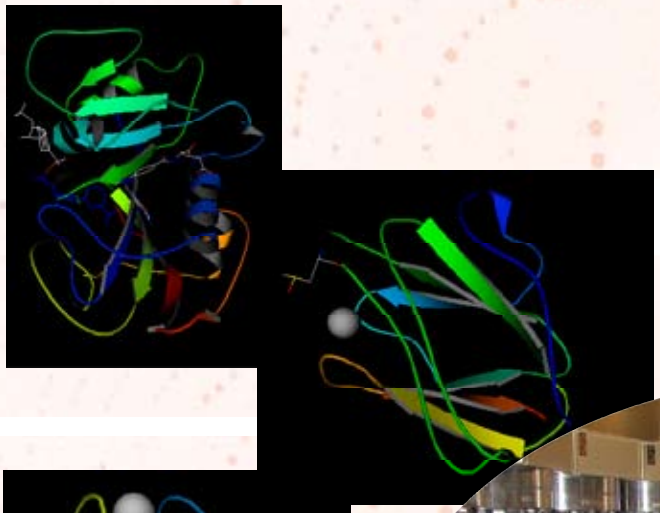
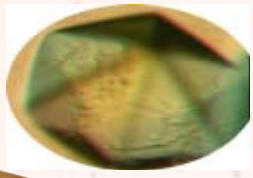
American Crystallographic Association

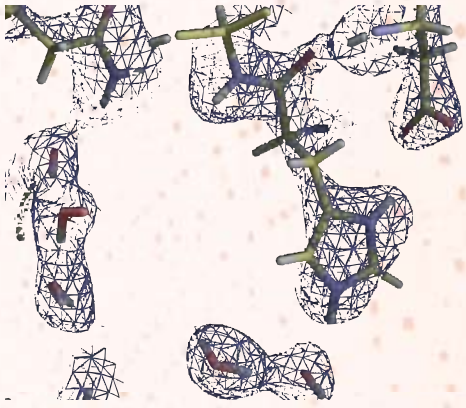
NEWSLETTER

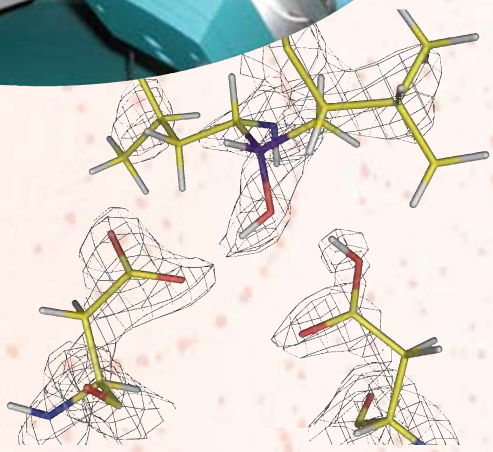
Number 4

Winter 2005









ACA 2006
The Future of Neutron Crystallography

American Crystallographic Association
NEWSLETTER

On the Cover

2006 ACA Transactions on the Future of Neutron Crystallography.
***On The Cover* article, page 12.**

ACA HOME PAGE http://www.hwi.buffalo.edu/ACA/

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Deadlines for contributions are: February 1 (Spring), May 1 (Summer), August 1 (Fall) and November 1 (Winter)
Articles by e-mail are especially welcome.

ACA Newsletter (ISSN 1958-9945) Number 4, 2005. Published four times per year in the spring, summer, fall and winter for the membership of the American Crystallographic Association, P.O. Box 96, Ellicott Station, Buffalo, NY 14205-0096. Membership in the ACA includes a non-deductible charge of $1.75 from membership dues to be applied to a subscription to the ACA Newsletter. Periodicals postage paid at Buffalo, New York. POST-MASTER: Send address changes to ACA, c/o 700 Ellicott St., Buffalo, NY, 14203.

There have been several natural disasters during the past year – a tsunami, an earthquake and several major hurricanes. People continually volunteer to help others recover from these major catastrophes. It is heartening to see such compassion throughout the world. There have also been some positive events. The ACA Annual meeting in May in a beautiful location, Orlando, FL, was very successful. The Twentieth Congress and General Assembly of the International Union of Crystallography was held in Florence, Italy in August. This was also a superb location and outstanding science was presented at the meeting. Congratulations to Phil Coppens of the State University of New York in Buffalo for winning the seventh Ewald Prize of the IUCr. The organizers of the IUCr meeting provided an excellent example of how to organize a relatively large meeting; approximately 3000 participants were provided lunch within the time period of one hour every day! In 2005 Argentina and Brazil were accepted for Latin-American Country Membership in the ACA; we welcome them to this new category of membership and look forward to increased participation in the ACA by researchers from these countries.

This is my last column as President and it has been a pleasure to work with so many very fine people. Lisa Keefe, Secretary, does an excellent job taking the minutes of Council meetings. Doug Ohlendorf, Treasurer, helps to keep us financially stable. S. N. Rao, Financial Officer, negotiates meeting site contracts and takes care of the investment portfolio. Lee Groat, Canadian Representative, reports on activities in Canada. Bill Duax, Chief Executive Officer and President of the IUCr for the past three years, keeps us informed, especially about international affairs. Thank you, Fran Jurnak, for your leadership and other contributions to Council during the past three years and best wishes in the future. I wish Bob Bau success as he takes over as President in 2006; I welcome his guidance and believe that he will continue to do an excellent job on Council. I am very grateful to our ACA staff Marcia Colquhoun, Patti Coley and Tammy Colley for all of their efforts. A special thanks also goes to newsletter editors, Judy Flippen-Anderson and Connie Chidester who organize and assemble the quarterly ACA Newsletter, which is so interesting and so professionally done.

Next year the ACA Annual meeting will be held at the Sheraton Waikiki Beach in Honolulu, Hawaii from July 22-27, 2006. Charles F. Majkrzak is the winner of the Bertram E. Warren Award and Helen M. Berman is the winner of the Martin J. Buerger Award. The *Transactions* Symposium concerns neutron diffraction of small molecules and macromolecules. Outstanding scientific sessions are being organized by the SIGS and the Program Chair, Judith Kelly, and local activities are being handled by Charles Simmons and Karl Seff. I look forward to seeing you in Honolulu in 2006. Aloha.

Louis Delbaere

Letters to the Editor

Dear Judy,

Ed and I and our family have settled just east of Charlottsville, Virginia for the time being. We have visiting professorship appointments at the University of Virginia. I am working in Milton Brown's drug discovery lab in the chemistry department. I have been awarded funds from Howard Hughes Medical Institute for this "sabbatical". Ed is teaching an online class for UNO. We put our kids in the local public schools and we are living in the summer home of a relative on Lake Monticello. We love living in Virginia. We have approached this whole thing as an adventure and a life experience. We got to live in a very nice place for a while and have made some great friends. My children had never seen the fall colors, lived in the country on a lake, or learned to water ski. I have even heard that there is a ski area about an hour from here. We don't have that in New Orleans! Xavier University declared a state of financial exigency and has layed off almost half (13 faculty members) of the chemistry faculty since they only expect 50% of the students to return. As Chair of the department along with all of the other stuff that I do, I am fortunate to have been offered a contract to stay. Both Xavier and UNO plan to open in January and Ed (also the chemistry dept Chair) and I will be there. (We would definitely consider other offers but we have found two body employment problems to be difficult). The kid's schools even plan to open in January as Charter schools. Our house had two feet of water in it. At this point, the downstairs has been just about fully gutted. All appliances, cabinets, furniture, etc. have been removed. The sheetrock and insulation have been removed and the place has been sprayed with bleach and fungicide to kill the mold. The second floor is fine. The house is not livable at this time but we should be able to repair it. The roof and awnings were damaged by the hurricane but most of the damage was caused by the flood. We will probably have to live in a FEMA trailer for a little while until we can get the house livable. Since there was so much property damage in the city, there is very little rental property available. Do you have an extra copy of the newsletter? Since the Universities closed, we have not gotten any mail at all.

Cheryl (Klein Stevens – eds@mindspring.com)

Dear Judy:

Bob Stewart and I hope that you will consider this historical material on Leroy Alexander and the Pittsburgh Diffraction Conference for publication in the Newsletter.

Leroy Alexander joined the staff of the Mellon Institute in Pittsburgh in January 1946. His involvement with the Pittsburgh Diffraction Conference began with the fourth Conference which was held in December, 1946. Thereafter, he was active in the affairs of this annual Conference until his retirement from the Mellon Institute of Carnegie-Mellon University in 1976. Throughout these thirty years he took part in the Conference in two different ways. First he became a regular among the Conference organizers. Second, he joined in the presentation of research that came from a growing x-ray group at the Mellon Institute. Harold Klug and Leroy Alexander were the leaders.

Crystallographers at the Mellon Institute, 1966: Front-from left - Harold Klug, Leroy Alexander. Behind-from left: Wayne Orr, Bob Stewart, Sid Pollack, Maurits Nothold, Maureen Sullivan. Absent - Gordon Smith, Roger Pettersen, Gardner Sumner, Patricia Brown, John Beres. Note: The biologist Roy Worthington had a separate small-angle x-ray laboratory.

Now that the Pittsburgh Diffraction Conference (PDC) is in its 63rd year, with a history older than that of the ACA, it is important to recognize the work of Leroy Alexander in gathering and preserving records that go back continuously to the first PDC. This took place at the University of Pittsburgh in 1943 (during the siege of Leningrad; now St Petersburg). Leroy made use of his archival material in his account of "Surhain Sidhu and the Early Pittsburgh Diffraction Conferences" which appeared in abbreviated form in the ACA Newsletter, December 1992 and in full on the website, ***www.pittdifsoc.org***. Leroy includes his own stories of those early years. His article points out that the early PDCs drew audiences of hundreds and were attended by leading figures such as Sir Lawrence Bragg, Isadore Fankuchen, Charles Barrett and David Harker.

Bryan Craven and Robert Stewart

ID NewsUpdate - from the Editors Desk

The Editors feel that it is important for ACA members to be aware of what is going on in some states where 'intelligent design' initiatives have been proposed. Following is an update on what is happening in a number of states and an article by Susan Spath, public information project director at the National Center for Science Education (NCSE). Sources for this column were *Science,* 4 Nov., 2005, p 754 & 787; the NCSE website: ***www.ncseweb.org;*** the National Public Radio website: ***www.npr.org***; and the AAAS website: ***www.aaas.org/news/press_room/evolution/.***

Pennsylvania: On November 8th, voters in Dover replaced eight pro-"intelligent design" incumbents on the Dover Area School Board with candidates that had taken a firm stand on the inappropriateness of teaching intelligent design in science classrooms. This happened a few days after the close of testimony in ***Kitzmiller v. Dover,*** the first legal challenge to the constitutionality of teaching ID in the public schools.

Kansas: Also on Nov. 8th, as expected, the Kansas state board of education voted 6-4 to adopt the draft set of state science standards that were rewritten, under the tutelage of local "intelligent design" activists, to impugn the scientific status of evolution. The new standards change the state's definition of science to move it beyond the search for natural explanations of the natural world and to allow for supernatural explanations. As a tactic to delay implementation of these standards, the NAS and the National Science Teacher's Association have denied permission to use materials in their copyrighted set of science standards (from which the board had borrowed extensively). The board will now have to completely rewrite the 123-page document. This delay may prove effective because 4 of the 5 board seats up for election in 2006 are held by ID proponents.

Michigan: House Bill 5251, introduced September 29th, would require the Board of Education to revise science standards. The bill aims to ensure that students will be able to "use the scientific method to critically evaluate scientific theories including, but not limited to, the theories of global warming and evolution." The Michigan Science Teachers Association promptly issued a statement denouncing the bill.

Alabama: Biology textbooks have included a disclaimer describing evolution as a "controversial theory" since 1996. The Board of Education adopted a softer disclaimer when they revised science guidelines in 2004, describing evolution as one of several scientific theories. But on Nov. 10th, the board voted to require the original disclaimer language.

México: In his *Science* essay "Teaching Evolution in México: Preaching to the Choir" (4 Nov. 2005, p. 787), Antonio Lazcano, a university biology professor in México, comments that many people in the US believe that México's strong Catholic background must have led to opposition to teaching Darwinian evolution. He emphasizes that this is absolutely not true, and says "Only twice during my 30 years of teaching about evolutionary biology and research into the origins of life have I encountered religious-based opposition to my work. In both cases, it came from evangelical zealots from the US preaching in México."

Intelligent Design - Get Involved

Like many biology majors in the 1970s, I was introduced to structural biology by *The Structure and Action of Proteins*, by Richard E. Dickerson and Irving Geis (Harper & Row 1969). This classic book showed me that the structures of complex proteins were both beautiful and interesting and could elucidate biological function at the molecular level. Furthermore, the text showed that comparing amino acid sequences and the structural features of proteins could yield deep insights into the evolutionary histories of living organisms. The section called "The History of a Protein," for example, explained that cytochrome c was an ancient, highly conserved protein found across the living world, an observation beautifully consistent with evolutionary theory. The study of macromolecular structure and function demonstrated that the special nature of molecules from living systems is not that they evade the standard laws of chemistry and physics, but rather that they are products of history, of evolutionary change over billions of years.

Meanwhile, in the past thirty years, opposition to evolution as an explanatory theory has continued to flourish among the general American public, especially in some conservative Christian communities. In 2005, the National Center for Science Education has recorded anti-evolution activity in 24 states, from middle-school teachers telling students the earth is 6000 years old to state legislators introducing bills that call for "alternatives" to evolution to be taught.

The most recent challenge to evolution education has come from the so-called "intelligent design" movement. Proponents of this movement have taken the dazzling advances in our knowledge of molecular structure as an opportunity to relocate special creation by God to the molecular level. In particular, the phrase "molecular machines" has captured the imagination of anti-evolutionists who proclaim that the intricacy and efficiency of these structures cannot be accounted for by evolutionary processes and, hence, must reflect the work of an "intelligent designer." The dangerous potential of this movement is illustrated by recent events in Kansas, where the state Board of Education is currently controlled by intelligent-design supporters. On November 8, the board approved a set of science standards containing misleading, incorrect, and downright bogus statements about evolution.

Crystallographers can help to counter the impact of anti-evolutionists, especially of "intelligent design" proponents. Some ways to help are:

- Featuring sessions on evolution at annual meetings and publishing special issues of research journals with a focus on evolution.
- Making sure that evolution is included in your undergraduate teaching, whether as a special topic or integrated theme.
- Reaching out to high school science teachers -- offering to answer questions or to visit a high school science class.
- Sharing your excitement about your work with the public by giving special lectures for the public and appearing on radio shows.
- Recognizing that many members of the public fear that evolutionary theory leads to atheism and treating this concern with respect.

Perceptions of beauty and design have stimulated scholars and scientists from the ancient Greeks to the present to try to understand the underlying structures (and physiological responses) that lead to wonder and delight. Crystallographers may well know this better than anyone. The public has much to gain from learning about the evolutionary history that contributes to the structural elegance of biological molecules. Crystallographers have much to offer to that endeavor and much to gain by countering anti-evolutionism.

Susan Spath

Fall Meeting of the AIP Governing Board

The Governing Board met on 6 November in Gaithersburg, MD. Although the fall meeting is generally focused on rather dry, budgetary issues, there are several continuing issues that interest a wider audience. Chairman Millie Dresselshaus reported on a recent European trip. Physics appears to be healthier in Europe than it is in the US. Britain has a periodic review of its physics establishment by outsiders every five years, and Millie attended that function. She reported on the widespread perception that US leadership in physics is slipping badly, to the extent that the US is no longer considered by many to be even "among the leaders". Thus, although it is sensible to expect the rest of the world to catch up with the US, the perception is that this trend has more than caught up with us. International collaborations are slipping away from US scientists. Visa and export controls have degraded this situation seriously while things elsewhere are moving in the opposite direction. No appropriate remedies were suggested, beyond changing the political environment. Especially troubling was the perception, shared by US physicists, that even though physics BA and PhD graduates are taking industrial positions in ever larger percentages, it is the industrial physics community in the US that is taking the biggest hit.

Open Access to publications is moving more rapidly than anyone expected, especially among younger scientists, and physicists allied with the biomedical sciences. Mark Brodsky reported that this trend has brought with it a serious problem with the multiplicity of "published" versions and the attendant difficulty of maintaining authoritative published copies of papers and the related problem of establishing priority. The NIH open access initiative is not working well; only 2-3% of authors are complying with the voluntary submission. Mark also mentioned how important he thought it had become to read carefully the copyright transfer arguments required for publications. These, too, are changing rapidly and not favorably for authors.

Physicists around the world are flabbergasted by the growth of the Intelligent Design advocacy in the United States. While this response is largely one of disbelief, it is also mixed with concern. ID has apparently also taken root solidly in Australia. I may have more to say on this in the Spring *Newsletter*. Discussion of this issue led naturally to the broader issue of how the AIP is to respond

to pressing requests for support of letters for example, endorsing policy initiatives outside the AIP. A temporary policy was agreed to such that whenever such a document is deemed by four resident members of the AIP Executive Board to be consistent with the stated policies of any member societies, it will be possible for those four to decide to endorse it. This initiative has ramifications to member societies as it underscores the importance of having clear statements within the ACA of policy issues on which there is a desire to have the AIP join in support.

Finally, it is relevant to point out that crystallographers enjoy a unique advantage with respect to their interactions with colleagues from the rest of the world, because of the exquisite balance that exists between the regional affiliates and the IUCr. Physics in general appears to have difficulty using its International Union to deal with this problem, because the IUPAP is relatively impotent, in part because it has no business model arising, for example, from publications.

2006 Art in Crystallography Prize

The *ACA Newsletter* Editors are accepting entries to the ***2006 Art in Crystallography*** contest in the form of images emailed to either of the us (**conniechidester@earthlink.net** or **flippen@rcsb.rutgers.edu**). Entries should be accompanied by a paragraph explaining the science and the method of producing the image. A photo of the artist would be appreciated but is not required. Prizes consist of a small monetary award and a banquet ticket at the annual meeting. Winning entries will be posted on the web and will also be displayed as printed images at the ACA Meeting. (Winners are not, however, required to attend the meeting). We will also feature images in the *Newsletter* from time to time. Judging will be by a panel appointed by the Editors; please let us know if you are interested in being a judge.

Call For Nominations for 2007 ACA Awards

The Elizabeth A. Wood Science Writing Award, established in 1997, is given to authors of books or articles that bring science to the attention of a wide general audience. Nominations are due by March 1, 2006.

Nominations for the ***Fankuchen Memorial Award*** and for the ***Kenneth N. Trueblood Award*** are due by May 1, 2006.

Nominations for the ***Margaret C. Etter Early Career Award*** are due by September 1, 2006.

Full details describing the criteria for all ACA awards can be found on the website (***www.hwi.buffalo.edu//ACA/***) and on page 12-13 of the Fall 2005 *Newsletter.* All Nominations should be sent the ACA office (***marcia@hwi.buffalo.edu***)

Nominations for ACA offices for 2007

In the fall of 2006 we will elect a new vice-president, treasurer and one person to each of the ACA Standing Committees (Continuing Education, Communications, and Data, Standards and Computing). Suggestions (due by February 1, 2006) may be sent to any member of the Nominating Committee: ***Kathy Kantardjieff (Chair, kkantardjieff@fullerton.edu), Fran Jurnak (jurnak@uci.edu) and Marilyn Olmstead (Olmstead@chem.ucdavis.edu).***

Local and Program Chairs selected for 2007 and 2008

2007 Meeting in Salt Lake City, UT

Local Chair: ***Chris Hill (U of Utah)***
Program Chair ***Jill Trewhella (U of Utah)***

2008 Spring Meeting in Knoxville, TN

Local Chair: ***Jason Hodges (Oak Ridge Nat'l Lab)***
Program Chairs: ***Paul Butler (NIST) & Dean Miles (Oak Ridge Nat'l Lab).*** Dean will be responsible (mainly) for matters regarding macromolecular abstracts and for interacting with the macromolecular SIG, while Paul Butler will handle the other abstracts and will be interacting with the other SIGs

Dues are Due

Invoices for 2006 dues have been mailed. Please renew promptly and remember to support your favorite ACA Award Funds.

