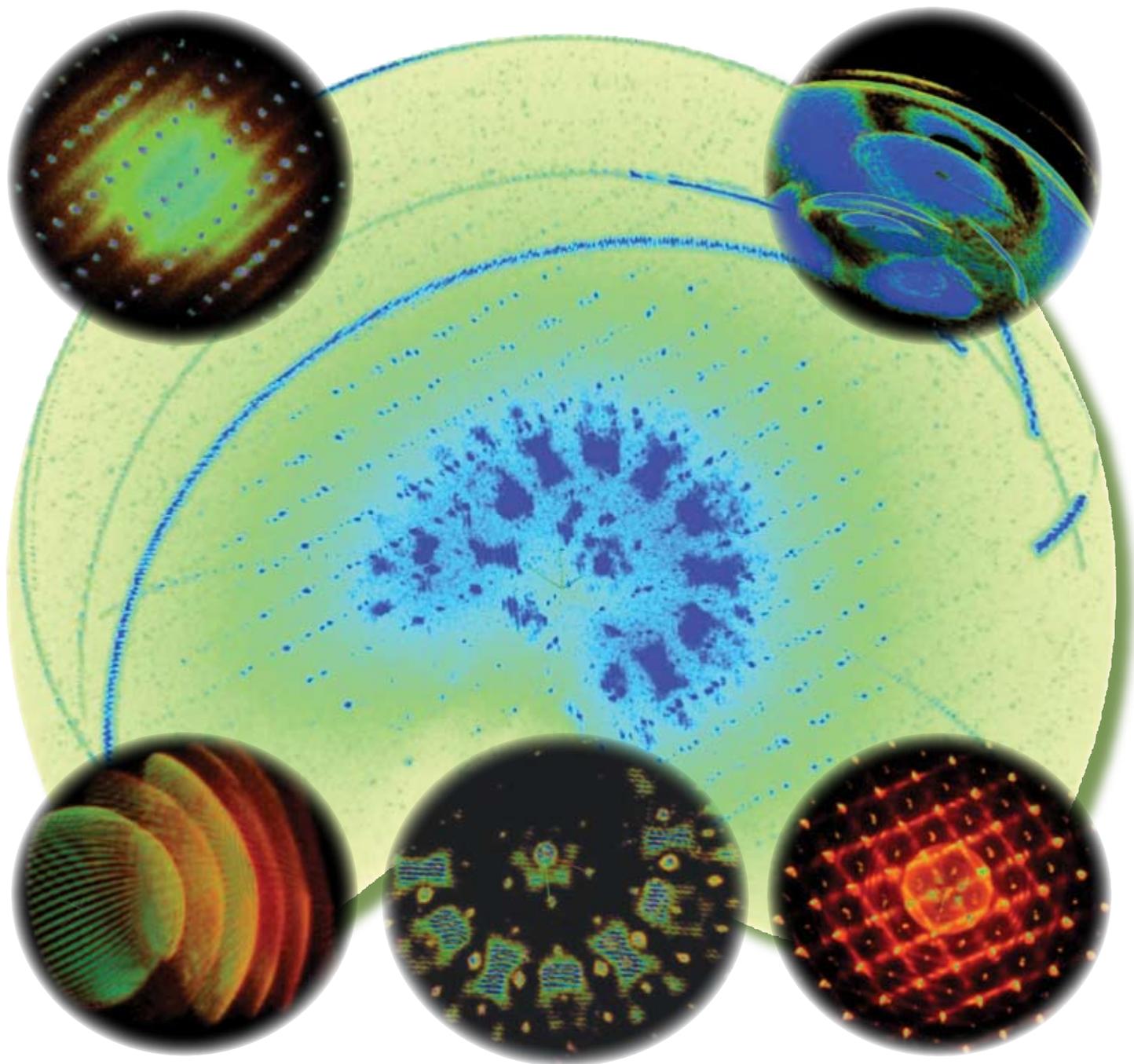


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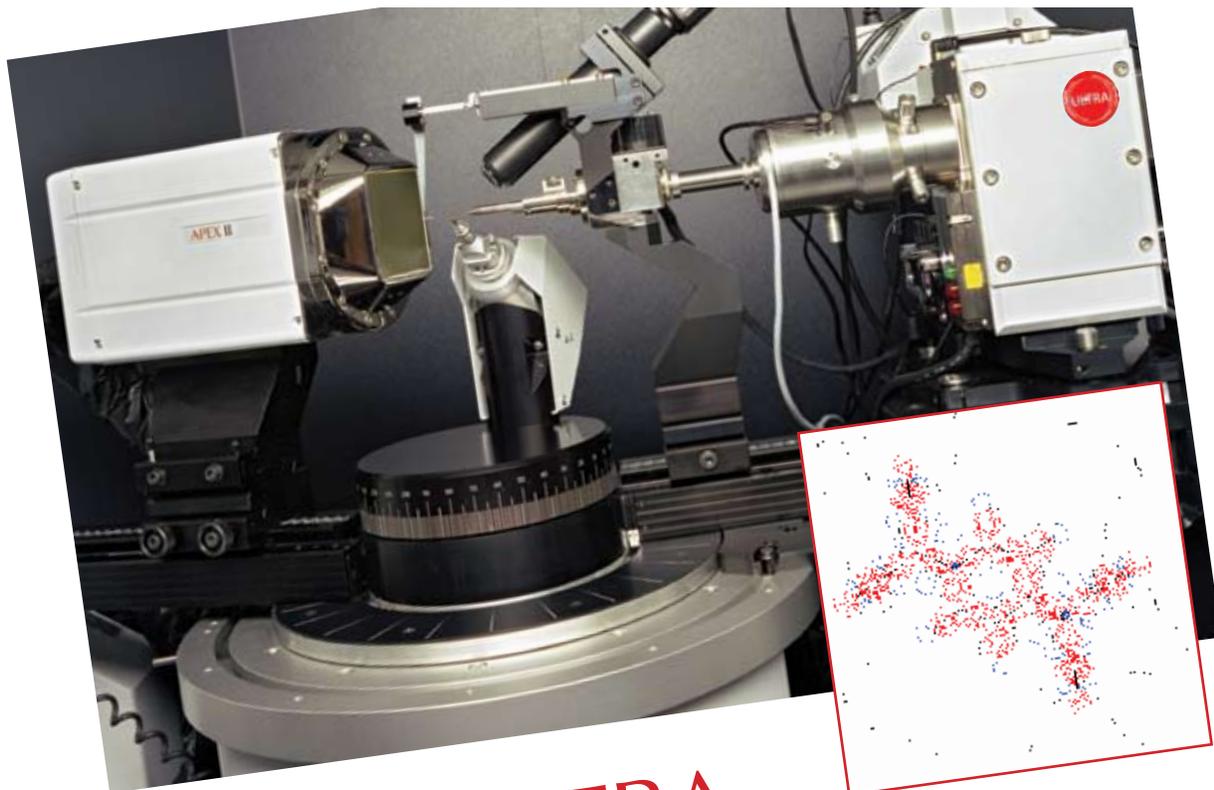
*American Crystallographic
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Number 4

Winter 2006



*ACA 2007
Transactions Symposium
Diffuse Scattering*

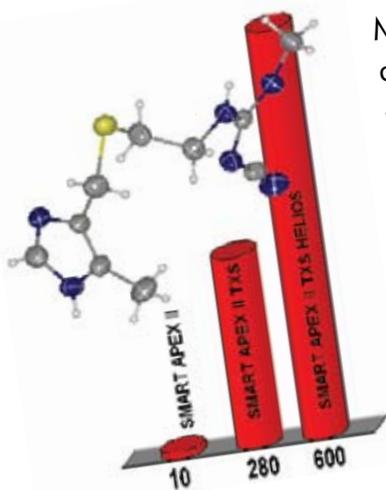


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2007 ACA Transactions Symposium on Diffuse Scattering
See What's on The Cover - page 64.

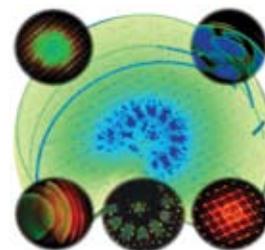


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Deadlines for contributions are: February 1 (Spring), May 1 (Summer), August 1 (Fall) and November 1 (Winter)

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The Future of Education in Crystallography

For quite some time now I have been concerned about the future of university courses in crystallography, especially from the point of view of a "small-molecule" crystallographer (I am going to limit my comments exclusively to graduate-level education). For the past two or three decades it has become increasingly evident that upon the retirement of structural chemists like myself, with research programs having their main thrust linked to crystallographic structural analysis, chemistry departments in

universities across the country are not replacing those positions with junior tenure-track appointments in the same area. I find this very ironic given that yet another Nobel Prize has been awarded (Roger Kornberg, Chemistry, 2006) for which crystallographic results provided the critical underpinning to his overall research. One has only to look at the rapid growth in depositions to all the structural databases to know that this situation is not unique. Yet, we are producing new generations of scientists who rely on crystallographic equipment and techniques, but have little knowledge of the underlying theory, technology or its limitations. Who will push the state-of-the-art?

Who will teach crystallography courses in the future? I used to offer a graduate-level course once every two years, but as the use of single-crystal analysis has become more widespread in the past 10 years or so, I've been asked to offer this course on an annual basis.

However, as I said earlier, what happens when people like me retire? Many universities now offer x-ray courses taught by professional crystallography staff members, most of whom do a really fine and excellent job. This will of course significantly help "plug the gap", but this practice is by no means universal.

In the macromolecular crystallographic community, with a user base of investigators that is continuing to expand, the situation is just as mixed, ranging all the way from universities that offer crystallography courses on a regular basis, to institutions in which graduate students who use crystallography as a tool simply "pick up" a working knowledge of the technique informally from more senior members of their research groups (typically postdocs), with the research director offering guidance and suggestions when difficult structures appear. In addition, many websites now offer "self-help" internet-based instructions on how to solve a protein structure.

One reason for the present state of affairs, of course, is the undeniable fact that as computers become more and more powerful, and as programs become more and more sophisticated, it is becoming easier to take a "black box" approach to the

solving of a crystal structure without fully appreciating the scientific principles behind what one is doing. This is true in both small-molecule and macromolecular crystallography, and I suspect that it is also true for other related fields such as powder diffraction.

However, it is education in the *fundamentals of crystallography* that I'm worried about. I'm sure that I am by no means the first to express concern about this issue; Dick Marsh and many others have worried about this increasing reliance on a "black box" approach to solving a structure. There is no easy solution to this problem. The IUCr and other institutions (including many synchrotron and neutron diffraction facilities as well as Cold Spring Harbor) help out immensely by having summer schools and "hands on" workshops. The ACA has been trying to address this issue with summer courses covering small molecules (organized by Bryan Craven and Charles Lake) and macromolecules (originally organized by B. C. Wang and his group and currently being run by Andy Howard) and with workshop such as the one on "Crystallographic Educational Policies for the Physical and Life Sciences" organized by Katherine Kantardjieff and the ACA Continuing Education Committee for the Orlando meeting in 2005. At this point I am simply tossing this topic up for discussion, and perhaps we could get our readers' reaction in the form of "letters-to-the-editor" in future issues of *Reflexions*.

Bob Bau



ACA Council: Rear - Louis Delbaere, N. Rao, Lee Groat, Middle: Doug Ohlendorf, Marcia Colquhoun, Bill Duax, Front: Alan Pinkerton, Lisa Keefe, Bob Bau

2007 Art in Crystallography Prize

ACA *RefleXions* Editors are accepting entries to the **2007 Art in Crystallography** contest in the form of images emailed to either editor (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 ACA *RefleXions* from time to time. Judging will be by a panel appointed by the Editors; please let us know if you are interested in being a judge.

Nominations for 2008 ACA Awards

The **Elizabeth A. Wood Science Writing Award**, established in 1997, is given periodically to authors of books or articles that bring science to the attention of a general audience. Nominations are due by July 1, 2007.

Nominations for the **A. L. Patterson Memorial Award** are due by May 1, 2007.

Nominations for the **Margaret C. Etter Early Career Award** are due by May 1, 2007.

Full details describing the criteria for all ACA awards can be found on the website (www.AmerCrystalAssn.org) 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 2008

In the fall of 2007 we will elect a new Vice-President and one person to each of the ACA Standing Committees (Continuing Education, Communications, and Data, Standards and Computing). Suggestions (due by February 1, 2007) may be sent to any member of the Nominating Committee: **Brian Toby** (Chair, brian.toby@anl.gov), **Bob Bau** (bau@usc.edu) and **Jeanette Krause** (jeanette.krause@uc.edu).

The Canadian Division of the ACA will also be electing a new representative to council. Suggestions (due by February 1, 2007) may be sent to **Louis Delbaere** (louis.delbaere@usask.ca).

2007 Dues are Due

Invoices for 2007 dues have been mailed. Please renew promptly and remember to support your favorite ACA Award Funds. **NOTE: It is now possible to renew online at www.AmerCrystalAssn.org**

2007 ACA Margaret C. Etter Early Career Award to Cora Lind



Cora Lind (U of Toledo) received her PhD in 2001 from Georgia Tech where her thesis described her synthetic studies of negative thermal expansion materials using novel sol-gel methods and her extensive characterization of the structural behavior of these compounds vs. temperature and pressure. As a post-doc at Cornell her research focused on the synthesis of complex nitrides and platinum complexes for use in fuel cells. She joined the U of Toledo faculty as an assistant professor in 2003. Her research program, already thriving and productive, is described at her web site (www.chem.utoledo.edu/FAC_INFO/Lind/SOURCE.htm). As an educator, Cora has gained the respect of her colleagues for her enthusiasm and professionalism. She revised the curriculum of the graduate x-ray crystallography course, that had historically emphasized small molecule studies, to include theory and application of several additional methods such as powder diffraction and Rietveld analysis. Since she was called upon to organize a session for a Gordon conference that conflicted with the ACA meeting in Hawaii she was unable to attend but did send two of her PhD students one of whom received a Pauling Prize while the other was a runner-up for the IUCr Prize. As the resident crystallographer at the U of Toledo she also manages the x-ray facility which includes a new powder diffractometer that was obtained through her efforts. Others have already recognized her doggedness, energy and accomplishments; she was recently awarded a CAREER grant from NSF.

