and was a NATO Postdoctoral Fellow at Cambridge University in 1989. Lee is currently co-Editor of *American Mineralogist*. His research interests include the crystal chemistry of minerals and X-ray and neutron powder and single-crystal diffraction.

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

On May 19th CLS had the honour of hosting Her Majesty Queen Elizabeth II and His Royal Highness the Duke of Edinburgh as part of the Royal Visit commemorating Saskatchewan's centennial. While at CLS the Queen met met several synchrotron scientists conducting research related to cancer, Alzheimer's disease, and zoonotics, and His Royal Highness was shown images of a protein structure mapped using synchrotron radiation as well as a simulation of an environmental sample being analyzed at the hard x-ray beamline. An estimated 1,000 people came to view the royal couple upon their exit from CLS



Electron density map for ATP from data collected at CLS (courtesy of Louis Delbaere)

On February 8th, Jeff Cutler was appointed Associate Director of Research for Industrial Science, and Emil Hallin was appointed Phase II Beamline Development Leader. On March 1st Thomas Ellis joined CLS as Director of Research. The Canadian Light Source is currently looking to fill a number of Beamline Scientist positions.

The Canadian Photoelectron Research Spectromicroscope (CaPeRS) and the PEEM staff scientist Uday Lanke moved to CLS in mid-April after a successful three-year operation at the Synchrotron Radiation Center in Wisconsin.

During the second week of May CLS welcomed their first user, Allen Pratt from NRCAN's CANMET Labs. In addition to helping christen the Plane Grating Monochromator beamline, Allen's research could lead to more environmentally friendly ways to separate gold from ore.

On May 11th CLS hosted a workshop entitled "Frontiers in Bio-Metals: Probing Metal Ions in Biology with x-ray Absorption Spectroscopy."

The 88th annual Canadian Chemistry Conference will be held in Saskatoon from May 28th to June 1st. This meeting will showcase the broad array of disciplines within the field of chemistry. This year's theme of "Illuminating Chemistry" is appropriate given the completion of the CLS. Sessions with specific synchrotron content include "Frontiers in Biophysical and Bioanalytical Chemistry", "Femtosecond Diffraction Dynamics with x-rays and Electrons", "Application of Synchrotron Science to Environmental Chemistry", "Mercury in the Environment and in Human Health", and "Solid State Functional Materials". In addition, there will be a symposium in honor of one of the builders of the Canadian synchrotron community, G. Michael Bancroft, FCIC, entitled "The Birth of a Dream: A Synchrotron Light Source in Canada". Also scheduled is a workshop is entitled "Introduction to Soft X-Ray Synchrotron Science of Soft Matter" concerning X-ray spectroscopy of low-density materials.

The 8th Annual User's Meeting and Associated Workshops will be held November 18-20th on the Saskatchewan Campus.

Birdseye view of booster and storage ring (courtesy of CNL, Inc. U. of Saskatchewan)

The international light source community recently launched the first website dedicated to providing the media, general public and scientific community with the latest news and information on the world's accelerator-driven light sources (synchrotrons and free-electron lasers) and the science they produce. The web site (***www.lightsources.org***) was developed and is jointly maintained by the Light Source Communicators Group, whose members represent the world's light source facilities in Europe, North America and Asia. Funding for the project is provided by science funding agencies of many nations

During the ACA meeting in Orlando it was decided that at the next ACA meeting (Hawaii 2006) the Canadian Division will hold a half-day session in collaboration with the Synchrotron Radiation and the General Interest SIGs on crystallographic research that will be available at the CLS..

Lee Groat

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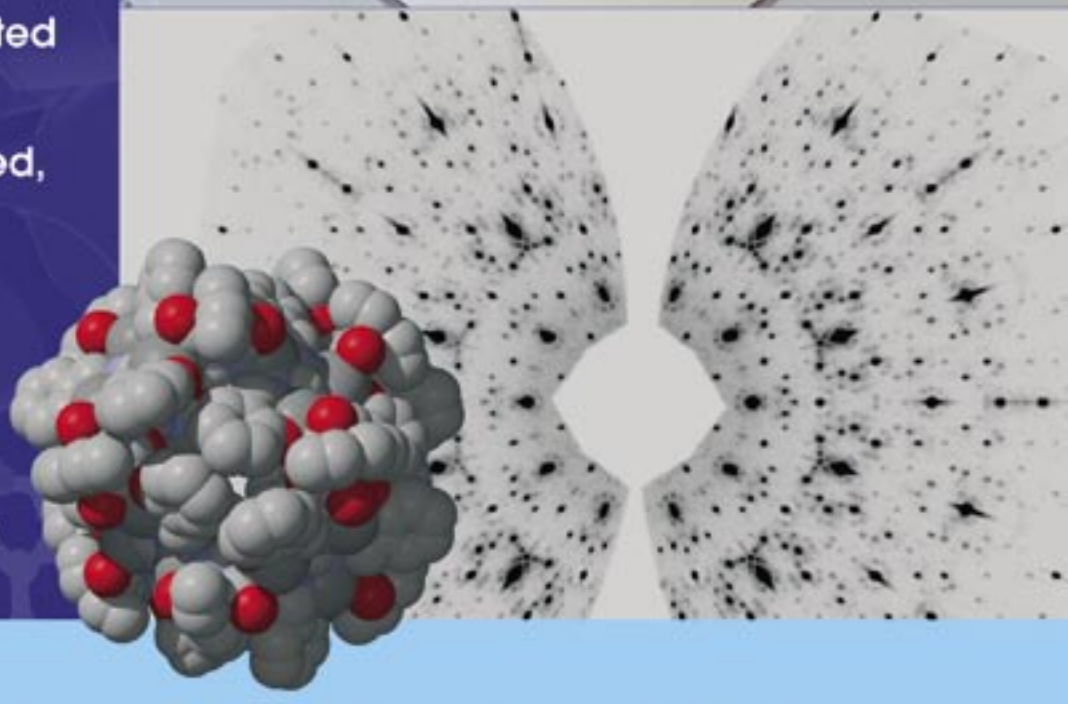

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2006 ACA Bertram E. Warren Award

The recipient of the 2006 Warren Award is Charles F. Majkrzak of the National Institute of Standards and Technology (NIST). He is being cited for his seminal contributions to the development of neutron reflectivity and for his pioneering work in the exploration of many issues in interface science using this technique.

His unusual technical and scientific creativity have profoundly advanced neutron reflectometry and the theory for polarized neutron reflectometry, and have led to the development of important new methods of data analysis. While his contributions to this technique are widely recognized, of particular note is how he designed, optimized, and made creative use of supermirror polarizers, integrating them into neutron instruments that attain very low backgrounds and consequently the highest signal-to-noise achieved anywhere. This point is crucial to achieving the widest possible wave vector range of data, and thereby providing the highest spatial resolution and thus the most detailed and reliable structural information available.

In the tradition of Bertram E. Warren, Charles applied his ideas and methods to a wide range of scientific problems of both fundamental and technological importance. He led a seminal study of Gd/Y rare-earth multilayers that revealed an oscillatory exchange coupling spanning non-magnetic layers. This research provided the basis for interpreting similar effects in transition metal multilayers that exhibit giant magnetoresistance (GMR), which is now the heart of present-day magnetic read heads in hard disk drives. His scientific foresight enabled him to recognize that neutron reflectometry would be an extremely powerful method with which to study biological and soft matter systems. He performed a classic series of neutron reflectometry experiments on the surface-induced ordering of block copolymers, and has more recently explored the structure of biological and biomimetic membranes. The structure of self-assembled biological membranes, particularly with proteins and other molecules inserted into the lipid bilayers, poses a significant new challenge because, unlike previous systems where the basic structure is controlled and known, the basic structure of the self-assembled system is not known *a priori*. Refinements of the structure of these new systems using the dynamical theory of diffraction can lead to significantly erroneous results because of the phase ambiguity.

To address this problem, Charles and his collaborators developed an exact, first-principles method to analyze specular reflectivity data. The culmination of their efforts was a solution to the phase problem for neutron reflectivity that allowed the direct inversion of the reflection amplitude, using the Gel'fand-Levitan-Marchenko integral solution, to obtain the scattering length density profile uniquely within the dynamical theory of diffraction. This method involves the use of a layer, a substrate, or fronting material that can be used as a reference, and is of immense importance for neutron reflectivity studies of unknown structures.

These extraordinary contributions to the field of neutron reflectometry and diffraction physics are the result of a rare blend of scientific, engineering, and technical talents that richly qualify him to continue the outstanding traditions of the Warren Award.

Warren Award selection committee:
Winnie Wong-Ng, Chair, Doug Dorset, Takeshi Egami, and John Tse

2006 ACA Martin Buerger Award

The recipient of the ACA Buerger Award in 2006 is Helen Berman, Board of Governors Professor of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey.

The Buerger award recognizes a mature scientist who has made a contribution of exceptional distinction in an area of interest to the ACA. The award recognizes her lifetime work in the pioneering development of information services for the global community of researchers who both produce and use macromolecular structural data. Her vision, persistence and hard work have ensured that this vital and expanding field of science has the infrastructure needed for archiving and retrieving the structural information on which so much of its future depends.

Helen played an influential role in the conception and early development of the Protein Data Bank, advocating an open access model of operation and uniform standards to ensure that the database could be used for systematic analysis. She pioneered new methodologies in the creation and maintenance of the Nucleic Acid Database and has made innovative use of both databases to show their value in analyzing structural properties.

Under her leadership the Research Collaboratory for Structural Bioinformatics (RCSB) assumed responsibility for the Protein Data Bank in 1999. She was also instrumental in working together with the Macromolecular Structure Database at the European Bioinformatics Institute (MSD-EBI), and the Protein Data Bank Japan (PDBj) to form the Worldwide PDB (wwPDB). This will ensure the existence of a single uniform and continuously updated standard database that covers both the original archive and all new depositions resulting in an unparalleled data resource for the systematic analysis of biological structure.

An important part of her work extended beyond the Protein Data Bank itself. She pressed hard for the development of the macromolecular Crystallographic Information File (mmCIF) which provided the ontology that underlies the archive, and she has worked persuasively with her collaborators in other countries to ensure integration of macromolecular structural informatics both world wide and with related fields in molecular biology.

Over the years she has served the ACA in many roles. She served on various committees and was on council from 1987-1989 (President in 1988). She was the program chair for the ACA meeting in Austin, TX in 1987 and she co-organized the *Transactions Symposium* on "Structural Informatics" in 1997.

Buerger Award selection committee:
I David Brown, Chair, Carol Huber, Jim Ibers and Alex McPherson

2005 Margaret C. Etter Early Career Award

Jennifer Swift (Georgetown University, Washington, DC) is the recipient of the 2005 Etter Early Career Award.

The ACA criteria for this award emphasiszes Peggy Etter's teaching of undergraduates, her role as a mentor, and "her love for people, for science, and especially for people who do science."

All the supporting letters for Jennifer's nomination stressed how closely she comes to these ideals. She is quoted as being a skillful and original experimentalist. Her approach to the problem of kidney stone formation is novel, employing atomic force microscopy techniques that have only relatively recently been applied to the study of crystal growth processes, and not often to pathogenic crystals. Her experimental approach allows the mechanisms of crystal growth under simulated physiological conditions to be studied in real time. This work will almost certainly take on a more pronounced, direct biomedical relevance once natural kidney stone pigments can be isolated and tested.

She has also demonstrated a deep committment to undergraduate education both inside and outside the classroom. Her classes tend to be large lecture and/or laboratory organic courses and she has already developed new and innovative experiments that cover fundamentally important concepts in organic chemistry providing a clear and exciting link to how chemistry impacts everyday life. At the Orlando ACA meeting Jennifer delivered the Etter Award lecture on "Growth and Dissolution of Cholesterol Crystals."

The call for nominations for the 2006 award was published in the fall issue of the ACA *Newsletter.*

SER-CAT Outstanding Science Award

Lorena Beese, Duke University Medical Center, received the first annual SER-CAT Outstanding Science Award presented at the 2nd Annual SER-CAT Symposium, "Practical Aspects of Structure Determination Using Synchrotron Radiation," (see review on page 17) This award recognizes her contribution to the SER-CAT scientific program in regard to her studies of DNA polymerase as published in *Nature* and *Cell*.

B. C. Wang presenting the Award to Lorena Beese

The award criteria included a review of high-impact publications by a panel outside of the SER-CAT membership. Two of Beese's articles were judged to have the highest scientific impact out of all papers considered, specifically in molecular biology and in the understanding of cancers and aging: "Error-prone replication of oxidatively damaged DNA by a high-fidelity DNA polymerase," G.W. Hsu, M. Ober, T. Carell and Lorena S. Beese, *Nature* **431**, September, 217-221 (2004) and "Structures of Mismatch Replication Errors Observed in a DNA Polymerase," S.J. Johnson and Lorena S. Beese, *Cell* **116**, 803-816 (2004).

This Award was designed to recognize important scientific accomplishments carried out at SER-CAT during the previous year and is open to any researcher or research group carrying out experimental activities at SER-CAT. The Young Investigator Award was also introduced in 2005, to recognize work by a young investigator (within two years of his/her Ph.D. degree) at, or of benefit to, SER-CAT. The first Young Investigator Award was presented to ***Nicole LaRonde-LeBlanc*** of the National Cancer Institute, as reported in the last issue of the ACA *Newsletter*. Nominations are currently being accepted for the 2006 SER-CAT Science Awards.

SER-CAT is the acronym for Southeast Regional Collaborative Access Team, an organization consisting of 23 member institutions. The facility operates an ID and BM beamline, located at Sector 22, Advanced Photon Source (APS), Argonne National Laboratory. For more information on SER-CAT, please visit their website,***www.ser-cat.org***.

Lisa Horanyi

Presidential Award for Excellence

ACA member ***Steven Watkins*** (LSU) has been named as one of the nine winners of the Presidential Award for Excellence in Science, Mathematics & Engineering Mentoring.

The award ceremony was presided over by John H. Marburger III, director of the White House Office of Science & Technology Policy. Each winner received a presidential commemorative certificate and a $10,000 grant to apply to mentoring activities.

The award, administered by the NSF, "honors individuals and institutions that have enhanced the participation of underrepresented groups--such as women, minorities, and people with disabilities--in science, mathematics, and engineering education."

Steven, an associate professor and director of graduate studies at Louisiana State University, "is considered an indispensable force in their programs that produce the largest number of African American chemistry doctorates of any university in the country." During an interview about the award Steven said he delights in helping students cope with the rigors and anxieties of university life. "The one-on-one contact, the successful resolution of bureaucratic or personal problems, the growth of independence and confidence, and the final success of the degree--it's like being a parent and watching your child succeed - There is no greater reward than that."

National Academy of Sciences (NAS) News

ACA member ***John Kuriyan*** is the recipient of an NAS award for outstanding scientific achievement. The Richard Lounsbery Award, a medal and cash prize, was one of the awards presented at a ceremony during the 142nd annual NAS meeting. The Lounsbery Award is given annually in recognition of extraordinary scientific achievement in biology and medicine, alternating between young American and French scientists. The 2005 prize went to John Kuriyan, Howard Hughes Investigator and Chancellor's Professor in the Dept of Molecular and Cell Biology, UC Berkeley. John was chosen for his critical role in revealing the structural mechanisms underlying processivity in DNA replication and the regulation of tyrosine kinases and their interacting target

proteins. The award, established by Vera Lounsbery in memory of her husband, has been presented since 1979.

New NAS Members : During their142nd annual meeting in April The NAS elected of 72 new members and 18 foreign associates from 14 countries in recognition of their distinguished and continuing achievements in original research. Election to Academy is considered one of the highest honors that can be accorded a U.S. scientist or engineer. Those elected bring the total number of active members to 1,976 and the total number of foreign associates to 360.

Crystallographer ***Axel Brunger*** (Howard Hughes Medical Institute, and Professor, Department of Molecular and Cellular Physiology, Stanford University) was among the 72 distinguished scientists elected to the Academdy.

April 13, 2005 - Nanotechnology Grant Recipients Announced: The National Academies Keck Futures Initiative (***www7.nationalacademies.org/keck/***) announced the 2005 recipients of its Futures grants. Fourteen research topics were awarded a total of $1 million -- in sums of $50,000 or $75,000 -- to support interdisciplinary research on nanoscience and nanotechnology (***www4.nationalacademies.org/news.nsf/isbn/04132005c?OpenDocument***).