New ACA E-Publication for 2006

To support younger crystallographers, the ACA Council has initiated a new, reviewed e-publication titled "Etter Lectures of the American Crystallographic Association", which will publish the *Transactions* of the Margaret C. Etter Early Career Award Symposium as well as papers presented by the winners of the Etter Student Lecturer Awards. The Margaret C. Etter Early Career Award is presented every year by Council to recognize outstanding achievement and exceptional potential in crystallographic research to an individual in the early stage of an independent career. Subsequently, a symposium is organized at the annual ACA meeting to honor the award winner. In addition, Etter Student Lecturers are selected from submitted abstracts by elected officers of the various SIGs and then invited to present their work as an oral presentation at the annual ACA meeting and subsequently as an e-publication. In order to be included in the e-publication a manuscript, reflecting the contents of the oral presentation, must be submitted at the time of the ACA meeting. Before printing, the manuscript will be reviewed by selected members of the ACA.

Fran Jurnak

Carrie Wilmot Selected for the 2006 ACA Margaret C. Etter Early Career Award

Carrie Wilmot (U of Minnesota) is a structural biologist who has pioneered exciting new technology that combines macromolecular x-ray crystallography, anaerobic single crystal kinetics and spectroscopy, as well as cryo-capture to identify, stablilize and characterize intermediates in complex oxidation reactions. Her work breaks new ground and moves previously unrecognized post-translational modifications of amino acids to the forefront of catalysis. The work in essence produces high-resolution 3D molecular structures as well as movies of complex enzymatic reactions. Her work is exceptional in that she examines biological reactions at the atomic level and develops experimental strategies to proble the complexities of fundamental enzymatic processes. She came to Minnesota after she received her PhD at the University of London and spent time as postdoctoral fellow at the Scripps Research Institue in La Jolla, CA. Although still an assistant professor, she has recently been named the Director of the Kahlert Structural Biology Laboratory at the University of Minnesota in recognition of her unique talents.

Excerpted from the nomination letters

ACA Members Selected as Outstanding Young Scientists

At a symposium, held at the 2005 American Chemical Society national meeting in Washington, D.C., eight graduate students and postdocs, selected from more than 50 nominations, were named Inorganic Young Investigators. Each award recipient received $500, a plaque, and the opportunity to give a 20-minute presentation on his or her research. Two of the eight honorees are ACA members.

Robin T. Macaluso, (Argonne National Lab) described how crystal structure can affect local and itinerant electronic behavior in inter-metallic magnetic and superconducting materials. She carried out the work while a graduate student in Julia Y. Chan's lab at Louisiana State University. She used x-ray diffraction along with magnetic and electronic property measurements to study Ce_2PdGa_{12}, $Ce_2MIn_{3n}{}^{+2}$ (M = Co, Rh, or Ir; n = 1 or 2), and other intermetallic systems made by heating stoichiometric amounts of the pure elements at high temperatures (*Chem. Mater.* 2003, 15, 1394). In particular, she has investigated structural trends that result from the presence of f electrons in the electronic structure of these materials, and how certain structure types favor "heavy-fermion" superconductivity. Heavy-fermion materials are those in which conduction electrons have a greater effective mass because they strongly interact with the localized magnetic moments of f electrons in the crystal lattices.

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Tamara D. Hamilton (University of Montreal) discussed research she performed in Leonard R. MacGillivray's group at the University of Iowa) involving the synthesis of tetrapyridylcyclobutane ligands that self-assemble into molecular frameworks when treated with transition-metal ions. These assemblies can take on various structures, including 2-D polygons and 3-D polyhedrons, that could serve as hosts to stabilize chemical intermediates, mediate chemical reactions, or be useful building blocks for larger molecular-scale devices (*Cryst. Growth Des.* 2004, 4, 419).

Preparation of the metal-organic assemblies was designed to mimic template-directed processes in nature, such as DNA-directed synthesis of proteins. Treating the ligand with Cu(II) ions, for example, forms a polyhedron structure made up of six copper ions and six ligand molecules. The ligand is unsymmetrical because it contains both 2-pyridyl and 4-pyridyl groups such that one set of pyridines can be "turned off" during the self-assembly process, allowing access to a wider variety of assembly geometries.

Excerpted from the article describing the awards in C&E News, October 3, 2005, pp 40-42

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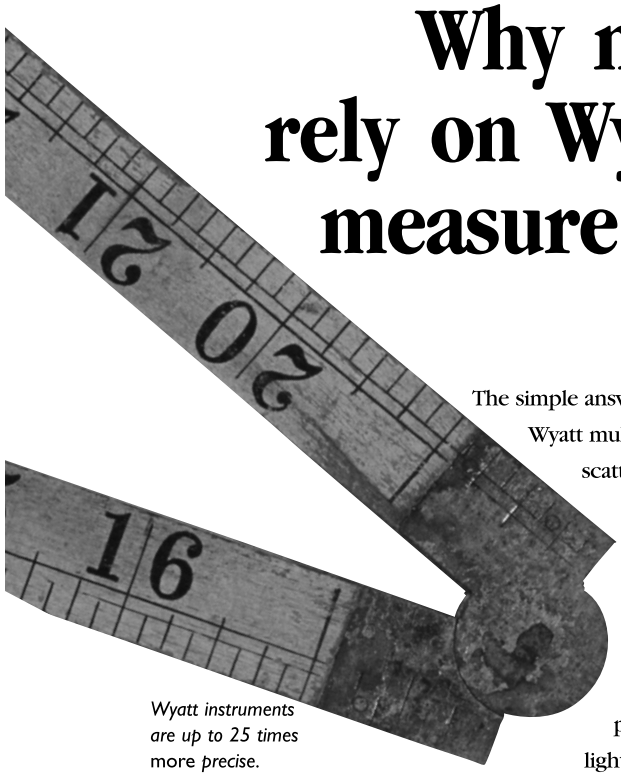

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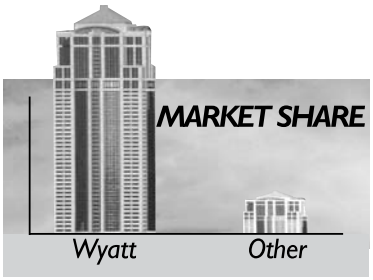

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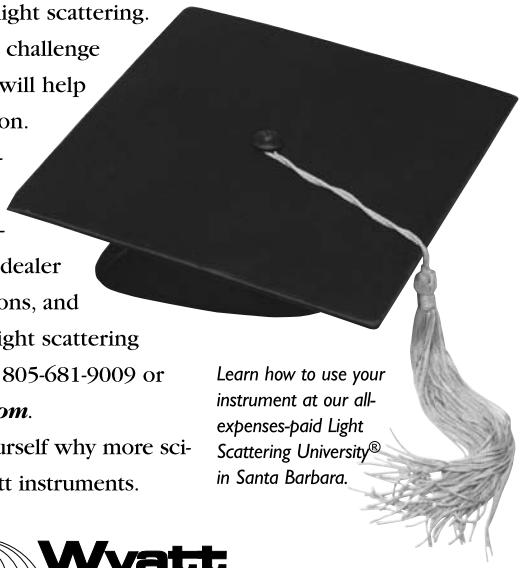

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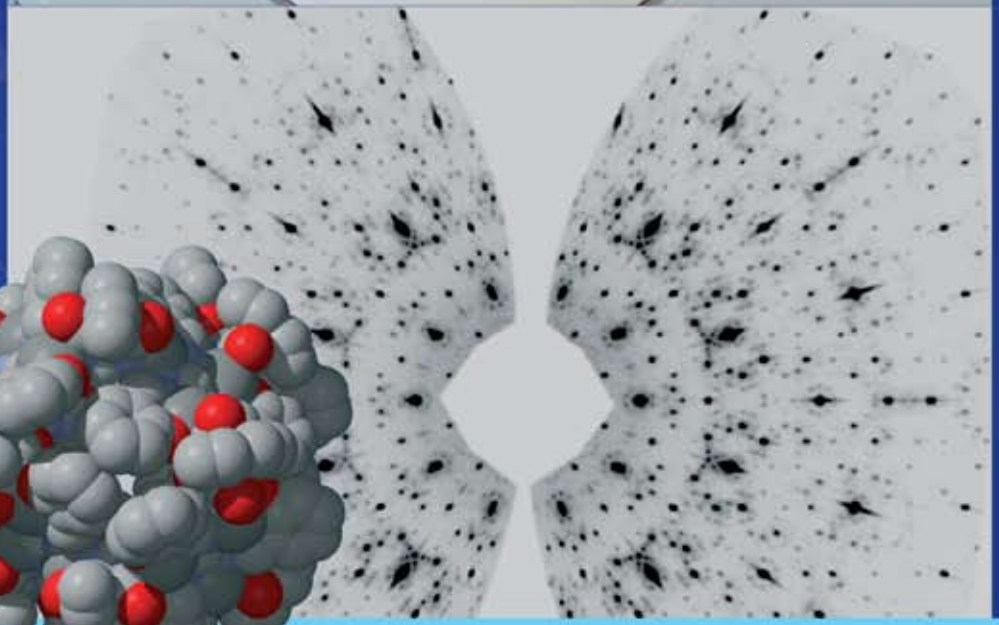

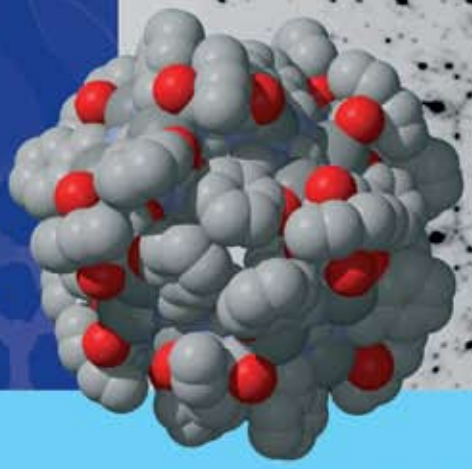

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On November 9th, the Hauptman-Woodward Board held a gala awards dinner in their new building. Bill Duax (seen on the right with Herb Hauptman) was honored with the Harker Award for contributions to crystallography and Herb Hauptman (seen on the left with his wife Edie) received the Koepf award for contributions to science. The Harker award has only been given twice previously, to Philip Coppens in 1995 and to George Jeffrey in 1999.

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7. I certify that the statements made by me above are correct and complete. (Signed) Marcia Colquhoun for American Crystallographic Association, Inc.

Web-Watch - Winter 2005

Science is for every age. This Web Watch column will direct you to a number of web sites that are targeted at kids. Whether you are interested in directing your child (or someone else's!) to science activities, images or age-appropriate articles, these sites can provide a good starting point. Some of them have resources for teachers. A few of them are offered in Spanish as well as in English.

scorescience.humboldt.k12.ca.us/fast/kids.htm is a site that has links to a number of general sites, some with appropriate grade notations, as well as to previously featured sites. For instance, one site tells you about the physics of roller coasters, lets you design your own, and tells you how well you did. One of the general sites noted is ***www.chem4kids.com*** which offers many relatively short descriptions of basic chemistry in a kid-friendly manner. Rader also offers the similar ***www.bio4kids.com*** site. Each has a site map that will allow you to find topics you are interested in exploring.

It shouldn't be a surprise that the American Chemical Society has developed a web site for children: ***www.chemistry.org/kids.*** This site offers many activities that show how chemistry fits into life – kids can learn to make an indicator, paint a fresco, go on a magnet hunt and pursue many, many other activities.

The BBC offers a number of sites: ***www.bbc.co.uk/schools/gcsebitesize/chemistry*** and ***www.bbc.co.uk/schools/gcsebitesize/biology*** both offer many topics and quick exams to test your understanding of the topic. The core curriculum for AS level biology, for instance, is covered in ***www.bbc.co.uk/education/asguru/biology/intro.shtml.***

Federal agencies are also interested in promoting science for children. Two examples are ***www.niehs.nih.gov/kids/home.htm*** and ***kids.earth.nasa.gov/.*** The first is mounted by the National Institute of Environmental Health Sciences and focuses on environmental issues. Besides its own content, it provides links to a number of non-NIEHS sites. The latter is a NASA site that is mostly an earth science enterprise.

For children that like to read, ***www.sciencenewsforkids.org*** offers illustrated articles that also provide bibliographies. The site offers puzzles, games, an archive of articles and more. One can also sign up for a free, weekly *Science News for Kids* newsletter.

The San Francisco Museum of Science, Art and Human Perception is "… an experimental, hands-on museum designed to spark curiosity—regardless of your age or familiarity with science." Its web site, ***www.exploratorium.edu***, does just that: it sparks and feeds curiosity. There are myriad topics explored, for instance music, cooking, gardening; and there is a good microscope imaging station with little videos.

The web site ***www.northvalley.net/kids/science.shtml*** contains links to science and math web sites for kids. Some you probably won't see elsewhere, such as the one to Grossology – the Science of Really Gross Things. ***www.sciencemadesimple.com/*** is a source of projects for kids to carry out.

A science teacher, mother and former science fair organizer has put together a site, ***faculty.washington.edu/chudler/fair.html,*** that tells how to put together a successful science fair project. It will help a child understand the steps he or she must go through in thinking about starting this process. She has also provided links to other science fair related web sites.

Do you have a favorite web site? Is there a web site that you could not live without? Have you come across a web site that you think would be of interest to your colleagues? If so, please share it by sending the web address (and a 1 or 2 sentence description) to ***Kay Onan (k.onan@neu.edu).***

Kay Onan, Louis Delbaere, Cathy Drennan
Annie Heroux

Sweeping Online Changes by the Journal Science Make Career Support and News Freely Available

Based on a merger of ***ScienceCareers.org*** and Science's Next Wave, the journal *Science* has announced a new Web site that is believed to be the single most comprehensive, freely accessible source of online science-career support currently available for scientists, teachers, students, career counselors and the public.

The debut of free online career support coincides with a sweeping redesign of the *Science* family of Web sites and the journal's decision to make newly published content on its *ScienceNOW* daily news site freely accessible to the public. The *Science* Web sites are published by AAAS, the nonprofit science society.

The newly tooled ***ScienceCareers.org*** offers job listings, a grants directory and other resources for the many facets of a young scientist's career, all in one place. Free to everyone and easy to navigate, the site also provides career advice, a CV database, meetings and events calendars, information about funding opportunities, advice on cover letters, interviews, career development, and more. Users will also find special topic portals, including the Minority Scientists Network and the Postdoc Network.

Stories on *ScienceNOW*, the daily news service, will also become freely available. Science's news team posts three to five news stories at ScienceNOW every work day, covering new developments in science research, policy, funding, exploration and technology. Users will be able to read these stories without a subscription for four weeks after each story is posted.

Natasha Pinol - npinol@aaas.org

MSA Grant for Research in Crystallography, Mineral Physics or Chemistry and Mineralogy

The Mineralogical Society of America announces the 2007 MSA Grant for Research in Crystallography, Mineral Physics or Chemistry, and Mineralogy from the Edward H. Kraus Crystallographic Research Fund with contributions from MSA members and friends. The grant comprises up to $5000 for research in crystallography. Students, including graduate and

undergraduate students, are encouraged to apply. However, all proposals are considered together. The award selection will be based on the qualifications of the applicant, the quality, innovativeness, and scientific significance of the research, and the likelihood of success of the project. The only eligibility requirement for the grant is that the applicant must have reached his or her 25th birthday but not yet have reached his or her 36th birthday on the date the grant is awarded, and that the person is not an MSA Counselor. There are no restrictions on how the requested funds may be spent, as long as they are used in support of research. Travel to meetings, conferences, short courses, non-research fieldtrips, etc. are not considered suitable uses of research money. Proposals that make such requests will not be considered further.

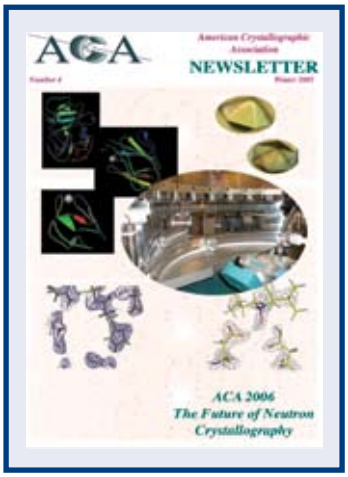
The next award will be made in January, 2007. Completed applications must be returned to the MSA Business Office by June 1, 2006. Application forms for the grant may be obtained from Dr. J. Alex Speer - Mineralogical Society of America - 3635 Concorde Pkwy - Ste 500 Chantilly VA 20151-1125 USA - Tel: (703) 652-9950 - Fax: (703) 652-995 ***- j_a_speer@minsocam.org***

Where are all the Crystallographers & Diffraction Facilities?

Only a small minority of science faculty are employed at PhD granting institutions and such institutions produce only a minority of the undergraduates who go on to get their PhDs in the sciences. This is especially true for those faculty and students from groups historically underrepresented in the sciences. The STaRBURSTT CyberDiffraction Consortium, ***www.starburstt.org/***, is a national effort whose central goal is to increase the quality, scope, and scale of utilization of diffraction methods by faculty and students at Predominantly Undergraduate Institutions (PUIs), Community Colleges (CCs), Historically Black Colleges and Universities (HBCUs), Hispanic Serving Institutions (HSIs), and Tribal Colleges (TCs). As part of our ongoing efforts in areas of crystallographic research and education, we are developing a comprehensive database of faculty with crystallographic training and/or interests and a crosslinked database of diffraction facilities at PUIs, CCs, HBCUs, HSIs, and TCs. We are also beginning to build a related database of other diffraction facilities can make available substantial blocks of time on their instruments to our faculty and students for "hands on" access, either local and/or remote. We ask the ACA membership's help in identifying such PUI, CC, HBCU, HSI, and TC crystallographers and diffraction facilities and also in identifying government labs as well as future PhD granting, non-profit, and industrial affiliate institutions for our consortium. Please send any suggestions to Allen Hunter, the director of the STaRBURSTT-CDC, at ***adhunter@ysu.edu.*** Remember, we are the source of most of your future graduate students and employees!

Allen Hunter

What's on the Cover



Background: A time-of-flight Laue neutron diffraction pattern collected from the commercially important enzyme D-xylose isomerase on the Protein Crystallography Station (PCDS) at Los Alamos Neutron Science Center (LANSC) by aa team of researchers from the University of Tennessee and Fox Chase Cancer Research center led by Gerry Bunick.

Center: The DOE-OBER funded PCS at LANSC, the first protein crystallography beam line in the world to be built at a spallation neutron source and the only neutron protein crystallography beam line in north America

Upper left: Top - The important drug target enzyme dihydrofolate reductase (DHFR) whose neutron structure, in complex with the anti-cancer drug MTX, has been determined on the PCS at Los Alamos Neutron Science Center by a team of researchers from the University of Tennessee led by Chris Dealwis. ***Center*** - A blue copper protein involved in electron transport whose neutron structure has been determined on the PCS at Los Alamos Neutron Science Center by a team of researchers from the Argonne National Laboratory and the Universities of Washington and Mississippi, led by N. Sukumar. ***Bottom*** - The iron binding protein rubredoxin whose neutron structure has been determined on the PCS at Los Alamos Neutron Science Center by a team of researchers from the University of Southern California led by Bob Bau.

Lower left: Neutron scattering density in the catalytic site of the commercially important enzyme D-xylose isomerase showing the protonation state of an important residue and the coordination of water molecules. The density was calculated from diffraction data collected on the PCS at Los Alamos Neutron Science Center by a team of researchers from the University of Tennessee and Fox Chase Cancer Research center led by Gerry Bunick.