2006 ECM Perutz Prize to Eleanor Dodson



The 2006 Perutz Prize was presented to Eleanor Dodson (Univ. of York) at the ECM meeting in Leuven, Belgium in August of 2006 for developing, implementing, teaching and applying the best tools available to produce macromolecular structures of highest quality.

Eleanor Dodson is an internationally known scientist who has made unusual and remarkable

contributions to crystallography. Since her early years working on insulin together with Dorothy Hodgkin, she has been at the center of the mathematical side of macromolecular crystallography and has been developing, implementing, teaching and applying the best tools available to produce science of highest quality.

Throughout her career she been engaged in the methodology of macromolecular crystallography, developing, implementing and applying mathematical and statistical methods for data collection and phasing (molecular replacement), refinement (maximum likelihood refinement of protein structure), and structure validation.

Eleanor is also recognized as one of the leading scientists

involved in the creation and development of the CCP4 program suite (Collaborative Computational Project No. 4 of the UK Research Councils) for macromolecular crystallography, which is now widely used by the crystallographic community throughout the world and has had a global impact on crystallographic science. She regularly tends to queries placed on the CCP4 bulletin board by students and postdocs needing help and has also been a frequent and excellent teacher at a large number of crystallographic schools. She has had a tremendous impact on many young scientists that have had the privilege of learning from her teaching, her experience and from her always open heart and friendly attitude.

Ray Davis Honored on his Retirement from the University of Texas at Austin

Ray (2003 ACA President) and about 40 of his former students, along with family and friends celebrated his 40-year career with a symposium on crystal engineering followed by a banquet/party in Ray and his wife Sharon's honor at the UT Club in Austin April 29th. The symposium, organized by **Bobby Barnett** and **Joel Oliver**, was opened by **Al Tulinsky** (Ray's PhD supervisor) and closed by **Joel Bernstein**, a fellow graduate student and long-time collaborator. Former students and colleagues presented a mix of science and nostalgia during the symposium. The abstracts along with contributed stories and photos were published in a souvenir program booklet (for photos and more information, see bioinst.cm.utexas.edu/davis_sympos/). Ray had a distinguished teaching career during his 40 years at UT-Austin. He co-authored a very successful freshman chemistry text, has been recognized with numerous teaching awards, and was selected as an inaugural member of UT's Academy of Distinguished Teachers. Although this event marks Ray's retirement from teaching, he will continue both to update his popular textbook and his studies on the packing in molecular crystals, with the goal of developing new techniques for organizing molecules in supramolecular arrays. Congratulations Ray!

Marv Hackert



Row 1: Walter Henslee, Bobby Barnett, Ray Davis, Al Tulinsky, Joel Oliver Row 2: Joel Bernstein, Robert Willcott, Hugo Steinfink, Kenneth Nicholas, Ning-Leh Chang Row 3: Robb Wilson, Christer Aakeroy, Pat Rafalko, George Stanley, Evan Kyba, Kraig Wheeler Row 4: Paul Riley, Khalil Abboud, Vince Lynch, Richard Harlow, Mark Frentrup. Photo by Marv Hackert (inset)



IUCr Wins Prestigious International Award for Publishing Innovation

The International Union of Crystallography (IUCr) has won the 2006 Award for Publishing Innovation of the Association of Learned and Professional Society Publishers (ALPSP).

The Award, for Data Exchange, Quality Assurance and Integrated Data Publication (CIF

and *checkCIF*), recognizes the involvement of the IUCr in the development of the Crystallographic Information Framework and its applications, for example:

- standard data definitions for crystallographic information archive and interchange.
- submission format for structure report articles in crystallographic journals.
- standard format for depositing supplementary structural data accompanying publications.
- automated checking of the integrity and self-consistency of crystal structure models (the web *checkCIF* service).
- use of *checkCIF* as a peer review tool.
- dissemination of crystal structural models in online publications and automated visualization.

The judges felt that in developing CIF and *checkCIF*, the IUCr has established an important example of data quality assurance with potential applications in other scientific, medical and social sciences publishing.

The crystallographic information file (CIF) and associated data dictionaries allow the seamless transfer of information from experimental apparatus, through computational analysis, to database deposition and publication. CIF also allows the definition of quality standards for data deposition and publication and the deployment of mechanisms for checking compliance with such standards, via the *checkCIF* web-accessible service. The main features of the standard are its well-defined machine-readable syntax, large collection of individually defined data names and the formalism that allows automatic validation of certain attributes of data. The standard has been extended to assist with routine aspects of editorial checking and peer review, which can now take place with much increased speed and confidence.

The judges were impressed with the way in which CIF and *checkCIF* are easily accessible and have served to make critical crystallographic data more consistently reliable and accessible at all stages of the information chain, from authors, reviewers and editors to readers and researchers.

The development and maintenance of CIF and *checkCIF* is sponsored by several publishers but it is freely accessible to all. The IUCr already works closely with other related structural

science communities and is looking to extend this cooperation.

“The IUCr is honored by the 2006 ALPSP Award for Publishing Innovation,” said Peter Strickland, Managing Editor, IUCr Publications. “The award recognizes the hard work and dedication of our publishing staff and academic collaborators, and the role that learned societies can play in introducing novel and valuable contributions to scientific information exchange. The Crystallographic Information Framework owes much to the special nature of crystallography and its relatively compact community of practitioners but we hope that this award will encourage other scientific disciplines to follow similar approaches to integrating research data and literature, and to extending the tradition of peer review more deeply into the supporting data.”

Brian McMahon (left), IUCr R&D Officer, receives the award from Bernard Donovan, ALPSP President at the Association’s annual dinner.

For more information about CIF and *checkCIF*, please visit www.iucr.org/cif and checkcif.iucr.org.



Andrea Sharpe

Rutherford Medal to Ted Baker

Ted Baker (Director, Maurice Wilkins Center for Molecular Biodiscovery, Auckland, New Zealand) has been awarded the Rutherford Medal, the highest accolade presented by the Royal Society of New Zealand.



Early in his career Ted was a postdoc with Dorothy Hodgkin working on the structure of insulin. Later, after returning to New Zealand, he established the country’s first structural biology program and became the first person outside Europe and America to complete a protein structure.

His current research focuses on *Mycobacterium tuberculosis*, the cause of TB. His group has produced at least 12 new TB protein structures is also developing high-throughput methods of protein expression and crystallization, including the use of robotics.

Ted has also made substantial contributions to the international scientific community by serving as President of the IUCr (1996-1999) and on the advisory boards of the RCSB Protein Data Bank, the World Wide Protein Data Bank (wwPDB) and BIOXHIT.

Ted’s response to hearing about the award was to say “I am delighted to receive this award. It is a great honor for me to be recognized by the Royal Society, and it is a reflection of the great team I work with. Drug discovery is a collaborative effort and is not possible without the excellent science available at the Wilkins Centre and through our international partners.”

James D. Jorgensen (1948-2006)

Jim Jorgensen, a pioneer in the use of pulsed neutrons for diffraction and a scientist with a remarkable gift for penetrating to the heart of the physics of every material he studied, passed away September 7, 2006, after a long battle with cancer. In spite of his illness, he never lost his enthusiasm for the science he loved but continued to be active until the very end, vigorously discussing new results and planning new research directions. His friends and colleagues at Argonne will long remember the dignity with which he conducted himself throughout his final year, never letting his struggle diminish his intellectual drive or sap his keen sense of humor. He will be sadly missed.

Jim was born in Salina, Utah, in 1948, and graduated as Valedictorian from the Brigham Young University College of Physical and Engineering Sciences in 1970. He was awarded the Outstanding Dissertation of the Brigham Young University Department of Physics and Astronomy in 1974. It was then that he joined Argonne National Laboratory in a post-doctoral position, beginning a productive association with the DOE laboratory that lasted for over thirty years. This was a particularly exciting period in neutron scattering at Argonne with the construction of the prototype of a new generation of pulsed neutron sources. During his tenure at the CP-5 research reactor Jim came to appreciate the advantages of the time-of-flight technique for high pressure studies even at steady state neutron sources. On the strength of such experience he directed the design and construction of the first time-of-flight powder diffractometers at ZING-P' and then IPNS, as well as adapting the Rietveld technique to time-of-flight data. The Special Environment Powder Diffractometer (SEPD) that he commissioned in 1981 continues to be an extremely productive instrument to this day, and was responsible for some of the most influential structural studies of the last twenty years. The new generation of powder diffractometers developed at ISIS and SNS are a testament to his vision and foresight.

However, Jim is best known in the condensed matter community not for his instrumental designs but for his scientific achievements. He wasn't interested in solving crystal structures *per se*, but in understanding the insights they gave into a material's properties. His systematic work in exploring the link between structure and the superconducting properties of the cuprates played a critical role in advancing the entire field of high temperature superconductivity. Through this work, he became one of the 100 most cited physicists and was in constant demand as an invited speaker at international conferences, where the clarity of his presentations and the depth of his insights were much admired. He conducted equally penetrating investigations into magnetic superconductors, negative thermal expansion compounds, CMR

manganites, ceramic membranes, and, most recently, the sodium cobaltates.

Among the many honors he received, was the prestigious Bertram E. Warren Award from the ACA, the Charles E. Barrett Award for "outstanding research contributions in powder diffraction," the US. Department of Energy Materials Sciences Research Competition Award for "sustained outstanding research in solid state physics" (twice), and the University of Chicago Award for Distinguished Performance. He was a Fellow of the American Physical Society, a member of the IUCr Neutron Scattering Commission and Vice President of the Neutron Scattering Society of America. As a section leader at Argonne he nurtured the diverse interests and inclinations of the scientists in his group. Perhaps more importantly, he was an inspiring mentor for the many young scientists who came from around the world to work with him. They will ensure that his skills and insights continue to be a vital part of the heritage of the scientific community in the US and the world

Gian Felcher

Martha L. Ludwig (1931-2006)

Martha L. Ludwig, acclaimed scientist at the University of Michigan (UM), died on November 27, 2006. Author of over 70 publications, she was the J. Lawrence Oncley Distinguished University Professor of Biological Chemistry and Senior Research Professor in the Biophysics Research Division. Among her accomplishments during her distinguished career as a protein crystallographer and biochemist were: participation in solving the first enzyme crystal structure in the United States, determining the structure and mechanism of the first vitamin B₁₂-containing enzyme, and development of a new synchrotron beamline for future generations of crystallographers. She is survived by her husband of 45 years, Frederic Hoch, who is Professor Emeritus of Internal Medicine and Biological Chemistry at University of Michigan. Martha was respected and beloved by colleagues and students, and leaves a lasting impact on scientific research at UM and in the field of protein crystallography.

Martha was born in Pittsburgh in 1931 and received her undergraduate degree in chemistry from Cornell University in 1952. She attended the University of California, Berkeley where she received a master's degree in biochemistry in 1955, and earned a PhD from Cornell University Medical College in 1956 under the mentorship of Donald B. Melville. She then moved to Harvard University where she worked as a postdoctoral fellow with



Margaret Hunter and J. Lawrence Oncley. In 1962, following reports of the first protein crystal structure, she “became an early convert to three-dimensional structures” (Hitt, E. (2004). Biography of Martha L. Ludwig. *Proc Natl Acad Sci USA* **101**, 3727–3728) and, in order to learn crystallography, joined the research group of future Nobel laureate William N. Lipscomb. She and her colleagues calculated 2.8 Å and then 2.0 Å-resolution structures of carboxypeptidase A, located the substrate-binding site, and proposed the catalytic mechanism.

Martha moved to UM in 1967 to join the Department of Biological Chemistry and the Biophysics Research Division then chaired by J. Lawrence Oncley. Martha’s research interests included the structural basis of cofactors and metals in enzymes. As an assistant professor, she began collaborating on the first structures of flavodoxin with Vincent Massey whom she considered one of her primary influences (Hitt, E. 2004). Her later structural studies focused on ferredoxin, superoxide dismutase, thioredoxin, flavin dehydrogenase, and phthalate dioxygenase reductase.

In 1991, Martha and Rowena Matthews (Biological Chemistry, UM) began a productive collaboration that continued to the present. In 1994, they published the structure of the vitamin B₁₂-binding module of the multi-domain enzyme methionine synthase. To fully understand how the methylated B₁₂ interacts with the other three domains of the protein to carry out catalysis, individual structures were subsequently solved of the S-adenosylmethionine-binding domain and the homocysteine- and methyltetrahydrofolate-binding domains together. These latter studies also demonstrated how a single mutation in the human methionine synthase elevates homocysteine levels and increases the probability of heart disease.

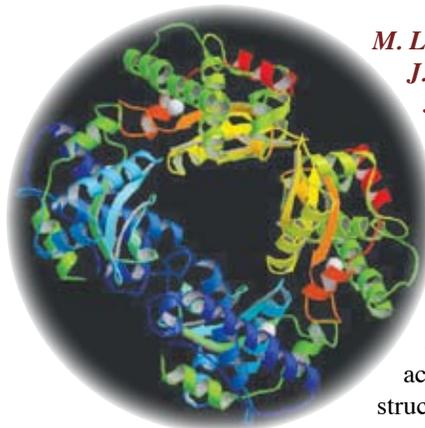
In recognition of her many accomplishments, Martha received the Distinguished Faculty Achievement Award from the University of Michigan in 1986, was elected Fellow of the American Association for the Advancement of Science in 2001, selected as a member of the US National Academy of Sciences in 2003, and as a member of the Institute of Medicine in 2006. She had a strong commitment to training students in molecular biophysics. In addition to serving as chair of the Biophysics Research Division from 1986–1989, Martha initiated the NIH-funded Molecular Biophysics Training Program in 1985 for UM graduate students and directed it for 20 years.