April 30, 2005 – Statement on International Cooperation in Science: The Council of the NAS has always been opposed to academic boycotts, and continues to call on the members of the world scientific community to support freedom in the conduct

of science and cooperative scientific exchange. As outlined in an August 2002 statement "The Critical Importance of Continuing International Collaboration in Science ," (*www4.nas.edu/nas/nashome.nsf/urllinks/NAS-5CXJ84?OpenDocument*) the Council firmly believes that scientists provide a voice for rationality and moderation in political affairs, and that they can and should work to build strong bridges of understanding between cultures. Two years after formally endorsing the establishment of the Israeli-Palestinian Science Organization (IPSO), the NAS Council is heartened to learn that IPSO now has the formal endorsement of 25 national academies, and that it has received more than 60 proposals from Palestinian and Israeli scientists who want to carry out joint research. These positive developments reinforce our belief that scientist-to-scientist and institution-to-institution interactions between Palestinians and Israelis are possible, and indeed vital to the future success of the region. It is especially unfortunate in light of this progress that there are renewed threats, from organizations outside the region, to academic exchange with Israeli universities.

May 10, 2005 - High-Quality Grad Students Integral to U.S. Science and Engineering: To maintain America's leadership in science and engineering research, a comprehensive effort is needed to improve the recruitment, education, and training of a cross section of U.S. students for careers in these fields, while at the same time continuing to attract the most talented scholars worldwide, says a new report (*books.nap.edu/catalog/11289.html)* from the NAS. These two goals are critical, given increasing global competition for quality graduate students and researchers

Conference on Research at the Interface of the Life and Physical Sciences: Bridging the Sciences

The meeting, held on November 9, 2004 in Bethesda, MD, was sponsored by the NIH Institute of Biomedical Imaging and Bioengineering and the NSF. It was planned by an Interagency Coordinating Committee and was intended to be a meeting of scientific researchers to obtain community input on how to bridge the life and physical sciences.

To meet this objective, the following three questions were considered:

1. What are high-priority issues and opportunities that will ultimately require the combined application of the physical, computational, social, and life sciences to address?

2. What are major challenges and barriers to bridging the sciences?

3. What actions or approaches are necessary to bridge the sciences and realize the potential benefits?

A total of about 170 people attended including 29 invited primary discussants from the life, physical, and interface sciences; investigators from a broad range of scientific disciplines; Congressional staff; and representatives of universities, technical societies, media, foundations, and Federal agencies. The one-day program consisted of two sets of breakout and plenary sessions aimed at addressing the three questions and developing consensus results.

The following topics were identified by the conference participants as high-priority opportunities that will need to be addressed by collaborations among the sciences: ·

Large-scale global problems - Climate change, national security, complex diseases, emerging diseases, environmental remediation, energy production and distribution, and food production.

Healthcare in the 21st Century - Personalized medicine, disease prediction, disease prevention, early diagnosis, early treatment, regenerative medicine, and reparative medicine.

Multi-scale phenomena - Bridging the vast scales of time, space, and organization in biosystems and natural systems - discovering physical principles that govern multi-scale phenomena and linkages.

Molecular-level measurement tools - Understanding fundamental biological and physical processes - measurement and imaging tools that provide molecular-level spatial resolution in living cells and temporal detection of chemical species in a single living cell.

Predictive understanding of biological systems - Quantitative approaches/computational models to analyze "omics" data to gain fundamental insights into biological processes.

Biological complexity - Understanding living systems will enable understanding the basis of health and disease.

Integrating biological and physical systems - The ability to integrate organic and inorganic systems will enable advances in a broad range of applications including manufacturing, medicine, environment, and energy.

The following areas were identified as contributing to challenges and barriers to bridging the life and physical sciences:

Education and training at all career levels –Insufficient investment of resources to develop researchers experienced in both the life and physical sciences who are able to work comfortably at the interface.

High-risk, long-term research – Opportunities and administrative mechanisms for support of high-risk, long-term research characteristic of basic scientific investigations in the physical sciences are inadequate and are eroding especially when biomedical applications are not initially apparent.

Problems to coalesce scientific communities - Scientific disciplines are presently too compartmentalized and do not have sufficient opportunities and incentives to encourage and sustain collaborations.

Research infrastructure - Facilities and tools, communication and interaction opportunities, and information management capabilities dedicated to supporting collaborative research and "team" science are inadequate.

Cultural differences across disciplines – Experts in scientific disciplines often have an inadequate appreciation for the expertise and potential of other disciplines and an imperfect ability to communicate with them.

Participants identified the following as novel actions that could catalyze, support, and sustain collaborations among scientific disciplines:

Identify and support well-defined, large-scale, complex problems (i.e., "big" research problems or grand challenges) that will drive multi-disciplinary research and nucleate the broad scientific community.

Increase support and develop appropriate mechanisms for long-term, high-risk research

Develop and maintain infrastructure required to support multi-disciplinary research and provide opportunities and support for multi-disciplinary education and training programs at all career levels aimed at ensuring a sustainable workforce of investigators equipped with the necessary technical expertise, appreciation of the physical and life sciences, and problem-solving abilities to conduct research at the scientific interface .

One of the suggestions for implementing the actions identified at this conference was a national effort aimed at bridging the sciences. Such an effort will require strong coordination and cooperation among academia, industry, national laboratories, technical societies, and Federal agencies and should not adversely impact existing programs that encourage and support collaborative research.

Complete information about this meeting is available at ***http://www.nibib1.nih.gov/Events/110904Conf/index.htm .***

Text excerpted from the Executive Summary prepared by Richard Swaja (NIBIB), Bruce Hamilton (NSF), Ken Dill (UCSF), Claire Fraser (TIGR), and Jose Onuchic (UCSD) February 4, 2005

Editors Note: The ACA has joined with other professional scientific societies to form a "Briding the Sciences Coalition." See the President's column and the article by Ken Dill on page 7 in the Fall '04 ACA Newsletter.

Contributors to this issue

Cele Abad Zapatero, Dan Anderson, I David Brown, Chris Cahill, Charlie Carter, Marcia Colquhoun, Bryan Craven, Durward Cruickshank, Louis Delbaere, Dave Duchamp, Howard Einspahr, Roberto Fornari, David Goodsell, Lee Groat, Lisa Horanyi, Andy Howard, Allen Hunter, Tom Koetzle, Jim Kaduk, Kathy Kantardjieff, Lisa Keefe, Chuck Kissinger, Edgar Meyer, Bill Pennington, Alan Pinkerton, S Narasinga Rao, Janet Smith, Ron Stenkamp, Peter Sun, Bob Sweet, Jack Tanner, Brian Toby, Iris Torriani, Winnie Wong-Ng.

Crystallography in Peru

A course on applications of x-ray diffraction and Rietveld refinement was recently organized at the Universidad Nacional Mayor de San Marcos, in the city of Lima, Perú. The site of this event is known to be the oldest University established in Latin America, founded by the Dominicans in 1551. The course was offered in March (7 – 18), 2005 and was attended by over 55 participants (students and teachers). The course was initiated by young researchers who graduated abroad and are interested in sharing the knowledge they have acquired. It also revealed the existence of a community that is active and interested in crystallography and will certainly grow. (***www.unmsm.edu.pe/sanmarcos/index.htm***)

The objective of the course was to give a solid base for theoretical and experimental aspects of powder diffraction and the refinement of crystal structures by the method of Rietveld.

Topics covered included:

- Introduction to x-Rays: historical aspects. A brief review of the different types of spectrometries (EXAFS, SAXS, ZANES, etc.)
- Generation of x-Rays: conventional methods (tube and rotating anode). synchrotron radiation.
- Properties of x-Rays: dsispersion and polarization.
- Diffraction of x-Rays: powder diffraction and Bragg-Brentano geometry.
- Determination of crystal structures: indexing of crystals, distortion effects of the cell.
- Methods of x-Ray diffraction: powder methods data treatment.
- Refinement Rietveld methods: fundamental theory of the method, important parameters and refinement of structures.

Iris L. Torriani

ACA Country Members

Both Brazil and Argentina have become Country members of the ACA in 2005.

The Argentinian membership has been sponsored by Aluar Alumino Argentina SAIC.

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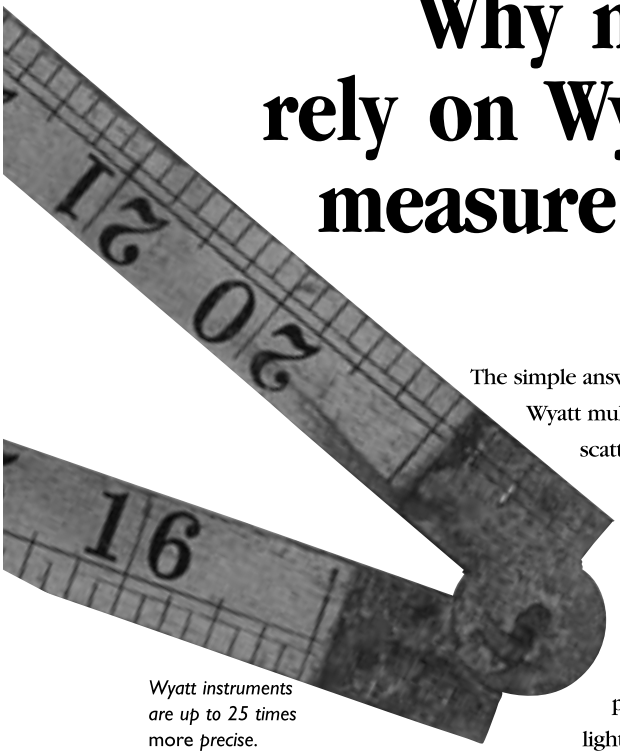

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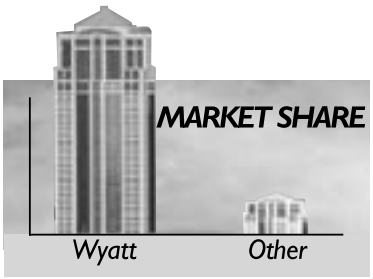

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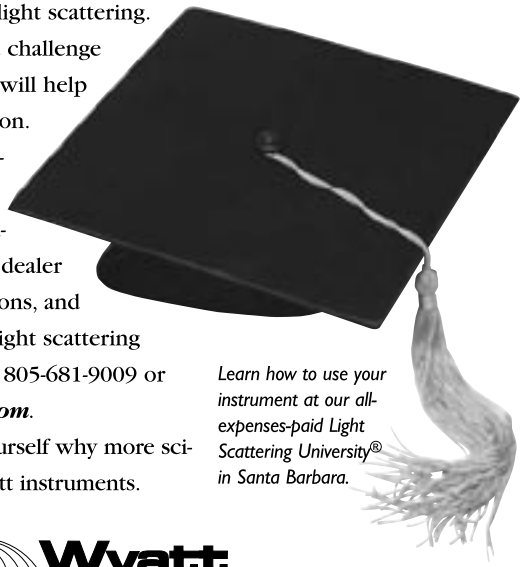

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Crystal Growth under the Popocatepetl

The *IUCR Commission on Crystal Growth and Characterisation of Materials* closed out the 2002-05 triennium with an international school which took place in Puebla de los Angeles (Mexico) between the 7th and 11th of March 2005. The **International School on Crystal Growth: Fundamentals, Methods and Applications of Biological and Nano-crystals** was co-chaired by ***Maria Eugenia Mendoza*** (Institute of Physics, Univ. Puebla) and ***Abel Moreno*** (Institute of Chemistry, UNAM) and sponsored by the International Union of Crystallography (IUCr), Sociedad Mexicana de Cristalografia, Universidad Autonoma de Puebla, Universidad Autonoma de Mexico, Bruker, Spectramex, Zeiss and Presidencia Municipal de la Ciudad de Puebla.

Abel Moreno and Maria Eugenia Mendoza, co-chairs of the International School on Crystal Growth, holding the school's ensignia.

The school was specifically aimed at young researchers, PhD and Master students working in the area of materials science and biological crystallization. The main objective was to provide basic crystal growth concepts along with an overview of growth technologies. Furthermore, the program included a series of tutorial lectures on specific subjects such as, for example, computer modelling of growth processes, epitaxy of semiconductors, bulk growth of oxides and semiconductors, organic materials for NLO, ferroelectric materials, solution growth of biocrystals, structural studies and defects in real crystals. Though the program may appear extremely broad, both lecturers and participants recognized that it was useful in order to overcome the strict borders of each one's field of activity and to stimulate discussion.

The school was attended by 45 participants, most of them from Mexico, but with a good representation from other Latin-American countries as well. The truly international character and the friendly behavior of participants and lecturers provided a nice and stimulating atmosphere for scientific as well as general discussions. The interest of participants in the subjects of the school was shown by the high level of attendance at each lecture. In addition to the official school program, poster presentations were organized during the one-hour breaks in the morning and afternoon. The poster presentations were highly appreciated as they proved to be useful to promote new contacts and strengthen relations among participants.

The school was altogether superbly organized, lectures and students were accommodated in two beautiful hotels in the historical center of Puebla, a colonial city some 120 kilometers from Mexico city, rich in magnificent buildings, museums, baroque churches, lively streets and cultural sites. The lectures were held in the central building of the 400 year old University. The 16 lecturers from Canada, France, Germany, Uruguay, Mexico, Spain, Switzerland and USA had the nice surprise of being awarded with a "Reconocimiento" (Acknowledgment) by the Mayor of Puebla for having contributed to the development of the scientific culture in Mexico.

The list of lectures and other information are available at the address: ***www.ifuap.buap.mx/ISCG05/school.html***

R. Fornari, Chair

IUCR Comm on Crystal Growth and Characterization of Materials

USNCCr News

IUCR General Assembly in Florence:

The U. S. National Committee for Crystallography (USNCCr) is the body which represents the United States to the IUCr, on behalf of the National Academy of Sciences (NAS, which is the Adhering Body to the Union). One of the most public way this representation occurs is at the IUCr General Assembly since it is the USNCCr that elects the delegates to represent the U.S. at the Assembly. The XXth IUCr General Assembly will take place on several evenings during the Florence IUCr Congress. The U. S. delegation will be chaired by Jon Clardy (Harvard Medical School and Chair of USNCCr). Other members are Jim Kaduk (BP Innovene, USNCCr Vice Chair), Judy Flippen-Anderson (RCSB), Katharine Kantardjieff (Cal State Fullerton), and Brian Toby (NIST). The alternates are Robert Bau (USC) and Fran Jurnak (UC Irvine).

The General Assembly (GA) agenda usually includes such items as amendments to the statutes and by-laws, applications for membership in the Union, withdrawal of Adhering Bodies, and changes in names and/or categories of Adhering Bodies. In recent years, there has been considerable discussion on what to do about countries that have fallen behind in their dues payments to IUCr. We can expect this General Assembly to continue to try to strike the right balance between involving all crystallographers and maintaining income.

There will be a report and discussion of the finances of the Union. If anyone wishes to ask a question about IUCr finances, please relay it to the delegation. The GA receives reports of the various IUCr Commissions, reviews their work, and considers proposals for new commissions. Reports are also received from representatives of Regional and Scientific Associates, and from representatives of bodies which do not belong to the Union.

One of the main tasks of the General Assembly will be to determine the date and place of the XXIInd General Assembly in 2011 (XXI will be held in Osaka, Japan in 2008). Spain and Brazil have been mentioned as potential sites for the IUCr meetings 2011 and 2014. If this comes to pass then North America could be considered for the 2017 meeting. We should start thinking about hosting an IUCr meeting while it would still be possible to take advantage of the institutional memory of those who planned the 1996 meeting in Seattle.

The appointments of editors for IUCr publications are made by the Executive Committee, and ratified during the General Assembly. The various National Committees have already sent suggestions to the IUCr Executive for members and chairs of the various Commissions. The Executive Committee uses these suggestions, hopefully keeping both geographic and gender balance issues in mind, to put together a list of candidates for election at the General Assembly.

The climax of the General Assembly is the election of the Officers of the Union and members of the Executive Committee. As they did with suggestions for Commission members the National Committees submitted nominees for these positions to the Executive Committee. Bill Duax, current President of the IUCr, will automaticallly serve another three years as Past-President.

The Executive Committee then presented the following slate of candidates for election during the General Assembly:

President:
Y. Ohashi (Japan)
General Secretary and Treasurer:
S. Lidin (Sweden)
Executive Committee - Six-year terms:
P. Coleman (Australia)
G.R. Desiraju (India)
C. Gilmore (UK)
M. Kovalchuk (Russia),
C. Lecomte (France),
M. Perez-Mato (Spain)
Executive Committee: Three-year term:
I. Torriani (Brazil)

It is interesting to note that, as put forth by the Executive Committee not all positions have multiple candidates nor are there any candidates from North America. It is possible to nominate additional candidates during the Congress. The USNCCr favors a policy of having multiple candidates for all position on the Executive Committee and welcomes your input on this issue. (jdb20@cornell.edu).

Stated so plainly, much of the business of the General Assembly must seem boring. But, since the decisions made there influence the operation of the Union for the next 3 years, they are important, and could affect every crystallographer. The U. S. delegation welcomes your input on any of these topics.