Upper right: Crystals of the DHFR/MTX complex . The protein was perdeuterated at the Biological Deuteration Laboratory at Los Alamos Neutron Science Center in order to increase its neutron scattering efficiency in the PCS by a team of researchers from the University of Tennessee led by Chris Dealwis.

Lower right: Neutron scattering density in the catalytic site of the enzyme endothiapepsin in complex with the transition-state analogue inhibitor H261. The density was calculated from diffraction data collected on LADI at the Insitut Laue Langevin by a team of researchers from the University of Southampton including Leighton Coates and Jon Cooper.

Bridging the Sciences: Where are we now?

As the Bridging the Sciences Initiative approaches its third year of existence, it has already had a significant impact. Born from the conviction that increased funding in the physical, mathematical and computational sciences would result in research that could significantly impact biomedical research, the initiative's goals were to determine how best to fund such research, and then find a way to make that funding source a reality.

In the spring of 2003, 6 societies agreed to participate. Most represented the biological sciences. It has non grown to 16 groups, including 14 professional societies that cover biology, chemistry, instrumentation, computer science, physics, and mathematics, representing over 280,000 research scientists.

Through meetings with members of Congress and their staff, and with officials at the federal agencies, the Coalition's ideas have gained recognition and traction. In 2004, NIH and NSF held a joint meeting to discuss ways the federal government could facilitate research at the interface of the life and physical sciences. In 2005, draft legislation to reauthorize NIH included a bridging the sciences demonstration program.

In addition, other groups have picked up the ideas expressed by the Coalition and gone to Congress with similar messages. The Council on Competitiveness's National Innovation report, (December 2004), called for the federal government to increase its investment in basic science research in order to keep the United States competitive globally. The October 2005 National Academies study recommends that policymakers increase federal investment in the physical, computational, and mathematical sciences by 10% per year for the next seven years. The report states that many advances in biomedical research are based on advances made through research in these other fields. Both reports also cite the need to fund more innovative research - not just research that will pay off in two to three years.

Unfortunately, the current federal funding environment is tougher than it was when we started this initiative. NIH is slated to receive an increase that does not keep pace with inflation, and NSF is slated to receive less than it did in 2004. Some may naturally ask, why pursue a funding stream for the bridging sciences now? Why not focus on protecting the "piece of the pie" we already have?"

While the funding environment has changed, the reality that biomedical research advances depend on advances in mathematics, physics, chemistry, and computational science has not. The difficulty of finding funding for research at the interface of the biological sciences and the physical, mathematical and computational sciences remains.

The Coalition has made great strides in creating an awareness of the need to fund research at the interface. While the funding situation now appears bleak, it will eventually be brighter. Now is the time to lay the groundwork to ensure that we will be ready when the time comes and to make the Bridging the Sciences concept a reality.

Ellen Weiss

News from Canada

CNCC Web Page - The Canadian National Committee for Crystallography (CNCC) webpage is viewable at www.cins.ca/cncc/. The site includes information, awards and financial status of the Larry Calvert Student Travel Fund, as well as general information on the CNCC.

Canadian Light Source News (from the CLS E-News, www.lightsource.ca) - Message from ***Bill Thomlinson***, the Executive Director: "It is hard to believe that a year has passed since our official opening and all of the exciting and memorable events that surrounded it. In the time since then, performance of the CLS has steadily improved in a manner similar to other synchrotrons around the world, meeting and in many cases exceeding expectations. With the completion of a month-long shutdown period for routine maintenance and upgrades, the staff is turning its attention to continued user operations and beamline commissioning. By the end of this year the CLS will have scheduled 20 experiments conducted in 140 experimental shifts, with 53 users visiting the CLS from across Canada and as far away as Germany. Requests for beam time are soaring, with over 900 experimental shifts sought. In order to accommodate the increasing demand, CLS is moving to "24/7" operations for much of the remainder of this year and continuing into next year."

Tom Ellis reports: "As research activity at the CLS ramps up, it is vital to develop a clear Strategic Research Plan. Such a plan will be the centerpiece of all other strategic planning at the CLS. We will launch a comprehensive and inclusive consultation process for the Plan on November 16th at our "Experts Day". It is timed to occur just before the Scientific Advisor Committee meeting and the Annual Users Meeting. A number of opportunities to provide input over the next few months will follow, so stay tuned for more details."

Jeff Cutler reports on the Industrial Science Program: "We are now conducting experiments for clients on our experimental floor using about 30 experimental shifts across the facility over the last 6 months. Projects for a variety of industries, ranging from kimberlite indicator minerals for the diamond sector to looking at the transformation of starch and proteins in seeds during feed processing, to examining nickel on air filters are on-going at the CLS and other synchrotrons.

The 8th Annual User's Meeting and Associated Workshops were held November 18-20 at the University of Saskatchewan. The meeting included workshops on: (1) Building Time Resolved Experimental Programs at the CLS; (2) Applications of Micro-Tomography in Science; (3) Pioneering Research in Plant Science Using Synchrotron Light; (4) Synchrotron Applications in Palaeontology and Archaeology. A prize (worth $1,000) was awarded for the best poster by a graduate student or postdoctoral fellow.

The Canadian eScience Workshop took place November 21-

22 at the University of Saskatchewan (see ***www.lightsource.ca/uac/escience/***). There are several ongoing initiatives both within synchrotrons and the wider scientific community to develop eScience systems which permit remote access to national and international scientific facilities. This workshop examined a recent eScience initiative being undertaken to provide remote access to synchrotrons and other national facilities, as well as the use of grid computing to support the programs hosted at these facilities. The use of Software Oriented Architecture (SOA), the CA4Net, and Websphere were emphasized.

ACA 2006: A session on Canadian Synchrotron Science and Instrumentation is planned for the Hawaii meeting, tentatively Wednesday morning July 26th"

C2 Neutron Powder Diffractometer, Chalk River: With the recent withdrawl of the NIST powder neutron diffractometer from their user program, the Canadian C2 neutron powder diffractometer in Chalk River, Ontario is now the only reactor-based powder neutron diffractometer available to the crystallographic community in North America; it is freely available to scientists (from both North and South America) publishing openly in the peer reviewed literature via a rolling peer review proposal system: ***neutron.nrc-cnrc.gc.ca/beamtime.html.***

Sixth Canadian Powder Diffraction Workshop, May 8-10, 2006 -The Workshop will be held at the University of Waterloo on the 8th to the 10th of May, 2006. It will cover basic powder diffraction, Rietveld analysis using GSAS, and Pair Distribution Function/Total Scattering Analysis. Lectures in the morning, hands on practical in the afternoon. A limited number of bursaries will be available for Canada and USA based students: ***/www.cins.ca/cpdw/.***

2006 Release of the Cambridge Structural Database -After serving as the Cambridge Crystallographic Data Centre's representative for the distribution of the Cambridge Structural Database to Canadian sites for many years, George Ferguson has now handed this task over to Kathryn E. Preuss of the University of Guelph Chemistry Department ***(preuss@uoguelph.ca).*** See also ***www.chembio.uoguelph.ca/preuss/PreussHomePage.htm.***

Member News -The first to respond to a request for news from Canadian members was ***Endel Aruja***, who reports that "I'm afraid I am out of physics for some time now and at 94 I am happy if I can understand some bits in the journal. Yours is the first letter I have seen from our rep at ACA and I think that some good may come from reminding the Canadian wing of ACA of its existence." Thanks Endel!

George Ferguson (University of Guelph) reports that "I am enjoying an "active" retirement as Editor of *Acta Cryst Section C* and am trying to find time to write up the large number of crystal structures which are maturing in my files."

Lee Groat

Selections from the Report of the Canadian Delegation to the XXth General Assembly of the IUCr, Florence, Italy, August 2005

The Canadian delegates were ***Louis Delbaere*** (Chair), ***Susanne Fortier*** (center), and ***Stan Cameron*** (left). The alternate was ***Lachlan Cranswick*** There were 62 delegates from 39 countries. As a category III member, Canada had three delegates, 4.8% of the total number. There were nine Canadians appointed to the 18 commissions and three major committees. Given that there are 129 commission members, Canadians are represented in excess of their expected proportion. In addition, one Canadian (***H.A. Dabkowska***) is the Chair of the Commission on Crystal Growth and Characterization of Materials and another Canadian (***I.D. Brown)*** was re-appointed as the chair of the Committee on the Maintenance of CIF Standards. ***George Ferguson*** is Editor in Chief of *Acta Cryst C* and there are four Canadian co-editors (out of ~120). There are currently no Canadian representatives on the executive. The Canadian National Committee will be proposing more Canadian names for membership of the commissions and will be attempting to persuade some commissions to adopt appropriate Canadians as consultants; this is often a first step to being appointed to the commission itself.

Substantial reports received from several countries concerning the history and activities of crystallography in that country have been published as major items in the *IUCr Newsletter* during the past three years. It was noted that that the CNC, in consultation with Canadian crystallographers, would be providing at least one such report to the *IUCr Newsletter* during the next triennium.

It was noted that ACA has established a "Latin-America Country" membership category. In early 2005 both Brazil and Argentina had asked to join this category. ***Louis Delbaere*** noted that the 2006 ACA conference would be held in Honolulu and he hoped to see members of the Asian Crystallographic Association in Hawaii. IUCr President Bill Duax then added that this time the ACA President's report had come from a Canadian, and that at some time in the future the ACA report could well be presented by a Brazilian or an Argentinian.

The Canadian National Committee for Crystallography has established a sub-committee to see if a bid to hold the 23rd Congress in Montreal in 2014 is possible. Since, in the general rotation of meetings through the regions of the IUCr, the 23rd congress should be held in North or South America, this suggestion was generally well received.

Stan Cameron

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XVII Meeting of the Brazilian Crystallographic Association

The 17th Meeting of the Brazilian Crystallographic Association (SBCr 2005) was held at the Campus of the National Synchrotron Light Source (LNLS) in Campinas, São Paulo, Brazil from 23-25 February, 2005. The scientific program included plenary lectures, invited lectures, oral communications and poster sessions. The third day of the meeting was dedicated to a symposium on the structure of polymers.

Several lecturers from abroad were invited for the occasion: ***Wim Brass*** (ESRF) opened the event with a lecture on "Scattering experiments of samples in extreme conditions." ***Katherine Kantardjieff***, (California State, Fullerton) presented a lecture on "Computational Molecular Modeling and Docking*: in-silico* experimentation to guide drug discovery and probe fundamental biochemistry." ***Bernhard Rupp*** (LLNL) talked about "Experimental and *in-silico* approaches to structure guided design of antimycobacterial drugs."

Invited lectures and oral presentations were grouped around the following subjects: biomolecules, small molecules, materials science, soft matter, powder methods, theory/ methods/instrumentation, teaching and history of crystallography. The

posters were organized around the same topics, and prizes were given to the best poster presentations.

The third day of the meeting was dedicated to a symposium on the structure of polymers. The participants were researchers from the physics and chemistry of soft materials. Especially invited for this occasion, ***Rufina Alamo*** (Florida State), presented a review of his important work on crystallization of poly(propylenes).

Interesting presentions by researchers from France, Argentina and Brazil were: "Correlated disorder in random block-copolymers" by ***Harry Westfahl*** (LNLS); "Crystallization of Poly(propylenes): The Role of Chain Microstructure" by ***Rufina, Alamo***; "A Powerful Tool for the Characterization of Polymers" by ***E.R. de Azevedo, , G.L. Mantovani and T.J Bonagamba,*** (IF-SC-USP); "Soft condensed matter experiments at the ESRF" by ***Wim Bras***; "Morphological Characterization of Polymer Blends" by ***Elias Hage Jr.*** (UFSCAR); "Self-assembling and Phase Behavior of Block Copolymer Melts and Solutions" by ***Daniel A. Vega*** (Univ. Nacional del Sur, Argentina); and "Novel Physical Properties of Polymers and Their Correlation with Morphological Structure" by ***Roberto Mendonça Faria*** (IF-SC, USP).

During this congress, the General Assembly of the SBCr dealt with matters that concern the Association and the local crystallographic community. Several proposals were discussed to improve interactions among crystallographers in Latin America. The affiliation of Brazil as a country member of the American Crystallographic Association was confirmed.

The 17th Meeting was attended by more than 130 participants. A total of 98 papers were presented. Eight participants from Latin American countries were awarded travel grants provided by the Brazilian National Research Council (CNPq - PROSUL program). The São Paulo Research Foundation (FAPESP) sponsored the meeting and covered expenses of three lecturers from abroad. After three days of very enthusiastic scientific interaction, the 17th Meeting of the SBCr left a very positive impression.

Photos: from top to bottom: - All participants at the meeting. crystallographers from Macelo, at the conference dinner and crystallographers from the state of Alagoas.

Iris L. Torriani - Presidente da SBCr

ACA Country Member Argentina: A one-day meeting of the newly formed Argentinean Crystallographic Association, held on September 30, 2005, included three plenary lectures. Iris Torriani (Campinas Synchrotron Faculty in Brazil), described the determination of the three-dimensional structure of the complex multidomain amyloid precursor protein by combining SAXS/WAXS data on the entire assembly with crystallographic and molecular modeling studies of individual components. Pedro Alzari (Pasture Institute in Paris, France) described structure functional relationships in the trypanosomal sialidases, a large family of multifunctional proteins responsible for diseases of relevance to South American countries. Pedro also described the plan now underway to establish a macromolecular crystallographic center in a new Pasture Institute in Montevido, Uruguay. Bill Duax described a monovalent cation transport through nanotubes formed by the d,l peptide gramacidin A. He discussed correlations, conflicts and ambiguities in the complexed and uncomplexed forms of the antibiotic in solid and solution as measured by x-ray and NMR techniques.

Twenty-two posters displayed around the lecture hall described the application of single crystal, powder and other scattering techniques to the study of inorganic, organic and pharmaceutical compounds and proteins. Authors of posters presented 10 minute talks at their poster in 4 sessions throughout the day. Four posters were selected to receive IUCr prizes.

Planning for the future:

SIGs: Six special interest groups were created; the subjects and the people responsible for each are: Donations – ***Daniel Vega***; Electron Microscopy – ***Alejandra Flores;*** Powder Diffraction – ***Gabriela Leyva***; Protein Structures – ***Gaston Paris;*** Small Angle Scattering – ***David Banchick***; and Crystal Growth – ***Griselda Polla.*** Anyone interested in participating should communicate with the coordinator of the chosen group. The aim is to exhange information and experiences, share equipment, discuss common needs, propose teaching courses, etc.

Committees: ACA Grant Committee (***Gaciela Punte, Griselda Narda , Guillermo Cozzi)*** and the Teaching Committee ***(Silvia Cuffini, Ricardo Baggio ,Oscar Piro***)

Future meetings: The AACr will organize a second meeting during the 2nd semester of 2006 (preferably in August), in Puerto Madryn. The organizing committee is composed of ***Miguel Harvey, Graciela Punte, Diego Lamas, Ricardo Baggio and Aurora Sagua.*** All those who want to help are welcomed.

It was asked that invited talks should deal not only with the specific subject of interest of the lecturer but also include a brief background of the techniques involved in the talk.

Membership dues: An annual payment of 50 pesos was decided for active members and of 25 pesos for students (named adherents). Any graduate or post-graduate student pursuing a degree in any university can be an adherent member.

Corporations are welcomed to become members, ahough it was not established how such membership will be accomplished as no legal inscription of the AACr has yet been completed.

Daniel Vega

Crystallography in Peru: IUCr Past Presidnent ***Bill Duax*** spent four days in Lima Peru where he gave presentations to 20 members of the faculty of San Marcos University (founded in 1551 by the Jesuits) including the director of International Relations, 20 members of the physics faculty, 100 undergraduate chemists, 100 undergraduate physicists, 65 undergraduate engineering students and the president of the Biophysics Society of Peru. While there he had the opportunity to talk with dozens of scientists at the Peruvian University of Cayetano Heredia, probably the most advanced and modern research institute in Peru. They are focused on the study of the structure and function of natural products and are keenly aware of the need for crystallographic capabilities in Peru to pursue their studies.

Armondo Perez, a young crystallographer at San Marcos University in Lima who studied for his PhD in Brazil with ***Iris Torriani*** and had a postdoc in Houston, organized the visit. Armondo organized a powder diffraction school for 40 people in Lima in March with no help from industry, the CCPD, the IUCr or the ACA. He is planning his next powder diffraction school in 2006. Bill promised to help him make the contacts he needs to secure support for future Schools of Crystallography in Peru.

Bill's formal presentations in Peru included descriptions of the programs of the IUCr and ACA, a talk on "Crystallography and the Nobel Prize" (delivered twice in Lima) and a talk on the crystallography of ion transport antibiotics. For the presentation to the Physics Department about the IUCr/ACA Latin American Initiative a translation was provided by Armondo that was very effective. Another staff member in the Physics Department provided a translation of the Nobel-related talk. (A copy of the text and slides were also published in a local newsletter).

There is excellent potential for Peru to form a Crystallographic Association that will strengthen its interdisciplinary research in the study of a wide range of mineral, plant, insect, aquatic, animal, bacterial and viral compounds that are unique to Peru. Just as there has been an avalanche of new structures coming from China and to a lesser extent from Malaysia and Turkey, the countries of South America possess untapped resources of structural diversity that can enrich all structural databases. Continuation of ACA efforts to increase our interactions with our Latin American neighbors will benefit all parties involved.

Crystallography in Chile: While in Chile, Bill visited five laboratories in three Universities, including Medical, Biochemical, Biophysics and Bioinformatics Departments where the need for and interest in macromolecular crystallographic analysis was expressed. His presentations ranged from individual interviews to informal discussions with small groups of staff and postdoctoral students. Discussions in each laboratory concerned ACA and IUCr programs and the merits of organizing a National Crystallographic Association that would improve the scientific infrastructure of the country.

The Physics Department of University of Chile has the most advanced crystallographic program in Chile. They provide single crystal and powder diffraction services to dozens of academics and industrial groups in Chile and Argentina. ***Maria Theresa*** heads the laboratory and ***Andres Ibanez*** is responsible for day-to-day operation of service crystallography. The department has a remarkable crystallographic history. In the 50's ***Martin Buerger*** hand delivered a precession camera to the department. He spent a month there while writing this classic book on the precession method. The book was typed on a remarkable "Siamese twin" typewriter (alphabet on the left, Greek and math symbols on the right joined by a common carriage). Bill's host in Chile, ***Oscar Whittke***, was present at the time of Buerger's visit and also recalled the visits from other prominent crystallographers of the day including ***Linus Pauling***. More recent visitors have included ***Tom Blundel and Mario Amzell.***

Excerpted from the IUCr Past Presidents report to the ACA Council and the USNCCr

John Kasper (1915-2005)

John Simon Kasper died peacefully on October 1, 2005 in Scotia NY. He was born in Newark, NJ on May 27, 1915, son of John F. Kasper and Josephine Naujalis Kasper. He earned his bachelor's degree in Chemistry in 1937 and his PhD in 1941, both from the Johns Hopkins University. John taught chemistry for a year at Washington University in St. Louis, MO and then worked on the Manhattan Project at Columbia University until the end of World War II. In October, 1945 he joined the General Electric Research Laboratory in Schenectady, NY, and worked there and at the GE Research and Development Center until he retired in 1980, although he continued as a consultant for GE for several years after that.

John (on the right) with two other past-presidents of the ACA: Walter Hamilton (President in '69) and Sidney Abrahams (Prsident in 1968)

John was a charter member and president of the ACA (in 1967, the year that ACA met in Atlanta and in Minneapolis). He was also on the USA organizing committee for the IUCr meeting in Stony Brook, NY in 1969. He edited, along with Kathleen Lonsdale, Volume II of the International Tables for X-ray Crystallography (Mathematical Tables).