Martha was an outstanding mentor both to students and faculty, and patiently worked with them to overcome scientific or personal problems. She had high expectations for her lab



members and derived much pleasure from their accomplishments. As a teacher, she prepared detailed, handwritten explanations of crystallographic concepts to challenge students in the classes she taught. One of her former students said, “Regardless of rank, all students and Fellows in the Ludwig laboratory receive superb training. No computer program is ever treated as a black box.... She spends enormous amounts of time with each of her students. I remember many five to six hour-long meetings, where we would sit down and write a paper together, or try to figure out why a crystallographic refinement was not working. Graduate students were included in brainstorming sessions about future experiments, as Martha encouraged us to think creatively about her projects. In addition to the training, Martha provided us with many opportunities to speak at national meetings and to network with well

established scientists.” Martha loved looking at and interpreting function in protein structures—marveling at the side chains and carbonyl bulges resolved in early self-contoured maps of carboxypeptidase A, or sitting at the computer display and animating the motions of methionine synthase.



*M. L. Ludwig et al. (1991)
J. Mol. Biol, 219, 335-358. PDBID = 3MDS*

As demand for synchrotron facilities increased in the 1990s, Martha recognized the need to secure adequate beamline access for future Michigan structural biologists. She led a consortium of crystallographers from Michigan institutions and Northwestern University to raise the multi-million dollar funding needed for construction of the LS-CAT beamline at the Advanced Photon Source, Argonne National Labs. Soon to be operational, this project serves as a legacy to her dedication and unselfish commitment to improve the research facilities available to current and future crystallographers.

In conclusion, Martha’s quiet determination, leadership, patience, modesty, and empathy influenced everyone around her and she will be greatly missed.

Mark A. Saper

News from Canada



Canadian Light Source (CLS) News (www.lightsource.ca)

The first CLS Corporate Annual Report, covering the 2005-2006 fiscal year, is now available from the CLS website.

The CLS User's Advisory Committee (UAC) has 12 members with staggered terms. **Grant Henderson** (U of Toronto) and **Ramaswami Sammynaiken** (U of Saskatchewan) were recently elected to three-year terms and Regan Wilks (U of Saskatchewan) was elected as a student representative for two years. **Dean Chapman, Stefan Kycia, and Michele Loewen** have recently completed their terms.

From August 26th to 30th, 2007, the CLS will host the Medical Applications of Synchrotron Radiation (MASR2007) conference (www.lightsource.ca/masr2007). MASR is the premier event of the international synchrotron medical imaging community. This meeting is expected to attract nearly 200 medical research experts from around the world and will be a great opportunity to showcase what will be the most exciting synchrotron medical infrastructure in the world, the BioMedical Imaging and Therapy (BMIT) beamline at the CLS.

Beamlines expected to be operational by January, 2007 include the Far-IR, the XAFS endstation on HXMA (Hard X-ray MicroAnalysis), Mid-IR, PGM (Plane Grating Monochromator), and SGM (Spherical Grating Monochromator).

Two new beamlines (the Canadian Macromolecular Crystallography Facility, CMCF1, and Soft X-ray Spectromicroscopy, SM) are now accepting Letters of Intent from researchers desiring an opportunity to perform exploratory experiments as the beamline is being commissioned (www.lightsource.ca/experimental/intent_letter.php).

Michel Fodje has been hired as a new Beamline Scientist for the second protein crystallography beamline (CMCF08B1), which is a bending magnet beamline being specifically designed for high throughput macromolecular crystallography. Members of the beamline design team have been collecting single-wavelength data sets on the small gap undulator beamline 08ID-1 since May.

A pilot program of the University of Saskatchewan is broadcasting a synchrotron course across Canada. **Ingrid Pickering and Graham George** (Dept. of Geological Sciences) are recording lectures presented for this term's undergraduate/graduate three-credit course. So far they have 33 remote participants from British Columbia to Nova Scotia! The course describes the physical principals, experimental techniques, and data analysis of synchrotron x-ray absorption spectroscopy. Lectures include frequent reference to practical examples in diverse research areas and a review of relevant synchrotron technology. This will equip the student or researcher with a practical working knowledge of the technique and its capabilities (www.usask.ca/its/apreso/geol498_898/).

The CLS received 58 proposals during the last call for proposals (11 for Mid-IR, 19 for HXMA, 6 plus 4 renewals for PGM, and

22 plus 12 renewals for SGM). The proposals will be reviewed by the Proposal Review Committee (PRC) in mid-November with applicants notified soon after.

The CLS welcomed **Bruce Bunker** (Notre Dame) as a new member of the PRC. The PRC evaluates and scores General User proposals for the use of CLS experimental facilities emphasizing the excellence of science based on the quality of scientific research in the context of the field (merit), the suitability of CLS resources being allocated relative to the proposed research (suitability), and the quality and capability of the researchers based on their track record (capability). Committee members serve a two-year term and the Chair serves a three-year term. The other members of the PRC are **Adam Hitchcock** (Chair; McMaster), **Bob McKellar** (NRC Stacie Institute for Molecular Sciences), **T.K. Sham** and **John Tse** (U of Western Ontario), and **Jeff Cutler** (CLS).

The CLS signed a Memorandum of Understanding (MOU) with the new French Synchrotron SOLEIL during a special ceremony held October 5th. "This is the first step towards creating scientific understanding that will be of mutual benefit to both facilities, as there are many unique opportunities at the Canadian Light Source that do not exist at SOLEIL." This is the third MOU to be signed by the CLS and another synchrotron in the last 18 months. Other agreements have included an MOU with the Australian Synchrotron involving research into medical imaging and applications of synchrotron light to the mining sector, and an agreement with the Italian 'Sincrotrone' ELETTRA for the development of a life science imaging program (www.lightsource.ca/media/media_release_20061012.php).

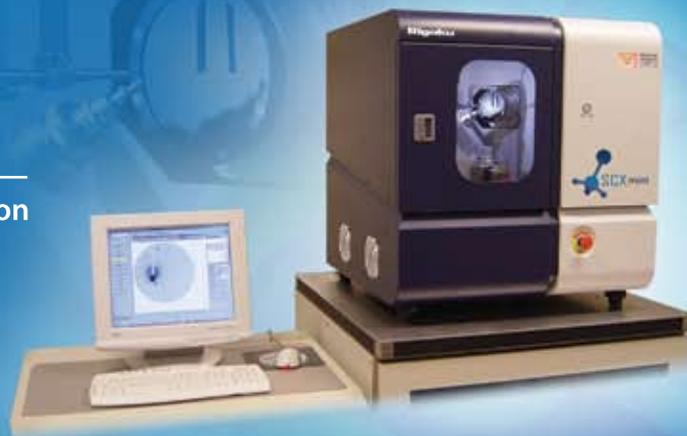
The 10th Annual User's Meeting and Associated Workshops will be held June 16th to 17th, 2007, at the University of Saskatchewan in conjunction with the Canadian Association of Physicists Congress taking place June 17th to 20th.

The Buffalo-Hamilton-Toronto (BHT) 15th Annual Regional Symposium

The Symposium took place on November 3rd at McMaster University. While kept for historical purposes, over the past 15 years the name BHT has become outdated, as groups also participate from Queen's University, Guelph, Western Ontario (London), Rochester, and York University (Toronto). Attendance this year numbered over 100. As in past years, the morning session was a discussion of a technical topic of interest to the community. This year **Bob Liddington** (Burnham Institute) spoke on "Protein Complexes/Protein-Protein Interactions". After his talk, Bob was joined by a local panel consisting of **Gil Privé, Frank Sicheri, and David Rose**, which effectively convinced the audience that there is no guaranteed recipe for attacking this problem crystallographically. While there are a number of techniques for identifying and quantifying association partners, getting them to embrace each other in a crystal lattice is another matter. The afternoon session featured presentations of some very impressive results from trainees, and also provided an opportunity for some new investigators in the region to introduce their programs. Trainees **Dona Ho** (Privé lab), **Des Shahinas** (Christendat), **Andrew Willems** (Junop), **Vladena Hlinkova** (Ling), **Patricia Taylor** (Junop), **Shao-Yang Ku** (Howell),

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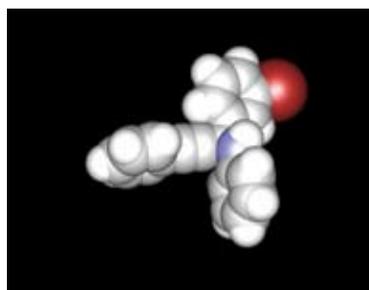
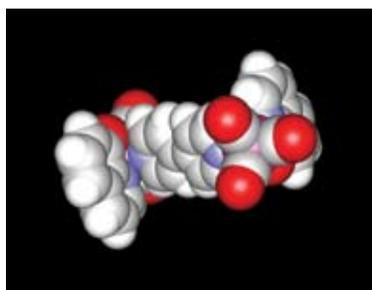
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William Bauer (Umland), **Andrew Torelli** (Wedekind) and **Danielle Simmons** (Malkowski) gave talks on their work. **Gerald Audette** (York) and **Matthew Kimber** (Guelph) gave their first presentations to the community. There was active participation from the commercial sponsors, Rigaku, Bruker AXS, Formulatrix, Qiagen, Axygen, VWR, Molecular Dimensions, and Hampton Research, whose booths were the locations of lively discussions, give-aways and contests.

Member News



Melanie Adams (Supervisor; Z. Jia) was awarded a Governor General's Academic Gold Medal during Spring Convocation at Queen's University. Her thesis was entitled "Structural Approaches to the Functional Annotation of *Escherichia Coli* Proteins". Melanie is now a Postdoctoral Fellow at the Scripps Research Institute in California.



The Canadian National Committee for Crystallography (CNCC)

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

*L.D. Calvert CNC/IUCr Trust Fund
Canadian National Committee for Crystallography
c/o Dr Marie Fraser, Treasurer
Department of Biological Sciences
University of Calgary
2500 University Drive NW,
Calgary, Alberta T2N 1N4*

Travel awards to the Florence 2005 IUCr Congress were granted to **Sung Yeun Choi** (U of Toronto), **Jason Dwyer** (U of Toronto), **Jason Thomas Mayne**, (U of Alberta), and **Elitza Tocheva** (U of British Columbia). More information on the Calvert Trust Fund may be obtained at www.cins.ca/cncc/calvert.html.

The CNCC (www.cins.ca/cncc) met in Ottawa on June 2nd, 2006. The meeting included a report on the XXth IUCr General Assembly and an update on the CLS (**Louis Delbaere**), a report from the Canadian representative to the ACA Council (**Lee Groat**), a report on the Canadian Travel Awards and Poster Prizes programs (**Marie Fraser**), and a report on the decision to propose Canada as the site of the 2014 IUCr General Assembly (**Joe Schrag**). The Committee decided to contact convention facilities in Montreal, Toronto, and Vancouver. This was followed by a broad discussion on support of the crystallographic community by NSERC, CIHR, and CFI. The Committee resolved to draft a letter to the Prime Minister on the lack of funding for technical staff. The meeting ended with nominations of Canadian representatives to IUCr Commissions.

On October 17th representatives from Montreal, Toronto, and Vancouver gave presentations to the CNC in Ottawa. The Committee decided that Montreal would be the best venue to propose for the 2014 IUCr General Assembly. We are now waiting for permission from the National Research Council before moving forward (all international meetings must go through the NRC since they sponsor all of the Canadian National Committees). Documents are being prepared for the NRC President to approve. These include a description of the crystallographic community in Canada, a brief description of what the meeting is about, an evaluation of the financial feasibility by NRC Conference Services, and a description of the organization of committees for putting the bid together and planning and running the meeting.

If everything comes together the proposal will be put forward at the next General Assembly in Osaka, Japan in 2008.

Lee Groat



Web Watch

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

Grant Application Websites in the USA:

National Institutes of Health

grants1.nih.gov/grants/

National Science Foundation

www.nsf.gov/

Petroleum Research Fund

www.chemistry.org/portal/a/c/s/1/acsdisplay.html?DOC=prf/index.html

Camille and Henry Dreyfus Foundation (www.dreyfus.org)

www.rescorp.org

Grant Application Websites in Canada:

Canadian Institutes of Health Research

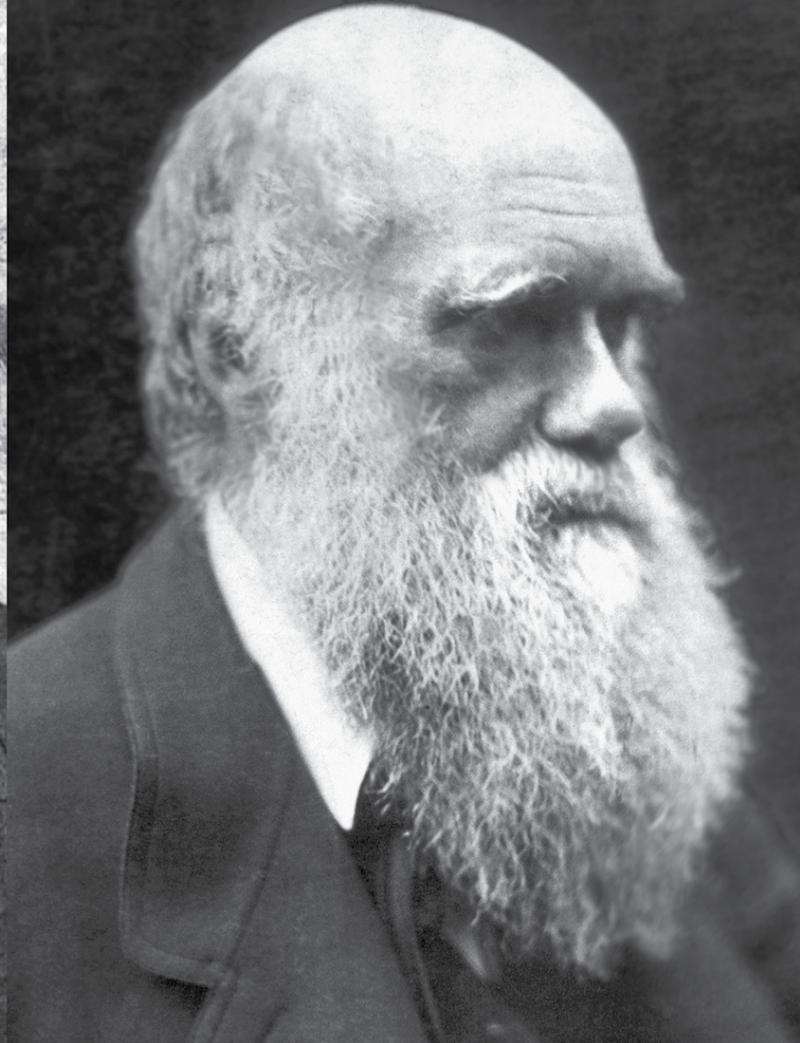
www.cihr-irsc.gc.ca/

Natural Science and Engineering Research Council

www.nserc.ca/

Canadian Foundation for Innovation

www.innovation.ca/



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US National Committee for Crystallography

The Committee met on November 11, 2006 in Washington, DC at the National Academies' Keck Center. The members in attendance were **Jim Kaduk** (chair), **Bob Bau**, **Joel Brock**, **Chris Cahill**, **Bill Duax**, **Frank Fronczek**, **Katherine Kantarjieff**, **Scott Misture**, **Doug Ohlendorf**, **Matthew Redinbo**, **Miriam Rossi**, **Bernie Santarsiero**, **Ronald Stenkamp**, **Cheryl Klein Stevens**, **Brian Toby**, **Victor Young**, **Peter Vekilov**, and NRC staff member **Kathie Bailey Mathae**.