USNCCr spring meeting:

The agenda for the U. S. National Committee meeting on 28 May in Orlando included a discussion of the recent NIH decision to discontinue the subsidy for academic users of the Cambridge Structural Database in the U.S. This decision will raise the annual price of a yearly subscription from $400 to approximately $1300. Other topics for discussiono were what the influence of the NIH policy on open access to results will have on the crystallographic journals, and how the proposed FY2006 budget could negatively impact operations of national user facilities. While as an organization we cannot be overtly political, each crystallographer can express a personal opintion to help ensure that the interests and needs of our science are communicated to our respective members of Congress.

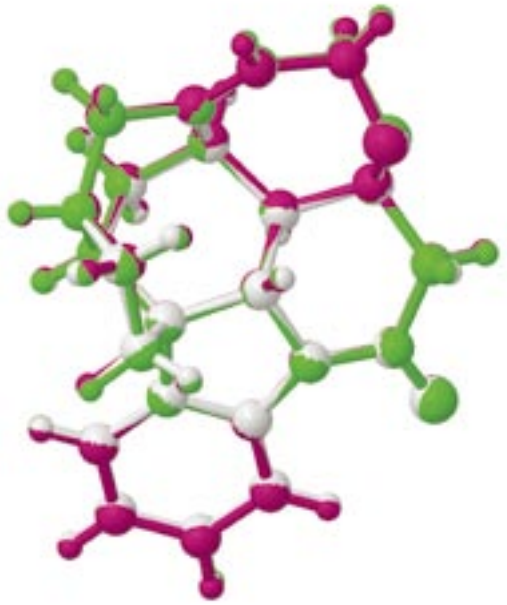
More detailed reports on both the IUCr General Assembly and the USNCCr meetings will be published in forthcoming issues of the ACA *Newsletter*.

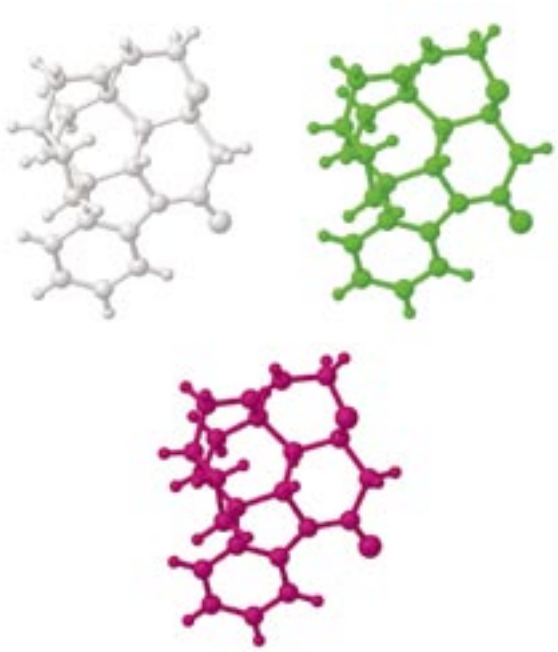
Jim Kaduk

Crystmol 2.1

The latest version of CrystMol was announced at the Chicago ACA meeting. CrystMol was developed to facilitate in-depth analysis and visualization of experimental crystallographic results for both small molecules and macromolecules. CrystMol provides easy-to-use access to most tools for analysis and display of crystal and molecular structure, including: various three-dimensional structure displays; bond distances; bond angles; torsion angle;, built-in space group symmetry; anisotropic thermal parameter;, CIF files; PDB files; standard deviations; best planes; hydrogen bonding; packing displays; molecular mechanics; protein secondary structure assignment; and QuickTime movies. CrystMol contains many capabilities useful to practicing crystallographers. It's also designed to be used by scientists and science students not familiar with crystallography. It can function as a teaching tool in undergraduate and graduate college courses.

The Chicago talk focused on new CrystMol tools for comparison of multiple experimental determinations of the same and similar molecules. Multiple molecules in the asymmetric unit of small molecule structures may be compared with each other very easily via a one-click overlay. Polymorphs of the same molecule may be automatically matched also. CrystMol does the hard part of the work via two new software algorithms. One matches molecules topologically according to their bonding arrangements (referred to as their "molecular graph"), and the other moves molecules as rigid bodies to find the best overlay. Non-identical molecules require manual set-up of matching atoms. A command is available for manually switching enantiomorph when multiple molecules in the asymmetric unit of centrosymmetric structures have different handedness. Root mean square displacements between matched atoms are calculated to provide details on the exactness of match. CrystMol's automatic matching algorithm was used to create the strychninium ion overlay shown below.





Overlay and spread views of strychninium ions from three different strychnine salts - perchlorate monohydrate (gray), hydrogen sulfate dihydrate (green), and dihydrogen phosphate dihydrate (magenta). RMS deviation was 0.4 Å for the 25 non-hydrogen atoms, indicating an excellent match. Data is from the CIF file for Acta Cryst. (2005). C61, o161-o164.

Macromolecular overlay is illustrated below by two overlaid monomers of the insulin dimer.

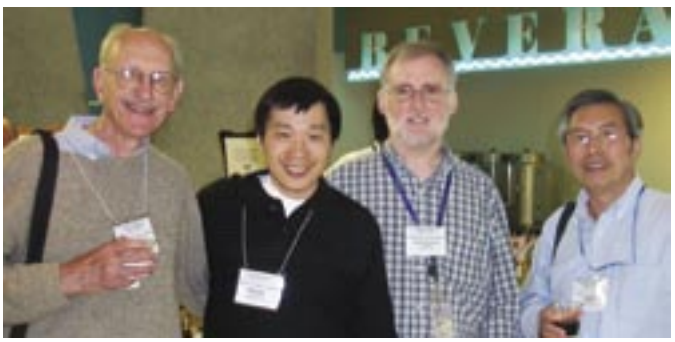
Overlay view of the two monomers of the porcine insulin dimer. RMS deviation was 0.5 Å for the 45 (of 51) residues that matched closely. Data is from the PDB file 4INS from Philos. Trans. Royal Soc. London (1988) Ser. B 318, 369.

CrystMol is available in Windows and Macintosh versions. Documentation (three manuals) is included with the program. There is a nominal charge for a license. More information is available on the CrystMol web site ***www.crystmol.com***.

Dave Duchamp

35th Mid-Atlantic Macromolecular Crystallography Meeting

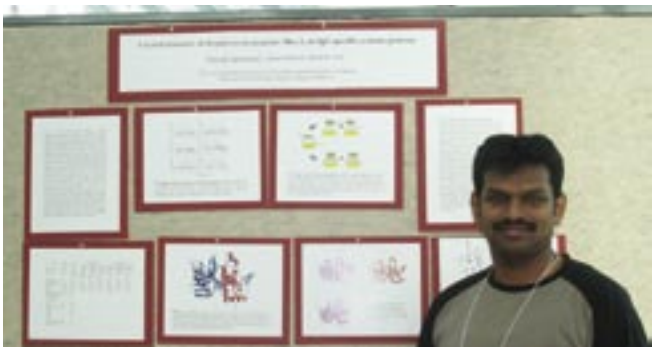
This year's meeting, held at NIH on May 11-13, was organized by ***Peter Sun*** and ***David Garboczi*** of NIAID and ***Mario Amzel*** (Johns Hopkins). The meeting attracted about 200 regional participants. This year's keynote address was delivered by ***Robert Stroud*** (UCSF) (pictured below) on their structural work on aquaporins and ammonium transporter, which are integral membrane proteins. After the keynote speech, participants enjoyed a lively reception with wine and beer, followed by a buffet dinner. On May 12, the scientific sessions started with ***Philip Anfinrud***'s (NIDDK) talk on visualizing structural dynamics in myoglobin using time-resolved Laue crystallography, and ***Irene Weber***'s (Georgia State) talk on the joys of atomic resolution structural studies of enzymes. Among the highlights of the meeting were the two talks given by ***Robert Kretsinger***, the founding member of the Mid-Atlantic Crystallography meetings, and ***Alexander Wlodawer*** on the historic perspective of the society and on the early development of synchrotron radiation in protein crystallography. Kretsinger reflected on his personal notes and communications from the early years of the meeting, which started in 1970 with a dozen or so participants. He also urged the present and past organizers to join his effort to archive the history of the annual meetings. Wlodawer, in his talk on early application of synchrotron radiation to protein crystallography, reminded us of the era when diffraction data were routinely recorded using precession camera on film. Other presentations on the second day included ***David Garboczi***'s talk on the structure of *Plasmodium* P25, an essential protein for transmission to mosquitos and ***Mark Mayer***'s (NICHD) talk on a glutamate receptor ion channel.



David Davies, Peter Sun, David Garboczi and Xin-hua Ji

Among the dozen commercial vendors participating in the meeting, Roche, Genecopoeia, Nextal and Fluidigm presented their newest technologies related to protein expression and crystallization. The poster session featured ~ 40 posters and was well attended. The day ended with another social gathering.

On the last half-day of the meeting ***Jae Young Lee*** (NIDDK) presented a Linchpin model for type II restriction endonucleases based on the structural studies of MutH complexed with hemi- and unmethylated DNAs. ***Brad Nolen*** (Yale) talked about crystal structures of Arp2/3 complex with bound nucleotide. ***Miguel Garcia-Diaz*** (NIEHS) offered structural insights for the Pol lambda catalytic cycle on normal and misaligned substrates.



Agniswamy Johnson and his poster on mac-1

Progress on structural genomic frontier was reported by ***Kinlin Chao*** (CARB) presenting the structure of *E.coli* YdcF, a nucleotide-binding protein and by ***Vivian Stojanoff*** (BNL) talking about ultra-high resolution and high throughput at the NIGMS East Coast Structural Biology Facility. ***Haijun Qiu*** reported on current progress of PepcDB project at the Midwest Center for Structural Genomics and reviewed up-to-date results from the other eight structural genomic centers.

Hua-poo Su and his poster on poxvirus L1 protein

Irene Weber, Robert Rose and Alex Wlodawer

The 35th annual Mid-Atlantic Meeting showed again that it is very much alive and vibrant as it brought together the growing community of crystallographers of the East Coast and reflected on changes and new directions in this field of research.

Peter Sun

17th West Coast Protein Crystallography Workshop

Over 300 attended the West Coast Protein Crystallography Workshop held at the Asilomar Conference Center in Pacific Grove, California March 20-23, 2005. ***Mary McGrath*** and ***Bob Stroud***, along with their staff, did a wonderful job organizing this workshop, the 17th in a series started by Jens Birktoft 35 years ago at Warner Springs near San Diego. The traditional "bar-PI" rule was in effect (with few exceptions), so nearly all of the talks and posters were presented by post-docs and students. The weather (rainy and stormy) limited the beach excursions, but it didn't affect the high quality of the science in the presentations.

crystals, the peptides take on an extended β-strand conformation and line up to form β-sheets that extend across the crystal, making their crystal structure even larger than the virus reported by Steve Larson (UC Irvine) or the vault protein reported by Dan Anderson (UCLA).

The remainder of the talks covered developments in new and old techniques and software. One interesting technology under development for several years is the Free Mounting System described by ***Joe Ferrara*** (MSC). He showed the effects of dehydration on protein crystals, both in terms of external mor-

Scenes from Asilomar: Discussions at a poster session, views of the Pacific and (left-to-right) Clare Peters-Libeu, Isolde Le Trong, and Gye Won Han

The Sunday night session started with a plenary lecture by ***Dick Dickerson*** (UCLA), who described the fundamental steps in our understanding of protein and DNA structures. His recent book aoubt this, "Present at the Flood. How Structural Molecular Biology Came About", includes reprints of important papers in the field dating back to the 1930s.

Sixty-nine percent of the 39 talks focused on structural results and covered a broad range of biological systems. The smallest and largest structures reported were for two amyloid-related peptides. ***Rebecca Nelson*** (UCLA) described a project in Dave Eisenberg's lab involving two peptides (NNQQNY and GNNQQNY) with sequences found in the yeast prion protein Sup35. Amyloid fibrils form in solutions of these molecules, and with suitable manipulation, microcrystals of the peptides can be obtained. Diffraction data collected using the microfocus capabilities of the ESRF extend to 1.3 and 1.8 Å for the two peptides. In the

phology and quality of their diffraction patterns. He showed a video of crystals shrinking and expanding as the humidity of an airstream passing over them decreased and increased. He also showed, using still photos, how the quality of the diffraction pattern could be optimized by adjusting the humidity. In some cases, substantial improvements in resolution can be achieved.

This Asilomar meeting was another in the long series of wonderful West Coast workshops. Several vendors participated in the meeting and contributed to its success in various ways. This year, prizes were awarded to the best of the 100^{+} posters presented during the meeting. Mary and Bob did a fine job organizing the meeting. ***Andy Karplus*** and ***Dick Brennan*** are the co-chairs for the next one scheduled for the spring of 2007.

Ron Stenkamp

Second Annual SER-CAT Symposium

The symposium, "Practical Aspects of Structure Determination Using Synchrotron Radiation," was held at St. Jude Children's Research Hospital in Memphis on March 18, 2005. It brought in a diverse group of ~ 50 participants from senior scientists to graduate students. In addition to the scientific program, attendees had the opportunity to tour the facilities and learn more about the history of St. Jude Hospital.

The scientific program began with a presentation by ***Irene Weber*** (Georgia State), who presented atomic resolution crystal structures of HIV protease mutants and described how these findings will be used in the development of new antiviral inhibitors.

method for protein crystallization which allows screening of up to 100 conditions while using a minimum amount of protein. Participants also learned how *in-situ* annealing, or "flash-annealing," can be used to improve the diffraction quality of macromolecular crystals. This method has been proven to produce better signal-to-noise ratios, which ultimately leads to the detection and measurement of higher resolution data.

K.R. Rajashankar (MSKCC) offered practical advice with "Getting the best data and getting the best out of your data." He summarized his experiences and general knowledge on ways of collecting good data sets and means of making the best use of it. Rajashankar is currently a scientist at the Memorial Sloan-Kettering Cancer Center in New York City, but has previously worked

John Chrzas (SER-CAT) followed with, "Did I collect the data I need to solve my problem?" which highlighting practical solutions for making the most efficient use of the SER-CAT facility. He also gave an overview of new beamline features that will be provided by the SER-CAT Operations Team, including automated tools for data processing, structure solution and refinement.

Andy Mesecar (UIC) focused on the technique of time-resolved x-ray diffraction studies. His lab is currently studying the structure and function of enzymes and receptors involved in cancer chemoprevention, cancer cell proliferation, cell longevity (aging), bacterial and viral pathogenesis, and bioremediation. Time-resolved x-ray crystallography is one of many tools from the fields of chemistry, biology and physics that are used in these studies. Mesecar presented an overview of time-resolved x-ray diffraction using the Laue method, a technique routinely used by his group at the Advanced Photon Source.

Pappannan Thiyagarajan (IPNS, ANL) and ***Dean Myles*** (ORNL) gave an overview of neutron macromolecular crystallography (NMC) at the Spallation Neutron Source (SNS) being developed at Oak Ridge National Laboratory. NMC can be used to provide accurate information on positions of protons and water molecules in the active sites of enzymes that will enable the elucidation of the mechanistic details involved in their function. Participants also learned of proposed plans to develop a dedicated high throughput and high resolution time-of-flight single crystal macromolecular neutron diffractometer (MaNDi) that will be used to exploit the high neutron flux that will become available by 2006 at the SNS.

Joanne Yeh (Brown) illustrated methodologies used by her lab in protein crystallization and diffraction of macromolecular crystals. She described an easily adaptable, manual nanoscale

at both Brookhaven and Argonne synchrotron facilities.

Brenda Schulman (SJCRH) presentedways to cope with the problem of poor electron density in several crystals that diffracted moderately at the SER-CAT facility. She gave an overview of a selenomethionine-scanning mutagenesis technique and described how it was used to solve the structure of the 110 kDa ternary complex between human SPPBP1-UBA3 and a 26-residue peptide corresponding to the N-terminal region of Ubc12.

Participants also took part in a hands-on workshop, entitled "A New Approach to Structure Determination Applicable to SER-CAT and In-house Operations" led by U of Georgia researchers ***Zhi-Jie Liu, Zheng-Qing Fu and Wolfram Tempel.*** An overview was given on techniques recently used to solve five structures in 23 hours during a visit to the SER-CAT facility. Attendees learned the techniques used in preparation, data collection and structure determination as well as the combination of technologies used behind the scenes.