Probably John's most important contribution to crystallography was that in order to solve the structure of decaborane ($B_{10}H_{14}$) he thought of using Cauchy Inequalities to get around the "phase problem" which had baffled crystallographers for 50 years. The result was that he and David Harker derived "Harker-Kasper Inequalities" (see the following note by Jenny Glusker).

John's research using x-ray diffraction spanned a wide range of materials: the structures of metals and intermetallic compounds, and unusual forms of many elements. Materials formed at very high pressures by Francis Bundy included artificially produced industrial diamonds that John was able to prove by their x-ray diffraction patterns to be true diamonds. Over a period of about 3 years John spent some time at the Brookhaven Laboratory using neutron diffraction to study antiferromagnetism. One of his great pleasures was that for many years he had graduate students working with him on their research projects. They were mostly from Rensselaer Polytechnic Institute in Troy, NY, but some also came from the State University of New York at Albany.

On leave from GE in 1957 he was a visiting professor at the University of Bristol, England, where he worked with F. Charles Frank on complex alloys and their closest packing. In 1975-76 he was visiting professor at the Université de Bordeaux, France, in the department headed by Paul Hagenmuller, working principally with Roger Naslain along with Michel Pouchard, Christian Cros, Jean Etourneau, Jean Michel Quinnisset and others in the study of composite materials. John's collaboration with that group of French scientists continued from the mid 1960's until the time that he retired. Patrick Cassoux of the Université de Toulouse, France, spent some months at GE and John enjoyed working with him.

John was a wonderful person with great patience and a twinkle in his eye and a great sense of humor. He delighted in his children and grandchildren. He played a social game of golf to relax and loved to play bridge. He was a good musician and continued to enjoy classical music even after his stroke approximately 10 years ago. Even after the stroke he retained some long term memory so that we were able to recall many happy past occasions

He is survived by his wife, Charlys Lucht Kasper, whom he married in 1951, his daughter, Marion O'Keefe and granddaughter Colleen O'Keefe, a son, Robert Kasper (wife Theresa), 3 grandsons; David, Daniel and Joseph Kasper, granddaughter, Colleen Belharrat, grandson, Timothy Kasper and 2 great grandsons. His older son, Frederick, died in 2000.

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Charlys Kasper

Harker - Kasper Inequalities

John Kasper's contribution to phase determination in x-ray diffraction studies is described in two important papers, both with his colleague David Harker and the second also with his future wife, Charlys Lucht. The main article entitled "Phases of Fourier Coefficients Directly from Crystal Diffraction Data" by D. Harker and J. S. Kasper (*J. Chem. Phys.* 15: 882-884, 1947; *Acta Cryst.* 1: 70-75, 1948) is short but very significant. The authors were at General Electric Company, Schenectady. New York. They pointed out that one can measure intensities but not

relative phases of diffracted x-ray beams (the "phase problem") but that they had found a way to help solve this problem. They used "unitary atomic-structure factors," $U_{hkl} = (F_{hkl})/f$, where F is a structure factor and f represents scattering factor(s). By application of "Cauchy's inequality" they found $|U_{hkl}|^2$ is less than or equal to unity. [Cauchy's inequality is $(\Sigma ab)^2 < \Sigma a^2 \Sigma b^2$, unless a and b are proportional to each other. The corresponding inequality for integrals is due to Schwarz and Buniakowsky.] Harker and Kasper showed that if the crystal has a center of symmetry then $U_{2h,2k,2l}$ is probably positive or zero (phase angle of 0 degrees) if the absolute value of U^2_{hkl} is greater than or equal to one half. Several other relationships arising from further symmetry were then identified by them. Harker-Kasper inequalities are considered to be based on the non-negativity of the electron-density function.

John described this discovery with Dave Harker as follows: "I became intrigued with the fact that the straightforward squaring of a real structure factor, F_{hkl} (with cosine terms) contained, in part, the sum of modified cosine squared terms. These latter could be rewritten, by virtue of the relation $2\cos^2 A = 1 + \cos 2A$ as components of $F_{2h,2k,2l}$. A relation then exists between F^2_{hkl} and $F_{2h,2k,2l}$, but also with the summation of cross terms. I did not know what to do with the cross terms and so I put the thing aside. Some days later (in 1947) it occurred to me that Schwarz's inequality would deal only with the desirable summation of cosine^2 terms. Accordingly, one morning at work I wrote down the relationship between F^2_{hkl} and $F_{2h,2k,2l}$ resulting from the application of Schwarz's inequality. No sooner had I written this down, when Dave walked in the office and looked over my shoulder. "What is that?" Dave asked. "That is the result of applying Schwarz's inequality to a structure factor," I replied. After satisfying himself that what I had written was correct, Dave became quite excited and remarked: "You can determine signs with that." "That's right," I replied." Charlys shared the excitement of the moment, writing: "It was an event one doesn't forget."

Dave suggested using the unitary atomic structure factor . This enabled treatment of more general situations. John continued "For the next few weeks Dave was immersed in the applications to various symmetries and space groups, and other ramifications, such as sum and difference formulas. He also produced an elegant write up of the work. I concentrated on its application to the Decaborane problem which was uppermost in our minds."

The method was first applied to the crystal structure of decaborane, $B_{10}H_{14}$, a small molecule of unknown structural formula, space group *Pnnm* (J. S. Kasper, C. M. Lucht and D. Harker, "The Crystal Structure of Decaborane, $B_{10}H_{14}$." *Acta Cryst.* 3: 436-455 (1950)). Robinson Burbank described the work in his 1976 ACA past-presidential address. He had heard the report on the determination of the crystal structure of decaborane by Kasper, Lucht and Harker at a meeting in 1948 and wrote: "As luck would have it they had unknowingly chosen the most intractable problem in the entire field of boron hydrides. They had been bedeviled by micro twinning, high specimen volatility, and a host of other technical difficulties. More importantly, the entire structural concept of the boron hydrides was dead wrong! This meant that every conceivable model that might be postulated was doomed to failure. Finally, in desperation John turned back to the phase problem and in a moment of inspiration discovered that it was possible to deduce something about the signs of the structure factors using the Schwarz inequality. David pounced on this breakthrough and it was rapidly developed into the tool that solved the decaborane structure. The open clam shell configuration defined by an incompleted icosahedron is now in freshman chemistry books but until that paper, it had never penetrated the mind of man." The authors derived many inequalities, based on symmetry elements of the space group of decaborane. In addition, it was necessary in several cases to add or subtact two U's before applying Cauchy's inequality ("addition-subtraction" relations). In the years that followed many crystallographers used Harker-Kasper inequalities to help solve structures until the now commonly used "direct methods", partly inspired by this work, were developed.

Jenny Glusker

Second Max Perutz Prize - Call for Nominations

The European Crystallographic Association (ECA) invites nominations for the second Max Perutz European Crystallographic Association Prize to recognize a significant achievement or discovery in crystallography in the past 5-10 years. Nominees should be affiliated or identified with the European crystallographic community, as broadly defined in the charter of the ECA (see the ECA-news site: www.ecanews.org) The prize, including a monetary award and certificate of recognition, will be awarded at the opening ceremony of the 23rd European Crystallography Meeting (ECM-23) to be held in Leuven, Belgium, 6-11 August 2005.

The previous laureates are:

2000 (1st ECA Prize) Ada Yonath

2001 (2nd ECA Prize) Jochen R. Schneider

2003 (3rd ECA Prize) Carmelo Giacovazzo

2004 (1st Max Perutz ECA Prize) George M. Sheldrick

Nominations for the prize should include a statement of the contribution for which the prize is to be awarded and, if possible, a short cv of the nominee. They should be sent by e-mail or by regular mail postmarked no later than ***February 28, 2005*** to: Anders Liljas, Molecular Biophysics, Center for Chemistry and Chemical Engineering, Lund University, Box 124, SE-221 00 Lund, Sweden Fax: +46-46-222 46 92
e-mail: ***anders.liljas@mbfys.lu.se***

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Macromolecular Structure Validation

From left to right: Kim Henrick, Jorg Hendle, Bernhard Rupp, Roberto Steiner, Kyle Burkhardt, Jane Richardson, Dave Richardson and Duncan McRee.

Complementing the CCP4 workshop and Gerard Kleywegt's presentation in the Patterson Award session, this workshop, organized by ***Bernhard Rupp*** and ***Katherine Kantardjieff***, expanded on the theory and practice of macromolecular structure validation. Given the excellent tools now available, it is becoming easier to deposit well validated, consistently prepared structure coordinate files that are practically free of model building errors and do not contain formal or nuisance errors. ***Roberto Steiner*** and ***Bernhard Rupp*** provided foundations of refinement theory, explaining the origins and sources of errors that make validation necessary. ***Kyle Burkhart*** from the RCSB PDB presented highlights of the automated *ADIT* deposition and validation tools, and ***Kim Henrick*** from the EBI-MSD demonstrated services to determine the proper oligomeric state or quaternary structure assembly from PDB files, which is not always a trivial task. ***Jörg Hendle*** from SGX presented his comprehensive, data base linked, industrial strength protein and ligand validation suite, ***Validate***. In the afternoon hands-on sessions, ***Jane and David Richardson*** worked with students on their atom clash detection and validation program, ***Molprobity***, which is largely integrated in ***MI-Fit***, the successor of ***XtalView/Xfit***, written and presented by ***Duncan McRee***.

Bernhard Rupp

CCP4 "A Protein Crystallographic Toolbox"

CCP4 (Collaborative Computational Project No.4) is a UK initiative based at CCLRC Daresbury Laboratory. It provides a suite of programs used for macromolecular structure determination by x-ray crystallography. The objective of the workshop was not to teach crystallography but rather to show the students how to use some of the key programs distributed with the CCP4 package to process their data and solve their structures. The format included presentations by both software developers and expert users from the UK and Europe to give presentations on different aspects of the software.

The workshop attracted over fifty delegates ranging from graduate students to experienced crystallographers having differing levels of familiarity with the software. Coupled with the breadth of the CCP4 suite, which goes from data processing to structure validation, this was a challenging workshop for delegates and speakers alike.

The first session concentrated on giving a broad overview of the CCP4 suite, intended for novice users and to lay the foundation for the later talks. ***Peter Briggs*** outlined many of the technical non-crystallographic aspects of the software, including the graphical user interface CCP4i and the gory details of MTZ files. ***Johan Turkenburg*** used a number of real-life examples in his tour of the crystallographic functionality of the suite from a user perspective, introducing a number of programs which even some more experienced users might be unfamiliar with, and also stressing the compatibility between CCP4 and other software suites such as SHELX and ARP/wARP. ***Maria Turkenburg*** then gave an overview of the broad range of technical and scientific help available in the CCP4 suite and the website.

Back Row: Peter Briggs, Roberto Steiner, Maria Turkenberg, and Stuart McNicholas. Front Row: Johan Turkenberg, Harry Powell and Paul Emsley.

The remaining sessions focused on practical aspects of running some of the flagship programs. ***Harry Powell*** talked in detail about data processing, integration and scaling using MOSFLM and SCALA, focusing in particular on practical aspects such as how to tell if your data processing is working, and how to address warnings and problem cases – something that many people found extremely useful. ***Roberto Steiner*** covered the background theory for REFMAC5 and gave a live demonstration of various features such as the use of TLS parameters and the generation of restraints dictionaries – both key to getting the best from your refinement.

Finally demonstrations were given by ***Stuart McNicholas*** and ***Paul Emsley*** of the two aspects of CCP4's molecular graphics project, CCP4MG and Coot respectively. The former currently focuses on providing presentation-quality representations of molecular models, while the latter is a platform for powerful model building tools. The entertaining "double-headed" demonstration of Coot was particularly popular, generating "oohs" and "aahs" from a rapt audience as they watched side chains wriggle their way into the correct density.

Feedback from the workshop was very positive, with many people reporting that they found the presentations helpful and that they would be trying out the software afterwards – something that was borne out by the people who visited the CCP4 exhibition booth after the workshop. There were also requests

for a longer workshop with more hands-on demonstrations and more examples of real-life problems, things which we will aim to address in future.

The workshop organizers ***Maeri Howard and Peter Briggs*** wish to thank the ACA for the opportunity to run the workshop, the speakers for their presentations and the delegates for attending. We also wish to acknowledge the help of ***Ed Collins and Marcia Colquhoun*** in setting up the workshop. Financial support for the workshop was provided by CCLRC (from CCP4 industrial income) and by the ACA.

Finally, the materials from the workshop can be found online at ***www.ccp4.ac.uk/courses/ACA2005/ACAworkshop05.html.***

Peter Briggs

Young Scientist Special Interest Group Meeting Report

The YSSIG is grateful for the continued support of the ACA community; special thanks to ***Marcia Colquhoun, Khalil Abboud, and Tom Selby*** for fantastic event planning assistance. YS-SIG Events in Orlando included:

Mixer: It was held at the Lake Terrace, Swan Hotel with an estimated attendance of around 200. Nextal Biotechnologies helped sponsor the mixer. The event was very successful and Nextal Biotech, equally pleased, has agreed to participate at next year's meeting.

Mentor-Mentee Dinner: The dinner was held at Disney's Rainforest Café. 60 people participated (20 mentors) and as can be seen in the photos below a good time was had by one and all. Due primarily to limited choice of venue, this year's dinner was quite a bit more expensive than usual cost of approximately one thousand dollars. We expect to substantially reduce the cost per head at next year's meeting. We are also considering changing the event to a breakfast or lunch.

YSSIG Session: Chandra Patel chaired the session that had an attendance of ~75 people. The session was reviewed in the fall issue of the *ACA Newsletter.*

YSSIG Business Meeting: It was held immediately after the YSSIG day session and was attended by 20 people (a record number indeed!).

Session chairs for the 2006 meeting will be ***Peter Horanyi, and Ashwini Nadkarni*** (both from UGA).

Chad A. Haynes, YS-SIG Chair 2005

Each year the ACA uses funds raised from a number of sources to support the travel of young scientists to attend the annual meeting. These are their stories.

I would like to thank the ACA for the travel grant to present my research in Orlando. This was my first ACA conference, and it was very informative and enjoyable. The poster session provided an excellent platform to discuss and exchange ideas with other scientists in a relaxed atmosphere. As a result, I received many helpful suggestions concerning my research.

In addition to the poster sessions, there were many presentations of interest to me. I particularly enjoyed the session on "Difficult Structures" because it reminded me that, although a problem may seem insurmountable, with continued effort a solution can be found. "New Horizons in Structure-Based Drug Design" was also an excellent session. Although I do not work in drug design, I have always been fascinated with this subject. This session inadvertently gave me insights and ideas regarding my own research. I also attended many talks on the practical aspects of protein crystallography, such as the talks about new software and improvements to current software. I had the opportunity to discuss my problems with the people who actually develop the software, which was an invaluable experience. Hence, I once again would like to express my gratitude to the ACA for making this experience possible. As a first time attendee and someone new to the field, the meeting exceeded my expectations. I felt welcome and accepted into a close-knit community of crystallographers who were enthusiastic about helping a novice.

Miranda Byrne

I would like to take this opportunity to express my sincerest gratitude to the organizers of the Orlando meeting for the opportunity to attend and present my research. This was my first attendance at an ACA meeting and I was thrilled to be able to present my research both in poster format and as an invited speaker. I am particularly grateful to the selection committee for the RCSB Protein Data Bank Poster Prize for the honor of being an award recipient.

I wish to offer my appreciation to Chad Haynes for the invitation to speak at this year's meeting. I would also like to offer my congratulations to the other speakers in this session on their accomplishments. I was very impressed with the quality and depth of research exhibited in this session, as well as throughout the three poster sessions.

I found many of the sessions to be of tremendous interest and have taken many suggestions and tips home with me to apply to my ongoing research. I was able to attend the presentations of many giants in our field whose tireless efforts have facilitated macromolecular structure determination and refinement beyond measure. I look forward to attending many more ACA meetings in the future and again offer my deepest thanks for my selection to be a travel award recipient

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Melanie Adams

I would like to thank the ACA for giving me the opportunity to attend ACA 2005 and to present my work to an international audience. This was my first ACA meeting and I found it to be very beneficial and informative. I had a tremendous opportunity to talk and discuss different topics with other young scientists as well as with several leading scientists in protein crystallography. I am glad that I was able to listen to interesting talks, especially the ones included in the Patterson Award Symposium. Unfortunately, at the same time another interesting session ("Topics of Interest to the Young Scientist") was running in parallel, so I didn't have a chance to hear it. The poster sessions allowed me to gain useful tips and encouraging remarks on my research. Also, I really liked the idea of a Young Scientist mixer because it facilitated networking between upcoming fellow scientists.

Overall, I really enjoyed this meeting and I am grateful to the ACA for its generous support. I would also like to thank Dr. Walter Keller, who is both my mentor and a co-author on the work I presented, for his continuous support, patience and encouragement. I am looking forward to attending again next year.

Tea Pavkov

I would like to thank the ACA for the travel grant that allowed me to attend the Orlando meeting. It was my first ACA meeting and it was a great opportunity to present my work to a varied and international scientific audience. In my research work on crystallographic studies

of enzymes, I am using a combination of high resolution neutron and atomic resolution x-ray analysis. I enjoyed the fruitful discussions, valuable comments and suggestions at the poster session. The different poster sessions were an excellent opportunity to establish contacts with scientists of wide-ranging interests. The scientific program of the meeting was excellent, with a great variety of topics and a high level of research. I really enjoyed this meeting and I am grateful to the ACA for its generous support.

Flora Meilleur

I would like to extend my gratitude to the ACA for providing funding which allowed me to attend the great conference in Orlando. As this was my first ACA meeting, it was a pleasure to finally meet so many of the names I have read about in the literature in the area of x-ray crystallography. On the academic front, attendance by both well established and young scientists provided for an interesting environment in which to learn about new techniques and 'tried and tested' methodologies. In addition, the industry sponsored exhibit was an excellent resource for learning about new advancements in the areas of crystal mounting, data collection, and solution refinement which are currently being developed.

As research in the Shimizu lab is focused primarily on the self-assembly of small molecules into extended networks, it was particularly nice to see symposia dedicated to research in crystal engineering. I would like to thank the coordinators of all the symposia for their time and efforts in organizing such an interesting series of presentations. As I am nearing the end of my Ph.D. studies, it was an excellent opportunity to meet and talk with potential post-doctoral supervisors and I hope that I will get the chance to continue relations at future ACA meetings.

Lastly, I would like to thank The *Journal of Chemical Crystallography* for their generous poster prize and the numerous judges for their time donated to reviewing the great research being done by young scientists.

Sean Dalrymple

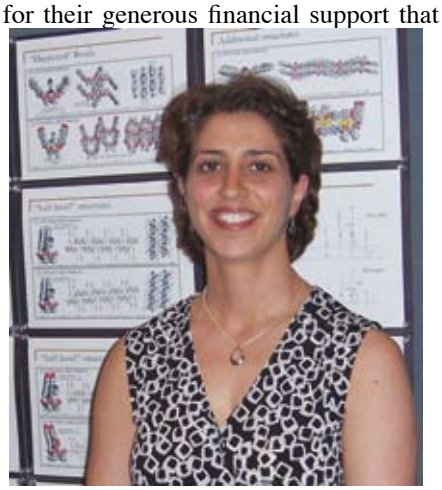
Many thanks to the ACA for awarding a travel grant to me for the 2005 meeting. I enjoyed listening to the various seminars and am in awe of the amazing discoveries being made in our field. Michael Rossman's movie of the T4 bacteriophage infection has forever changed the way I will think about viral infection. Drug design is my particular interest. I was impress by Tom Blundell who gave an inspiring opening seminar to this year's session on structure-based drug discovery. Using chromium radiation to collect anomalous data is a new crystallographic technique I learned about at ACA. Paul Emsley dazzled everyone with his model-building program, Coot, which has been implemented in our lab and makes model-building a breeze.

The meeting's location was excellent and the facilities were beautiful. My stay in the Swan Hotel exceeded my expectations. Although we didn't venture out into Walt Disney World, both Goofy and Pluto stopped by to say hello during dinner at Gulliver's and we could see the fireworks from the Magic Kingdom's nightly parades.