This was the last meeting for **Joel Brock**, **Frank Fronczek**, **Matthew Redinbo**, and **Robert Bau** (ACA President). **Chris Cahill**, **Cora Lind**, **Joseph Ng**, and **Brian Toby** were elected to serve three-year terms as At-Large Members. **Doug Ohlendorf** was elected to succeed **Joel Brock** as Secretary/Treasurer.



From the left: Ken Doxsee (NSF), Frank Fronczek, Cheryl Klein-Stevens, Vic Young, Scott Misture, Brian Toby, Peter Vekilov, Bernie Santarsiero, Doug Ohlendorf, Miriam Rossi, Jim Kaduk, Ron Stenkamp, Chris Cahill, Matt Redinbo

The meeting's agenda focused on two major topics: initiating the process to modify the by-laws of the IUCr and a discussion with **Ken Doxsee**, NSF Program Officer and Acting Program Director, Organic and Macromolecular Chemistry Program, on NSF's perspective on crystallography.

The goals of the proposed changes to the IUCr's by-laws are (i) to add elected representatives of the regional associates to the IUCr Executive Committee, and (ii) to recognize that the General Assembly (GA) is the sovereign body of the IUCr by ensuring that GA holds elections for all the members of the Executive Committee. The USNCCr approved wording for suggested changes to the by-laws, and will begin discussions with other national committees and with the IUCr Executive Committee. These proposed changes will need to be voted on during the next Congress in Japan in 2008 and, if enacted, would take effect at the following Congress in 2011.

Ken Doxsee began with the statement that "X ray crystallography plays a central role in determining unprecedented complexity at unprecedented speed. It is the "eyes and ears" of modern chemistry." His brief overview of the Chemistry Divisions' award portfolio exhibited the breadth and depth of NSF's continuing support of crystallography. Of course, this support is always in the context of a fiscal balancing act juggling instrument acquisition, instrument development, technique development and applications. However, NSF's mission to support basic research is unique among government agencies.

A particular challenge for crystallographic proposals is that our science contributes to all traditional disciplines and does not fall within any single program office. A focus of recent USNCCr efforts has been the development of the curriculum recommendations outlined in *Crystallography Education Policies for the Physical and Life Sciences: Sustaining the Science of Molecular Structure in the 21st Century*. Included in the NIH proposal which funds the math and physical sciences National Committees is a plan to hold a workshop to bring together experts from different crystallographic-related disciplines to discuss ways to better incorporate crystallography in the K-16 curriculum and make more students aware of it as a career choice. Ken encouraged the USNCCr to seek ways to fund its educational outreach efforts, and build on the work so far.

The USNCCr and the US National Committee for IUPAC have made initial contacts, and are beginning to explore some joint projects, especially educational projects. A joint committee meeting next November is likely. Additional interactions with CODATA are also planned. It is important that the USNCCr represent all facets of crystallography-related research. Accordingly (in addition to representatives from the American Association for Crystal Growth, the Microscopy Society of America, and the International Centre for Diffraction Data), the USNCCr will invite the Neutron Scattering Society of America to appoint a representative.

Joel Brock and Jim Kaduk

From the Editor's Desk – The Evolution of *Reflexions*

For some time we have wanted the quarterly ACA publication to become more than ‘just’ a *Newsletter*. While we have no intention of abandoning our core content we do want to expand our coverage into new areas such as, for example, invited feature articles and topic oriented material. Changing the name of this publication to *ACA Reflexions* is part of the process. The first general topic we have taken up is the Anti-Science movement that is trying to infiltrate our public schools with the teaching of creationism. Inspired by discussions at the ACA meeting in Orlando (2005) and Charlie Carter's report on AIP discussions on creationism (summer 2005 *ACA Newsletter*) Connie followed with an editorial on this issue in the fall of 2005 and we have published update columns in every issue since then. The ACA has also become a participant in the Coalition on Teaching Evolution. This issue of *Reflexions* has an article on energy and the environment that Judy asked *Jeff Deschamps* to write after having seen *Al Gore's* movie "An Inconvenient Truth". Jeff has been very active in conservation activities for a number of years and we would like to see him continue to share ideas on this topic. In this issue of *Reflexions* Marc Brodsky presents the AIP position on copyright transfers, another timely topic. We are interested in your opinions on and suggestions for the evolution of *Reflexions* so please send us your comments. We promise to pay attention to all suggestions (including criticism) so don't be shy.

Judy Flippen-Anderson and Connie Chidester

Anti-Science Movement Summer 2006

Only one of five candidates for superintendent of education in *South Carolina* believes that only science should be taught in science classes. The others believe that bogus “critical analysis” and “intelligent design” are OK, with one saying “[evolution] is an active attempt to destroy Christianity.” Two bills up for vote encourage students to “critically analyze” scientific theories. These bills were introduced by the same state senator that last year introduced a bill to allow “alternatives” to evolution to be taught in public school science classes.

In *Kentucky*, the state board introduced the scientific terms “CE” and “BCE” into draft curriculum guidelines for high school and middle school social studies classes. Anti-science attackers insisted that the board also retain the religious notions of “AD” and “BC” alongside the scientific notations.

In *Ohio's* upcoming school board elections, a strong creationist is now being challenged by both a mainline democrat and a green party candidate who may split the liberal vote.

A bill in *Wisconsin* that would have confirmed intelligent design as an unscientific idea not suitable for public school science classes died in the last general session of the state's legislature. A similar amendment within a bill in the Minnesota legislature was introduced but was eventually stripped out before the vote.

An amendment within a bill in *Michigan* that would have made students unfairly learn evidence “for and against” evolution while being required to “critically evaluate” scientific theories was introduced in January 2006 but eventually stripped out.

Two bills were introduced in *Alabama* this session that would have protected the rights of teachers “to present the full range of [sic] scientific views” and that students should not be “penalized in any way because he or she may subscribe to a particular position on any views.” These bills were not confirmed by the end of the legislative session.

A senator in the *Missouri* House's Elementary and Secondary Education Committee introduced a bill this session that would allow the teaching of intelligent design in Missouri. A similar bill was introduced in the senate. The bills eventually died, but are expected to be introduced again in 2007.

A speaker from Answers in Genesis, a fundamentalist Christian group that disputes the theory of evolution and supports a strict Biblical interpretation of creation, spoke to high school and middle school science classes in a *Missouri* town in May. The superintendent was not there, but said that the speaker only spoke about science.

In *Maryland* a legislative initiative would have pushed discussion of “intelligent design” creationism from science classes to humanities classes in public schools. Another bill would have protected teachers presenting the “full range of scientific views, including intelligent design.”

A grassroots initiative to amend the *Nevada* constitution to require public schools to teach “[that] parts of evolution are unproven theories” and various specific points are disputed by “some” scientists was dropped because they could not get enough signatures

Ohio board considers having students learn politically motivated objections to scientific consensus. The Ohio State Board of Education received a proposal to have students critically analyze evolution, global warming and stem cell research. The words “critically analyze” are carefully-chosen keywords by the anti-science movement, who wish students to learn selected arguments against the evidence in evolutionary theory. This proposal was sent in by the same school board member who had previously proposed that students be required to hear about “intelligent design” in science classes. AIP worked with its member society government relations colleagues to develop messages that would help the Ohio board understand the proper teaching of science. Three societies -- AAS, AAPM and OSA - sent a joint letter. AGU prepared a separate letter to send to the Ohio school board, but this letter was put on hold when the board received a new proposal to consider an even more vague definition of “critical analysis” that would still have students learn to criticize established scientific principles inappropriately. While AIP was analyzing this new proposal in order to work with member society GR staff to develop a united strategy, the committee voted to drop the entire issue for the rest of the year.

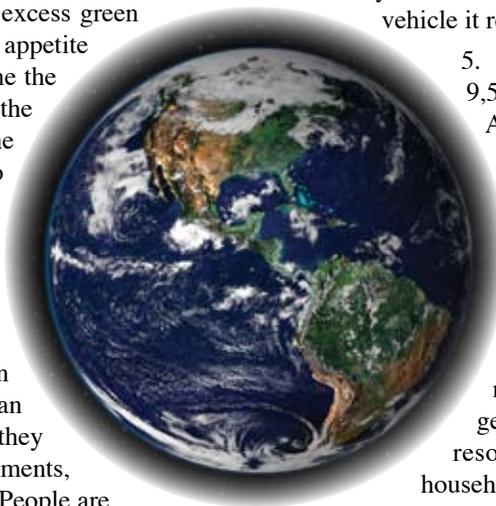
Martha Heil - AIP

Energy, the Environment and the Future

A local workshop on energy held in a Maryland suburb of Washington, DC was well attended and even got some coverage in the local press. This was no surprise – in Maryland many utilities have raised their rates substantially in the past year. The workshop was sponsored by a chapter of the Izaak Walton League of America. The League was formed in 1922 to save outdoor America for future generations. It is one of the oldest conservation organizations in America and almost every major, successful conservation program that America has in place today can be traced directly to a League activity or initiative. Saving energy is more than just a way of reducing your monthly electric bill. In this country fossil fuels (coal and oil) are the source of most of our electric power and are in limited supply. A cornerstone of many League initiatives is sustainability and our current consumption of fossil fuels is not sustainable. The world is facing critical shortages in both renewable and nonrenewable resources. We can not extract and consume these resources at present rates and have any hope of leaving sufficient resources for future generations. The League promotes policies that “generally reduce demand for and consumption of scarce resources” and “encourage resource recovery, recycling, and reuse”. These policies work can work for us as individuals, as well for governments and corporations.

The problems associated with our current use of fossil fuels are not limited to sustainability. Most of the acid rain and atmospheric mercury are the result of burning fossil fuels, and then there are the green house gases. The problem of excess green house gases is intimately linked with our appetite for energy. The more energy we consume the more green house gases are released into the atmosphere. As scientists we recognize the need to change our behavior if we hope to slow or reverse the effects of green house gases in the atmosphere. However, most of us look at this problem as something on which only national governments or large companies can have any real effect.

Since its inception the Izaak Walton League has recognized that people are an integral part of the natural world. As such they are subject to the same natural laws, requirements, and controls as all other animal species. People are unique in that we can alter the biosphere over a relatively short period of time, and we can recognize (sometimes) the consequences of our impact. Despite our preconceived notions there are things we can do as individuals to at least slow the accumulation green house gases. There are many steps you can take to reduce your own energy demands and contribution to emissions of green house gases. A few of these are given below, they are relatively painless, and may also save you some money.



1. Recycle – Landfills generate methane (a greenhouse gas) and waste valuable resources. Thus, recycling will not only recover valuable resources for reuse, but also reduce the production of methane. In some cases, most notably aluminum, recycling is more energy efficient than producing the same material from natural resources. Many cities offer curbside recycling. If your hometown does not have curbside recycling you can work towards getting a program started.

2. Conserve energy – Consider replacing incandescent bulbs with more energy efficient compact fluorescent lights (CFLs). CFLs will cut your energy use for lighting by 75%. When replacing old or worn out appliances look for new models that meet the Energy Star standards. According to the EPA if every American household changed a single light bulb to an Energy Star bulb, it would provide enough power to light more than 2.5 million homes.

3. Plant trees – Trees remove carbon dioxide from the atmosphere as they grow. Combine this with planting perennials and removing part of your lawn and you will save time mowing every week AND reduce the use of a really polluting device, your lawn mower!

4. Buy a more fuel efficient vehicle – Look for models with good gas mileage such as the gas-electric hybrids, which can get up to 50 miles per gallon. Ford, Toyota, GM, and Honda all offer hybrid models, including SUVs that get 30 miles per gallon. The hybrids are also cleaner than their conventional counterparts, so even if your new hybrid only gets the same mileage as the vehicle it replaced it will produce less pollution.

5. Drive less – A typical mid-sized car emits 9,500 pounds of carbon dioxide per year. According to EPA leaving your car home just one day a week can reduce your yearly carbon dioxide emissions by almost one ton. If mass transit isn't for you try telecommuting. Studies have shown that telecommuting improves worker productivity.

6. Buy green power – Some utilities now allow consumers to buy electricity generated from wind and other renewable resources for at least a portion of your household's energy needs.

In order to live in harmony with our natural world we need to develop a sustainable society. In the League's Conservation Policies book sustainability is defined as "...a system that meets the basic needs of all people without compromising the ability of future generations to meet their own life-sustaining needs". To find out more about the Izaak Walton League and their environmental policies and programs (or to join) go to www.iwla.org

Images: 'Earth rise' as seen from the moon and a computer enhanced satellite image of planet Earth downloaded from the NASA website.

Jeff Deschamps

Update - Bridging the Sciences Coalition

The Bridging the Sciences Coalition has made major progress in 2006, with Bridging the Science Programs included in legislation for the National Science Foundation (NSF) and the National Institutes of Health (NIH). In addition, the coalition has been discussing with staff at the National Institute of General Medical Sciences (NIGMS) how to design a mechanism to replace the R21 high-risk grants. While a mechanism to fund research at the interface of the life and physical, mathematical and computational sciences that currently is overlooked has yet to be created, the coalition has successfully raised awareness for the need for such a program and is well on its way to realizing that goal.