SER-CAT Science Awards: Two new awards, designed to recognize important scientific accomplishments at or of benefit to SER-CAT were announced at the symposium. The SER-CAT Outstanding Science Award was presented to ***Lorena Beese*** (Duke), recognizing the scientific impact of her work in DNA polymerase studies related to the understanding of cancers and aging (see page 7). The SER-CAT Young Investigator Award, open to researchers within two years of a Ph.D. degree, was presented to ***Nicole LaRonde-LeBlanc*** (NC I) recognizing her work on RIO serine kinases, which was recently published in *Structure*. The next SER-CAT symposium will be held in March 2006. Details are available at ***www.ser-cat.org.***

Lisa Horanyi, SER-CAT

GM/CA CAT at APS to be Dedicated

This summer a new facility for macromolecular crystallography, known as GM/CA CAT, is being dedicated at the Advanced Photon Source (APS). The GM/CA CAT facility, based at APS sector 23, includes two beamlines from insertion-device (ID) sources and one from a bending-magnet source. The powerful ID beamlines are produced by dual canted undulators that reside in one straight section of the storage ring. The APS undulator has been a highly successful x-ray source for macromolecular crystallography at other APS sectors because it produces a brilliant, parallel beam. The ability to produce two independently tunable undulator beams in one straight section is a major technical advance achieved by APS scientists and engineers. At present, the two undulator beamlines have been built. User experiments are underway on one beamline, and will begin on the second beamline in fall, 2005. The bending magnet beamline will be completed in 2006.

The goal of GM/CA CAT is to operate a streamlined, user-friendly facility where data can be collected from samples of variable size and quality. All beamlines are rapidly tunable, and the facility is capable of multiwavelength anomalous diffraction (MAD) experiments over a wide energy range from 3.5 keV to 35 keV (wavelengths of 3.54 Å to 0.35 Å). In addition to rapid tunability, the facility emphasizes use of small, stable beams for experiments with small crystals (or small regions of larger crystals). Small beam sizes are achieved by focusing mirrors (20 mm x 80 mm for the undulator beams). Feedback systems stabilize the position and intensity of the x-ray beams. Specialized goniometry allows accurate and reproducible positioning of samples that are less than 10 mm in size. Optical alignment of crystals is aided by a permanently mounted microscope to view samples directly along the x-ray beam. The Blu-Ice user interface, developed at SSRL, is used for experiment control. The ALS sample-handling robot is being adapted for the GM/CA CAT beamlines.

The figures show results from bacteriophage HK97 obtained by Lu Gan and Jack Johnson (The Scripps Research Institute). Gan and Johnson obtained data well beyond the previously observed diffraction limit of crystals of the HK97 virus. The data allowed them to visualize the unusual chemical crosslink of lysine and asparagine side chains that the virus uses to interlock subunits and form its stable and rigid shell.

The GM/CA CAT dedication is the culmination of a partnership of the National Institute of General Medical Sciences (NIGMS, or "GM") and the National Cancer Institute (NCI, or "CA"). These two Institutes at the National Institutes of Health (NIH) established the GM/CA Collaborative Access Team (CAT) because their sponsored projects need the most advanced methods for rapid data collection, and structure determination at the highest available resolution for a wide range of sample types. ***Janet Smith***, University of Michigan, is the Director of GM/CA CAT. ***Robert Fischetti***, GM/CA-CAT Project Manager, heads up the 12-member GM/CA-CAT staff, which is based in the Biosciences Division of Argonne National Laboratory.

Beam time at GM/CA CAT will be allocated for several categories of users. When all three beamlines are operating, the largest single share of beam time will be for general users, who will apply through the APS central system. Another share of beam time will be set aside for projects within targeted programs of the two sponsoring NIH Institutes. For the NIGMS, the targeted program is the Protein Structure Initiative (***www.nigms.nih.gov/psi/***). The targeted programs of the NCI will discover molecules with anti-cancer or cancer-preventive activity. In addition, beam time is set aside for research projects of GM/CA CAT and of members of the GM/CA Synchrotron Advisory Board.

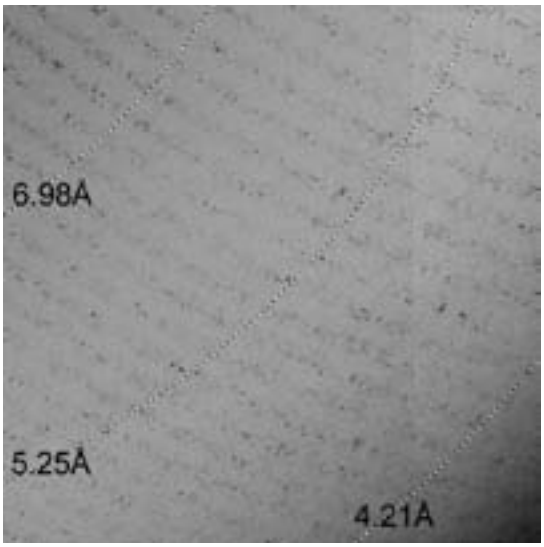


Figure 1. Part of a diffraction image from crystals of bacteriophage HK97. Spots are well resolved for the 1000-Å unit cell using x-rays of wavelength 0.688 Å focused to ~25 μm x ~90 μm on GM/CA-CAT beamline ID-23$_{in}$. The 0.25° oscillation image was recorded on a Mar mosaic detector 681 mm from the sample.

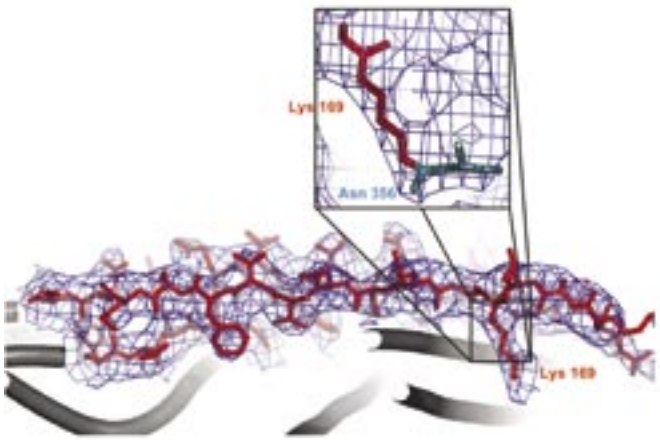
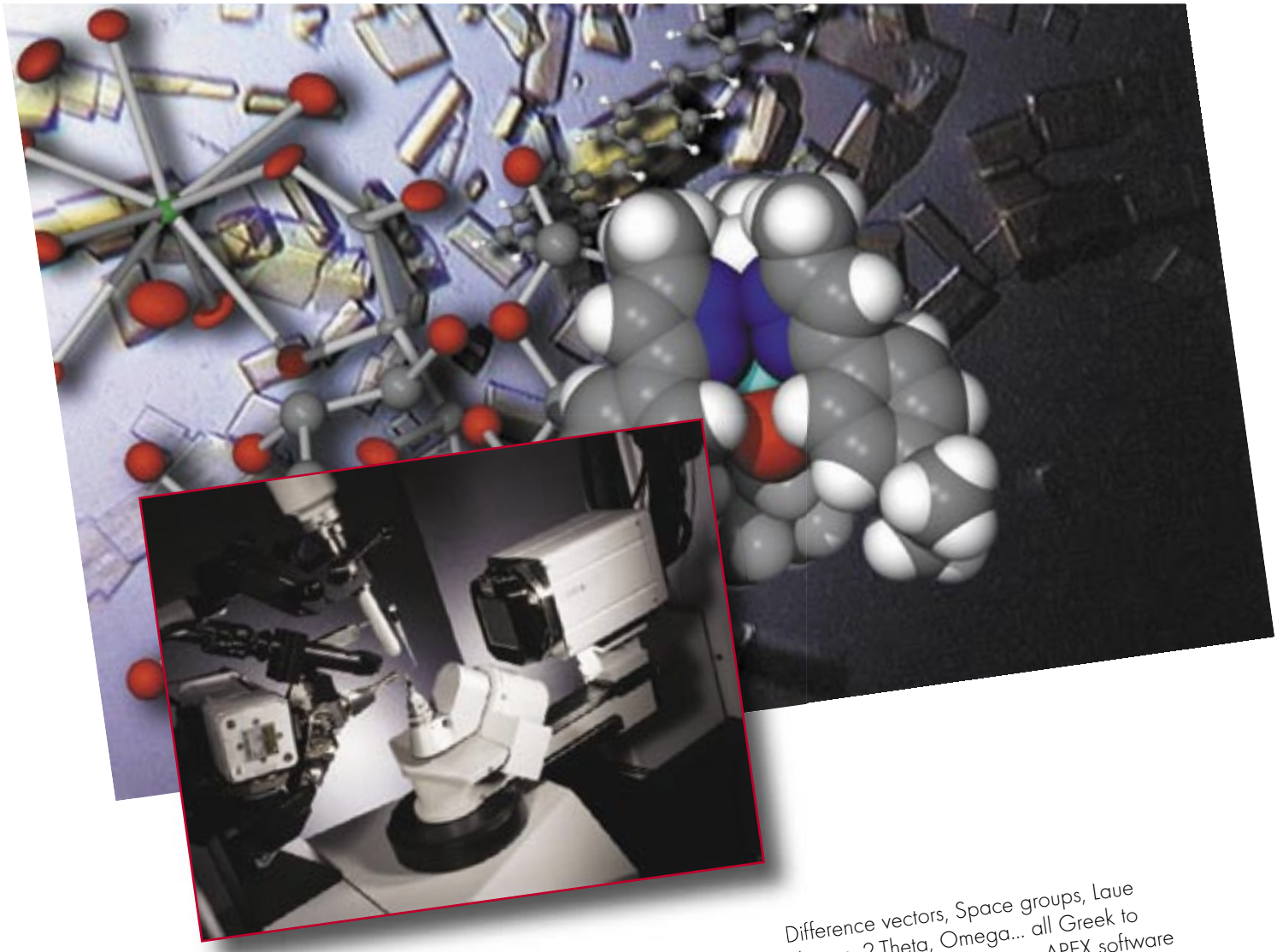


Figure 2. Electron density for the crosslinked region of bacteriophage HK97. The long loop including residue Lys 169 is shown in 3.9-Å electron density contoured at 1.5 times the RMS level superimposed on a ribbon diagram of the protein in gray. The polypeptide (red stick rendering) is built into the density. The insert shows the chemical crosslink between Lys 169 and Asn 356 (cyan) in another subunit. This crosslink, repeated 420 times in the virus capsid, rigidifies the shell and interlocks the subunits much like the links of a chain.

Janet Smith



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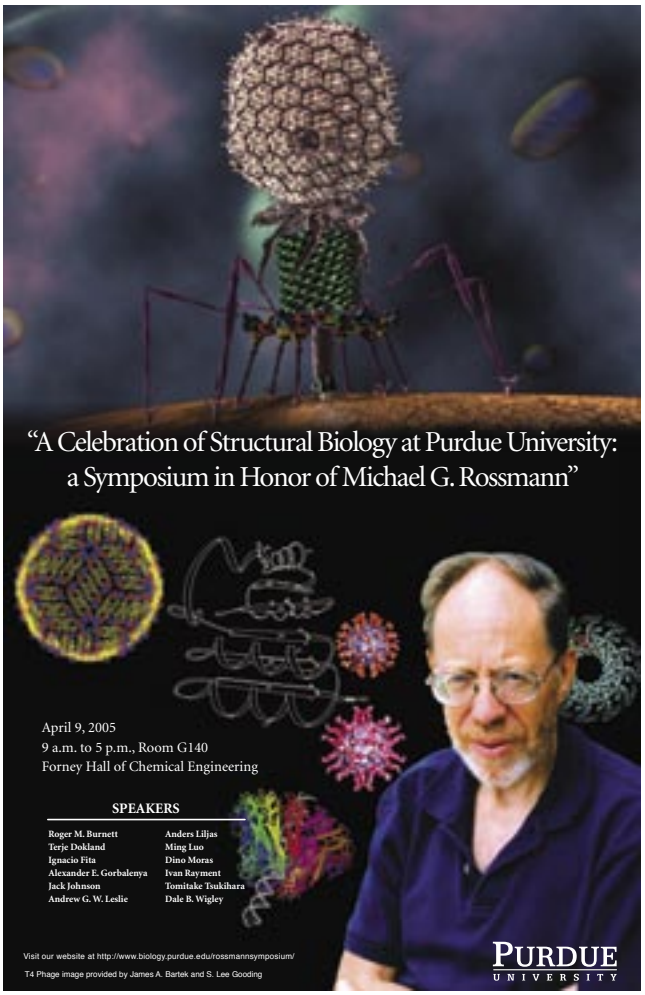
Notes of a Protein Crystallographer - Homage to Prof. M.G. Replacement: A Celebration of Structural Biology at Purdue University.

Macromolecular crystallography has developed into an extremely powerful technique to determine the three-dimensional structure of the molecular components of living systems. Its place among modern scientific disciplines is now well established. However, this was not so forty years ago when the pioneering heroes of protein crystallography were beginning to conquer, one by one, the structures of the icons of our field: myoglobin, hemoglobin, lysozyme and the others that followed. In fact, the future of the field was not clear in the mid 60's as the MIR method pioneered by Perutz for the structure of hemoglobin failed to yield rapid successes when applied to other proteins.

At that time in the history of the field, 1964 to be exact, Prof. M.G. Replacement moved from the MRC in Cambridge to Purdue University in West Lafayette, Indiana, in the heart of the American midwest. To commemorate the 40th anniversary of that event and to celebrate also the achievements of structural biology during those forty years, a symposium was organized at Purdue University on April 9, 2005. Naturally, the purpose of the meeting was also to honor the man behind it, ***Michael G. Rossmann***.



The date also corresponded approximately to MGR's 75th birthday so it was a memorable occasion for several reasons. An earlier meeting ten years ago also honored Michael (New directions in Protein-Structure Relationships. Symposium in Honor of Professor M.G. Rossmann's 65th Birthday. Purdue University, Oct. 21, 1995). On this occasion the symposium was more encompassing of the science and had a much more global character. The scientific topics and the featured speakers addressed advances in vast areas of structural biology. They came from the four corners of the world to share their work with the new generation of structural biologists currently being trained at Purdue.

A detailed report of the meeting has been published recently in *Structure* (Abad-Zapatero, C. (2005) *Structure,* **13**, 1-4). An abridged version is presented here to convey the excellence of the science discussed, the ambiance of the meeting and the camaraderie among all participants. Readers are encouraged to consult the published meeting review for a complete technical summary.

The symposium opened with brief comments by ***Jeff Vitter*** (Dean) and ***Richard Kuhn*** (Department Chair). The morning session, chaired by ***Jeff Bolin,*** (Associate Dean of Research) focused on Proteins and Complex Assemblies.

Dale Wigley (London Research Institute, London, UK) formerly a visiting scientist in MGR's lab discussed helicase structures in detail, focusing on the quaternary complex of RecBCD bound to a DNA hairpin duplex. ***Andrew Leslie*** (MRC, Cambridge, UK) a former postdoc at Purdue and member of the virus group in the late 1970's , reviewed the main structural and functional features of the multimeric structure of the ATPase as unveiled in the last ten years combining the structural data with the results of the dynamic fluorescence studies of Yoshida and coworkers in Japan.

After the coffee break, ***Anders Liljas*** (University of Lund, Sweden) one of Michael's postdocs during the heroic years of LDH, addressed some of the still unanswered questions about protein synthesis. He suggested a more integrated, five-pronged approach where x-ray, NMR, cryoEM, theoretical (computational) chemistry and physical chemistry would be needed to understand the most complex problems in molecular biology. ***Tomitake Tsukihara*** (Osaka University, Japan), a member of the group that solved Southern Bean Mosaic Virus (SBMV) in the late 1970s, presented the results that the group in Japan has been obtaining during the last decade on the structure and reaction mechanism of cytochrome c oxidase. Given the sheer size of the oxidase (13 subunits) and the complexity of the reaction catalyzed by this enzyme, one is constantly reminded of the subtlety of the conformational changes required to transfer protons or electrons by such a large multimeric enzyme across the mitochondrial membrane.

In perfect consonance with the spirit and intensity of the honoree, the organizers allowed the attendees only a brief break for a lunch that was packed with anecdotes and recollections from a few persons whose lives intersected with Michael's at critical times in their careers. Over a background of images of the French Alps and MGR in full hiking gear provided by ***Janet Smith*** (University of Michigan, Ann Arbor), ***Don Bilderback***

(CHESS, NY) reviewed the impact that the crystallographic work on rhino virus played in the development of synchrotron radiation for virus crystallography. as ***Alwyn Jones*** (Institute of Cell and Molecular Biology, Uppsala, Sweden) in his own inimitable style, captured the audience with his recollections of the impact of the early days of computer graphics on macromolecular crystallography.

It was a very special moment when ***Sharon Wilder***, MGR's personal assistant and factotum, told the story of how she found her way to Michael's office for her job interview. The rest is history. Outsiders will probably never realize what a unique role Sharon has played. She was anonymous and unassuming yet always extremely competent and knowledgeable in a myriad of tasks. She always orchestrated the routine of the laboratory with a gentle but effective harmony. The audience recognized her unique contribution with a standing ovation at the end of her brief presentation. By taking care of so many odd-jobs she allowed MGR to concentrate on the important tasks needed to revolutionize the field. This is indeed a major contribution.