The ACA meeting helped me to put faces with names and provided many enjoyable opportunities to interact with other crystallographers and vendors. I am most grateful for the opportunity to tell others about my research at the poster session and learn from others about their research. I am looking forward to all the new discoveries and seeing everyone in Hawaii in 2006.

Tommi White

I would like to sincerely thank the American Crystallography Association for their generous financial support that

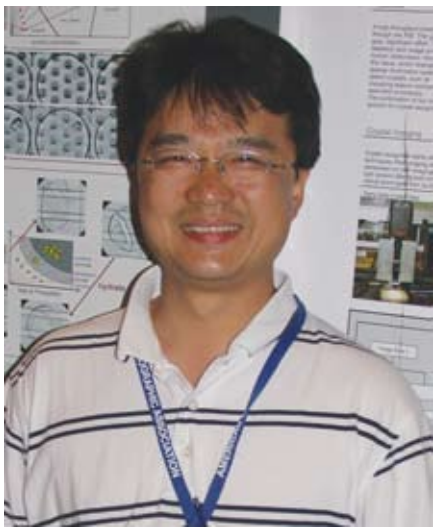


facilitated my attendance at the 2005 annual meeting. Even though I have attended a number of meetings, nationally and internationally, this was my first ACA meeting. The organizers have done a wonderful job all around. The quality of the talks was world class and I was glad to have the opportunity to interact with

a number of outstanding scientists. The crystal engineering and metal-organic symposia were particularly stimulating as the presenters highlighted some wonderful results. A wide range of interesting topics was presented, which provided some great forums for discussion. The poster session was equally superb and I had some interesting discussions with a number of people that provided invaluable comments and suggestions. The fabulous location of the meeting was particularly attractive as it facilitated our leisure time as well. Thank you ACA for the opportunity to attend the meeting and present my work.

Heba Abourahama

I would like to thank the ACA for giving me the travel grant and a chance to present a poster in Orlando. I presented "The Phase Chip: High Throughput Screening with Microfluidics." As can be seen from the title, it is very hard to meet other people who are working on similar research because it is a new born research area. The ACA meeting gave me very nice opportunities to meet other people working in research institutes and industries. It was a great experience to share some very recent information and behind the scenes stories.



I also found the meeting was very fruitful and informative. During my poster session I was asked many useful questions and received encouraging comments about my research project. Also, I enjoyed the "Topics of Interest to the Young Scientist" which was particularly designed for graduate students and post-docs to provide information about their future careers. The meeting took place on Walt Disney World. which provides lots of really good places to look around. I enjoyed them at night as well.

I really appreciate the support from the ACA, which made my travel possible.

Jung-uk Shim

I would like to thank the ACA for their generous support which allowed me to travel to the annual meeting. It was a wonderful to be in the presence of

crystallographers with more experience. I was able to learn a lot from the talks that I attended as well as from being able to talk to speakers and exhibitors. The meeting allowed me to expand my knowledge of small molecule crystallography and also enhance my limited knowledge of protein crystallography. I want to thank the ACA for this opportunity and I look forward to future meetings.

Lauren Borkowski

I would like to thank the ACA for awarding me a student travel grant. The grant enabled me to attend ACA 2005 and to present my research work to a wide audience. The conference also gave me the opportunity to meet researchers from different parts of the world whom I had only known from discussion boards but had never actually met in person. It was very inspiring to listen to the research of more experienced and famous crystallographers. The sessions on "New Structures", "Difficult Structures", "Structure-Based Drug Design" and "Biomolecules and Membrane proteins" were very informative and interesting. Being a graduate student who is about to graduate, my poster session provided me with the opportunity to make new contacts and meet possible future research partners. Overall, attending the ACA annual meeting

was a great experience both academically and socially and I thank the ACA for their generous support.

Akanksha Nagpal

I would like to thank the ACA for the generous funding for the 2005 meeting. It was an exciting experience and has a special meaning to me. It was my first time to attend the ACA meeting, first time to present a talk before experts from all over the world, first time to win an award, and first time to the magic of Disney World.

As a second year graduate student, I have just started my journey into the exciting field of crystallography. I was so lucky to get the great opportunity to present a talk entitled "Structure of an Antimicrobial Compound in Complex with AT-rich DNA Decamer at 0.95Å Resolution" in the "Ultra-high Resolution Structures" session and to receive a Margaret C. Etter Student Lecturer Award (Great thanks to the Synchrotron Radiation SIG). For a beginner, this experience was a wonderful gift and a great encouragement.

This meeting also provided me precious opportunities to listen to interesting talks, watch cool program demos, see attractive posters, and talk with other young scientists as well as several leading scientists in the field. I enjoyed most of the sessions I attended, especially the "New Structures", and "Difficult Structures" session, and the Patterson Award Symposium. It was truly a pity that I could only attend part of the sessions since they overlapped. These cutting-edge talks greatly opened my horizons and attracted me more than ever to the fantastic three-dimensional world of protein crystallography. Besides learning technologies and gaining knowledge from the talks, I was also inspired by the great stories behind some talks and by the spirit of scientific research.

Thank again to the organizers for their hard efforts and the wonderful meeting. Hope to meet you again in the near future.

Yuan Lin

First, I would like to thank the ACA for giving me the opportunity to present my work in Orlando. This was my first attendance at a major crystallographic meeting and I really enjoyed the wide variety of topics presented.

As a postdoc in fiber diffraction, I particularly liked the session on "Advances in Neutron Fiber Diffraction". This provided me the opportunity to interact with other fiber diffractionists as well as crystallographers, and to make connections with them. I appreciated all of the helpful and encouraging comments. The poster sessions were also of high quality and allowed me to continue interesting discussions about my research.

Finally, I would like to thank the ACA for providing funds that allowed me to attend to this unforgettable meeting.

Ingrid Parrot

This was my third ACA meeting and I very much enjoyed it although it was a busy one! I was delighted to have the opportunity to present some of my work on radiation induced redox changes during x-ray data collection in a great session chaired by Keith Moffat. I also gained valuable experience chairing the Margaret C. Etter Early Career Award Symposium in which it was really exciting to have several graduate student and postdoc presenters. One of the nice things about chairing a session is that you get to pick really interesting abstracts and all the talks were as good as I had hoped.

Other highlights this year included the YSSIG session and social events, especially as, unlike last year, I hadn't had to organize them! The pool-side party was particularly enjoyable and has me looking forward to next year in Hawaii!

One of my favorite things about the ACA meeting is being able to catch up with friends and colleagues and this year was no exception. It was fantastic to hear about their latest work and plans for the future. So, many thanks to the ACA for providing me with a travel award which enabled me to attend.

Arwen Pearson

First of all, I would like to thank the ACA for the travel grant that allowed me to attend the Orlando meeting. Attending a meeting with close to 1000 participants working in areas closely related to mine has always been of great interest for me. The atmosphere at ACA was wonderful for presentation of scientific results. I presented a talk on "A thiamine diphosphate-dependent enzyme with a small product trapped in the active site" in the 'Interesting Structures and Computing Techniques' session. It was very beneficial to me to hear the comments and suggestions about my work from the learned audience. I enjoyed the friendly atmosphere of the meeting as fellow researchers were excited to exchange ideas and were eager to discuss their work-past, present and future.

The sessions at the meeting were incredible and many days were difficult to schedule due to concurrent sessions on very interesting topics. I found the sessions on new structures, difficult structures, ultra high resolution structures, and time-resolved diffraction extremely interesting. Some of the talks in other sessions were also of interest to me even though they are not related to my research area.

I sincerely appreciate the efforts that went into organizing the "Topics of Interest to the Young Scientist" session. The speakers offered important tips on career development, and the future of science publishing. I also enjoyed the topics of many fantastic posters and the latest instrumentations exhibited by vendors. Thanks once again to the organizers for their efforts and hard work. Overall, it was been academically a stimulating and motivating experience.

Asim K. Bera

I'd like to thank the ACA for providing me with the travel bursary that allowed me to attend the meeting in Orlando. My father always told me that if I applied myself to science, I would go to great places and meet important people. I bet he

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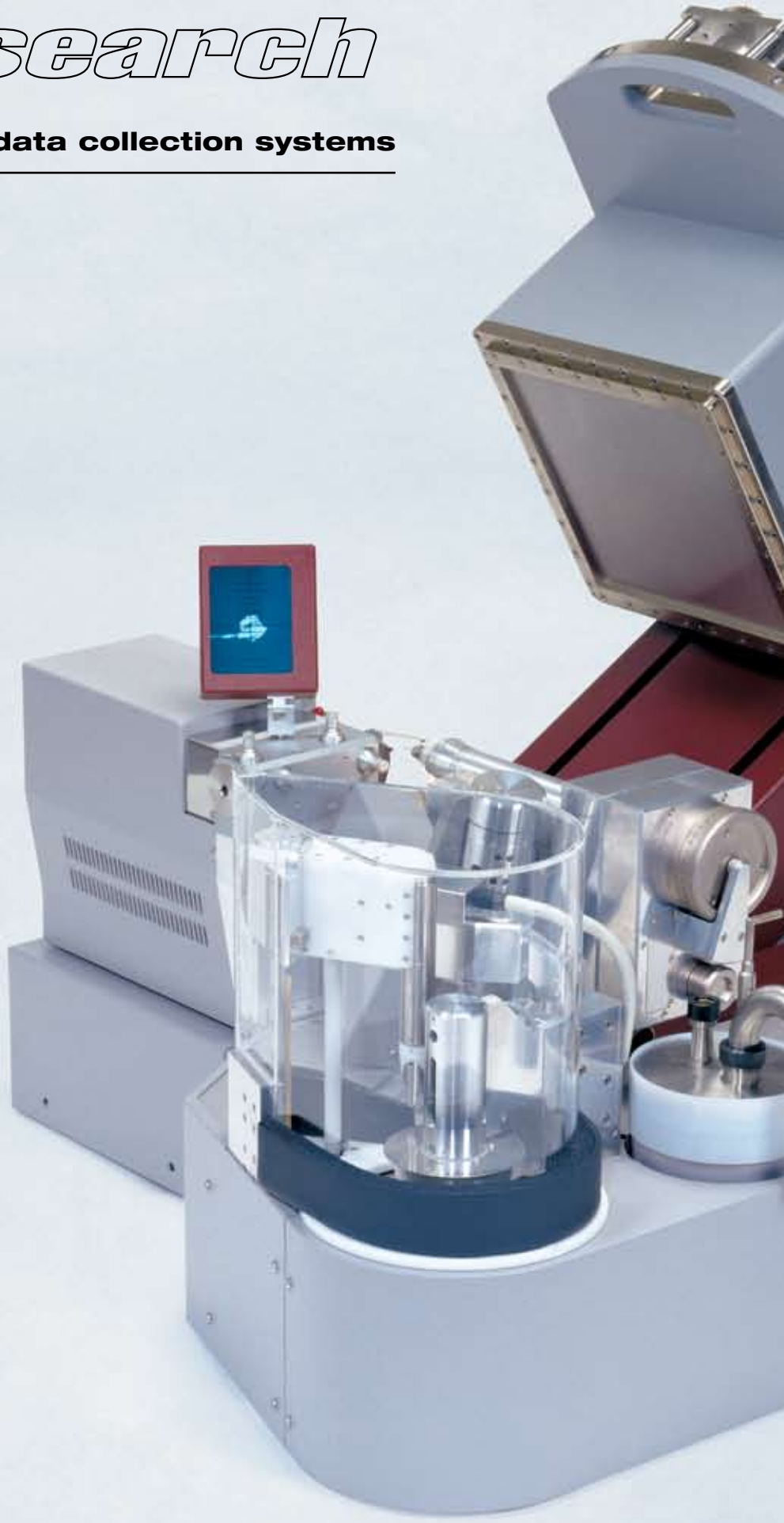

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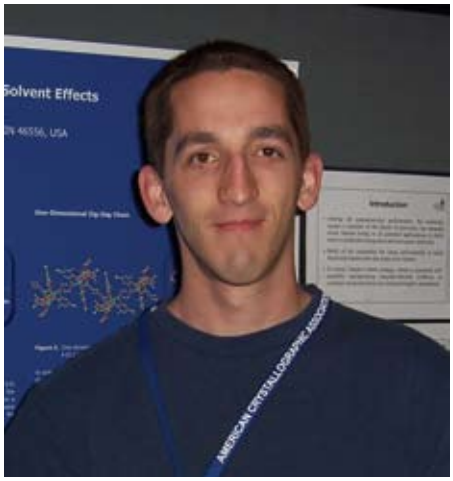
never imagined the zenith of my research would be a trip to Disney World to meet Mickey Mouse! Aside from the inevitable trips to the fun parks, there was also a little spare time to squeeze in a bit of chemistry. All of the sessions I attended covered interesting topics and were well attended. Of particular relevance to my own research were the "Microporous Metal Organic Framework" symposia. As the recipient of a 2005 Margaret C. Etter Student Lecturer Award I had the opportunity to give an oral presentation of my work to some of the leading luminaries in the field. The evening poster sessions were a great opportunity to meet other graduate students and also talk to the experts on a less formal footing. Additionally, the vendor exhibitions were a welcome distraction that gave an eye opening insight into the state of the art equipment currently available.



All things considered, I had an excellent time and would thoroughly recommend the event to any student interested in the solid state.

Dugald MacDougall

I would like to thank the ACA for the travel grant that allowed me to come to Orlando. It was my first ACA meeting and also my first time in the USA.

It was an amazing time. I met lots of people and shared many good experiences. The conference gave me a fantastic opportunity to talk with other young scientists as well as with several leading scientists in the crystallographic field. I have just finished my PhD. I also had the opportunity at this meeting to present my work in an oral talk as well as in a poster session.

All of the sessions I attended were very interesting and informative. Of course, the magical Walt Disney World ambience gave a particular taste for the 2005 ACA meeting. In this way, I came back to Brazil with lots of good memories and new ideas.

Once again, I really enjoyed this meeting and I am grateful to the ACA for its generous support, which made my participation possible at this wonderful event.

Cristiano Oliveira

I would like to express my gratitude to the ACA, organizers, and sponsors for the opportunity to attend the 2005 meeting in Orlando. It was with this travel award

that I was able to attend my first ACA meeting. The meeting hosted a large and diverse number of professionals and it was a privilege to present my work to such an audience as an oral presentation. In addition to the many useful conversations I had with numerous attendees of the conference and the excellent feedback I received, I also learned about new crystallographic techniques, handling methods, and synthetic preparations of single crystals. The poster sessions were also excellent as I learned a great deal of new information particularly in the field of protein crystallography. The exhibition also proved to be a valuable event as I had the opportunity to discuss new advancements, hardware, and equipment with numerous engineers and sales representatives. On the whole this was an excellent conference with impressive representation from a multinational audience. In addition to the excellent organization and superb mixers, the venue in the Walt Disney Swan resort was beautiful and enjoyable. I met with many fun, exciting, and interesting people throughout the conference and am grateful for the opportunity to have done so.

Brett Chandler

I would like to thank the organizers of the 2005 ACA meeting for giving me the opportunity to attend and present my work to the international audience.

I presented a poster of my research entitled "Ultra-high Resolution Protein Crystallography & Electrostatic Interaction Energies Computation." This was my first ACA meeting and I found the meeting very beneficial and informative. The variety and quantity of posters was incredible. The poster sessions allowed me to gain useful and encouraging remarks on my research. The meeting allowed me to interact with many interesting people, and to keep contact with some of them.

Thanks again to the organizers for their efforts and hard work on this well arranged meeting. The Mentor/Mentee mixer and dinner and the banquet added a pleasant touch to the meeting. These dinners gave me a tremendous opportunity to talk with other young scientists in the crystallography field.

The organization and scientific program of the meeting was excellent. I particularly

liked the "Biological Macromolecules" session. Sessions such as "New Horizons in Structure-based Drug Design", "Structural and Bioinformatics Approaches to Evolution" and "Ultra-high Resolution Structures" were very interesting.

My attendance and participation at the meeting was made possible by a generous travel grant from the ACA and the International Union of Crystallography. The meeting was an enriching experience and I would like to convey my sincerest appreciation to the ACA and the IUCr for their generosity.

Angelique Lagoutte

The USNCCr used funds left over from the 1996 IUCr Congress in Seattle to support travel to the Congress in Florence for 31 young scientists studying and working in the US. Several sent comments on their experiences:

I wish to express my gratitude to the USNCCr for financial support to attend the IUCr congress. It was an invaluable opportunity to present my work and interact with colleagues that would not have happened without their assistance.

The sessions at the meeting were incredible, and many days were difficult to schedule due to concurrent sessions on very interesting topics. Portions of the conference that I found intriguing and helpful included the current state of structural genomics, new refinement and molecular replacement strategies, crystal growth and handling techniques, complementary approaches and the interplay of EM and crystallography, time resolved diffraction experiments, and information on crystallographic teaching (including many helpful pointers and web addresses).

There were also excellent keynote speakers, in particular David Sayre on single particle diffraction (shortly followed by D. Shapiro), Michael Parker on pore-forming toxins, Janet Smith on cytochrome b6f, Gerhard Klebe on probing and cataloging cavities in proteins and Harry Kroto on fullerenes, which was particularly welcomed as I am working on virus capsid structures, which are essentially protein fullerenes.

The setting for the meeting was wonderful and allowed us to experience some of the culture of Italy. While we never made it to the Uffizi, we were enthralled by the statue of David at the Galleria Accademia and various scientific "artifacts" including Galileo's telescopes at the Museo di Storia della Scienza. In the evenings there was time to catch up with colleagues and friends and share superb local wine and food. Overall, while the meeting was very demanding it was also very rewarding, and I am grateful to the USNCCr for this opportunity.

Christina Bourne

I am a third-year PhD graduate student at SUNY Stony Brook, and am working with Prof. Clare P. Grey in the Chemistry Department on the crystal structures of cathode materials for Li ion batteries.

I would like to thank the USNCCr for their generous support in assisting me to attend the XX IUCr Congress in Florence. I had the opportunity to give my first oral presentation at a conference and it was an unforgettable experience. The remarks and comments following my talk will be extremely useful for the end of my PhD studies. In addition to hearing many excellent talks and posters in so many different interesting research areas (it was often hard to choose which talk to attend at a particular time), I renewed old friendships and created new ones. This conference was of course a great opportunity to discuss my work with current leading researchers in the field of crystallography and to learn new state-of-the-art techniques and synthetic methods. I was inspired in so many ways by these discussions and came back with a lot of memories from the conference and the beautiful Tuscany region. Thanks again to my advisor, the IUCr organization committee, and the USNCCr for this great opportunity.

Julien Bréger

The XX IUCr Congress in Florence has been for me a great experience. Not only because of the location (of course, Florence and the beautiful landscape of the Tuscany countryside did play an important role), but also because of the high quality of both the scientific program and the social events. Even though my main interest lies in crystallography of biological macromolecules, I was

really fascinated by discovering that crystallography can be applied to so many different fields, of which microsymposia such as "Crystallography and Cultural Heritage", and "Crystallography and Art" were good examples. This meeting gave me the opportunity to learn new

techniques, to talk to experts in the field and to discuss my data with them and get helpful suggestions.

I really want to thank the USNCCr for awarding me the travel grant which allowed me to participate in such a scientifically and culturally stimulating conference.

Barbara Calamini

I greatly appreciate the travel award granted by the USNCCr which made my attendance at the IUCr meeting in Florence, Italy possible. This was the first international meeting I have attended. It opened my eyes to the extensive use of the field of crystallography all over the world. It was very interesting to see the variety of research projects involving protein crystallography. The talks varied greatly from the dynamics and theory of the technique to the results of a specific project. I particularly enjoyed the session "When Bad Crystals Turn Good..." on the first day of the conference. This session offered useful hints and techniques that can be applied to many difficult crystallization projects.