National Science Foundation

HR 5356, the Research for Competitiveness Act, passed the House Science Committee in June. This bill includes a "Program to Foster Cross-Disciplinary Research" that would be run out of the NSF Director's office.

While HR 5356 was not passed by the House or the Senate this session, it is likely that competitiveness legislation will be reintroduced in a new Congress especially with the Democrats in a majority. The bill was held up in the House this year by a handful of fiscally conservative Republicans that objected to the authorization of any new programs that had money tied to them.

National Institutes of Health

H.R. 6164, the National Institutes of Health Reform Act of 2006, introduced by Chairman Barton (R-TX) of the House Energy and Commerce Committee, and passed by the committee and full House in September, includes a Bridging the Sciences Demonstration program as well. As at NSF, the Bridging the Sciences Demonstration Program would be housed in the Director's office. It was not clear, at the time this article was prepared, whether the Senate would act on the bill this year since there was so little time left in the Congressional session. ([see 'Breaking News on page 20](#)).

National Institutes of Health, NIGMS

The NIGMS staff is developing a replacement for the R21 high risk grants that were discontinued in March. The committee responsible for creating the new grant mechanism invited Ken Dill, co-chairman of the Bridging Coalition to be a part of that process and to present the Coalition's ideas for funding this type of research. Dill has stressed the need for shorter proposals, diverse review panels, and longer time frames for payoff. Those ideas stem from the meeting held by the coalition in 2004 focused on barriers to funding interdisciplinary and high risk research.

Moving forward, the coalition plans to continue its legislative efforts as well as work with staff at the NSF, NIH, and Department of Energy to create a mechanism to fund the bridging sciences.

Ellen Weiss - Biophysical Society

Fair and Useful Copyright

As Executive Director of the American Institute of Physics (AIP) I often dealt with intellectual property issues, particularly those pertaining to copyright. Earlier in my career, as an author eager to report my research results to colleagues, copyright was just one more form to fill out en route to getting my paper published. If I thought about it at all, I probably just assumed that the publisher, usually a society to which I belonged (over the years, I have been a member of six of AIP's ten member societies), needed me to transfer copyright in order to protect my work in some way. I probably thought it was for my benefit more than anyone else's. While that turns out to be true, it is also an oversimplification of what, in the modern world of electronic dissemination, is a very complicated and controversial issue.

Since coming to AIP in the fall of 1993, just as the first widely available web browsers stimulated electronic distribution of articles, I have learned more about copyright than any scientist or engineer should care to know. Nevertheless there are a few basic concepts all authors should understand because the future of their societies may depend on their decisions.

An important issue confronting learned society publishers and authors today is: Who should own the copyright of published articles and what rights should be given, by license or otherwise, for the pre- and post-publication use of those articles? There are many aspects of this issue, some legal, but others which are matters of policy, fairness, usefulness, economics and the viability of peer review and scientific publishing itself.

Aspects of copyright law, while complicated and often costly, are relatively simple compared to the policy and economic issues. The basis of copyright law in the United States stems from Article I of the U.S. Constitution which empowers Congress "To promote the Progress of Science and useful Arts, by securing for limited Times to Authors and Inventors the exclusive Right to their respective Writings and Discoveries." It is interesting to note the matched goals of this constitutional stricture to promote the progress of science and the AIP charter to advance and diffuse "the knowledge of the science of physics and its applications to human welfare, and to this end ... to undertake, among other measures, the publication of scientific journals." Internationally, the 1971 Berne Convention for the Protection of Literary and Artistic Works provides the basis for copyright law in most countries today. Congress and other legislatures throughout the world have created a system of property and moral rights for authors and their publishers. While granting exclusive rights to control reproduction and distribution of copyrighted works, there are exemptions for what is called "fair use" in the U.S. and "fair dealing" in the UK and parts of Europe. The most obvious fair use is the right to quote from or refer to published works. Also, copyright only protects original, tangible forms of expression and not ideas or data. Ideas or facts can be used by anyone, although in our fields it is expected that suitable attribution is always given. The Berne Convention gives a three-step test to countries that might want to allow some exceptions to copyright protection, namely: (i) if it is a special case; (ii) if it does not conflict with a normal exploitation of works; and (iii) if it does not unreasonably prejudice the legitimate interests of owners of rights.

So what exceptions are fair and reasonable and legal?

For journals, some cases are easy. Most journals allow authors to distribute preprints or reprints of their articles to colleagues. Similarly if a scientist reads something of interest, it is generally acceptable to give or send a copy to a collaborator, student or colleague and say have a look at this. In lieu of a subscription, it is not fair use to regularly ask a subscriber to send copies of articles. It is not acceptable for organizations to make systematic copies for distribution to their employees, students or customers without permission of the rightsholder. There are many complicated issues in the middle ground. How often can one library subscribing to a journal copy articles for another that does not pay for a subscription? This is sometimes called "Inter-Library Loan" (ILL), analogous to loaning physical copies in the days before easy copying. Can a library charge for ILL? Can libraries sell copies (Documents Delivery or DocDel) to its patrons? Who is a library's patron? Is it anyone in the world making a request via the web? Who determines what rules apply?

While the pre-web era was somewhat more straightforward, even then there was controversy over just how much ILL was acceptable. Some voluntary guidelines were established in 1978 (*Final Report of the National Commission on Technological Uses of Copyrighted Works*, July 31, 1978, Library of Congress, Washington, DC 1979, pages 54-55). While helpful, these guidelines are not always well understood or followed. Realizing that the World Wide Web was enabling much easier use and reuse of copyrighted works, a new Conference of Fair Use (CONFU) was convened. After 2½ years of extended discussions and proposed guidelines, it was unable to reach a consensus between users who "thought the guidelines were over restrictive and copyright owners [who] thought they were giving away too much." It ended in failure in 1997 (www.utssystem.edu/ogc/INTELLECTUALPROPERTY/confu.htm). I think today, many in either group would be happy with such reasonable guidelines.

Legal issues aside, what is the value of copyright for learned societies? Does it help sustain the valuable role of society journals in promoting the dissemination of information to the widest possible audiences of interest?

In my mind there is no question that for AIP and its member societies, the transfer of copyright from author to publisher is a very positive ingredient for a scientific journal. It gives the society important freedom of action available no other way. For example, it reduced the fear of legal complications when we scanned, digitized and posted online the articles from all our journals back to Volume One, Issue One. While perhaps the risk to us was small, some publishers in other fields who only had licenses and not copyrights were sued when they digitized older articles (U.S. Supreme Court, *New YorkTimes Co. v Tasini* (2001); U.S. 11th Circuit Court of Appeals, *Greeberg v Nat'l Geogrpic* (2001)). In other cases, where some document delivery services were reselling articles from our journals, it was essential to have the copyright transfer forms in order to file legal cases to protect the journals. If instead of a transfer, journals only had a license, then protection against misuse would be much more difficult to pursue.

On the other hand, there are those who say that authors should retain copyright and only license certain non-exclusive rights to the publisher. Having viewed in detail some of the proposals

(For example, web.mit.edu/ocwhq/pres/facpack/Amendment_to_Pub_Agreement.pdf) they contain terms that would undermine the subscription value of a journal by allowing posting on any site for any purpose, commercial or not, that might compete with the journal. AIP and many of its Member Societies already grant many author rights, including postings of their own articles on free-access, non-commercial e-print servers (ftp.aip.org/aipdocs/forms/copyright.pdf).

But these are only illustrative details. The big picture is that much of the current discussion on copyright is intertwined with debates on open access, mostly driven by four very important forces:

- Libraries, whose budgets cannot keep up with growth of research and materials that they and their patrons want;
- Ideologues, who feel that "information should be free;"
- Funding agencies assert that if publications result from research they support, then they should be able to mandate free access to those publications without paying for the reviewing and editing costs incurred by publishers;
- Technologies, which lower some of the barriers to entry for publishing and which make it easier to post copies of almost anything. It is incorrect to assume that electronic publishing is cheaper than print publishing. The submission, review and editorial costs are the same. For AIP, the print-specific costs – printing, binding, shipping and mailing – total less than 15% of the overall production costs. Even if there were no print, the extra production costs for electronic-specific production, such as tagging and linking, more than eats up that 15%.

As a consequence of these forces, there are many who would like to see publishers of costly journals fail, and attacking copyright has become one element of a strategy towards that end. While not as costly on a per article or per page basis as most commercial publishers, learned societies journals are being swept along in the wave of populism that threatens copyright and the right to choose business models most appropriate for any given society journal.

As authors contemplate their reaction to requests to transfer or retain copyright, it pays to think about what problems we are trying to solve. Will author retention of copyright result in wider promotion, dissemination and acceptance of their results? The answer is not likely. This is because publishers not only add value by peer review and editing, but they also brand, market and distribute journals to audiences that recognize the value of reputable journals. Yes, these journals are costly to subscribe to. They are also costly to produce, distribute and maintain. AIP and its member societies have embraced new technologies and have launched many new pricing models which have kept prices as low as possible while sustaining the financial viability of our operations. The result is that more authors submit to our journals and more researchers, educators and students have access to them and use them more effectively than at any previous point in history. Copyright ownership by the societies has helped create that wide dissemination that advances our fields.

Marc H. Brodsky, Executive Director, AIP

Fall 2006 Meeting of the AIP Governing Board, San Francisco, November 11-12, 2006

The meeting, together with a meeting of the AIP Executive coincided with the annual meeting of the American Vacuum Society and the AIP co-hosted the Industrial Physics Forum on Nanotechnology in Society and Manufacturing (www.aip.org/ipf). I did not attend, but several of the featured topics were quite interesting, including the report from an MIT physicist who has exploited a previously unappreciated cranny in the theory of electromagnetic fields to produce non-radiative fields capable of transmitting energy into a room for the purpose of recharging batteries in laptops and other electronic devices. Although a stretch, it doesn't seem totally out of the realm of possibility that the ACA might at some point want to sponsor a similar forum in connection with one of its meetings.

The AIP is evolving significantly in several areas. The CEO of the AIP for the past 13 years, Marc Brodsky, who has transformed the organization in very positive ways. will be retiring next year. Among the many things that Marc accomplished was his rescue of the \$65 million publishing arm of the AIP from a downward spiral into restored profitability. They publish a dozen or so journals in many branches of physics. AIP journals, though of premier quality, were facing serious challenges from commercial publishers going through the rounds of cannibalism that seems to afflict almost all industries. Among other pleasant surprises, the AIP has had growing penetration into the market of publishing conference proceedings. They are doing both printed and online versions at very competitive prices.

The publishing industry is also faced with very significant intellectual property issues, because of the rapid growth of electronic access. Marc Brodsky has written an eloquent statement of both sides of the intellectual property issues (*see preceding article by Marc Brodsky*). These issues pose a serious dilemma and may eventually cripple scientific publishing.

The profitability of publishing during the last three years has meant that the AIP can devote more resources to its public service activities, which are the province of the Physics Resources Center. A major decision made in San Francisco was to endow and sustain a fund whose proceeds will eventually assure continuation of PRC activities, even if the publishing endeavor eventually shrinks.

PRC activities include several of interest to the wider community and hence to the ACA membership. The Society of Physics Students has initiated a program to have undergraduate members attend and report on the national meetings of member societies. The report for the Honolulu meeting arranged with the assistance of Katherine Kantardjieff and written by Jeremy Kowalczyk, is well worth reading. It can be found at: www.spsnational.org/meetings/reports/2006/aca06.htm. Jeremy's report is also included in the fall issue of *RefleXions*.

The PRC history website has several outstanding pages, including a very clear and comprehensive history of the discovery of global climate change by Spenser Weart: www.aip.org/history/climate/. At the same site, there are quite a number of celebrations of notable physicists, including Einstein and Heisenberg. These, too, are highly recommended.

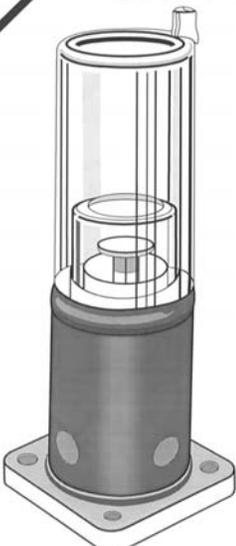
The Governing Board voted on the historic election of a black physicist, Quinton Williams, to serve as an At-Large Member. This question had been debated for several years. The National Society of Black Physicists (NSBP), after a decade or so of associate membership, actively sought status as an AIP member society, despite failing several of the constitutional requirements. At the long-range planning meeting of the Executive Committee in September, the NSBP made two presentations that served to identify a significant gap between what their constituency needed and what AIP was doing. Two initiatives, the nomination of Quinton Williams to an at-large membership of the Governing Board and the creation of a Physics Diversity Council under the Physics Resources Center, were approved. The NSBP has the personnel, contacts, knowledge, and ideas necessary to channel bright students from historically black colleges and universities into good PhD programs. The hope is that having Williams on the Governing Board will facilitate two-way communication that will help the NSBP grow toward full membership.

Several of the member societies already have active programs to serve minority constituencies, and these provided the initial context of the Physics Diversity Council. The ACA apparently does not have explicit programs to enhance diversity, and the Council might consider appointing a representative. The contact at the PRC is Jim Stith (jstith@aip.org).