John E. ('Jack') Johnson (Scripps Research Institute, California), a close associate of Michael for many years, concluded the lunch period with some candid anecdotes. He described his time at Purdue from the late days of the dehydrogenases (GPDH and LDH) project to his impact on the critical work on the Southern Bean Mosaic Virus (SBMV). The methods developed during those years are now mainstream in the area of virus crystallography.

The afternoon session was chaired by ***Carol Post*** (Purdue) and was devoted almost exclusively to virus work. Ming Luo (University of Alabama), former graduate student, presented structural genomics results of the South Eastern Collaborative for Structure Genomics. ***Roger Burnett*** (Wistar Institute, Philadelphia), MGR's first (surviving) graduate student, discussed the evolutionary implications of the finding that the structure of the major coat protein (P3) of bacteriophage PRD1 resembles that of the component of the human adenovirus hexon. ***Alexander Gorbalenya*** (Leiden University Medical Center, The Netherlands), a former visiting scientist, discussed his explorations into the classification and life cycles of various virus genera within the universe of RNA-containing virus.

Ignacio Fita (Institut de Biologia Molecular de Barcelona, Spain), former postdoc on the catalase project, presented the structure of a representative of the minor group of human rhinovirus (HRV2-V23) bound to the ligand binding repeats of its cellular receptor (VLDLR). ***Terje Dokland*** (University of Alabama, Birmingham), former postdoc associated with the lab, presented his results on the structures of the nucleocapsid and core proteins of two enveloped ssRNA^{+} virus of two different families. ***Jack Johnson*** (Scripps Institute, California) discussed the results of several structural techniques (i.e. crystallography, SAXS and intrinsic capsid fluorescence) to illuminate the nature of the particle maturation in the bacteriophage HK97.

It was most fitting to hear MGR himself at the of end the day, reviewing the myriad of scientific projects and achievements that have taken place in his laboratory since 1964 when he moved to Purdue until now and what might still be in store for the future. In closing, he emphasized once again what he wrote in the Foreword to *Crystals and Life*: 'It has been my privilege to host and work with many pre- and post-doctoral students with vastly different cultural backgrounds during almost forty years at Purdue University in Indiana. We have together enjoyed the pleasures of discovery and agonized over disappointments'. I think that I can speak for the majority of the attendees to the symposium when I say: Michael, it has been our privilege to work with you and to experience the pleasures of discovery and the anguish of the temporary failures along the way. You have enriched our personal and professional lives immensely.

After the official reception at the end of the meeting, it was time to honor another anonymous contributor to the field: MGR's wife ***Audrey***. From her early cartoons drawn to convey the meandering of the polypeptide chain in LDH, she has followed the breakthroughs of the laboratory. She hosted dinners and other social events for generation upon generation of students, postdocs, associates and collaborators. She also produced pottery masterpieces to mark each scientific milestone of the laboratory or the departure of friends or co-workers. The attendees flocked to University Place to present their tribute, friendship and homage to her. There were hugs and emotional exchanges with this remarkable woman who has played such an important role in the life of not only Michael, but also of every single person who has had the good fortune of interacting with her.

A beautiful sunset completed this momentous day of spectacular structural biology, excellent science, warm friendships, camaraderie and unforgettable memories. Based on what we observed during our visit, they are nowhere near finished yet.

Cele Abad-Zapatero

Acknowledgments

The author thanks the organizers of the symposium: R. Kuhn, J. Bolin, B. Fein, J. Johnson, J. Smith and Dana Neary. He also acknowledges the comments and suggestions of H. Berman, S. Wilder and M.G. Rossmann and the suggestions from all the speakers at the symposium. The illustrations were kindly provided by the organizers and M. G. Rossmann.

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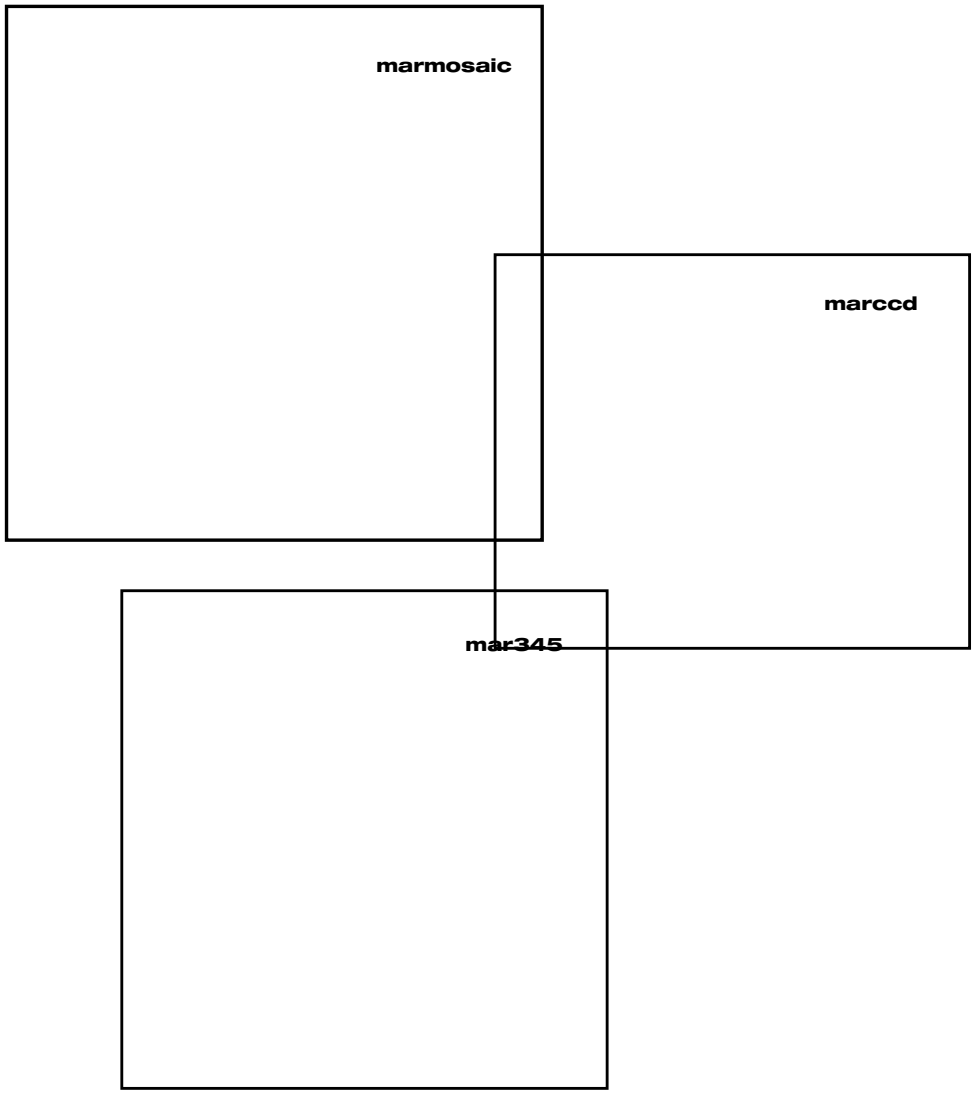

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Spring AIP Governing Board Meeting

The American Institute of Physics held its spring Assembly of Society Officers and its semi-annual Governing Board meeting from 7-9 April at the American Center for Physics, College Park, MD. Also present at the Assembly were Doug Ohlendorf, S. Narasinga Rao, and Bill Duax.

The Assembly met Thursday afternoon and Friday morning, and the Governing Board met on Friday afternoon and Saturday morning. The former is pretty much a forum for policy issue development; the latter is primarily an AIP business meeting. Following is a brief summary of both meetings, with special attention to issues of potential interest to the ACA community.

The AIP consists of two principal action-oriented management groups, one devoted to publishing of AIP journals and to publishing services in general, the other, the Physics Resources Center, to development, outreach, and science policy programs.

Assembly presentations

The presentations to the Assembly on Thursday afternoon and Friday morning were devoted to the funding environment, especially at NASA; to the growing influence of fundamentalist sources on secondary and undergraduate education, to online database searching with respect to publications, open access, and to intellectual property and intellectual freedom issues. All of these issues are likely to impact the ACA community, and the presentations were outstanding.

Creationism and its current implementation known by the phrase *intelligent design* have become a clear and present danger in recent years because of the substantial growth in private institutional funding for an aggressive campaign of misinformation and mis-education concerning secondary school teaching of geology and evolution. The AIP has asked support for, and the ACA Council has agreed to co-sign a Brief Amicus Curiae (Friend of the Court brief) regarding the case pending before the US Eleventh Circuit Court of Appeals on appeal from the US District Court for the Northern District of Georgia. The appeal has been brought by the Cobb County School District Board of Education to sustain its use of a disclaimer in all biology texts, saying briefly that:

"This textbook contains material on evolution. Evolution is a theory, not a fact, regarding the origin of living things. This material should be approached with an open mind, studied carefully and critically considered."

The brief is strongly and conservatively worded, drawing from several publications, including the NSF document, *Science and Creationism: A View from the National Academy of Sciences* (***books.nap.edu/html/creationism/***). It is motivated by concern for the low level of scientific literacy in the United States, and the important role of secondary school teaching therein. A copy of the brief has been posted on the ACA website. Its purpose is limited to expressing the views of the mainstream scientific community regarding the implications of the use in the disclaimer of the words "theory" and "fact", and the status of evolution in the scientific community, which are all broadly misleading, as well as the sense that the disclaimer has no pedagogical value or scientific merit. The ACA Council voted to add their signature to the list of amici, with reference to the membership and their activities investigating the structure of matter, including matter from living things.

The Physics Resources Center of the AIP is actively involved in monitoring state level activities of groups like the Seattle-based group "Discovery Institute". Anyone interested in participating in this activity can contact the AIP official in charge of it, Alicia Torres, ***atorres@aip.org***. Alicia directs the Committee on Media and Government Relations.

Open access publication was the subject of several presentations. One open access electronic journal, *Optics Express*, is evidently a significant success story that operates entirely without copyediting. They have a 52-day submission to publication time and publish entirely in XML. A representative from PNAS described the evolution of that journal. They have made all articles available for download 6 months after publication. 16% of authors overall and 20% of authors of Genetics and Immunology papers opt for open access publication from the date of publication. Norka Bravo, director of NIGMS, spoke on the NIH policy of urging voluntary submission of accepted manuscripts to be accessible through PUBMED. Discussion of this presentation was distinctly two-sided, as views of scientific consumers on the one hand, and of publishers on the other hand, were amply represented.

Mark Brodsky, CEO of the AIP, presented the status of a lawsuit against the Treasury Department (OFAC) over the right to transfer information to Cuba without a license and economic and trade sanctions involving intellectual property in general. This lawsuit is a big deal, and has been joined, for better or worse, by the recent Iranian Nobel Peace Prize laureate, Shirin Ebadi, who was refused an entry visa to the US because of her country of origin.

Charlie Carter

The following is excerpted form AIP FYI Number 70: May 18, 2005 (***www.aip.org/fyi/2005/070.html***)

Threats to the teaching of high-quality, peer-reviewed science continue to arise in school districts around the country. "Although the controversy focuses primarily on biology," National Academy of Sciences President Bruce Alberts warned Academy members earlier this year that "some who challenge the teaching of evolution in our nation's schools have also focused their sights on the earth and physical sciences" (see ***www.aip.org/fyi/2005/049.html***).

In cooperation with many of its Member Societies, AIP continues to track attempts around the country to dilute the science taught in science classrooms. In some instances, AIP and several Member Societies have initiated such responses as writing letters to school boards and state and local officials, encouraging individual scientists to testify at hearings, issuing news alerts, and encouraging other grassroots initiatives.

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION, INC.
BALANCE SHEET - December 31, 2003 and 2004

	CURRENT FUNDS (2004)		TOTAL	
	Unrestricted	Restricted*	All Funds	
			2004	2003
ASSETS				
Current Assets:				
Cash	141,055		141,055	32,532
Investments	442,268	336,602	778,870	760,609
Inventory	3,600		3,600	3,600
Total Current Assets	586,923	336,602	923,525	796,741
Fixed Assets:				
Computers and Printers	6,500		6,500	6,500
Office Equipment	1,300		1,300	1,300
Accumulated Depreciation	0		0	0
Total Fixed Assets	7,800		7,800	7,800
TOTAL ASSETS	594,723	336,602	931,325	804,541
Liabilities:				
Deferred Dues Income			0	0
Total Liabilities	0		0	0
Fund Balance:				
Unrestricted	594,723		594,723	486,260
Restricted		336,602	336,602	318,281
Total Fund Balance	594,723	336,602	931,325	804,541
TOTAL LIABILITIES & FUND BALANCE	594,723	336,602	931,325	804,541

*** Current Balances in individual restricted funds - as of December 31, 2004**

Buerger Award	33,751
Etter Award	60,186
Fankuchen Award	63,903
Patterson Award	36,356
Pauling Award	28,709
Supper Award	9,713
Trueblood Award	29,348
Warren Award	26,852
Wood Science Writing Award	47,784

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 14205-0096.

Howard Einspahr
Vice-President

Currently, Founding Editor, *Acta Crystallographica*, Section F; Research Fellow and Director, Macromolecular Crystallography, Bristol-Myers Squibb Pharmaceutical Research Institute, Princeton, New Jersey, retired.

Education: BA, Chemistry, Rice University (1964); PhD, Chemistry, University of Pennsylvania (1970) with Jerry Donohue; postdoctoral research fellow, California Institute of Technology (1970-1972) with Dick Marsh.

Professional Activities: Co-Editor, ***Acta Crystallographica***, Section D (1997-present); Council Member, International Organization for Biological Crystallization (2004-present); U.S. National Committee for Crystallography (1998-2003); Space Studies Board, National Research Council (2001-2004); Chair, Macromolecular Biotechnology Strategic Planning Committee, NASA (2001-2004); Chair, General User Program, Industrial Macromolecular Crystallography Association, Advanced Photon Source (1995-2003); American Crystallographic Association Service Award (1991); *ad hoc* member and chair of peer review panels for NIH (1987-2000) and NASA (1992-2003).

Research Interests: My first significant steps in science were as a small-molecule crystallographer, but during my tenure at the University of Alabama at Birmingham, begun as a postdoc with Charlie Bugg, I was fortunate to team with Bud Suddath and others to determine the structure of pea lectin. It was during this time that, along with the rest of the lab, I became interested in applications of macromolecular structure for drug design. In the mid '80s, Keith Watenpaugh and I joined the Upjohn Company to provide structures for its drug design programs and I continued this work for B-MS when I joined that company in the early '90s. The research interests that marked my later career continue: structural biology, macromolecular crystal growth, and drug design. Most recently, I've been especially interested in the nuclear hormone receptors as targets for drug design.

Statement: For as long as I've known it, the ACA has tried to serve the full range of diffraction and structural science interests. This has been one of its strengths and one of its challenges. The evolution of the SIG system has provided an excellent mechanism for assisting this mission by fostering the nucleation of new communities of scientific interest and by assuring that all the constituents within the ACA are heard by its leadership and are served effectively. The SIGs have also provided important opportunities for a committed membership to participate meaningfully in the organization and to identify and develop successive generations of new leaders. The ACA must continue to evaluate the success of its programs to assure that it fulfills the needs of the broader community while effectively serving the needs of its principal constituencies. This includes monitoring the health and welfare of our national facilities, journals, and databases, which are vital to continued progress and to assuring the impact and utility of our results. It also means playing an important part in supporting education initiatives that will help to identify and nurture the young scientists that are our future. Finally, the American Crystallographic Association has evolved to serve the scientists in two American countries and to do it well. Recently, however, we have seen the first steps toward widening the community the ACA serves to other countries in this hemisphere. I believe that is the right path toward the future and I urge the ACA to continue its leadership in this direction. Through prior service to the scientific community, notably the U.S. National Committee for Crystallography and the Journals Commission of the International Union of Crystallography, I have become especially attuned to international issues affecting crystallography and science in general. This perspective and the freedom to devote my efforts full-time to the benefit of the crystallographic community will help me to be an effective advocate for ACA programs and interests.

Candidates for ACA offices in 2006

The Nominating Committee has selected the following candidates for the 2005 elections for ACA offices in 2006

Vice-President: **Howard Einsphar and Alan Pinkerton and**

Secretary: **Lisa Keefe**

***Committees*:**

Communicatons: **William Pennington and John Tanner**

Data, Standards & Computing: **Andrew Howard and Brian Toby**

Continuing Education: **William Cahill and Allen Hunter**

2005 Nominating Committee:

Kathy Kantardjieff (Chair), Wayne Anderson and Ray Davis

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, 2005 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 2005.