This meeting not only gave me an opportunity to survey what is going on the field, but it was also held in a wonderful city. After attending the daily sessions, the city of Florence offered numerous attractions to explore. The poster sessions, although a bit crowded and hot, provided an excellent opportunity to talk about research in the field and meet fellow crystallographers. Finally, we attended the banquet held in the courtyard of Palazzo Pitti which was beautifully decorated. It was a wonderful way to end the conference, which included a nice dinner followed by a lot of dancing. Thanks again for this tremendous opportunity.

Jill Dombrauckas

I would like to express my gratitude to the USNCCr for their financial support to attend IUCR 2005 in Florence, Italy. Aside from being the most distant place I'd ever traveled to, it was also the first international conference I had the opportunity to attend. I was amazed at the health of the crystallographic community represented both by the number of people that were there and the diversity of work that I viewed. Even with a week to stretch out the conference I still often found myself deciding which of two fascinating concurrent sessions I would attend. My favorite sessions included those that highlighted new techniques for crystal growth and freezing as well as those that revealed the inner workings of macromolecular assemblies.

My own research on the catalytic intermediates of amine oxidase was well received and I fielded a number of questions from individuals interested both in my techniques and my results. I also enjoyed meeting some of the authors of the crystallographic programs that I've grown to love and use frequently, especially Paul Emsley who created Coot. Again I'd like to say thank you to the USNCCr for making the trip possible and I hope to be back in subsequent years.

Bryan Johnson

I would like to thank USNCCr for the financial support that allowed me to attend an international scientific meeting and to present my work to researchers from around the world. Not only did I benefit from talking about my project with others, I found the research from different students most impressive. The "Crystallography and Forensic Science", "Getting Function from Structure", and "High Throughput Technology in Structural Biology" sessions were most interesting and informative. I also enjoyed the art in crystallography displays and was amazed by the creativity of fellow scientists.

Not only was the meeting a huge success, I had such a great time in Florence Italy. When touring the city it was nice to see the familiar red backpack of other crystallographers.

The social banquet was absolutely amazing. The food was great, the location was wonderful and I had so much fun with the band after dinner. I thank you again for making this experience possible and one that I will never forget.

Sonia Larsen

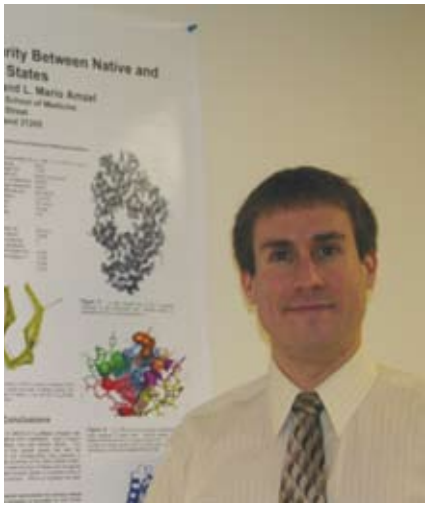
I would like to thank the USNCCr for giving me a travel grant which allowed me to attend the 20th IUCr congress. It was my first time to participate in such a large international scientific meeting. The conference was very well-organized, and there were many interesting talks and posters as well as social activities. I presented a poster titled "Synthesis and Structural Characterization of Novel Metal-Organic Frameworks," which describes my current PhD research. Throughout the conference, I was able to interact with many crystallographers to discuss my work as well as the current topics in crystallography.

There were a number of stimulating microsymposia. In particular, I enjoyed the talks given during "Powder Diffraction on Micro- and Meso-porous Materials" and "Inorganic-Organic Framework Materials" sessions. I was also very excited to learn new techniques and developments in x-ray diffraction and structure determination.

I was able to see the beautiful sights in Florence and experience the city's rich history and culture. I am very grateful to my advisor, Prof. J. B. Parise, the conference organizers and the USNCCr for giving me this wonderful opportunity. This conference was an excellent chance for me to enrich my research and scientific career. I hope I will attend more IUCr meetings in the future.

Hyunsoo Park

I would like to sincerely thank the USNCCr, in cooperation with the ACA, for their travel award which allowed me to participate in the 20th Congress of the IUCr in Florence, Italy. This was my first international conference and my first time in Italy; neither the event itself nor the venue was a disappointment.



I think the spirit of the conference was best summed up in the introductory remarks made by one of the co-chairs of the microsymposium on Non-covalent Interactions in Crystals of Small Molecules and Macromolecule: "The purpose of this microsymposium was to bring together the small molecule and macromolecular communities to learn from each other." "Conference" easily could have been substituted for "microsymposium" and any of the disparate crystallographic sub-disciplines might have been substituted for "small molecule"and "macromolecular". Indeed, talks and poster topics ranged from methods development to applications, from materials science to biological systems, from the use of crystallography in forensic science to its use in archaeology. I tried to take advantage of this diversity of topics by, on a couple different occasions, making a conscious decision to attend talks that didn't directly pertain to my own area of research. It was, however, the rule rather than the exception that a coin had to be flipped in choosing between which of two equally interesting talks to attend, and since I've returned to the lab, I've already begun putting to the test some of the knowledge acquired and new tools learned about at the conference. Just days ago, for example, I tried out the elNemo server (***igs-server.cnrs-mrs.fr/elnemo/index.html***), a site which generates multiple PDB files for use in molecular replacement trials, each output file representing a "point" along a normal modes trajectory of the input structure. As of this writing, AMoRe is crunching away on the resultant files.

The number of posters, like the number of talks, was overwhelming, and I'm sure I'll be thumbing through the abstract book for some time to come. As I'm presently nearing completion of my thesis work and entering the writing stage, all comments and suggestions received regarding my own poster were particularly helpful. In addition to the talks and posters, the conference provided a unique opportunity to meet not only established crystallographers from abroad who perhaps I would not have met at an ACA conference, but also to meet and share ideas with crystallographers at my own early stage in their careers. Hopefully these new friends and colleagues will remain into the future.

Italy was a great venue for the meeting, although admittedly it was sometimes difficult to sit through talks knowing that it may be a once in a lifetime opportunity to see Florence and surrounding Tuscany. In terms of food, I quickly realized that the Little Italy neighborhoods found in some large cities here in the States aren't that true a reflection of the real thing. Fellow manicotti lovers take note, I couldn't find any; whether manicotti is an American take on some platonic ideal of Italian food or I was simply looking in the wrong places, I still haven't determined. Surely my future recollections of this trip will also include time spent on the Ponte Vecchio in the early hours of the morning. Occasionally I would sit there among a crowd of people lining both sides of this famous bridge listening to Italian street performers who would play a popular Italian song and then follow it by a song such as U2's "Where the Streets Have No Name" at the crowd's request for rock. I'd then walk a short distance to the Uffizi gallery and hear American street performers playing the Eagles' "Hotel California." It was a surreal experience. The history, the architecture, the art, the people, the piazzas, the food - it was too much to take in during such a relatively short trip, so my strategy quickly became not to try, but rather assure myself that I would visit again someday.

It was a great experience all around, and again, I offer my sincere thanks to the USNCCr for the travel award which allowed me to have it.

Anthony Armstrong

The IUCr congress in Florence was a great showcase for the wide scope and great achievements in the field. The advances in technology rangeing from new crystal screens to robots to facilitate

all steps of structure determination to GUI-driven automated structure solution software have placed less emphasis on the hardships of structure determination

and more on structure understanding and interpretation. The poster sessions were one of the highlights of the congress. It was a great experience to be standing next to scientists from countries as different as China and Spain, although it did not feel at all strange, being that knowledge knows no boundaries and structure speaks no language. The most memorable moment of the congress for me was the keynote address by Dr. David Sayre. For a lot of us his name brings to mind one of the most mathematically involved chapters in crystallographic theory – Direct Methods and the Sayre equation. But the man behind the scientist was passionate for new and exciting research, generous with praise and credit for his young collaborator, with words of hope and motivation towards the new field of single particle diffraction. I do not think that I will be able to read the direct methods chapter in my book with the same detachment ever again!

Evi Strubel

I want to thank the USNCCr for helping to sponsor a wonderful trip to the IUCr meeting in Florence, Italy this summer. It was my first international meeting, and

it was great to meet crystallographers from a variety of scientific and cultural backgrounds. The different sessions covered a wide spectrum of topics, many of which were very accessible to newer crystallographers such as myself. The more challenging subjects left me with a motivation to learn more. The best talks were those that helped me see my project in a new way. Sessions that I especially enjoyed included: "When Bad Crystals Turn Good: Transforming Poorly Diffracting Crystals," "Combating Viruses," and "Large Protein Assemblies—Forming and Analyzing Complexes." The venue, Fortezza da Basso, with its doors thrown open to the Italian summer, allowed us to enjoy the beautiful weather and fresh air inbetween sessions and at lunch. The posters sessions were also very informative and, as usual, a great way to meet people and pick up new experimental ideas. The conference concluded with an amazing outdoor banquet in the Boboli gardens. The endless food, the magical lighting, and the overall beauty of the gardens concluded the week in Florence perfectly. I am very grateful for having had the opportunity to attend the IUCr conference this past summer.

Kiira Ratia

IUCr XX was a wonderful experience to be part of. With so many leaders in crystallography and related fields under one roof, there was no shortage of cutting-edge talks to attend and discussions to become involved in. Microsymposia that were particularly interesting to me included those on non-covalent interactions,

supramolecular chemistry, and controlled building of crystals. The keynote lecture entitled "Synthetic Crystallography" was also very engaging. The opportunity to present my research brought many thought-provoking questions and contacts with new people. I would like to thank the USNCCr for providing this unique chance to interact with so many people active in different areas of crystallography in such a beautiful place as Florence.

Tamara Hamilton


American Crystallographic Association

2005 ACA Small Molecule Summer Course

Faculty and students from the 2005 ACA Small Molecule Summer Course: Back Row: Jim Kaduk, Nate Schultheiss, Ray Sachs, Marcos Navarro, Jahyr Theodoro, Nathan Takas, Guillermo Minguez, Curtis Moore, Charles Lake. Second Row: David Duchamp, Curtis Haltiwanger, Adam Beitelman, Sam Owens, Greg Hogan, Marvadeen Singh-Wilmot, Sarap Safran, Bryan Craven. Front Row: Paulo de Souza, Lee Daniels, Robert Stewart, Evan Hurly, Asli Ozturk, Van Nguyen Mai, Brian Toby, Lori Fields, Erica Tozzo. Missing: Chuck Campana, Charles Weeks, Bellam Sreenivasulu and John Woolcock.

The 2005 ACA Small Molecule Course was held August 7th through August 17th, on the Indiana University of Pennsylvania (IUP) campus in Indiana, PA. Over the past few decades, there has been a steep decline in the number of chemical crystallographers amongst university faculty. This is unfortunate because the demand for crystallographic information has steadily increased. Staff crystallographers and some industrial scientists have been trying to keep up with this demand, but unfortunately, this leaves them very little time for teaching crystallography. Today, technical training in the use of instrumentation is readily available at most diffraction laboratories, but actual scientific education in the basic principles of crystallography is lacking. The Small Molecule Course at IUP is designed to fill this need. The 10-day course included 8 days of instructions (lectures in the morning, workshops in the afternoon and computer tutorials at night), a day trip to Pittsburgh, PA to visit the University of Pittsburgh, the Carnegie Museum and the Church Brew Pub and a final day allotted for student presentations. This year, eighteen students representing six countries attended (4 from Brazil, 1 from Jamaica, 1 from Singapore, 2 from Turkey, 1 from the United Kingdom and 9 from the United States). Our teaching staff included 12 members from academia, national laboratories and industry. On the final day, 13 of the 18 students attending submitted a questionnaire to help evaluate the course and make future improvements. The questionnaire was rated on a scale of 1-5, with 5 being excellent. Those that submitted the questionnaire unanimously judged the course as highly successful and stated that they would recommend the course to others. Average scores for whether they enjoyed the course scientifically and socially were 4.85 and 3.92, respectively.

This year, Bruker-AXS and Rigaku/MSC used the summer course to demonstrate their latest instrumentation. Besides our in-house D8 Advance and CAD4 diffractometers, Bruker-AXS set-up an APEX II single crystal diffractometer (supported by ***Charles Campana***) and Rigaku/MSC set-up a SPIDER single crystal diffractometer (supported by ***Lee Daniels***) and a MINIFLEX powder diffractometer (supported by ***Lori Fields***). These individuals and instruments were tremendous additions to the course and made very positive impacts upon both the students and faculty! We especially wish to thank ***Susan Byram*** (Bruker-AXS), ***Joseph Ferrara*** (Rigaku/MSC) and ***Thomas McNaulty*** (Rigaku/MSC) for showing such strong support for crystallographic education. They clearly care about the future of the crystallographic community. We would also like to thank ***Scott Field*** (Cephalon, Inc.) for allowing us to recruit the indispensable services of ***Curt Haltiwanger*** whose assistance was truly appreciated.

The students rated the course administration a 3.85 for advanced publicity and a 4.62 for responsiveness to student needs. The majority of the students felt the duration of the course was just right (10 of 13). Surprisingly, the remaining 3 stated the course was too short! The students felt that Indiana, PA was an acceptable course location and gave it an overall score of 4.0.

Our lecture series consisted of 25 presentations covering a wide range of single crystal and powder topics. Students were given a hard copy of all lecture notes as well as a CD-ROM containing all notes, presentations, tutorials and course photographs. These materials were rated highly by the students. The lectures were well received and given a 4.62 in the category "did the lectures meet my needs", but only a 3.58 on the pace of the lectures. Clearly, the students felt that we disseminated too much information too quickly. This year, one of our workhorse lecturers was ***David***

Duchamp who proved to be a tremendous lecturer who willingly volunteered to pick up extra lecture duties due to unforeseen circumstances. We would also like to thank ***Robert Stewart*** for his excellent job explaining difficult mathematical concepts. He is without doubt a mathematical wizard! We also had the good fortune of having ***Charles Weeks*** from the Hauptman-Woodward Institute visit to give a guest lecture on Shake and Bake.

Our tutorials were a major improvement over the last two years. In the past, the computer lab scored a dismal 3.1, but this year that rating rose to 4.85! The students rated our tutorials highly and gave a score of 4.5 to "did the tutorials meet your needs" and a 4.31 to "did the tutorials have adequate supervision". The success of the tutorial sessions was not only due to the high quality of the computer lab, but also due to the tremendous work done by ***Curt Haltiwanger*** and the wonderful powder diffraction duet of ***Jim Kaduk*** and ***Brian Toby***. This year we had many tutorial topics including those involving the CSD and the PDF-4 in which ***John Faber*** of the ICDD donated one-month evaluation copies to the students. These databases were discussed by our resident expert ***John Woolcock***. Jim and Brian offered an excellent series of powder diffraction tutorials ranging from the use of GSAS/EXPGUI to Rietveld analysis and phase identification. These two seem to have a synergistic effect when they work together! Curt gave a tutorial on SHELX and spent numerous hours working with the students solving structures. ***Dave Duchamp*** gave a tutorial on his CRYSTMOL structure evaluation software and gave all participating students a licensed copy.

Our experimental sessions were much better received then previous years and 24 single crystal and powder data sets were collected. The evaluations on the experimental sessions were as follows "did they meet your needs" 4.33, "did you have adequate supervision" 4.42. These sessions were successful due to the indefatigable trio of ***Chuck Campana, Lee Daniels and Lori Fields***. These individuals worked with the students into the wee hours of the morning. Their contributions were indispensable!

The organizers are grateful for the direct financial support donated by the ACA, USNCCr, PDS, Bruker-AXS, Rigaku/MSC, IUP and Cephelon, Inc. who collectively donated $11,600 to the course. These generous donations allowed us to award 12 full scholarships to students. The USNCCr donation also covered travel awards to gifted South American scholars.

Lastly, we would like to thank IUP for its support in making the course successful. The university provided excellent lecture and computer facilities and allocated two university vans for student transportation. We would also like to thank ***Pat Craven*** for organizing the course picnic at the Cherry Ridge alpaca farm and finally, we would like to thank ***Raymond Sachs*** (IUP Physics graduate student) for volunteering for the thankless duty of driving the van back and forth to the airport.

Overall, we feel that the course was very successful and we are planning to offer the course again in the summer of 2006.

Left to right: Bob Bau (ACA), Peter Vekilov (American Assoc. for Crystal Growth), James Zuo (Microscopy Society of America), Ken Downing, Joel Brock, John Parise, Miriam Rossi, Frank Fronczek, Frank Jurnak (ACA), Cheryl Klein Stevens, Matt Redinbo, Kathy Kantardjieff, Jon Clardy, Brian Toby, Doug Ohlendorf (ACA), Julia Chan, Ron Stenkamp and Bill Duax (IUCr). Missing: Phil Bourne, Peter Kuhn and Jim Kaduk.

Report on the 20th General Assembly of the IUCr, Florence, Italy

The US delegation were (left ot right) Kathy Kantardjieff, Jon Clardy (Chair), Judy Flippen-Anderson, Jim Kaduk , and Brian Toby. ***Kathie Bailey Mathae*** from the National Academies accompanied the group.

The first General Assembly (GA) meeting largely accepts recommendations from the IUCr Executive Committee (EC) and reports from the various Journals and Commissions. The EC had met for several days prior to the GA to go over the reports in more detail.

A number of comings and goings of various adhering bodies to the IUCr were approved. Some were straightforward while others were more complicated and rooted in financial issues. The GA voted unanimously to approve Greece as a new member of the IUCr. Argentina's membership had been suspended at the 19th GA in 2002 for nonpayment of dues. With the help of the USNCCr, the ACA and the Spanish Adhering Body, Argentina's back dues were paid, and the Argentine government has agreed to pay all future dues. As a result, the suspension on Argentina's membership was lifted. The EC recommended that the memberships of Ukraine and Bulgaria, which had been suspended prior to the 2002 meeting, be canceled, and the GA concurred. While it sounds unlikely, cancellation is actually a way to get both nations back into membership as it has the effect of canceling the unpaid dues – somewhat akin to declaring bankruptcy. The Ukrainian government has agreed to pay dues when Ukraine is readmitted as a member but not the past dues, which date to 1996. The membership of Bulgaria was also canceled, for essentially the same reasons. The Brazilian adhering body was reduced from Category III to Category I at their request, while the Russian adhering body was increased from Category IV to Category V. These changes mean that Brazil will get one vote instead of three and Russia will get five votes instead of four. The class of membership, and number of votes, is fundamentally determined by how much a country is willing to pay in membership dues and, as such, does not necessarily reflect the importance of a country's contribution to crystallography.

The Secretary-Treasurer, ***S. Larsen***, reported that the finances of the IUCr are "in a reasonably healthy position" and, therefore, the unit contributions will remain at the present level.

The report from the Journals Commission also found the situation to be "positive". The challenges posed by the "open access" requirements from both the NIH (US) and the Science and Technology Parliamentary Committee (UK) were noted by the retiring Editor-in-Chief, ***John Helliwell***. The IUCr, like other scientific publishers, does not have a clear plan of how to generate revenues in an open access world.

Many of the Commission reports noted the increased importance of crystallographic education and the general decline internationally in formal opportunities for such education. Ironically the Commission on Crystallographic Teaching was effectively nonfunctional during the last triennium. It did not meet for the first two years and slowly lumbered into action during the last year. "Action" means getting together by email to decide on a program for the Congress and to meet during the Congress to come up with plans for the next triennium. Katherine Kantardjieff, a member of the USNCCr, will serve as a consultant to the Commission. Commissions in general were urged to strive for geographical balance, gender balance (to the extent that it is represented in the discipline), and to involve younger people. Accountability was also stressed.

The second meeting of the GA was devoted to confirming the site for the next meeting and hearing presentations about possible sites for the meeting after that. Thus Osaka was confirmed as the site for the 2008 meeting, The Statutes and Bylaws of the IUCr require this quaint procedure. The bulk of this session was devoted to presentations from the Prague and Madrid groups that would like to organize the 2011 meeting.