Charlie Carter

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ACA 2006 Election Results

Vice President
Marv Hackert

Treasurer
Bernie Santasiero

Communications Comm.
Alice Vrielink

Continuing Education Comm
Bill Furey

Data and Standards Comm.
Winnie Wong-Ng

Canadian Division
Chair: David Rose

SIGS

Biological Macromolecules
Chair-elect: Carrie Wilmot
Secretary: John Tanner

General Interest
Chair-elect: Allen Oliver
Secretary: Jeanette Krause
At-Large: Nathan Coker

Industrial
Chair-elect: Herbert Klei
Secretary: Sue Byram

Materials Science
Chair: Branton Campbell

Powder Diffraction
Chair-elect: Cora Lind

Service Crystallography
Chair-elect: Peter Mueller
Secretary: Bruce Noll

Small Angle Scattering
Chair: P. Thiyagarajan
At large: Alec Sandy

Small Molecules
Chair-elect: Kraig Wheeler
Secretary: Allen Oliver

Synchrotron Radiation
Chair-elect: Richard Gillilan

Young Scientist
Chair-elect: Peter Horanyi
Secretary: Mark Collins

Synchrotron SIG Constitutional
Amendment: passed

Marv Hackert, Vice-President


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

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

Statement: I am honored to have been elected as your next Vice-President. The ACA means a lot to me – it is both an important scientific organization and a fraternity of scientific friends and colleagues. In the nearly forty years that I have been part of the ACA, I have seen it grow from a relatively small, low-budget operation that met on university campuses where attendees were housed in

dorms, to a larger, more professional organization with over two thousand members and annual meetings attended by nearly 1000. Our larger size has enabled us to hire staff responsible for taking care of many of the day-to-day business matters of the organization, thereby enabling the Vice-President and President to concentrate on administrative and policy decisions.

In addition to being a member of the ACA Council the Vice-President serves as an ACA representative on the USNC/Cr, assists the ACA President in making policy decisions, provides input for the site selection for our annual meetings, and assists with appointments to various ad-hoc committees.

As your Vice-President, I will use my breadth of research and administrative experience to assist the ACA in meeting its goals while at the same time working to ensure that the ACA serves the needs of all its members. The ACA has always been an inclusive organization – recognizing the central role that structure determination plays in a wide variety of fields and appreciating the benefits that we all gain from our interactions with each other at our annual meetings.

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

Our annual meetings need to remain the centerpiece of our efforts. Their success has always been due to the dedication of our members who readily step up to the plate when asked to help organize sessions, serve on committees, and volunteer their time and expertise in a variety of ways. My experience on the local committees of two ACA meetings will serve me well when making future decisions to ensure that our annual meetings are intellectually stimulating, a good value for our members, and a means to attract new members. I will work to promote joint meetings involving other organizations as appropriate.

The ACA needs effective means of communicating to ensure that its members can

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

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

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

Bernie Santarsiero - Treasurer



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

Research Interests: My research spans four major themes: structure-based drug design of therapeutics against disease, identification of natural products

as chemopreventative and anti-cancer agents, manipulating of enzymes to modify specificity, stability, and reactivity, and the development of enabling technologies in biological and chemical crystallography for high-throughput structural genomics.

Statement: The ACA Treasurer serves the membership by overseeing the financial commitments of the organization and as a member the council. The ACA must be fiscally stable. We should continue to keep dues and conference costs as low as possible while still providing the resources necessary to host interesting meetings by choosing sites wisely and organizing excellent scientific programs. The council should continue to broaden the appeal of membership in the ACA, and to foster physical, chemical, and biological crystallography education on a national and international scale. I am a strong advocate for education, sustained government support of our research, and the continuing vision of molecular structure as a unique portal towards the understanding of function, reactivity, and energetics in physical, chemical, and biological systems. On a personal level, I have been a member of the ACA for over twenty years, and thoroughly enjoy attending the annual meetings with long standing colleagues and new acquaintances. I was honored to be nominated and look forward to "giving back" something to the organization.

Winnie Wong- Ng Data, Standards and Computing Committee



Ceramics Division, National Institute of Standards and Technology (NIST).

Research Interests: Crystallography, crystal chemistry, phase equilibria, and structure/property relationships of high temperature materials; standard reference materials; reference x-ray powder patterns; single crystal and powder diffraction crystallography; high-temperature x-ray diffraction; superconductors; thermoelectric materials.

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

In my view, four particular activities would be important to pursue: 1) due to the advent of computer technology, an increasing amount of crystallographic software is available, and it is important for developers to maintain adequate documentation and to make source code available so users can modify it for local needs; 2) in addition to the availability of macromolecular information from high throughput techniques, a vast volume of other diffraction data will soon be available due to the increasing importance of the combinatorial approach in materials research, an area that I am also involved with. To be able to access this large volume of diffraction data, various computational strategies and standards are critical for data collection, storage, transport and exchange; 3) communication and cooperation between creators/producers of crystallographic databases and those responsible for databases of other properties are important in order to maximize research opportunities for users; 4) user training in utilizing various databases, in recognizing existing standards and in using various crystallographic computing software, is critical for crystallographers in today's computerized world.

I plan to work with the Committee and the ACA to push forward the above activities, namely, to encourage cooperation between the various database producers, encourage software developers to maintain good documentation, promote crystallographic informatics as an area of importance, and encourage the ACA to

continue organizing workshops/symposia to address applications and issues related to data, standards and computing topics, in both macromolecule and small molecule crystallography.

Bill Furey, Continuing Education



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

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

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

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

Alice Vrielink, Communications



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

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

Statement: I am honored to have been elected to the Communications

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

The NIH Reauthorization bill, “National Institutes of Health Reform Act of 2006,” passed the Senate on December 8, 2006. The bill includes two demonstration programs of special interest to many ACA members.

“Bridging the Sciences Demonstration Program” authorizes the Secretary of HHS, acting through the Director of NIH, in consultation with the Director of the NSF, the Secretary of Energy, and other agencies, to award grants for demonstration projects for biomedical research at the interface between the biological, behavioral, and social sciences with the physical, chemical, mathematical, and computational sciences.

“High Risk, High Reward Research” project for NIH to allocate funds to award grants, contracts, or engage in other transactions that foster scientific creativity and increase fundamental biological understanding leading to the prevention, diagnosis, and treatment of diseases and disorders.

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Second Meeting of the AACr (Asociación Argentina de Cristalografía), Puerto Madryn, Chubut, 25-27 October, 2006

Approximately 40 participants gathered for the AACr II meeting in Puerto Madryn (a city in the province of Chubut in Argentine Patagonia). The place had been chosen during last year's assembly because of its natural beauty and to accomplish the aims of the association: to disseminate crystallography around the country, to promote its understanding and to strengthen already existing groups, especially those working far away from the main scientific centers.

The meeting was scheduled on a rather flexible basis; invited speakers delivered top level short courses that alternated with more in-formal talks where students and younger scientists showcased their achievements and conveyed their enthusiasm. Afternoons were mostly dedicated to poster sessions.

The invited speakers were **Eduardo Granado** (LNLS and UniCamp, Campinas, Brazil), **Iris Torriani** (Vice-president of the IUCr, LNLS and UniCamp) and **William Duax** (HWI and Immediate Past President of the IUCr). Participants were disappointed to miss Bill Duax as a last minute inconvenience prevented him from attending.

Eduardo Granado gave a short course, "Solving and refining crystal structures with high-resolution synchrotron x-ray powder diffraction data", covering some of the possibilities opened up by using synchrotron radiation to study crystalline powders. He discussed several relevant aspects of the geometry, data collection and analysis, and applications of synchrotron x-ray powder diffraction, using examples taken from his experience at the XPD beam line at LNLS. He described aspects and capabilities of the LNLS beam line, including possible sample environments for *in-situ* phase transformation studies. He used the *ab initio* determination of the $\text{BiMn}_2\text{O}_{5w}$ crystal structure to describe some freeware programs that can be used to find accurate peak positions, determine the space group, analyze the profile lines, and solve the structure from direct methods. He showed how the analysis of the temperature-dependence of the powder diffraction profile of $\text{BiMn}_2\text{O}_{5w}$ revealed subtle lattice anomalies that could be related to a ferroelectric/antiferromagnetic transition at $\sim 37^\circ \text{K}$. With this example he illustrated the usefulness of high-resolution synchrotron data for studying the subtle structural transformations that may be associated with electronic and/or magnetic phase transitions, and how such transformations may give important

clues on the physics of the studied compounds.

Iris Torriani also gave a short course: "Small and Wide Angle Scattering: Applications in Materials Research". She started from the very beginning and went through the fundamental principles of monochromatic x-ray elastic scattering produced at low angles when samples contain inhomogeneities (particles) in the 1-100 nm scale range. Then, she discussed the potential provided by synchrotron radiation dispersion and diffraction techniques, especially when combined with other techniques, to study the structure of matter at the atomic level, to analyze macromolecular systems, biological molecules and polymeric materials. To illustrate her points she discussed some real-time experiments, especially designed in her group at the LNLS to detect phase transitions, to perform 2D detection in macromolecular systems

when the samples present some type of orientation and to simultaneously obtain x-ray scattering data (at small and wide angles), calorimetric (DSC) measurements, and experimental data resulting from applying magnetic fields. She showed that this combination of methods and measurements proved to be very important in the development of new materials.

Miguel Harvey (graduate student from Universidad Nacional de la Patagonia San Juan Bosco) talked about "Coordination compounds of group XII metals complexed to sulfur(VI) oxoanions and nitrogenated ligands: a systematic study". He used the structural characterization of approximately 20 newly synthesized compounds to describe his efforts to find regularities in the coordination spheres and packing schemes. Starting with well developed concepts like the *Bond Valence* he arrived at a new model extending the scope of the original ideas, the so called "Vectorial Bond Valence Model", that could lead to a simpler description of complex binding geometries and he showed its applicability to simple systems.

Máximo Barrera and Sebastián Klink (graduate students from Fundación Instituto Leloir, Buenos Aires, Argentina) enthusiastically talked about their experiences in "Protein X-ray crystallography: combining molecular biology, chemistry, physics, statistics and heavy computer calculations". They presented all the steps involved in the process from genes to the final structures. They focused on gene cloning, protein expression and purification, crystallization, sample preparation, x-ray diffraction measurement and processing, structure solving and manual and computational refinement. Additionally, they described their experiences at the Brazilian (LNLS) and the



Brookhaven (NSLS) synchrotrons.

Daniel Vega (Grupo Materia Condensada, Centro Atómico Constituyentes, Unidad de Actividad Física, Comisión Nacional de Energía Atómica, Buenos Aires) spoke on: "Application of PXRD in the quantification of polymorphs of pharmaceutical interest". He called attention to the current use of different aspects of crystallography in the pharmaceutical industry. He discussed detection and quantification of polymorphs, both in small laboratory samples and commercial products. He gave examples related to generating standards, identifying the so called *analytic peaks* and the different analytic methods used to evaluate the results obtained. He also presented the advantages and disadvantages of each of the methods in relation to the pharmaceutical products under study in his group.



Two evening talks were dedicated to invited sponsors. **Oswaldo Maldonado** (Bruker AXS) presented some technological innovations in XRD and **Iris Torriani** took the audience back to the founding of the IUCr and the launching of *Acta Crystallographica* and the *International Tables of Crystallography* to the time that the first crystallography laboratories were established in South America. Her talk was enhanced by some remarks by Maria Benyacar, one of the pioneering crystallographers in Argentina. Mary was a member of the old Argentina Crystallographic Committee and she worked with Galloni who, as far as we know, was the first one in Argentina to publish a paper on a crystal structure.

Very enthusiastic explanations and interesting discussions took place at the poster session; there were 35 posters covering diverse topics: preparation, characterization and properties of nanostructures, nanopores, nanotubes and films; irradiation damage; geological and archeological investigations; new drugs; bio-materials and protein and enzyme structure determination.

The General Assembly, though informal because a main power shortage forced a move to the cafeteria facing Golfo Nuevo and its deep blue sea, was nonetheless very productive. Main topics addressed were: ACA membership and its benefits, which laboratories will be awarded with a one year subscription to the IUCr Journals, and the necessity of taking the proper steps to become an official Association including deadlines for the approval of the by-laws. The convenience and difficulties of meeting every year were discussed and it was decided to continue with annual meetings at least until the association grows in strength and numbers. The next meeting will be San Luis because of its central location. It was decided that the best solution for continuing the program of expanding crystallographic education for researchers far away from the main scientific centers

would be the development of a web course followed by a week of laboratory training. Many of the participants were eager to be involved in that project. The outcome of the meeting could not have been better, and the enthusiastic response of the attendants forecasts many more successful meetings to come.

An unplanned summit took place the day after the closing remarks when most of the participants could be seen riding boats at Puerto Pirámides and enjoying the marvellous blue of the sea and the splash of the offspring of Southern Right whales jumping around their mothers.



Meeting organizers: Sergio Baggio, Graciela Punte and Ricardo Baggio

Many thanks to the sponsors (ANPCYT (Agencia de Promoción Científica y Tecnológica, Argentina), IUCr, CLAF (Centro Latinoamericano de Física), Bruker AXS, and ALUAR (S.A) for the financial help that supported almost 60% of the participants in their travel and lodging expenses. Local academic centers, CENPAT (Centro Nacional Patagónico) and UNPSJB (Universidad Nacional de la Patagonia San Juan Bosco) kindly and disinterestedly provided the required infrastructure.

Seen in the inset: Iris Torriani talking things over with Griselda Polla, Patricia Konig and Gabriela Leyva.

Graciela Punte

2006 ACA Summer Course on Small Molecule Crystallography

The course was held on the Indiana University of Pennsylvania campus July 10th through July 19th, 2006. The 10-day course covered both single crystal and powder diffraction and included 8 days of instructions (lectures in the morning, workshops in the afternoon and computer tutorials at night), a day trip to Pittsburgh to visit Duquesne University, the Carnegie Museum and the Church Brew Pub and a final day allotted for student presentations. This year twenty students representing five countries attended (2 from Canada, 1 from Columbia, 4 from Brazil, 1 from Korea and 12 from the United States). Our highly dedicated teaching staff included 14 individuals from academia, national labs and industry. The major goal of the ACA course is to teach the basic principles of crystallography. This is sorely needed for there has been a steep decline in the number of chemical crystallographers amongst university faculty, but a rapidly increasing demand for crystallographic information. Technical training in the use of instrumentation appears to be readily available but a scientific education in the basic principles is not. The Small Molecule Course at IUP is designed to fill this void. On the final day, 17 of the 20 students completed evaluation forms. The feedback from these evaluations has been instrumental in the continuing growth and development of the course at IUP since 2003. 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.