A. Alan Pinkerton
Vice-President

Professor and Chair, Department of Chemistry, University of Toledo, Toledo OH 43606; joint appointments in the departments of physics and astronomy, and medicinal and biological chemistry

Education: Graduate, Royal Institute of Chemistry, UK (1966); Ph.D. University of Alberta, Canada (1971); PDF, University of Sussex, UK (1971-72); Fellow, Royal Society of Chemistry (1997).

Professional activities: Regional Crystallography Workshop organizer, Toledo, 1986; Co-chairman of Rare Earth Research Conference, 1986; Student Awards Committee, 18th Rare Earth Research Conference, 1988; Local Chairman for ACA Annual Meeting, 1991; ACA, Development Committee, 1989 – 1991; Secretary, UT Chapter of Sigma Xi, 1989-90; Chairman, ACA Small Molecule SIG, 1994 -1995; American Institute of Physics, Development Committee, 1995 – 1997; ACA Apparatus and Standards Committee, 1998 – 2000; ACA Nominations Committee, 1998-2000; Organizer, Siemens' Area Detector Users Group Meeting, Toledo, 1999; Organizer, Charge density and cryo-crystallography workshop, Toledo, 1999; USAMRMC, Review Panel, 2003; Pittsburgh Diffraction Society, President Elect (2004), President (2005).

Research Interests: Charge density studies, cryo-crystallography, methods development. All three of these topics are driven by the desire to obtain the most accurate information possible from diffraction experiments. Current charge density studies allow us to determine the electronic energy density distributions in explosives and propellants. A second project produces detailed maps of the electrostatic potential for steroids, and insight into their receptor binding. Our initial development of liquid helium cooling was for charge density applications, however, we have since become interested in its potential for abating radiation damage in protein crystallography, and in providing higher resolution data. Recently we have shown that charge density quality data at liquid helium temperatures is obtainable in less than a day with appropriate choice of modern in-house equipment.

Statement: I am honored to be nominated as a candidate for Vice-President of the ACA, and would be pleased to repay some of the many benefits that I received from my membership in the ACA over the years. I have been an active member of the crystallographic community for over thirty years, first in Switzerland, and for the past twenty years, in the US. During this time, participation in the business of the ACA, attending the annual meeting or other ACA sponsored activities, has played a major role in my professional life, and will continue to do so.

As the major professional organization for scientists using short wavelength diffraction techniques, the ACA must address the needs and concerns of a broad range of interests. I believe that I can closely relate to many of these based on the breadth of experience developed in my own research. For example, I have interests spanning solid state physics (e.g. the twinning of the low temperature - < 33 K – phase of $TbVO_4$) to macromolecular crystallography (e.g. abatement of radiation damage to xylose isomerase crystals at 15 K), from in-house crystallography to national facilities, from x-rays to neutrons. The ACA must also relate to other structural communities using non-diffraction techniques such as NMR, a field to which we have also contributed.

In looking at the membership of the ACA, I divide it into three groups. The first are the senior members on whose shoulders the rest of us stand. I am proud that the ACA recognizes their value to the discipline with numerous awards, and always makes them welcome at our annual meetings. That we have many senior members, long into "retirement", who still volunteer their time and expertise to the ACA, speaks highly of the respect with which the organization is held, and to the respect which the ACA accords them. The second group is the current membership of active researchers and teachers. These are the organizers of symposia, the generators of new science which our association represents, the backbone of our SIG's. The third group is the next generation of crystallographers. This is our future, and perhaps the heaviest responsibility of the ACA is to ensure their education and participation in our activities. I strongly support activities such as the Etter Early Career Award, The Young Scientists SIG, travel awards to students and the Pauling Poster prize. Continuing support of the ACA for the small molecule and macromolecular summer schools is also very important.

The ACA plays a key role in the international community, both as the regional affiliate of the IUCr, and by fostering interactions with our overseas colleagues, be it facilitating cooperation with underfunded laboratories to provide them access to modern diffraction data, or assisting with the development of major multinational laboratories. Having spent a significant part of my career in other countries (UK, Canada, Switzerland, France), and having a number of active collaborations with colleagues in other countries, I feel that I can play a significant role in our international relations.

Having served the ACA in a number of capacities over the years, I believe I have a good working relationship with the current staff of a dynamic, vital and efficient organization, and, if elected, would strive to represent the interests of all members of the association.

You must be an ACA member in good standing to be eligible to vote in the fall elections.

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Lisa Keefe
Secretary

Director, Industrial Macromolecular Crystallography Association Collaborative Access Team (IMCA-CAT), University of Chicago, at the Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439

Education: A.B. in Chemistry (1983) Vassar College; Ph.D. in Biophysics and Biophysical Chemistry (1992) The Johns Hopkins University School of Medicine; DOE Alexander Hollaender Distinguished Postdoctoral Fellow (1992-96) at the Structural Biology Center, Argonne National Laboratory and Brookhaven National Laboratory.

Professional Activities: Secretary, ACA Council (2003-present); member, ACA (1985-present); member, Steering Committee of Advanced Photon Source Users Organization (APSUO) (2001-2004); Chair, Young Scientist Special Interest Group (YSSIG) (1993-1994).

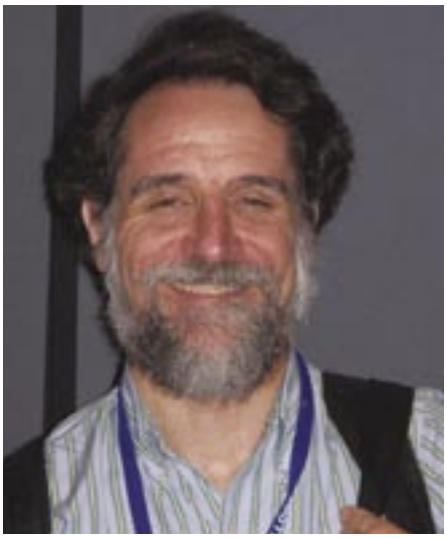
Research Interests: High-throughput data collection; automation and robotics; synchrotron radiation; molecular recognition; macromolecular crystallography

Statement: It has been a pleasure to serve as ACA secretary for the last three years. As secretary, I worked with council to manage the affairs of the ACA, recorded minutes and maintained records of the meetings, and communicated council news to the membership.

I remain committed to supporting all areas of crystallography and to representing the diversity of crystallographic disciplines. My crystallographic education began in small molecule crystallography, extended to macromolecular crystallography, and broadened to include synchrotron radiation. From my experience in working at synchrotron user facilities, I have worked with many researchers in academia and industry, understanding the variety of needs, issues, and concerns of the crystallographic community. I have developed a broad perspective regarding the endeavors on which the ACA can focus in order to best serve its constituency.

I enthusiastically welcome the opportunity to continue to serve the ACA and its membership.

Andy Howard
Data, Standards and Computing



Associate Professor of Biology, Illinois Institute of Technology, 3101 South Dearborn St, Chicago IL 60616 USADirector, Industrial Macromolecular Crystallography Assoc., Collaborative Access Team, Advanced Photon Source

Education: Ph.D. in Physics, UC San Diego, 1981, with Prof. Xuong Nguyen-Huu, B.A. in biophysics, Pomona College, Claremont CA, 1975.

Professional activities: member of ACA since 1980, Diffraction Methods in Molecular Biology Gordon Conference: vice-chair 1998; chair 2000, Advanced Photon Source Research Directorate: chair of CAT Directors' Council, 1998-2000

Research interests: Methods development in macromolecular crystallography, particularly data processing software and synchrotron beamline optics, structural genomics, pharmaceutical crystallography.

Statement: A variety of sources contribute to error and uncertainty in crystallographic measurements, including pilot error, sample inhomogeneities, software misfeatures and bugs, and documented or undocumented instrumental weaknesses. Teasing apart the contributions of these factors in a specific experiment is often difficult. The development of validatable and repeatable data standards will contribute to our understanding of where our errors come from. I would like to encourage the development of such standards, and the development of procedures to compare the results of various crystallographic software packages. My experience in running the ACA's Summer School in Macromolecular Crystallography, and the many years I have spent providing user support for my own software and for beamline operations, have given me a broad perspective on the ways to develop these standards and experiments.

Brian H. Toby
Data, Standards and Computing

Research Chemist and Crystallography Team Leader, NIST Center for Neutron Research, National Institute of Standards & Technology, Gaithersburg, MD 20899-8562.

Education: B.A., Chemistry, Rutgers University (1980). Ph.D., Physical Chemistry, California Institute of Technology (1986). Research Associate/Lecturer in group of Takeshi Egami, University of Pennsylvania (1988-1990). Principal Research Chemist, Air Products and Chemi-

cals, Inc. (1990-1995). Senior Chemist, Union Carbide Corp. (1985-1988).

Research Interests: Structural characterization from neutron and synchrotron powder diffraction; neutron Laue diffraction methods; improved neutron powder diffractometer techniques; powder diffraction software. Coauthor of ~90 refereed publications.

Professional Service: ACA: held several SIG Chair positions, session organizer at numerous annual meetings, unsuccessful candidate for this position; IUCr: former member COMCIFs and Neutron commissions; U.S. National Committee: member 2004-2006; ICDD: member, fellow and former task group chair. Principal developer of the powder diffraction crystallographic information file dictionary (pdCIF); principal author of software for reading and writing pdCIFs; Author of EXPGUI, front-end to the GSAS package and unprincipled author of several other widely used tools in powder diffraction crystallography.

Statement: If elected to the Data, Standards & Computing Committee, I will use what little authority (if any) that the position generates to advocate for the importance of volunteer software development within our field. I would also encourage wider availability of crystallographic databases -- particularly for crystallographic education. I have worked for nearly two decades in the development of our field's first effective standard for electronic communication of crystallographic data and results -- CIF. This standard is well accepted within our field, but still needs advocacy, for example to non-IUCr journals. I see this as an important role of this committee.

You must be an ACA member in good standing to be eligible to vote in the fall elections.

Have you paid your dues for 2005?

William T. Pennington, Communications

Professor of Chemistry, Clemson University, Clemson, SC 29634-0973.

Education: B.A. Chemistry, Hendrix College (1977); Ph.D. Inorganic Chemistry, University of Arkansas (1983) with A.W. Cordes; Postdoctoral Fellow, University of Illinois (1984-85) with I.C. Paul and D.Y. Curtin.

Professional Activities: Editor in Chief, Journal of Chemical Crystallography, Member of ACA, 1983-present.

Research Interests: Halogen bonding; polymorphism and polymorphic interconversions; gas-solid reactions; crystal design.

Statement: The objective of the ACA is to promote interactions among scientists who study the structure of matter at atomic (or near atomic) resolution, and the activities of the Communication Committee are key to this pursuit. The committee also provides an evolving interface to facilitate communication among an increasingly diverse community of crystallographers and solid state scientists. The ACA with the help of this committee has led the way in developing progressive and effective means of sharing information among its constituents. As editor of the *Journal of Chemical Crystallography* and frequent contributor to and reviewer for *Acta Crystallographica*, I am particularly interested in continuing to make the best use of developing technologies for the dissemination of results to the scientific community. Outreach to improve public perception and appreciation of our efforts is also an important function of the Communications Committee and one that is in all our best interests. I am honored to be nominated for the Communications Committee and I look forward to the possibility of being involved in these exciting endeavors.

Jack Tanner Communications

Associate Professor, Department of Chemistry, University of Missouri-Columbia, Columbia, MO 65211

Education: B.S. Chemistry, University of Missouri-Columbia (1983); Ph.D. Chemistry, Brown University (1988); Postdoctoral research in computational chemistry, University of Houston (J.A. McCammon, 1988-1991); Postdoctoral research in protein crystallography (University of Houston, K.L. Krause, 1991-1997).

Professional Activities: Member of the ACS and AAAS; Operations Committee member for ALS beamline 4.2.2; former secretary-treasurer and president of local ACS section; *ad hoc* reviewer for NIH BBCB study section, NIH Biophysical and Chemical Sciences IRG Postdoctoral Fellowships study section and National Centers for Biomedical Computing study section.

Research Interests: Protein structure and function, computational biology. Ongoing projects include proline catabolic enzymes, multifunctional proteins, anti-DNA antibodies and structural bioinformatics of protein-bound water.

Statement: It is an honor to be nominated for a position on the Communications Committee. I have been an avid supporter of the ACA for the past several years in terms of attending the yearly meeting, encouraging my graduate students to join the

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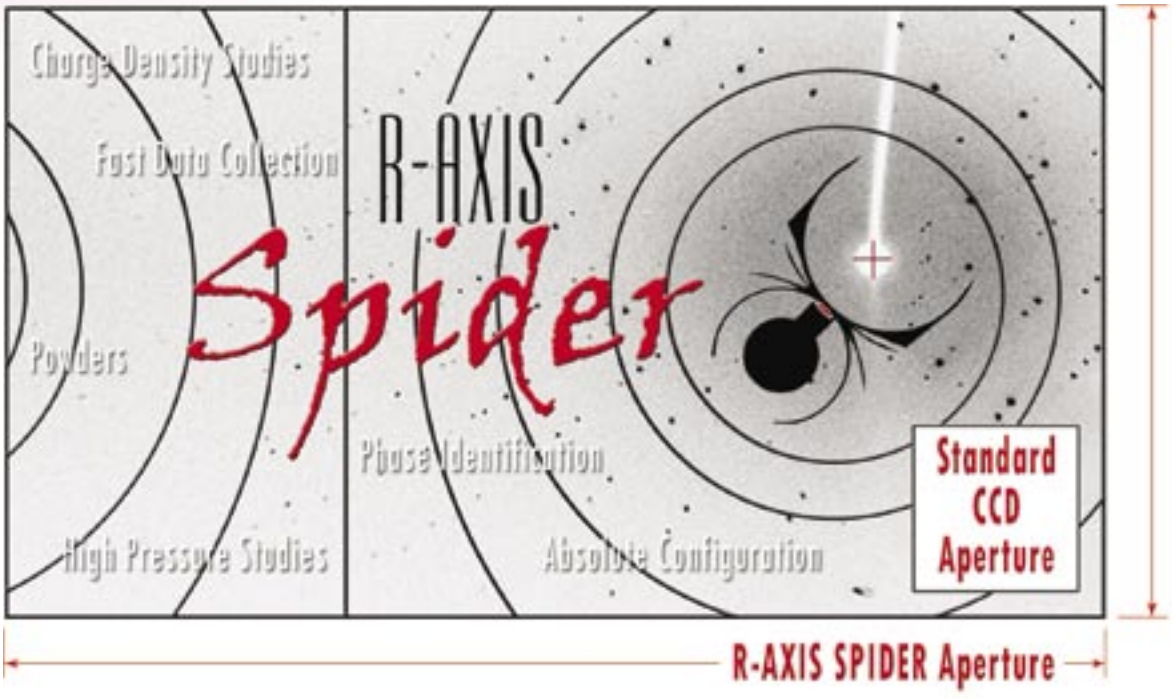

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ACA, writing for the newsletter and serving as a session Co-Chair at the Orlando meeting this Summer. I believe that service is an important part of professionalism and I look forward to serving ACA members in this new capacity, if elected

Christopher L. Cahill
Continuing Education

Assistant Professor of Chemistry, The George Washington University, Washington, DC 20052

Education: B.S. Geochemistry and Chemistry (1993) State University of New York- Fredonia; Ph.D. Inorganic Chemistry (1999) SUNY- Stony Brook (Advisor: John Parise).

Professional Activities: ACA Member since 1997; Member of ACS, Sigma Xi, Mineralogical Society of America, Geological Society of Washington.

Research Interests: Solid state chemistry, inorganic/organic hybrid materials, f-metal compounds, mineralogy, synchrotron studies.

***Statement*:** I am both honored and flattered to have been nominated to the Continuing Education committee. I look forward to working with this group and the ACA as a whole on a range of topics that I feel are of critical importance to this and future generations of crystallographers. At the core of my interest with respect to this committee is the mixed blessing of the increasingly user friendly instrumentation and software packages available to today's small molecule crystallographers. On the upside of these developments has been access of a previously esoteric activity (that is, data collection and structure analysis) to a wider variety of scientists and students. Both hardware and software have removed much of the 'mystique' of what we do and crystallography is arguably more accessible to students (including undergraduates!) now than ever before. On the downside of this can be an under-appreciation of the methods employed during crystal structure analysis and, ultimately, complacency with less than correct results.

To address these challenges, I envision organizing a component of a workshop dedicated to critical assessments of crystal structure refinements and data collection for the end user: students and faculty alike. Such efforts would challenge new users to think critically about their results and carefully examine structures for potential pitfalls. Coupled to this would be an effort to involve more faculty in crystallography education, especially those at primarily undergraduate universities. I will strive to foster communication between universities with diffractometers and those without, yet who are capable of collaboration, in part due to the technological advances mentioned above.