The third session of the GA is traditionally the one in which all of the important decisions are made. As these meetings go, it was unusually tense. The first vote was for the provisional site of the 2011 meeting. The GA voted for the Madrid site.

The next elections were for officers: the President, the Vice President, and the Secretary-Treasurer. At the USNCCr meeting in May, the slate of officers was incomplete, with only Ohashi (Japan) nominated for President and Lidin (Sweden) for Secretary-Treasurer. Later, Torriani (Brazil) was announced as the candidate for Vice President. The USNCCr was uniformly unhappy with the lack of choice offered by the nominations, and felt that every office should have a contested election. Other National Committees (NCs) had similar feelings and, as a result, a group of NCs (US, UK, Greece, The Netherlands, and Hungary) coalesced around a nomination from the floor for ***Maria Carrondo*** (Portugal), a sitting EC member, for President. Carrondo was viewed as an outstanding candidate because of her accomplishments in crystallography, her experience with the IUCr, and her connections with Latin America. Her nomination had originally been submitted to the EC by Italy, Hungary, and the Netherlands, but they did not put her name on the ballot. That she was a woman was not overlooked. The initiative for the Carrondo nomination started before the EC nominated Iris Torriani as Vice President. At the GA there were brief statements by the two candidates following the announcement of the slate, and several shorter statements. The latter ranged from eloquent support for Carrondo by ***G. Díaz-Delgado*** (Venezuela), to statements about the desirability of having contested elections by ***J.C.A. Boeyens*** (South Africa) and ***J. Flippen-Anderson*** (US), to supporting the 'status quo' by ***L. Aslanov*** (Russia). The election was won by ***Yuji Ohashi***, who began working hard to mend fences. ***IrisTorriani*** and ***Sven Lidin*** were also elected. For more on this topic see "From the Editor's Desk" in the IUCr Newsletter – Volume 13 Issue #3).

The next election was for regular members of the Executive Committee with full, six-year, terms. ***Chris Gilmore*** (UK), ***Gautam Desiraju*** (India) and ***Peter Colman*** (Australia) were elected on the first ballot. Because Ohashi was elected President, there was then an election to fill the rest of his term, a three-year term. That election went through several rounds and finally ended in a tie between ***Claude Lecomte*** (France) and ***M. Perez-Mato*** (Spain). President Duax had the difficult and unpleasant task of breaking the tie, which he did by selecting Lecomte.

Action items for the USNCCr in the next triennium.

1. Whether or not to bid, or to be part of a bid, for a meeting in 2014. The recent meetings have been in Europe and Asia so it would be time for a meeting in the western hemisphere. The last time the Congress met in Canada was in Ottawa in 1981 and the last US meeting, which was quite successful, was Seattle in 1996. The Congress has never convened in Latin America.

2. Work with other NCs to propose changes to the IUCr's Statutes and Bylaws to require contested elections for the officers of the Executive Committee.

Membership Update: for 2006-2008 ***Jim Kaduk*** will become Chair. ***Kathy Kantardjieff*** was elected Vice-Chair. ***Chris Cahill*** (George Washington U) was elected to fill out Kathy's term as a regular member and ***Cheryl Klein Stevens*** (Xavier University of Louisiana, ***Jennifer Swift*** (Georgetown U) and ***Victor Young*** (U of Minnesota) were elected to three year terms.

Coming to the US for a Meeting in 2006 - You Might Need a Visa

Advance planning by foreign travelers is critical. We recommend all foreign travelers keep in mind the following when making their plans to travel to the United States: As soon as travel to the U.S. is considered,you should identify whether a visa is needed. If you already have a U.S. visa appropriate for this travel, check the expiration date to make sure it will not expire before your planned travel date. Contact the U.S. Embassy or Consular Section inyour homeland to determine any additional visa procedures, the timeframe required to set up an appointment for the interview, and to schedule an appointment for the interview. An interview is required for most visa applicants. For most, the waiting time for an interview is a few weeks or less, but for some embassy consular sections it can be considerably longer. We recommend contacting the Consular Section via the Internet at: ***travel.state.gov/visa/questions_embassy.html***. You should start this process at least four months before you plan to leave for the meeting.

First Annual UK-Southeast USA Symposium

The First Annual UK-Southeast USA Symposium on Structural Genomics and Proteomics of Membrane and Metalloproteins was held at the University of Georgia on October 13-17, 2005. ***Bi-Cheng Wang*** (UGA) served as Organizing Chair. The meeting attracted about 100 participants from the southeast as well as participants from the UK, Japan and China. This symposium was created to expand international communications in structural genomics and proteomics, extend the boundaries of crystallography and increase gene-to-structure capabilities in these areas.

The participants enjoyed an opening reception at the UGA Atlanta Alumni Center. They were welcomed by former UGA VP of Research, ***Gordhan Patel*** (retired) and British Consul-General ***Martin Rickerd***. Guests then traveled to Athens for the scientific sessions, which were held at The UGA Center for Continuing Education.

The inaugural ceremony was opened by UGA President, ***Michael F. Adams***, followed by comments from ***C. Michael Cassidy***, President of the Georgia Research Alliance and British Consul-General ***Martin Rickerd***. The scientific talks were divided into five sessions: Genomics & Proteomics, Bioinformatics, Cloning & Expression, Mass Spectrometry and Biophysical Tools & Data Management. The first session was chaired by ***Bi-Cheng Wang***, who opened with an introduction and overview of current challenges in the fields of structural genomics and proteomics, followed by talks from ***Jim Naismith*** (Univ. of St. Andrews) and ***Seiki Kuramitsu*** (RIKEN), which focused on their experience in these fields and techniques used to reach the goals in their perspective funded projects. The session on Cloning & Expression was chaired by ***Jim Hartley*** (NCI/SAIC) who gave an overview on proteomics screening methods, followed by a presentation by ***Peter Horanyi*** (UGA) outlining the advantages of a novel parallel protein expression technique. ***Steve Baldwin*** (Univ. of Leeds)gave an overview of membrane protein expression in the genomic era. ***Lance Wells*** (UGA) provided some insight into the field of mass spectrometry, describing tandem mass spectrometry approaches used in his laboratory for the study of glycoproteins. A session on "Biophysical Tools and Data Management", chaired by ***Laurence Barron*** (Univ. of Glasgow), wrapped up the first day of talks. Barron's talk, focused on Raman Optical Activity and its usefulness in protein structure analysis, was followed by presentations from ***Anne Pajon*** (EMBI) on a laboratory information system designed for the BBSRC SPoRT Initiative and ***C.W. Yong*** (CCLRC Daresbury Laboratory), who described how to make the best use of high performance computers for molecular dynamics and quantum mechanical pictures.

The second day of the symposium included sessions on "Membrane Proteins," "Metalloproteins" and "Crystallomics & Crystallography." The "Membrane Proteins" session, chaired by ***Neil Isaacs*** (Univ. of Glasgow) and ***Larry DeLucas*** (UAB) began with a report on the Membrane Protein Structure Initiative (Mpsi) in the UK by ***Neil Isaacs***. ***Larry DeLucas*** followed with an overview of novel crystallization techniques for membrane proteins. ***David Puett*** (UGA) gave a presentation on G protein-coupled receptors. Two important contributors to this session, ***Zihe Rao*** (Chinese Academy of Sciences/Tsinghua Univ.) and ***Steve Sligar*** (UIUC) were unable to attend due to extenuating circumstances. ***Dawei Lin*** (UGA) filled in on short notice, giving a report on accurate detection of protein domain boundaries. The "Metalloproteins" session, chaired by ***Samar Hasnain*** (CCLRC Daresbury Laboratory) and ***Robert Scott*** (UGA) began with some examples on using combined x-ray approaches to

Left to right: John Chrzas, Zhongmin Jin, Robert Yu and Laurence Barron

study the functions and misfunctions of metalloproteins from ***Samar Hasnain***. ***Robert Scott*** followed with a report on x-ray spectroscopy in post-genomic biology, ***David Richardson*** (Univ. of East Anglia) gave a description of the structural resolution of the nitrogen cycle respirome, and ***Gary Sawers*** (John Innes Centre) ended the session with an overview on the maturation of metalloproteins. The last session, "Crystallomics & Crystallography," chaired by ***John Rose*** (UGA), focused on novel techniques in these fields. ***John*** gave a talk on a high-throughput crystallization pipeline for structural genomics applications developed for SECSG. ***SvetlanaAntonyuk*** (CCLRC Daresbury Laboratory) illustrated how cryo-annealing methods can be used to diffract crystals to atomic resolution, which has greatly increased the understanding of metalloprotein structure based mechanisms. ***Martin Caffrey*** (OSU/Univ. of Limerick) followed with a presentation on crystallizing membrane proteins in lipidic mesophases, and ***Joseph Ng*** (UAH) described the fundamentals of counter-diffusion as compared to traditional crystallization methods and its use in structural genomics. The day ended with a talk by ***Xiaodong Cheng*** (Emory Univ) focusing on five different structural folds of SAM-dependent methyltransferases and their involvement in membrane and/or metal (zinc) binding.

The last day of the symposium focused on tools and methodology for current and future use in genomics and proteomics. Talks were divided into three sessions: "High-Throughput & Novel Methods", "Scientific Aspects of New Diffraction Equipment" and "Next Generation Macromolecular Crystallography Methods". The first session, chaired by ***Zhi-Jie (James) Liu*** (UGA), began with his overview of the high-throughput structure determination pipelines at SECSG. ***Peng (George) Wang*** (OSU) followed with a talk on the mechanism of polysaccharide synthesis, which he termed the "last frontier on the biosynthesis of biopolymers." The first session ended with ***Robert Yu's*** (MCG) presentation on glycomics and glycolipidomics, which focused on the use of mass spectrometry in conjuction with proteomics/genomics to analyze complex glycoforms. The second session, chaired by John Chrzas (SER-CAT/UGA), was opened with an overview of the SER-CAT beamlines presented by ***Chrzas*** and ***Bi-Cheng Wang*** (SER-CAT Director). The remainder of the session focused on equipment options and included presentations from ***Jules Hendrix*** (Marresearch) on the mar555 flat panel detector, a description of a new high speed, large area photon-counting detector by ***Roger Durst*** (Bruker AXS), and a talk by ***Joe Ferrara*** (Rigaku Americas) on advances in SAD phasing in the home lab. The third session began with a talk by ***Zhi-Jie (James) Liu*** (UGA) on the novel technique of sulfur phasing in crystallography, followed by ***Zheng-Qing (Albert) Fu's*** (UGA) presentation on SGXPro, a user friendly computation environment developed for protein crystallography. ***Ming Luo*** (UAB) ended the session with an overview of a proteomic platform for expression of higher eukaryotic proteins, where he described how his group investigated over 10,000 open reading frames (ORFs) from *C. elegans* and human genomes through a robotic pipeline.

After the third day of talks, participants attended a poster session including contributions from junior and senior researchers as well as UGA graduate students. In conjunction with the poster session was a vendor show and an interactive demonstration of SER-CAT Remote Access, which combines AccessGrid (computer conference technology) with robotics at the SER-CAT beamlines to provide remote site participation by its users.

The symposium ended with a banquet featuring keynote speaker, ***Arnett Mace***, Provost and Senior VP of UGA. Participants also enjoyed some lively bluegrass music, pork barbeque and catfish with all the fixings served up southern style.

Following the symposium was a meeting of the Organizing and Program Committees, who all agreed the meeting was a worthwhile endeavor and served to form international collaborations to further benefit the field of structural proteomics. While the term "First Annual" is certainly optimistic, in this case it was quite fitting as it was agreed to hold the "Second Annual" UK-Southeast USA Symposium at the University of St. Andrews in Scotland in August 2006.

The symposium was a joint effort of the University of Georgia and the British Consulate and was sponsored by Rigaku Americas, Xenocs, Bruker AXS, Qiagen/Nextal, MarUSA, Marresearch, and The Center for Biophysical Sciences and Engineering at the University of Alabama at Birmingham. More details, including abstracts, are available at ***www.bmb.uga.edu/uk-seusa***.

Lisa Horanyi

FOX2D CU 25_25P
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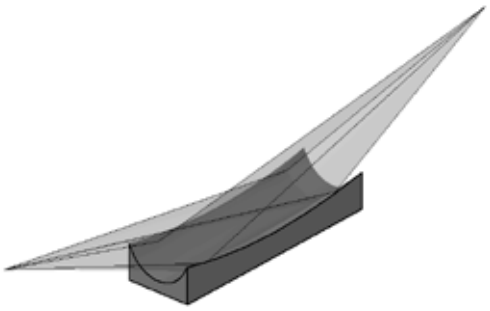
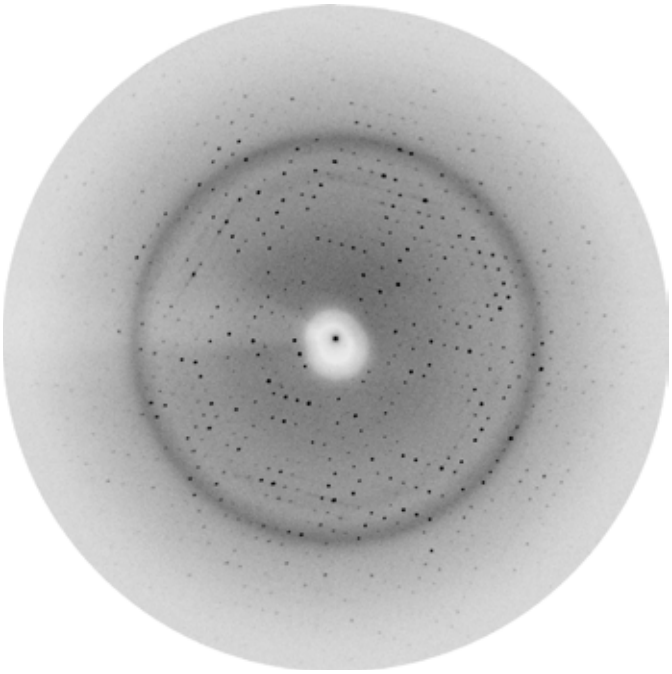
Based on Xenocs' innovative single reflection design, the new *FOX2D CU 25_25P* provides a **"clear improvement in data quality for small crystals"** even with your existing home lab x-ray source.





- enhanced useful flux with low background
- improved data quality
- enhanced lifetime
- lower cost of ownership
- easy alignment and integration
- compact mechanical design adaptable to all X-ray generators

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

The crystal belongs to space group C222 with cell dimensions a=72.1Å, b=97.4Å, c=191.0Å. Images were collected with an oscillation angle of 0.4°.
The crystal was a thin plate with approximate dimensions 200x75x50 µm³.
The generator was a Rigaku RuH3R running at 50kV, 100mA (300 µm focus) and the data were collected on a Mar345 image plate detector.

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

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A. Alan Pinkerton - New ACA Vice-President

Alan Pinkerton was born in Watlington, England in 1943 and received his Ph.D. from the University of Alberta, Canada in 1971. After graduation he gained experience in the field of crystallography by serving as a research associate in a number of prominent international universities in England, Switzerland, and France.

Alan joined the University of Toledo as a faculty member in 1984. He achieved full professorship is 1989, and is currently the Chair of the Chemistry Department. He has joint faculty appointments in the Department of Medicinal and Biological Chemistry and the Department of Physics and Astronomy, as well as an adjunct faculty position at Bowling Green State University.

Over the last 30+ years, he has published nearly 200 papers applying crystallographic ideas and applications to an incredibly wide variety of subjects. Research funding has been successfully acquired for projects involving such topics as lanthanide chemistry and charge density studies of biologically active compounds as well as energetic materials and cryogenic cooling of protein crystals. While maintaining an interest in many areas, his recent research has focused on methods development with respect to data quality in both small molecule and protein data on both "in-house" sources, as well as synchrotron sources, and on applying these methods to charge density studies, including the determination of energy densities.

He has been honored by the University of Toledo (1989, 1994), Sigma Xi (1996), CSUI (1997), and the Pittsburgh Diffraction Society (2004). He has served the scientific community as a member of the ACA Development Committee (1989 – 1991), Chairman of the ACA Small Molecule Special Interest Group (1994 -1995), member of the American Institute of Physics Development Committee (1995 – 1997), member of the ACA Apparatus and Standards Committee (1998 – 2000), member of the ACA Nominations Committee (1998-2000), member of the USAMRMC, Review Panel (2003), Pittsburgh Diffraction Society, President Elect (2004) and President (2005).

Damon Parrish

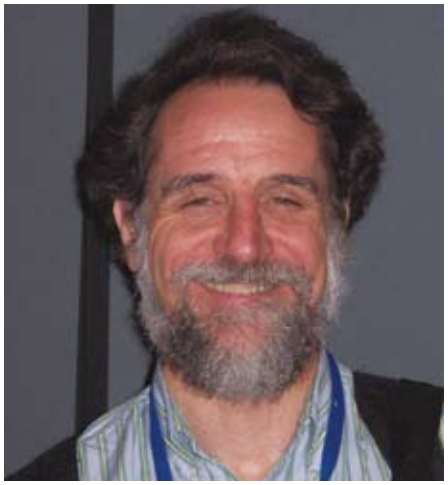
Lisa Keefe - Re-elected as ACA Secretary

The ACA membership has reelected Lisa J. Keefe, Director of IMCA-CAT at the Advanced Photon Source, as ACA Council Secretary. Lisa received an A.B. in Chemistry from Vassar College in 1983 before enrolling in the graduate program in Biophysics and Biophysical Chemistry at the Johns Hopkins University School of Medicine. Lisa worked in Carl Pabo's laboratory at Hopkins through 1989, when she moved to Ed Lattman's laboratory, where she earned her Ph.D. in 1992. She then received a DOE Alexander Hollaender Distinguished Postdoctoral Fellowship with a joint appointment in the Structural Biology Center (SBC) at Argonne National Laboratory and the Biology Department of Brookhaven National Laboratory, where she helped to develop the user program for SBC, first at the National Synchrotron Light Source (Brookhaven) and then at the Advanced Photon Source (Argonne). In 1998 Lisa joined the Industrial Macromolecular Crystallography Association Collaborative Access Team (IMCA CAT) at the APS as a user interface scientist and was promoted to User Program Coordinator in 2001. In July 2002 she was appointed to her current position of Director where she directs the CAT's technical and user programs with a staff of 9 for the 13 IMCA memberships (9 pharmaceutical companies). In January 2005 the IMCA contract and group moved to the University of Chicago.

Lisa has been active member of the ACA since 1985, was one of the organizers of the ACA Young Scientist SIG and was its first chairperson from 1993-1994. She has also been very active in the APS organization and has helped draft and implement current and past procedures for user safety and the proposal system for general user access to the APS facility. She was elected a member of the APS User Organization Steering Committee for 2001 – 2004.

I met Lisa when she joined Jenny Glusker's group at Fox Chase Cancer Center as a technician between her undergraduate and graduate studies and I was a Research Associate in Helen Berman's group. I need not go further in discussing her talents, achievements or organizational skills except to say we are married and have three great children.

Steve Ginnell



Data, Computing and Standards
Andy Howard

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.

Communications Committee
William T. Pennington

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 elected to the Communications Committee and I look forward to being involved in these exciting endeavors.

Continuing Education
Christopher L. Cahill

Statement: 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, these developments have provide access to a previously esoteric activities (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 substandard 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. These efforts will challenge new users to think critically about their results and carefully examine structures for potential pitfalls. Coupled to this will 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.

I hope I can provide 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 welcome the opportunity to participate in this capacity.