This year, Rigaku-Americas Inc. loaned a MiniFlex powder diffractometer (supported by *Lori Fields*) and an SCXmini benchtop x-ray crystallography system (supported by *Lee Daniels*) for use in the experimental sessions. The students and faculty are very grateful to *Joseph Ferrara* and *Thomas McNulty* (Rigaku-Americas Inc.) for showing such strong support. We also had access to a Bruker APEX II diffractometer located at Duquesne University (run by *Nathan Takas*) and our in-house Bruker D8 Advance powder diffractometer. Both companies loaned their proprietary software for use in the tutorial sessions. It is very obvious that Rigaku Americas Inc. and Bruker-AXS Inc. care about the health and vitality of the crystallographic community. We are also grateful to *Scott Field* (Cephalon, Inc.) for allowing us to recruit the indispensable services of *Curtis Haltiwanger*.

Our lecture series consisted of over 22 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 highly rated by the students. This year our workhorse lecturers were *David Duchamp* and *Jenny Glusker*. Their knowledge of basic crystallography and their abilities to disseminate this information is truly impressive! *Jen Aitken* not only allowed us to use the Duquesne APEX II instrument, but also took time out of her busy schedule to contribute to our lecture sessions. She presented an outstanding introduction to powder diffraction. This year, we were extremely fortunate to have *Sue Byram* visit to present a lecture on diffraction instrumentation. As always, she was a model of professionalism and competence. We were very pleased that she wished to contribute as a lecturer for she has been one of strongest supporters of the course since its inception in 1992. *Lee Daniels*, besides his many other contributions to the course, lectured on collecting accurate intensity data. *James Kaduk* and *Brian Toby* lectured on advanced topics in powder diffraction and showed their usual excitement and tremendous dedication to the field. We also had the good fortune of having *Bob Blessing* lecture on Shake and Bake and advanced topics in direct methods.

Front Row: Beth Leverett, Brian Toby (with the neon green hat!), Lori Fields, Jenny Glusker, Solemar Oliveira, Rogério Salloum, Il-Hwan Suh, Charles Lake Middle Row: Louise Dawe, John Woolcock, Nachiappan Arumugam, Peter Mueller, Karah Knope, James Kaduk, Chenguang Li, David Duchamp, Eric Diede, Corneliu Stanciu, Jonathan Lekse, Lee Daniels, Julie Collins, Adam Beitelman, Tayo Ikuton Back Row: Wenqian Xu, Lincoln Romualdo, Jose Luis Pinto, Curtis Haltiwanger, May Nyman, Bryan Craven



This year, our tutorial and experimental sessions were well received. We had excellent computer support provided by the IUP College of Humanities and Social Sciences. The success of these sessions was due to the tremendous work done by *Curtis Haltiwanger*, *Peter Mueller* and *Lee Daniels* who presented a very well received series of tutorials on SHELX and the amazing powder diffraction duet of *James Kaduk* and *Brian Toby* who ran a set of tutorials including indexing powder patterns, the use of GSAS/EXPGUI and Rietveld analysis. We would especially like to thank Brian for taking the time to assist us even though it was in the middle of his move to Argonne National Lab. Our resident database expert *John Woolcock* presented tutorials on the use of the CSD and PDF databases. *David Duchamp* gave a tutorial on his powerful CRYSTMOL structure evaluation software and gave all participating students a licensed copy. *Adam Beitelman*

presented a tutorial on Mercury with permission of the Cambridge Crystallographic Data Centre. The experimental sessions were highly successful due to the indefatigable duo of *Lee Daniels* and *Lori Fields* who worked with the students into the wee hours of the morning and made indispensable contributions!

The organizers and students are grateful for the direct financial support donated by the ACA, USNCCr, PDS, Bruker-AXS, Rigaku Americas and IUP. Their generous donations allowed us to grant scholarships to all graduate and undergraduate students who registered before the deadline. The USNCCr donation also covered travel awards to gifted South American scholars.

Many thanks to *Pat Craven* for organizing the class picnic and to *Jonathan Lekse* for being the dedicated grill master. Finally, thanks to *Adam Beitelman* and *Beth Leverett* (IUP Chemistry students) for volunteering to take care of the attendee's and providing van service to the students and faculty. Adam was also instrumental in setting up the computer laboratory for the tutorials. Overall, we feel that the course at IUP was very successful and achieved all its goals. In Summer 2007, we are planning on offering the Small Molecule Course again at IUP with the tentative dates of July 8th – 18th, 2007.

Charles H. Lake and Bryan M. Craven

2006 ACA Summer School in Macromolecular Crystallography:

The annual ACA Summer School in Macromolecular Crystallography was held at Illinois Institute of Technology (Chicago, IL) and the Advanced Photon Source (Argonne, IL) from Monday 10 July through Saturday 22 July 2006. The school is designed for upper-level graduate students and postdoctoral researchers, but we have accepted lower-level graduate students and industrial scientists successfully over the four years that the school has operated at IIT and the APS. The 2006 school included 22 lectures by eminent crystallographers and qualified graduates of our own program, plus extensive chemistry and crystallographic lab work and a minimum of three visits per student to macromolecular crystallographic beamlines at the Advanced Photon Source. Students worked on crystallizing their own proteins and learned crystallization techniques using commercial proteins; they also collected diffraction data at the APS on their actual research samples and on test crystals.

Most of the first week was spent at IIT, with time divided between lectures and lab experiences. The second week was held partly at IIT and partly at the APS, where students not only collected data but engaged in training experiences shepherded by the beamline staff scientists. For the first time, the APS visits included instruction in skills other than beamline and software usage: we provided overviews of cryo-cooling and heavy-atom derivatization techniques while we were at the APS. The schedule and the content of the lectures, labs, and beamline visits are listed on the school website. Social events were included in the school, and the students were allowed free time to visit Chicago's

attractions in the evenings and during the middle Saturday of the school.

The school's location in Chicago made it easy to recruit world-class scientists to lecture and lead lab demonstrations without having to pay travel expenses. Only two of our featured academic speakers, *William Furey* and *John Rose*, were from outside the Chicago area, and all the local speakers spoke without compensation. We engaged several industrial scientists as integral members of our teaching team, and for their employers, this school was a marketing opportunity and a chance to contribute to the scientific community.

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

Participants (from IIT unless indicated otherwise):

Lecturers: Spencer Anderson (BioCARS/U.Chicago), *Michael Becker* (GM/CA-CAT/Argonne), *Grant Bunker, Chuck Campana* (Bruker AXS), *Jim Cary* (NIU), *Chris Dankulich* (Fluidigm), *Bill Furey* (Pittsburgh VA/U. Pittsburgh), *Andy Howard, Tom Irving, Constance Jeffery* (UIC), *Jim Kaduk* (Innovene), *Gocha Khelashvili, Allan Myerson* (Provost, IIT), *Joseph Orgel, Jim Pflugrath* (Rigaku / MSC), *Narayanasami Sukumar* (NE-CAT / Cornell), *Jeff Terry*.

Lab Facilitators: Jim Cary (NIU), *Shih-Chia Chang, David Ehle, Andy Howard, Rebecca Howard* (UCSF), *Sireesha Ratakonda, Pauls Reinfelds, Greg Sahli*.

Administration and Technical Assistance: David Ehle, Rebecca Howard, Sandra Howard, Faith Kancauski.

Beamline Science User Support: Randy Alkire (SBC-CAT), *Spencer Anderson* (BioCARS), *Michael Becker, Michael Bolbat* (BioCARS), *Norma Duke* (SBC-CAT), *Albert Fu (SER-CAT), Frank Rotella* (SBC-CAT), *Ruslan Sanishvili* (GM/CA-CAT), *Ward Smith* (GM/CA-CAT), *Narayanasami Sukumar* (NE-CAT), *Zdzislaw Wawrzak* (DND-CAT).

Eighteen students attended the school. They came from every part of the US and from Canada, Croatia, and Poland. All applicants were accepted for admission to the Summer School this year. The attendees, except for *Faraz Hussain* (IIT), are seen in the group photo. In addition, two students had to withdraw from attending at a very late date, one because of difficulties securing a visa into the US, and the other because of illness.

Finances: The school is funded in part through a contribution from the ACA. Other sources of funding for the 2006 school were registration and housing fees from the students themselves, in-kind contributions from commercial vendors, and cash contributions from three vendors. The total budget, apart from in-kind contributions, was approximately \$19,750. Housing was moderately discounted. Students paid for their own food and long-distance transportation, so their costs for those purposes are not reflected in that amount. Chief among the in-kind contributions to the 2006 school were crystallization supplies (crystallization

trays, screening kits, and crystal-mounting gear) from Hampton Research and deCode / Emerald.

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

For the first time, the 2006 survey solicited the students' views on the specific lectures. We plan to take their opinions regarding the lectures into account in setting up the 2007 program.

grant from the USNCCr for scholarship and travel funds for Latin American students; unfortunately we received no applications from Latin America and we were unable to use those funds. We will request that the funds be carried over to provide similar opportunities to prospective Latin American applicants to the 2007 School. The computer cluster for the Summer School is now in essentially the same state it was in when we purchased it in 2003. We plan to upgrade it substantially for the 2007 school. At a minimum we will replace the monitors and video cards on all twelve processors and upgrade the memory on the machines from 512 MB to 1 GB each; if we can, we will also upgrade the processors themselves. We will increase the disk storage for the cluster and replace the old, slow removable disk drives that we bought for the first school.

We hope the school will continue to be an important resource for the crystallographic and biochemical community, and that it can serve to acquaint a wider circle of scientists with the realities of macromolecular crystallography.

Andy Howard



Plans for the Future: For 2007 the organizers hope to define the objectives of the wet-lab and computer-lab exercises more fully so the students have a better sense of where they are heading. We also plan to expand our instruction in cryo-cooling techniques. In 2006 we reinstated the practice of offering application seminars in addition to the core lectures; we believe this broadens the students' overall experience. We will extend this further in 2007. We have moved our crystallization lab to a less vibratory room, and we hope to borrow an automated crystal visualization system for the 2007 school, as we did for the 2005 school. We will provide all registered students with a comprehensive set of instructions on how to prepare for the School, and we will mail the course textbook to the students as soon as they pay their registration fees. We also believe that the school would benefit from more assertive marketing, and an effort to accomplish that is underway. We received a \$6000

Standing - from the left: Sireesha Ratakonda (TA), Tanya Bekyarova (IIT), Shiamalee Perumal (IIT), Rob Gruninger (U. Lethbridge), Rong Cao (UIUC), Hao Guo (NIU), Yvonne Lee (UCSD), Zoran Stefanic (Rudjer boskovic), Ryan McAndrew (Med. Coll WI), Amer Alanazi (UGa), Ravikiran Yedidi (Wayne State), Poramaet Laowanapiban (UNC), Onome Swader (U. Tenn), Grzegorz Dubin (Jagiellonian U). Kneeling, from left: Andy Howard (Faculty), Sean Taylor (Yale), Reba Howard (TA), Danielle Corgliano (NIU), Silvia Albillos (UUT/NCFST), Balarenuka Sankuratri (IIT)



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64th Pittsburgh Diffraction Conference October 26-28, 2006

The conference, hosted at Duquesne University in Pittsburgh, was presided over by Jennifer Aitken. It consisted of four discrete symposia over the three days. The 2006 Sidhu Award winner was **Peter Chupas** (Argonne National Lab). In keeping with PDC strong support for student participation the recipient of the Chung Soo Yoo Award was **Johnathon Lekse** (Duquesne University) - seen accepting the award from Jennifer Aitken in the photo.

In his Sidhu Award Lecture, Peter described the exciting advances he has made together with colleagues at the Advanced Photon Source performing *in-situ* studies of materials using the pair distribution function (PDF) method. Taking advantage of the high intensity, high energy x-rays (>60 keV) from an undulator source, new experiments become possible, including studies of materials *in situ* at high temperatures and high pressures, time-resolved studies to follow chemical reactions, and studies that probe structural variations in materials on the micron scale.

There was a full day session on the "Frontiers of Electron Diffraction", chaired by **Ken Downing** (Lawrence Berkeley Lab) and a second full day organized by **Bob Von Dreele** (Argonne National Lab) was dedicated to "In-Situ and Time-resolved Diffraction techniques".

Two half day sessions covered the "Challenges of Crystal Twinning" chaired by **Victor Young** (University of Minnesota) and the "Diffraction and Scattering of Amorphous Materials" chaired by **Peter Wildfong**.

The first session included a mix of some of the latest applications of electron diffraction and microscopy along with updates on several long-term projects that seem poised for significant payoffs. **Dwayne Miller** (University of Toronto) led off with a description of the latest developments and applications of ultra-fast electron pulse generation and the use of a fast laser pulse to synchronize data recording with the pulse. **Lawrence Marks** (Northwestern University) who has been investigating the use of precession in electron diffraction as a way to minimize effects of dynamical scattering described the procedure and some recent results. **Alwyn Eades** (Lehigh University) described the use of backscattering diffraction

patterns as a sensitive approach to characterizing materials. **J. M. Zuo** (University of Illinois Urbana-Champaign) talked about the characterization of nanotubes by "nanoarea" diffraction and high resolution imaging. **Eric Yearley** (University of Toledo), one of the student travel award winners, described collection and processing of data that have allowed him to develop a charge density model for dienestrol. **Ken Downing** (Lawrence Berkeley National Lab) talked about the application of electron diffraction and imaging at various size scales in studies of tubulin, microtubules, and the proteins and drugs with which they interact. **Howard Young** (University of Alberta) described formation of two-dimensional crystals of a calcium ATPase complexed with an inhibitor and imaging of the crystals to produce a map that identifies the location of the inhibitor. **Mercouri Kanatzidis** (Northwestern University) talked about his characterization of incommensurate superstructures in a series of polytelluride compounds. **Paul Voyles** (University of Wisconsin, Madison) discussed his use of nanodiffraction and "fluctuation microscopy" to investigate amorphous materials and to characterize variations in their short-range order. **Nathan Takas** (Duquesne University) another student travel award winner, described neutron diffraction studies that revealed a new phase of sodium monothiophosphate and transitions among the three known phases. Finally, **Simon Bates** (SSCI, Inc.) described some applications of x-ray powder diffraction for material characterization in the pharmaceutical industry.