In summary, I offer the following to the committee and the ACA in general: insight into what I consider to be issues of utmost importance to this generation of small molecule crystallographers and a commitment to expanding the roles of educators to address (and embrace!) these opportunities head-on. I have a particular fondness for this Committee as I was awarded a Graduate Student Travel Grant in 1998 to give a talk at my first ACA meeting. Since becoming a faculty member in 2000, I have sent four students to the ACA Summer School in Small Molecule Crystallography and am currently hard at work at raising the next crop of crystallographers at GW. I would welcome the opportunity to participate in this capacity.

Allen Hunter
Continuing Education

Professor, Materials Science, Department of Chemistry, Youngstown State University, Youngstown, OH 44555-36633

Education: B.Sc., University of British Columbia (1981); Ph.D., University of British Columbia (1985); Postdoctoral Fellow, Australian National University (1986) & University of Alberta (1987).

Professional Activities: Assistant Professor, University of Alberta (1987-1992); Associate Professor, Youngstown State University (1992-1998); Full Professor (1998-present). Founder and Director of the YSU-PUI Undergraduate Diffraction Consortium which employs local and remote diffractometer control to give access to the four diffractometers at Youngstown State University to faculty and students of other predominantly undergraduate institutions. Active in the development of crystallographic education materials, especially those designed for undergraduate students. Member of the editorial board of the *Journal of Chemical Crystallography*. Organizer of, and presenter to, crystallographic education symposia at recent ACA & ACS national meetings. NSF & ACS-PRF grantee and proposal reviewer. Member of ACA, BCA, PDS, ACS, & CUR.

Research Interests: Synthetic materials chemistry, applications of x-ray methods to structure determination, chemical & crystallographic education. I was primarily trained as a synthetic organometallic chemist. Since graduation, my group's research has emphasized the synthesis

and structure/property correlation studies of organometallic complexes, organic and organometallic polymers, and nanoscale organometallic materials. Over the last decade, I have also become increasingly active in the use of single crystal diffraction methods to characterize these species. I am also very involved in chemical education studies in several areas, including: professional writing, discovery research experiments, and the teaching of single crystal diffraction methods to groups as diverse as chemistry MS and high school students.

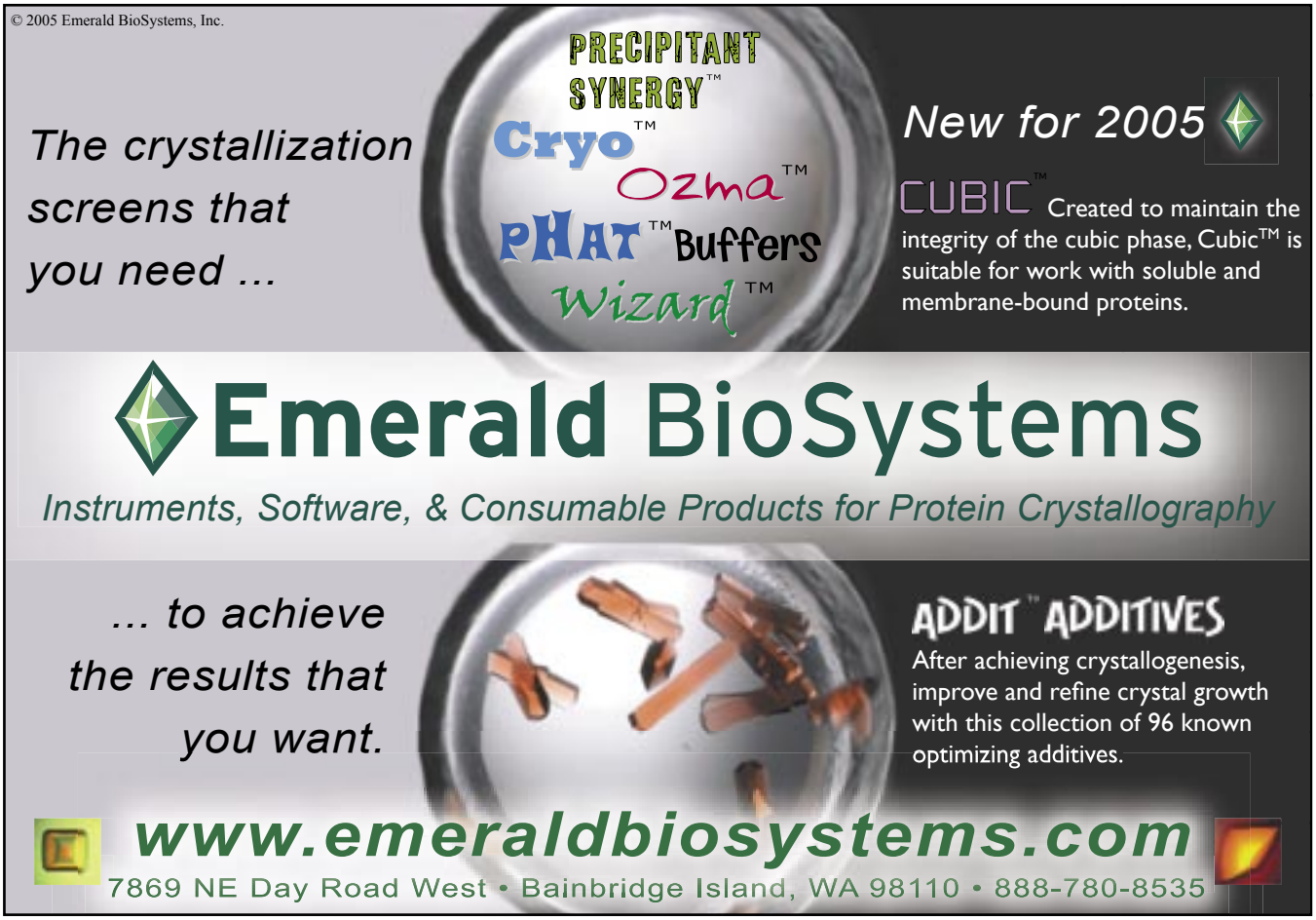
Statement: While the ACA must continue to play a central role in the education of professional crystallographers, I believe that it is *equally important* for the ACA to play a central role in developing, evaluating, and disseminating educational materials aimed at non-specialists. This reflects the reality on the ground that non-specialists are increasingly involved in crystal structure determinations. It also provides us with opportunities to show off the beauty and power of our technique and to recruit future crystallographers. To this end, if I am elected to the continuing education committee, I will concentrate my efforts on working with other committee members and the larger community in identifying, evaluating, and distributing exemplary materials, modules, and courses that can be integrated into non-crystallographic courses by both expert crystallographers and those earlier on the learning curve. In addition, I will work with the committee and others to increase the awareness in the community of funding opportunities to support these efforts and at funding agencies of the need for such grants.

63rd Pittsburgh Diffraction Conference - PDC '05

The 63rd Pittsburgh Diffraction Conference – PDC '05 – will be held on November 3-5, 2005, at Argonne National Laboratory.

An outstanding scientific program is in the works, featuring a symposium on "Frontiers in Neutron Scattering," together with symposia to honor the late Professors M. Sundaralingam and Leroy Alexander. Attendees at PDC '05 also will have an opportunity to tour Argonne experimental facilities.

For additional information please see the Pittsburgh Diffraction Society's website at ***www.pittdifsoc.org***.



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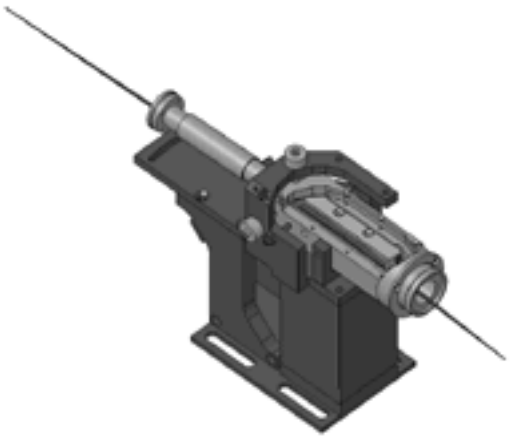
Data courtesy of R. Kahn, L. Nauton, IBS Grenoble

Before upgrade with classical confocal multilayer system	Lysozyme crystal 0.4x0.4x0.4 mm and Gd as a phasing agent Unit cell (Å) a=b=77.12 c=38.6	**After Upgrade** with Fox 2D single reflection multi-layer optic from Xenocs
3 Minutes Exposure	Data collection: 360 images at 1° steps	1 Minute Exposure
0.55	Mosaïcity	0.55
0.209	Rsym from 1.86 to 1.75	0.209
0.262	Rsym from 1.75 to 1.66	0.27
0.053	Rsym mean	0.048
0.053	Rfac	0.048
0.074	R ano	0.074
99.8	Completion	99.9
23.4	Multiplicity	23.3
9.0	Imean/Sig	10.2
2.5	I/Sig from 1.75 to 1.66	3.3



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RCSB Protein Data Bank – Update Summer 2005

Content and access

- In March 2005 the contents of the PDB passed 30000 structures (~6000 unique).
- 5360 experimentally-determined structures were deposited in 2004.
- Over 10000 scientists visit the PDB Web site every day; on average one structure is downloaded every second 7/24/365.

News

- Gary L. Gilliland has left CARB/NIST and taken a position with Centocor (a subsidiary of Johnson and Johnson). The PDB functions formerly performed at the CARB/NIST site have been assumed by the groups at Rutgers and UCSD/SDSC. The transition has been successfully completed.
- The beta site (***www.pdbbeta.org***) will become the production site on January 1, 2006.

New features already on the Beta Search Site

- Query by example
- Detailed help system
- Summary reports
  - Biology and chemistry
  - Materials and methods
  - Sequence details
  - Structural features
- Customizable reports

Current focus for development of new features

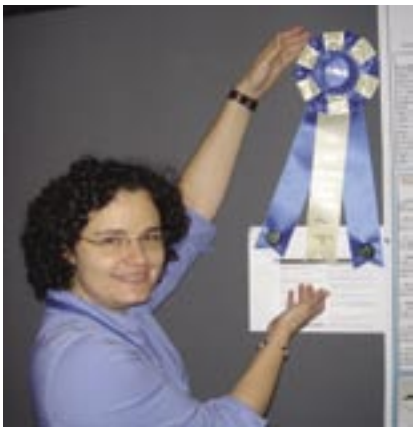
- Better description of ligands with stereochemistry.
- Better support for cryo-EM and NMR data.
- Description of the progress and results from structural genomics.
- Emphasis on fully exploring a single structure e.g., protein-ligand interactions and characterization of the functional role and integrating structure into a broader framework of sequence-structure-functional-disease relationships.
- The Art of Science traveling exhibit displays images of molecules in the PDB. Since its beginnings at a space dedicated to art exhibits at Rutgers University, the show has traveled to Texas A &M University; EMBL-Hamburg, Germany; University of Wisconsin-Madison; California State University, Fullerton; Purdue University; and Hyderabad, India. The latest display was at the ACS Mid-Atlantic Meeting (MARM) being held May 22-25 at Rutgers University in Piscataway, NJ.
- The Molecule of the Month feature continues to be widely recognized for its educational value.
- The RCSB PDB held an education and professional development session titled, "The Protein Data Bank in the Classroom and Beyond" at the 2005 ASBMB Annual Meeting in San Diego.

Global Issues

- wwPDB (***www.wwpdb.org/***) comprising PDBj (Japan), the MSD group at EBI (Europe) and RCSB PDB had its first official meeting in November 2004. The three sites are continuing to work together to create a uniform and consistent archive.
- They also agreed to support a single time stamped yearly contents of the archive on DVD. This first volume contains the current contents of the PDB at the end of 2004.
- RCSB will share an exhibit booth at IUCr XX with MSD and PDBj.

RCSB PDB at ACA Orlando

Kyle Burkhardt gave a talk on RCSB PDB validation tools at the Workshop on Macromolecular Structure Validation organized by Kathy Kantardjieff and Bernhard Rupp. The Workshop will be reviewed in the winter ACA *Newsletter*.



Kyle Burkhardt placing the prize winning ribbon on Melanie's poster

The RSCB PDB Poster Prize went to ***Melanie Adams*** (Queens University) for her poster on "Safety in Cycling: Novel Redox Proteins from *Escherichia coli*" co-authored with Zongchao Jia. Melanie will receive copies of "Biochemistry - Vol. I" by Donald and Judith Voet and "Introduction to Macromolecular Crystallography" by Alex McPherson.

RCSB PDB Staff

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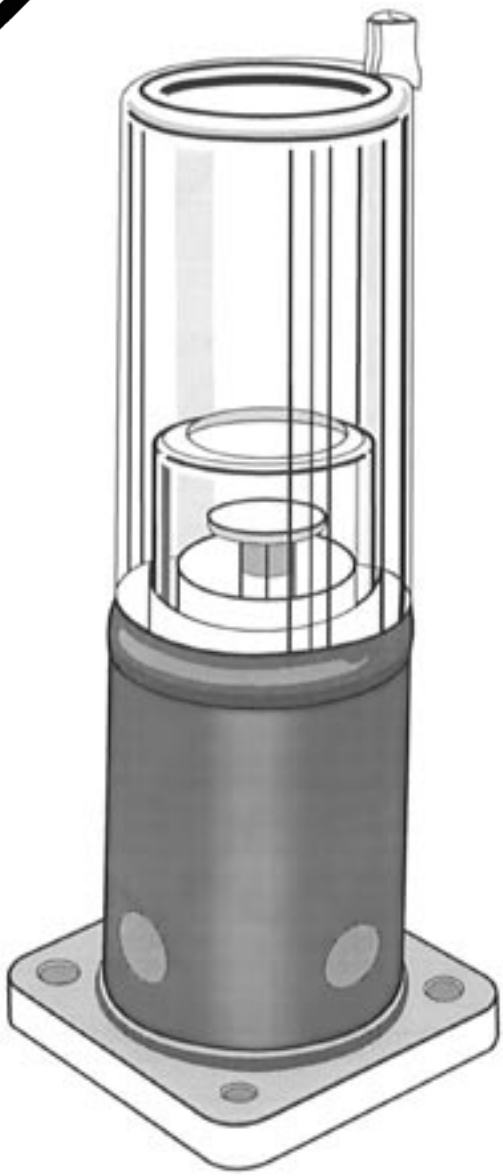

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Rapid Data Collection and Structure Solving at the NSLS: A Practical Course in Macromolecular X-Ray Diffraction Measurement

Once again this spring, nearly 50 budding crystallographers from around the world gathered at Brookhaven National Laboratory for RapiData 2005, a week-long course designed to introduce students to the best people, newest equipment, and latest techniques in the field of macromolecular x-ray crystallography.

The course is offered annually by Brookhaven's Biology and National Synchrotron Light Source (NSLS) departments, and is always a successful event for participants and instructors alike. This year, it ran from April 5 to 11.

The course began with two days of lectures and tutorials taught by scientists from Brookhaven, industry, academia, and other national labs. Then, the instructors and other participants guided the students through a marathon, 60-hour data-collection session on eight NSLS beamlines. Half of the 48 students came with their own specimens to analyze, while the other half learned as observers. Nearly a dozen students left with solved structures that may be publishable in scientific journals.

The course was organized primarily by the 24 members of the PXRR (the Biology and NSLS Macromolecular Crystallography Research Resource), a number of NSLS staff members, and about 16 volunteer outside teachers.

Topics covered in the lectures included: Diffraction Geometry for the Rotation Method (***Bob Sweet*** - BNL); Strategy vs tactics in data collection (***Zbyszek Dauter*** - NIH); Cryocooled specimen preparation for the synchrotron (***Sean Parkin*** - U. Ky); Data reduction with d*TREK (***Jim Pflugrath*** - Rigaku/MSC); Special properties of SR: polarization, bandwidth, collimation (***Lonny Berman*** -BNL); Data reduction with The DPS/Mosflm Package (***Frank vonDelft*** - Structural Genomics Consortium Oxford); Automatic control of data collection with the "dna" system (***Graeme Winter*** - Daresbury Lab); Modern CCD-based x-ray detectors (***Chris Nielsen*** - Area Detector Systems Corp); Are we MAD or are we SAD? (***Howard Robinson*** - BNL); Structure solving with SHELX (***Bram Schierbeek*** - Bruker AXS); Structure solving with SOLVE and Phenix (***Tom Terwilliger*** - LANL); Structure solving with autoSHARP (***Clemens Vonrhein*** - Global Phasing); A tutorial on FORTRAN Jiffies (***Mark Rould*** - UVM); Structure solving with Shake-and-Bake (***Chuck Weeks*** - (HWI); Data reduction with the HKL suite (***Wladek Minor*** - U. Va)

The majority of the funding for the course comes from the National Institutes of Health's National Center for Research Resources and the Office of Biological & Environmental Research within the U.S. Department of Energy's Office of Science. Funding was also provided by the International Union for Crystallography to assist half a dozen Latin American students in attending the course. This followed several years of generous contributions for this purpose from the U.S. National Committee for Crystallography. Additional support is provided by the NSLS and several equipment vendors and drug companies. For more information, go to: ***www.px.nsls.bnl.gov/RapiData2005/.***

Bob Sweet

The Jeffrey Awards, 2005

The Jeffrey Awards in memory of Professor George A. Jeffrey are intended to assist outstanding graduate students to attend the IUCr Congress. These awards are administered by the Pittsburgh Diffraction Society. For 2005, five awards were made. The award committee consisted of Helen Berman, Robert Stewart and Bryan Craven. Applications came from the US (3), Canada (1), Brazil (1), Hong Kong (1), Australia (3) and New Zealand (1). Judging was based on scientific merit, financial need and skills in English. All ten applicants had merit.The awardees are:

Jason Benedict, University of Washington, Seattle. "Spherulites for polar dye organization."