ACA 2005 SIG Election Results

Biological Macromolecules
Chair-elect:William Royer

Fiber Diffraction
Chair-elect: Joseph Orgel

General Interest
Chair-elect: Peter Mueller
secretary: Marilyn Olmstead

Materials Science
Chair: Claudia Rawn

Neutron Scattering
Chair-elect: Ian Swainson
Secretary: Thomas Proffen

Powder Diffraction
Chair-elect: Thomas Proffen
Secretary: Claudia Rawn

Service Crystallography
Chair-elect: Allen Oliver

Small Angle Scattering
Chair: Volker Urban
Chair-elect: David Londono
Secretary: Hirotsugu Tsuruta
Member at large: Pete Jemian

Small Molecules
Chair-elect: Xiaoping Wang
Secretary: Brian Patrick

Synchrotron Radiation
Chair-elect: James Holton

Young Scientist
Chair-elect:Anna Gardberg

The ACA gratefully acknowledges contributions to our award fund

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Rudolf Allmann
Helen M Berman
Abraham Clearfield
David R Davies
Karl F Fischer
Theodor Hahn
Hampton Research
Joseph Xiaomin Ho
Heinz Jagodzinski
Carroll K Johnson
Judith A Kelly
James R Knox
Rudolph K Kullnig
Bruce C Noll
Sean Parkin
James W Pflugrath
Clara B Shoemaker
Carla Slebodnick
Hugo Steinfink
Thomas C Terwilliger
Thomas Webb
Bernhardt J Wuensch
Shu-Cheng Yu

Etter

Christer Aakeröy
Paul W Baures
J Michael Bennett
Helen M Berman
Joel Bernstein
Lee Brammer
Doyle Britton
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Jose Miguel Delgado
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Dale E Tronrud

Patterson

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Erich F Paulus
James W Pflugrath
Edward Prince
Timothy J Rydel
David Sayre
W Robert Scheidt
Helmut W Schmalle
George M Sheldrick

Clara B Shoemaker
William C Stallings
Robert Stewart
Boris Strokopytov
Marianna K. Strumpel
David H Templeton
Thomas C Terwilliger
Dick Van der Helm
Thomas Webb

Pauling

Alfred E Attard
Paul W Baures
Helen M Berman
Joseph C Calabrese
Charles W Carter
Abraham Clearfield
Edward J Collins
David E Cox
David R Davies
Robert Degeilh
David J Duchamp
Drake S Eggleston
Paula M D Fitzgerald
J. L Flippen-Anderson
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Helmut W Schmalle
George M Sheldrick
Clara B Shoemaker
William C Stallings
Hugo Steinfink
Thomas C Terwilliger
Joseph E Wedekind
A P Wilkinson
D L Worcester

Student Travel

Robert Bau
Helen M Berman
Richard G Brennan
Roger M Burnett
Paul Butler
Christopher L Cahill
Connie Chidester
Ewa Ciszak
Abraham Clearfield
Fred Dyda
Ulrich Englich
Andrew J Fisher
J. L Flippen-Anderson
Frank R Fronczek
Judith C Gallucci
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John Richard Helliwell
Jason Hodges
Joseph A Hriljac
Thomas D Hurley
Doba Jackson
Richard D Kidd
Daniel R Knighton
Boris Kodess
Jeanette A Krause
Thomas Laube
Emil B Lobkovsky
Craig McLauchlan
Bruce C Noll
Sean Parkin
Erich F Paulus
James W Pflugrath
A Alan Pinkerton
Marc Lee Pusey
Frank J Rotella
Walter L Roth
Phil Rudolf
Timothy J Rydel
Helmut W Schmalle
George M Sheldrick
Carla Slebodnick
Dmitri Soldatov
William C Stallings
Hugo Steinfink
Göran Svensson
Thomas C Terwilliger
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wwPDB at IUCr Congress in Florence

The worldwide Protein Data Bank (wwPDB; www.wwpdb.org), established in 2003, consists of three member organizations that act as data deposition, data processing, and distribution centers for PDB data. The founding members are the Research Collaboratory for Structural Bioinformatics (RCSB) PDB (USA), the Macromolecular Structure Database at the European Bioinformatics Institute (MSD-EBI, Europe) and Protein Data Bank Japan (PDBj). The mission of the wwPDB is to maintain a single Protein Data Bank archive of macromolecular structural data that is freely and publicly available to the global community. The wwPDB exhibited at the IUCr Congress in Florence. All three sites ran demonstrations of their websites and were available throughout the exhibition to meet with PDB users. The wwPDB Advisory Board also met in Florence.

Kim Henrick (MSD), Helen Berman (RCSB PDB) and Haruki Nakamura (PDBj)

The wwPDB also had an active presence throughout the meeting, with presentations at sessions including the CCP4 Workshop, the microsymposium *Improving Structures Using Bioinformatics*, and the COMCIFS and Biological Macromolecules Open Commission Meetings. All three members of the wwPDB combined to host a Round Table on *Data Mining with the PDB* at which Helen Berman presented an overview of the wwPDB that was followed by Kim Henrick, Haruki Nakamura, and Philip Bourne (RCSB PDB) describing the various ways to mine the data available in the PDB archive through their respective websites.

Christine Zardecki

RCSB PDB Update

New Beta Site Replaces Current RCSB PDB Portal on January 1, 2006

The RCSB has enhanced and revised its web and FTP sites.to provide a powerful portal for studying the structures of biological macromolecules and their relationships to sequence, function, and disease,

Navigation has been improved based on user feedback and a new help system has been implemented to enable users to find structures of interest as well as information in the RCSB's significant number of curated web pages.

The new site, in public beta test since July of 2004, replaced the current production site at www.pdb.org and ftp.rcsb.org on January 1, 2006. Users can report bugs or navigation problems to info@rcsb.org. Comments as well as suggestions for future enhancements can be sent to the same address..

A short narrated tutorial (core1.rcsb.org/tutorial/), available in Flash, is provided to help explore new features. A jump menu allows one to watch sections of the tutorial without having to start at the beginning each time.

The intent of the new site remains to not only provide full details of each deposited structure and its associated experiment, but to also place structure in the context of a broader understanding of

biology that appeals to a wide audience of students, educators, and researchers from different life sciences disciplines.

Simple searching has been made more powerful. Structures can be found by browsing biologically meaningful concepts such as human disease terms, molecular functions, biochemical processes, structural classifications from SCOP and CATH, and more.

Using PDB data that has been remediated and standardized, new tools are available – improved ligand searching with associated viewing of protein ligand interactions is one example. Another is the mapping of structural features to sequence, which includes showing the relationship between the structure sequence and the proteomic sequence.

A new structural genomics portal offers target summary reports for each center, databases that track the progress of protein studies (TargetDB and PepcDB), and tools to explore the distributions of functions relative to the human genome found within PDB structures, structural genomics targets and homology models.

We hope that you find the new site useful and wish to thank everyone contributed to its development.

RCSB PDB Poster Prize in Florence

The prize went to *Proline isomerisation in stefin B: A crucial step towards amyloid fibril formation* by ***Sasa Jenko Kokalj***, Gregor Guncar, Eva Zerovnik, and Dusan Turk (Dept of Biochem and Mol Biol, Jozef Stefan Institute, Ljubljana, Slovenia). ***Maria-Arménia Carrondo*** chaired the selection committee

Looking Forward

In addition to other activities planned for 2006, RCSB PDB director ***Helen M. Berman*** will receive the Buerger Award at the ACA Meeting in Hawaii. The award symposium: "Structural Biology from All Angles" will feature, presentations by ***Helen, Jordi Bella, Stephen K. Burley, Wah Chiu, Paula M. Fitzgerald, Stephen Neidle and John Westbrook.***

Philip E. Bourne

Notes of a Protein Crystallographer: Robots in Crystallography: A Personal and Historical Perspective.

Whether we like it or not, robots have entered into crystallography with noticeable impact in all stages of our work. First, it was to remove some of the tedium of preparing solutions and doing screens. Later by setting up trays for crystallization. and more recently, robots are beginning to enter ('invade'!) the realm of crystal mounting, centering and automatic data collection at synchrotron stations and in-house laboratories.

The sequence of unrelated steps that brought this technology to protein crystallography and the impact on the future of the field have been briefly reviewed in a recent publication (Abad-Zapatero, *Acta Cryst.* (2005) D61, 1432-1435). Readers, especially students and younger crystallographers, are encouraged to read the entire article for a full historical perspective of the design process and the people involved. An abridged version is presented here to whet your appetite.

It would have appeared to be an impossible dream in the late sixties, when the field of protein crystallography first became established, just as the structures of myoglobin and hemoglobin were first unveiled. Even if somebody had thought about it in the early seventies, when protein crystallography was "coming of age", it would have still seemed utterly impossible or even a miracle. Yet, only thirty years later, here I am late at night putting a protein crystal in front of an extremely brilliant x-ray beam using a computer controlled robot to mount, center, orient and expose a protein crystal to x-rays emanating from a third generation synchrotron source. How did this all happen? Who were the people involved in these amazing technological advances? What are the implications of these developments for the future of the field?

There was a sequence of modest, somewhat unrelated changes in the way macromolecular crystals were handled that turned out to be tremendously import. A bit of historical background is necessary to put it in perspective. Besides having read about it in textbooks, new generations of protein crystallographers might never mount a protein crystal in capillary as it was done in the past. This was the critical observation by Bernal and Crowfoot in their 1934 *Nature* paper. Protein crystals need to be in equilibrium with their 'mother liquor' in order to retain their internal order and diffract x-rays, reflecting their atomic order. This translated into an elaborate crystal-mounting protocol. Crystals were 'sucked in' with a syringe or by an elaborate suction apparatus that was completely personal to the crystallographer, containing a mouthpiece, rubber or plastic tubing and a quartz capillary at the end. Sealing wax was carefully laid out on both ends of the capillary prior to the suction step. For some precious seconds the crystal was seen through the microscope in the spot plate and then disappeared into the capillary, floating within a minute amount of mother liquor. The crystal was separated from the mother liquor by various tricks (i.e. further suction, drying the surrounding liquid with filter paper, etc) and eventually the crystal and mother liquor were sealed and exposed to the

x-rays at room temperature. X-ray sources of the time started with sealed x-ray tubes and continued on with different types of rotating anodes.

I briefly reviewed the process for two reasons. First, it was tedious and elaborate and second, it was also eminently personal. The tools were individual and the different steps had a unique personal character that varied widely among crystallographers. I have never seen Max Perutz mounting a hemoglobin crystal but I am quite certain that he did it differently from the way Dorothy Hodgkin, David Blow or even 'Sage' (i.e. J. D. Bernal) mounted the crystals of their favorite proteins. Probably they all had their own set of utensils and used them in a unique way to break off crystals from a cluster or to manipulate and control them prior to the final mounting step. There was also the 'supreme moment' when that precious crystal disappeared from the center of the circular drop viewed through the microscope, to hopefully reappear in the capillary, immersed in a small amount of liquid. In one of those inexplicable connections of the human brain, at least mine, I have often associated all these events with the losing battle of the bull in the bullring. The bullfighter using his cape and other instruments to move the bull around in the ring, followed by the 'supreme' moment of the toreador in the middle of the ring, when after having had a deadly dance with the bull in the circle, faces him eye-to-eye for the ultimate sacrificial moment.

All this agony was prevented when the first description of the cryo-loop mounting method was presented by Teng, using small wire loops to immerse the crystal in a free-standing liquid film. There had been earlier insights and developments in the area of cryo-protection of protein crystals and data collection at subzero temperatures. Haas and Rossmann used a combined solution of sucrose-ammonium sulfate to freeze crystals of lactate dehydrogenase in liquid nitrogen and collected three-dimensional data at 3.5 Å resolution. They were able to show that the rate of radiation decay decreased by ten-fold and that the frozen crystals were isomorphous with the native unfrozen crystals. Further work by Petsko extended the method to other proteins using glycerol as the cryoprotectant. Hope later used methods for cryoprotection involving transferring the crystals to inert oil (or propane) with subsequent freezing in polyethylene glycol using a glass fiber for mounting. For the extremely fragile crystals of ribosomes, Hope, Yonath and colleagues crafted minute glass spatulas to freeze (85° K) and mount the delicate crystals of ribososomal particles achieving three-dimensional data collection to 4.5 Å at synchrotron sources. The immersion of protein crystals in small wire loops, suggested by Teng, was an amazingly simple and effective way of 'scooping' the crystal from the cryoprotectant solution to the X-rays bathed in a stream of liquid nitrogen.

There is still some of that agonizing moment when a crystal flies from the cryoprotectant drop onto the goniometer head, cradled in the rayon loop, but the process is so much simpler and effective that it actually almost never fails. These modest advances paved the way to automatic mounting, centering and exposing that we see nowadays all handled by computer controlled robots.

This engineering achievement is only one more of the developments in the field that is giving the sense that old skills are no longer needed. Some might argue that old-fashioned crystallographers are becoming redundant, obsolete or even plain unnecessary and superfluous. I would rather think that they have now been freed to utilize their hard-won skills in more imaginative and productive ways. All these thoughts came to me during one of those long nights at the APS (17-ID, IMCA-CAT) when our robot was mounting, centering, exposing, collecting and dismounting crystals with predictable and reliable motions and gestures, like a reliable old friend. Almost like a rigid mime, a dancer without music, only accompanied by the sounds of levers and mechanical actuators and the huffing and puffing of liquid nitrogen passing through valves and filling reservoirs. The robot will perform those required tasks obediently and flawlessly, even performing an annealing cycle on the mounted crystal without my having to move from my chair outside the hutch.

As with any other technological advance, there were other gloomier nights when both the robot and I had to learn to talk to and trust each other. In those earlier nights, I had to learn about his vocabulary, his moods and idiosyncrasies, pauses and unexpected interruptions. I also needed to observe his every move and document his flaws so that his behavior could be corrected in future encounters. From what we learned from each other in those sleepless nights, the robot has now become a true friend.

I also had to learn to be more trusting of my new friend and to give him a vote of confidence. I soon learned that I could allow this complicated piece of machinery to get close to my valuable crystals stored frozen in our 'pucks'. That I could abandon into his anonymous, mechanical hands those precious crystals that I would have otherwise carefully, even tenderly, mounted and aligned myself.

Thus questions arise: What will robot technology bring to macromolecular crystallography? What will be the implications of the widespread use of this technology in the field? What doors will this totally unexpected technology open? How will it affect future generations of students?

Some ramifications are easy to predict: higher throughput of samples and structures, faster screening for crystal quality that will be critical for some of the more difficult membrane protein structures, more efficient use of synchrotron beam time and the ability to tackle massive numbers of structures in the structural genomics projects. But what will be the effect in more unpredictable areas? What will be the impact on the student population that perhaps in a generation or so will take automatic crystal manipulation for granted? I will not even dare to make any further pronouncements. However, I will say that that these new tools should allow us to concentrate on what lies ahead: the design and development of novel experimental designs that would permit us further insights into the workings of the cell. Experiments that will allow us to explore by x-ray diffraction, scattering, spectroscopy, fluorescence or other means the order and structure of even larger and more complex aggregates. In the foreseeable future, they could also open a window into the subtleties of transient interactions of different molecular components of living organisms, into the cell's most ephemeral 'dissipative structures'. Time will tell and we will all have to thank the robots and their creators for it.

Cele Abad-Zapatero

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Meeting Calendar

JANUARY 2006

26-27 **Advances in Protein Crystallography, Conference & Exhibition,** South San Francisco, CA *www.ProtCrystConf.com.*

APRIL 2006

3-6 **DGL 2006 - Annual Meeting of the German Society for Crystallography,** Freiburg, Germany *www.dgk-2006.de/.*

MAY 2006

28-June3 **Ninth International Conference on Synchrotron Radiation Instrumentation**, Daegu, Exco, Korea *www.sri2006.org*

JUNE 2006

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

JULY 2006

22-27 **ACA Annual Meeting, ACA 2006, Sheraton Wakiki, Honolulu, Hawaii.**

AUGUST 2006

6-11: **ECM-23, 23rd European Crystallographic Meeting.** Universiteit Leuven, Belgium *www.lcm3b.uhp-nancy.fr/mathcryst/leuven2006.htm*

SEPTEMBER 2006

1-4 **EPDOC-10 - European Poweder Diffraction Conference,** University of Geneva, Geneva, Switzerland *www.ecm23.be*

JANUARY 2007

14-19 **International School on Mathematical and Theoretical Crystallography,**. The University of Havana, Cuba. *www.lcm3b.uhp-nancy.fr/mathcryst/havana2007.htm*

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 *www.crystalerice.org*

JULY 2007

21-26 **ACA Annual Meeting, ACA 2007,** Salt Lake City, Utah. Local Chair, Christopher Hill, Program Chair, Jill Trewhella

MAY 2008

31-June 5 **ACA Annual Meeting ACA 2008**, Knoxville, TN. Local Chair, Jason Hodges. Program Chairs, Paul Butler and Dean Miles

Contributors to this issue:

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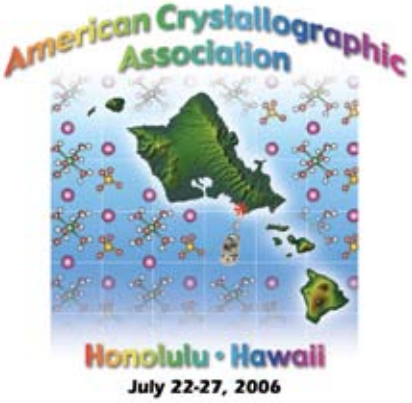

Abstract Deadline: March 1, 2006

Advance Registration Deadline: June 1, 2006

Advance Hotel Registration Deadline: June 13, 2006

On-line abstract submission instructions, on-line registration, and a preliminary meeting program are posted on the ACA website at: **www.hwi.buffalo.edu/ACA/**

The meeting will begin with workshops on Saturday, July 22. Symposia and sessions will begin on Sunday morning, July 23. Consult the Call for Papers, now on the ACA website, for detailed information.

Application procedures for acquiring visas for travel to the US have eased sometwhat over the past year, However, the best advice remains to APPLY EARLY! Applicants are currently advised to apply at least 3 to 4 months in advance.

The International Visitors Office of the National Academy of Sciences has very useful website (www7.nationalacademies.org/visas) that answers most questions pertaining to applying for a visa to attend the ACA meeting in Hawaii. It also provides links to State Department websites for further information.

2006 Local Chairs:

Charlie Simmons
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Karl Seff
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2006 Program Chair
Judy Kelly
judith.kelly@uconn.edu

Symposia

Transactions **Symposium: Neutron Diffraction (featuring its uses in studying biological macromolecules as well as small molecules and recent developments in neutron techniques), organized by Tom Koetzle, Paul Langan, and Alberto Podjarny.**

Buerger Award Symposium to honor Helen Berman, 2006 Awardee.

Warren Award Symposium to honor Charles Majkrzak, 2006 Awardee.

Workshops

Grazing Incidence Methods for Nanoscience and Biotechnology: Organized by the Small Angle SIG

Methods in Neutron Protein Crystallography: Organized by the Neutron SIG.

Management of Synchrotron Image Data: Organized by the Data, Standards and Computing Committee

Sampling of Scientific Sessions

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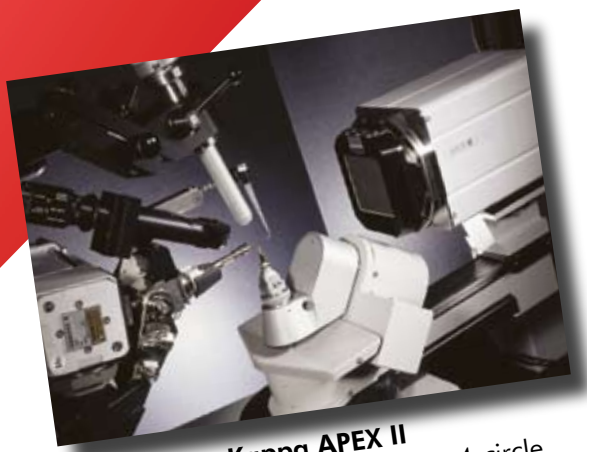

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