HaeJoo Kang, University of Auckland, New Zealand. "Structural studies on novel streptococcal virulence factors."

Shao-Yang Ku, Hospital for Sick Children, Toronto. "Structure of 5-methylthioribose kinase: mechanism & drug design."

Mihwa Lee, University of Sydney, Australia. "*E. coli* dihydroorotase: Loop movement and cooperativity."

Valeska Ting, Australian National University, Canberra. " Structural studies of...ordered perovskites."

Bryan Craven, Steward of the Jeffrey Fund

USNCCr Student Travel Awards for the 2005 IUCr Meeting in Florence, Italy

Anthony Armstrong - Johns Hopkins
Joseph Arndt, - Scripps Research Institute
Jason Benedict - U of Washington
Dominka Borek - UT Southwestern Med. Center
Christina Bourne - U of Oklahoma
Julien Breger - SUNY Stony Brook
Christian Burger - SUNY Stony Brook
Barbara Calamini - U of Illinois at Chicago
Jill Dombrauckas - U of Illinois at Chicago
Richard Felts - U of Missouri - Columbia
Yulia Frenkel - Rutgers
Tomislav Friscic - Univ. of Iowa
Tamara Hamilton - Univ. of Iowa
Daniel Himmel - Rutgers
Rebecca Hoeft - U of Minnesota
Marilise Hycacinth - U of Virginia
Bryan Johnson U of Minnesota
Pavol Juhas - Michigan State
Sonia Larsen - U of Illinois at Chicago
Ting-Wan Lin - UC Irvine
F. Marc Michel - SUNY Stony Brook
Jasmine Millican - Louisiana State
Hyunsoo Park - SUNY Stony Brook
Kira Ratia - U of Illinois at Chicago
Christina Rush - St. Jude Children's Research Hospital
Alex Smith - U of Illinois at Urbana-Champaign
Tony Sokolov - U of Iowa
Evi Strubel - Johns Hopkins
Evan Thomas - Louisiana State
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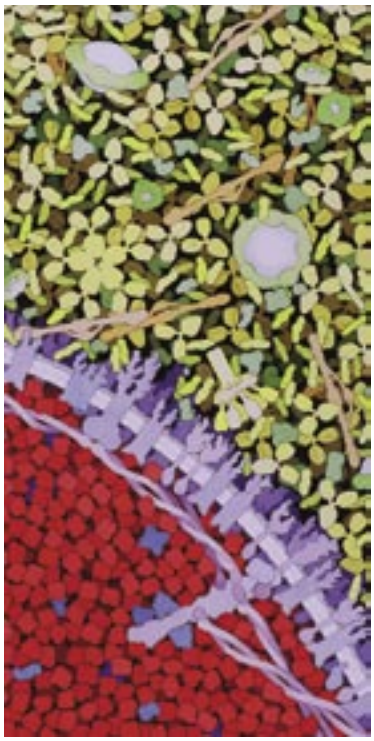
Art in Crystallography

The first ACA "Art in Crystallography" competition has been completed and the prizes have been awarded. All entries have been posted to the ACA web site and they were displayed at the meeting in Orlando. The images displayed in Orlando were put up for sale through a silent auction. Bids were received for all the images and bidding was quite lively for a number of the photographs. The proceeds from the auction were donated to the ACA Student Travel Fund. The winners of this years contest are shown below along with the text provided by the 'artists'. A cropped version of Blood 2,000,000X adorns the cover of this issue of the ACA *Newsletter.*

First Prize - David S. Goodsell: Blood 2,000,000X



This watercolor illustration shows a cross-section through the blood, with blood serum in the upper half and a red blood cell in the lower half. In the serum, look for Y-shaped antibodies, long thin fibrinogen molecules (in light red) and many small albumin proteins. The large UFO-shaped objects are low density lipoprotein and the six-armed protein is complement C1. The red blood cell is filled with hemoglobin, in red. The cell wall, in purple, is braced on the inner surface by long spectrin chains connected at one end to a small segment of actin filament.

Second Prize - Edgar Meyer: Cortisol

A photograph of a cortisol sculpture that was carved from laminated 3" blocks of walnut and finished with several coats of marine-grade polyurethane spar varnish. The model was made using coordinates from the cortisol ligand complexed with PDBID 1GS4 (Matias et al. (2002), *J. Med. Chem.*, **45**, 1439). The wood was so beautiful that the 'box' around the sculpture was kept.

Honorable Mention - Dan Anderson: Be Fruitful and Symmetrize

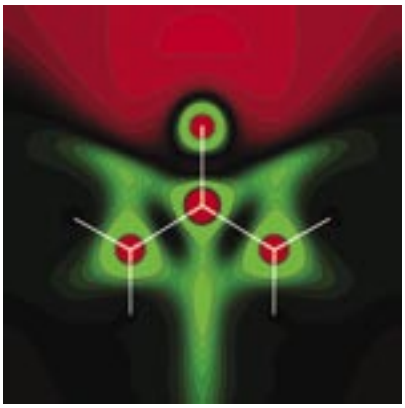
This photograph served as a low-tech introduction to the goals and problems of non-crystallographic symmetry averaging.

The foreground object is a "Kiwano Melon," a fruit that seems to have evolved specifically for this figure. I found it in the grocery store. In the background is a Navajo pot in my apartment. The structure in the crystal has concentric 24- and 48-fold non-crystallographic rotational symmetry, as exemplified by the patterns of varying periodicity incised into the pot. The averaged electron density (as of the Difficult Structures session at ACA 2004) was mostly patterned, but had spikes, bumps and holes. The Kiwano Melon looks like it's almost patterned. To try to improve the phases, I put atoms into the patterned density while avoiding the un-patterned features. I will try to present all this low-throughput work (without pointing at a melon) in the Difficult Structures session at ACA 2005.

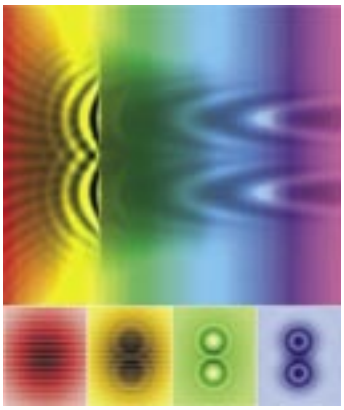
The light came from a studio flash to camera right. A 32 inch white reflector just left of the fruit eliminated almost all black pixels from the eventual image histogram. I used a flash meter and macro lens. Compensating for divergence of the T-stop away from the F-stop, I arrived at a flash energy of 308 Joules radiating into my favorite 36x48 inch diffuser. The image file came from a film scan.The collaborators were amused. The fruit was almost tasteless.

Background images: More 'Art in Crystallography" was used in this issue as backgrounds for some of the *Newsletter* pages. They were taken from the covers of *Acta Cryst* journals and used with permission of the IUCr.

D. Jayatilaka and D. Grimwood (2004) *Acta Cryst.*, **A60**, 111-119 "Electron localization functions obtained from x-ray constrained Hartree-Fock wavefunctions for molecular crystals of ammonia, urea and alloxan". An experimentally derived plot of the Fermi hole mobility function (FHMF) for urea. The FHMF can be interpreted as a potential energy surface for electron transfer. This plot was obtained from a Hartree-Fock wavefunction constrained to fit measuredx-ray diffraction structure factors, using the Tonto program.



W. Leitenberger, H. Wendrock, L. Bischoff and T. Weitkamp (2004) *J. Synchroton Rad.*, **11**, 190-197, "Pinhole interferometry with coherent hard x-rays." Simulation of Young's interference pattern (vertical line scan) in the 5-20 keV energy range (horizontal, colors indicate different wavelengths), see pages 190-197. Bottom: calculated area maps at different points of the spectrum. Owing to both the absorption of radiation in the thin foil containing the pinholes and the coherence properties of the x-rays, a double pinhole and a point diffraction interferometer are realized in a single set-up.



Mary Rosaleen Truter (1925-2004)

"Jackie" Truter (Lady Mary Cox) died from leukemia on 26 November 2004. Her career in x-ray crystallography began in 1945 and at her death she was still active as Visiting Professor in the Chemistry Department at University College, London. She was the widow of Sir Gordon Cox FRS.

Mary Rosaleen Jackman, "Jackie," attended Imperial College, London, where A.J.E. Welch, who had given excellent lectures on crystal chemistry, started her on research with x-ray powder photography. After hearing Sir Lawrence Bragg at the Royal Institution she "was hooked on crystallography." After graduation she got a job as Assistant Lecturer in the Department of Inorganic and Physical Chemistry at Leeds University advertised for someone with "an interest in, but no necessary knowledge of, crystallography." In 1947 she married Dr. Eric Truter, whom she had met as a chemistry student at Imperial College, a marriage that lasted until 1965.

She obtained her PhD degree, based on research to determine the crystal structure of nitronium perchlorate, from University of London as an external student while carrying a heavy teaching load at Leeds. With her research students she achieved a considerable reputation with a series of papers on trimethyl platinum compounds, arising from syntheses by R.C. Menzies dating back to 1928. She was promoted to Reader in Structural Chemistry in 1960.

In 1966 she was appointed Deputy Director of a new Agricultural Research Council (ARC) Unit of Structural Chemistry at University College, London, and was soon made a Professor. The charge for her Unit, considered a risky idea at the time, was to look for complexes of alkali and alkaline earth metal cations in order to understand and even emulate the discrimination shown between sodium and potassium. They were indeed able to make some complexes and subsequently to determine the crystal structures of several of Pedersen's crown ether complexes. (Pedersen, Nobel laureate 1987, had shown by 1967 that macrocyclic ethers extract metal salts into non-polar solvents and act selectively on these metals. He spent three months in the Unit in 1969.) Many papers were published including her 1973 review in *Structure and Bonding* "Structures of organic complexes with alkali metal ions" which was an ISI Citation Classic in 1989. She received a Chemical Society Award for Structural Chemistry in 1976. In 1977 the Unit was renamed the Molecular Structures Department and moved to new accommodations at the Rothamsted Experimental Station in Hertfordshire. The group had some very productive years, but in 1984 Mrs. Thatcher's cuts of research that was considered "too basic" could no longer be staved off. The group was dissolved and Jackie moved to University College where she did some teaching and continued her research.

Gordon Cox and Jackie Truter at the 1954 Paris IUCr

Jackie married Sir Gordon Cox, then Secretary of the ARC, in 1968. Gordon suffered increasing ill-health from 1992, and he died in June 1996. (He had retired from the ARC in 1971.) Jackie's own leukemia was first diagnosed in 2002. In periods of remission, she continued to visit the College. She died in November 2004.

Especially as a younger woman, Jackie cut an attractive figure, elegantly dressed and independently stylish. She was a founding member of the BCA, a past chairman of the CCG and a trustee of the CCDC. At Rothamsted colleagues were always impressed with her dedication to the work, to her staff and students and to the laboratory. Her many friends in the UK and around the world mourn her passing.

Durward Cruickshank

Editor's Note: The Truter obituary was excerpted, by permission, from the BCA Newsletter

Checkout the new look of the ACA website at www.hwi.buffalo.edu/ACA/

Travel Awardees

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Melanie Adams
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Purdue
Lauren Borkowski
George Washington U
Miranda Byrne
U of Alabama Huntsville
Brett Chandler
U of Calgary, Canada
S.A. Dalrymple
U of Calgary, Canada
Tomislav Friscic
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Mirta Mir Caraballo
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Scenes from ACA Orlando: Left to right - Top: Ray Davis and Gautam Desiraju, Frank Allen, Helen Berman (below Frank), Lisa Keefe, Steve Ginell and twins Keara (right), Keanan (middle) and Garrett. Second row: Janet Smith, Dan Anderson and Peter Meuller, Khalil Abboud and Marcia Colquhoun. Third Row: Michael Rossmann, Graciel Diaz de Delgado and Iris Torriani, just desserts, Simon Billinge. Bottom Row: Suzanne Fortier and Chris Gilmore, swans at the Swan, Connie Chidester and Christine Muchmore

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RCSB Protein Data Bank
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AUGUST 2005

23-31 **XX IUCr Congress**, Florence, Italy. Local Chair: Paola Paoli, **iucr@iucr2005.it**, Program Chair, Carlo Mealli, ***www.iucr2005.it.***

OCTOBER 2005

28-29 **Macromolecular Crystallography Symposium,** Nashville, TN ***structbio.vanderbilt.edu/xtal/symposium*.**

NOVEMBER 2005

3-5 **Pittsburgh Diffraction Conference, Argonne National Laboratory.** ***www.pittdifsoc.org***

DECEMBER 2005

6-7 **Crystallographic Society of Japan,** Himeji, Japan**.** ***www.sci.u-hyogo.ac.jp/crsj2005***

JUNE 2006

9-18 **The Structural Biology of Large Molecular Assemblies**, the 38th crystallographic course at the Ettore Majorana Centre, Erice, Italy.

JULY 2006

23-28**19th General Meeting of the International Mineralogical Association- Expansion to Nano, Bio and Planetary Worlds.** Kobe, Japan ***www.congre.co.jp/ima2006***

JULY 2006

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

Local Chairs: Charles Simmons (U of Hawaii-Hilo - simmons@hawaii.edu) and Karl Seff (U of Hawii - Manoa - seff@hawaii.edu)

Program Chair: Judith Kelly (U. Conn - judith.kelly@uconn.edu)

AUGUST 2006

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

SEPTEMBER 2006

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

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.**

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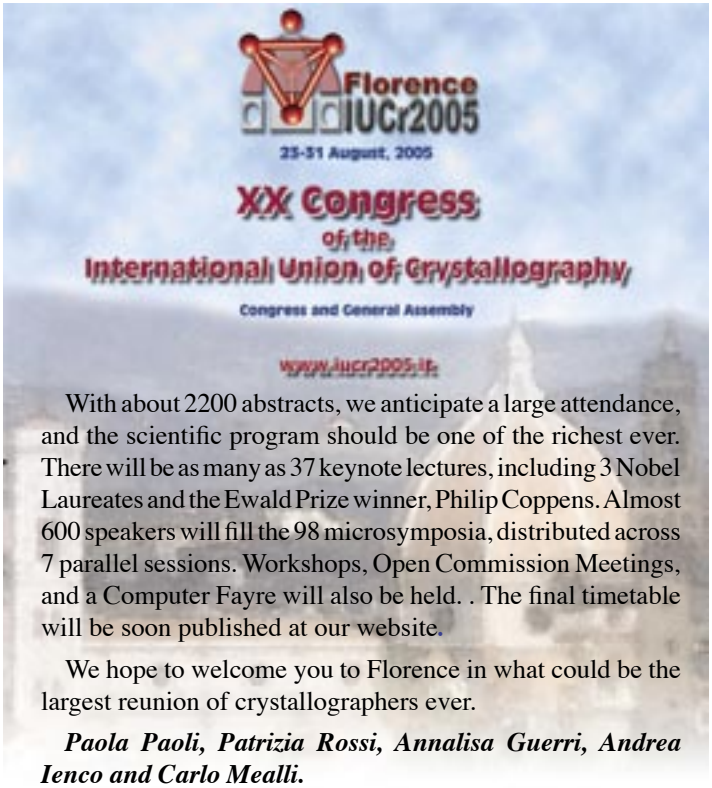

With about 2200 abstracts, we anticipate a large attendance, and the scientific program should be one of the richest ever. There will be as many as 37 keynote lectures, including 3 Nobel Laureates and the Ewald Prize winner, Philip Coppens. Almost 600 speakers will fill the 98 microsymposia, distributed across 7 parallel sessions. Workshops, Open Commission Meetings, and a Computer Fayre will also be held. . The final timetable will be soon published at our website.

We hope to welcome you to Florence in what could be the largest reunion of crystallographers ever.

Paola Paoli, Patrizia Rossi, Annalisa Guerri, Andrea Ienco and Carlo Mealli.

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