Lecturers in the Twinning Session: Jennifer Aitken, Chuck Campana, Zbigniew Dauter, Regine Herbst-Irmer, Lee Daniels, Victor Young

The symposium on "In-situ and Time-resolved crystallography" featured a very wide ranging series of talks

which in the morning session alternated between time-resolved single crystal studies of proteins and powder studies of oxides. It opened with a talk by **P. Anfinrud** on picosecond studies of CO interacting with myoglobin in which the electron density maps showed how the CO moves from place-to-place within the protein as it is liberated from the Fe binding site. The next talk by **Jon Hanson** (Brookhaven National Lab) switched the theme to *in situ* catalytic reactions including substrate binding on zeolites and the water gas shift reaction on Cu-CeO₂ and Au-CeO₂ catalysts. **Bill Royer** (University of Massachusetts Worcester) presented results on global allosteric protein transitions. He described a dimeric *Scapharca* hemoglobin



which produces a photolytic release of ligands following a 150ps flash. **John Parise** (SUNY Stony Brook) presented a complex double-lever mechanism for the structural phase transitions in silicotitanates and **I.N. Lokuhewa** (seen in the photo with **Tom Koetzle**) gave one of the Student Speaker/Travel Award lectures on *in situ* variable temperature powder diffraction studies of the SrCo₃/Fe₂O₃ system in CO₂, air and Ar. The afternoon session continued alternating themes with talks on x-ray powder diffraction in high magnetic fields by **V.K. Pecharsky**, the role of cryoprotectants for protein crystallography by **R. Thorne** and very high temperature powder diffraction with a thermal-image furnace by **W. Kriven**.



Bob Von Dreele presented some results on the effects of radiation damage on powder diffraction patterns of hen egg white lysozyme; followed **G.**

Whittaker spoke on the effects of microwave radiation on crystal structures and the session concluded with a student travel award lecture by **R. Haggerty**. Haggerty used the thermal-image furnace and a curved image plate detector to study oxidation of borides, an amorphous to crystalline transition of pollucite (Al₂O₃-Cs₂O-4SiO₂) and thermal behavior of mullite to 1700C in air.

The "Challenges in Crystal Twinning" session was structured to offer some basic instruction on twinning, as well as presenting a number of challenging crystallographic problems solved by the expert lecturers. The lead speaker was **Regine Herbst-Irmer** (University of Göttingen) who presented, "Non-Merohedral Twinning in Small Molecule and Protein Crystallography." She presented some basic instruction on twinning concepts, as well as examples of non-merohedral twins in both classes. The next speaker was **Zbigniew Dauter** (Argonne National Laboratory) who presented "Twinning in Protein Crystals." It was clear from his presentation that macromolecular crystallographers are making great strides in both the solution and refinement of non-merohedral protein twins. **Victor Young** then presented, "Low-Melting Organic Salts: Phase Transitions, Twinning, and Disorder". He discussed several enantiotropic phase transitions of this class of materials; they have complex relationships that include order-disorder phases, as well as twinning. **Charles Campana** (Bruker-AXS) followed with his presentation on "The Diagnosis and Treatment of Merohedral and Pseudo-Merohedral Twins: Examples from Chemical Crystallography." He demonstrated the strategy of examining the data critically when encountering these classes of twins. The final speaker of this session was **Lee Daniels** (Rigaku Americas Corp) who presented "Twinned and Modulated Lattices: Strategies for Success." He showed some really nice examples of non-merohedral twins and temperature-dependent incommensurate modulation in thiourea.

This final session in PDC 2006 brought four speakers together from a breadth of disciplines to discuss their work with diffraction from amorphous and disordered materials. The first speaker, **Simon Bates** (SSCI, Inc.), presented a survey of the emerging use of pairwise distribution functions to elucidate structural features in small molecule organic solids in the pharmaceutical industry.

In particular, he shared with us the use of PDF data to demonstrate differences in the structure of disordered materials prepared via various methods. **Stephanie Tristam-Nagle** (Carnegie Mellon University) presented her work with synchrotron x-radiation to interpret microstructural features of fluid phase bilayers.

Additionally, her presentation described the use of diffuse scattering data to correlate with mechanical moduli that result from these different structures. The third speaker, **Valeri Petkov** (Central Michigan University) provided a comprehensive overview of the use of pairwise distribution functions from high-energy synchrotron diffraction data to resolve the structures of various materials. He provided insight into some of

his work with nanocrystalline composite materials, particularly the resolution of structural features despite their highly disordered data. Finally, **George DeTitta** (Hauptman-Woodward Institute) concluded the session with a presentation describing the capabilities of his laboratory with respect to high throughput macromolecular crystallization. George recounted that at present the application of these fast screening techniques is experimentally quite successful, and that the greatest bottleneck lies with the analysis of the millions of images on record as the experimental databank continues to grow.

Allen Oliver

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(signed) Marcia Colquhous for American Crystallographic Association, Inc.

Workshop on Remote Data Collection at SSRL, Buffalo, August 4, 2006

The workshop, organized by *Aina Cohen* and *Clyde Smith* (Stanford Synchrotron Radiation Laboratory - SSRL) and *Edward Snell* (HWI), was held at the Hauptman-Woodward Medical Research Institute (HWI) in Buffalo. There were 34 US and Canadian investigators and graduate students in attendance. The workshop started with a presentation by *Aina Cohen* that introduced the macromolecular crystallography facilities available



at SSRL including the Stanford automated crystal mounting system and the associated cassette system used to transport samples. Exciting new developments on a standardized universal puck were also described. Following this a practical demonstration of the control, monitoring and data processing software was carried out by *Clyde Smith*. Crystals were mounted, fluorescence scans recorded and data collection initiated. The lecture hall watched as the Blu-Ice GUI displayed images from several video cameras and they saw the diffraction images as they appeared. The presentation included developments in Web-Ice, a remote data viewing application used for screening that combines scoring crystal quality with automatic indexing, resolution estimation, strategy determination and recently the ability to run RADDOSSE and BEST to optimize the data collection. Following this *Edward Snell* presented a talk on practical tips from the users point of view covering experiences from 10 remote data collection runs. A common theme, well known in Buffalo, is that ice (or in our case snow) is the enemy.

After a lunch break and taking great care to avoid the movie camera tracks that had been laid down, the practical sessions started. The workshop split into two groups. One group was led by *Clyde Smith* assisted by *Graeme Card* (SSRL). They made sure that the remote access software operated on the laptop computers attendees were asked to bring. *Geoff Franks* (HWI) was kept busy updating some of the computers to the latest X-windows software. The group then proceeded to take control of two beamlines at SSRL. They mounted crystals, moved detectors, changed wavelengths etc. They collected x-ray data and processed it in Stanford from Buffalo, probably setting the record for the most people controlling a beamline at any one time. Apart from a few wireless connectivity problems, the system was up to the task and worked well.

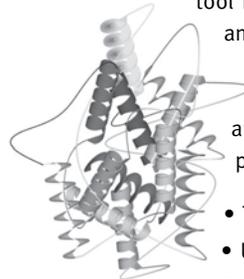
The other group started with a practical session run by *Aina Cohen* assisted by *Mike Hollenbeck* (SSRL). An example of what could happen 'when good pins have gone bad' was shown and then the kind of things to avoid and look out for was covered in detail. Then the fun started. The group donned safety shields and gloves and the liquid nitrogen came out. Everyone got a chance to mount at least one sample in the cassette and practiced the techniques involved. There were lots of lively discussions and many practical ideas were swapped.

After a coffee break, and avoiding the film crew and extras, the groups swapped. At the same time a group from Grenoble synchrotron (ESRF) watched from the SSRL end of the operations to learn from the SSRL experiences. The day concluded with a wrap up question and answer session, by which time everyone was exhausted. A few diehards stayed for dinner in the famous Anchor Bar, the place that invented Buffalo Wings, and then headed to Niagara Falls to see the water, lights and fireworks. Everyone made it home safely after the meeting, although in a couple of cases, the laptop power supplies left a little later and took a little longer to travel! It is hoped that a similar workshop will be held next year.

Edward Snell & Aina Cohen

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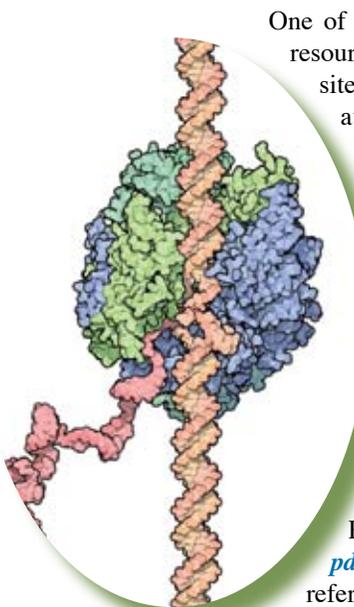
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www.PDB.org in the Classroom

As molecular biology continues its march into mainstream biology education and cyber infrastructure becomes more reliable, it is inevitable that online resources serving the research community will migrate from textbook footnotes into core curriculum activities. As part of its educational outreach program the RCSB Protein Data Bank is working toward having its archive more accessible and useable by this growing audience. Several new tools and a simpler query mechanism allow for educational and fun in-class activities that can provide a solid framework for that age-old question teachers face each year, "Why do I need to know this?"



One of the most popular educational resources on the RCSB PDB web site is the Molecule of the Month, authored by David Goodsell (Scripps Research Institute). David's contribution to this monthly column over the past seven years has produced a comprehensive documentary on the structural biology of over 80 important biological macromolecules contained within the PDB archive. Readers can access these publications through the main RCSB PDB web page (www.pdb.org). Each feature contains references to structural details and provides links to the data summary

page in the PDB database. The example illustrated here is RNA Polymerase II (PDB ID 1I6H a deposition from the laboratory of 2006 Nobel Lauerate Roger Kornberg, *Science* (2001) **292**, 1876-1882). The motivated reader can dig deeper on each topic using both the database itself and the list of references found at the end of each article.

The RCSB PDB web site also provides several hands-on bioinformatics activities targeting the introductory biology curriculum. The Green Fluorescent Protein module (image seen here is PDBID 1EMA by M. Ormo *et al.*, *Science* (1996) **273**, 1392-1395), downloadable from the educational resources page of the PDB site, provides a bioinformatics approach to understanding GFP from its gene to biological function, and includes medical and biotech applications. This activity utilizes the new RCSB PDB molecular

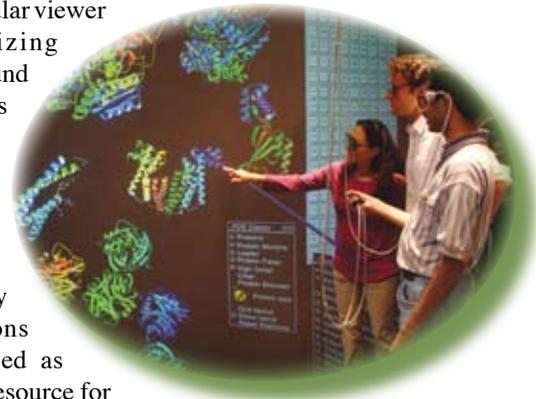


viewer, Protein Workshop, and guides users through advanced queries using the RCSB PDB search interface. Similar scenario-based tutorials are also available for teaching the biology of transcription, translation, bioluminescence, insulin, RuBisCO, and the function of antifreeze proteins. The low technical learning curve for these new web-based tools makes these modules excellent 'plug-and-play' activities that can be included in existing biology curricula.

The RCSB PDB has also developed several more informal activities for introducing proteins to younger audiences and the general public. Currently on display at the Steven Birch Aquarium in La Jolla, California, is an RCSB PDB exhibit showcasing the role of proteins in the every day life of marine organisms. The interactive software (requiring Flash) for this exhibit is also available from the RCSB PDB web site



ImmersivePDB, a virtual reality molecular viewer for visual-izing structures found in the PDB is runn-ing at the visualization lab at Calit2 on the UCSD campus. With almost daily demonstrations this has served as an excellent resource for introducing protein structure to a wide variety of audiences.



Each issue of the quarterly *RCSB PDB Newsletter* includes an "Education Corner" describing how educators at different academic levels use the PDB in their classroom. as well as many articles on other RCSB PDB educational outreach efforts. All issues of the *Newsletter* are available at the RCSB PDB website.

Comments and suggestions on educational resources at the RCSB PDB are welcome at info@rcsb.org.

Jeff Milton

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Erich Paulus
Tea Pavkov
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Carrie Wilmot

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ACA 2006 – Workshop on Methods in Neutron Protein Crystallography

The workshop, held on Saturday the 22nd of July 2006, was attended by over 50 participants from across the world. It was sponsored by the Neutron Scattering SIG and organized by **Paul Adams** (Lawrence Berkeley National Laboratory - LBNL) and **Paul Langan** (Los Alamos National Laboratory - LANL). Much attention has been given to the development of beamlines and techniques for collecting neutron protein crystallographic data at meetings over the past few years. However, there are several additional steps just as important as data collection involved in determining a neutron biomacromolecular structure. An aim of this workshop was to not only describe available facilities for data collection but also to make those wishing to use neutron protein crystallography aware of the methods involved in those other steps.

In a series of early morning short presentations, **Benno Schoenborn** (LANL), regarded by many as the founder of this field, **Leighton Coates** (LANL), **Nobuo Niimura** (Ibaraki University) and **Flora Meilleur**, (Oak Ridge National Laboratory), described how optimized methods for perdeuteration, crystal growth and sample freezing can greatly increase the chance of successfully collecting neutron diffraction data from crystals as small as a fraction of a millimeter in volume. Our ACA president, **Bob Bau** (University of Southern California), gave an overview of available neutron beamlines for protein crystallography; LADI at the Institut Laue Langevin, BIX at the Japanese Atomic Energy Research Institute and the PCS at LANL. The later sessions focused on structure refinement and in particular new computational tools for neutron protein crystallography that are being developed by a consortium between Los Alamos and LBNL funded by the National Institute of General Medical Sciences and directed by the workshop organizers. **Marat Mustyakimov** (LANL) and **Pavel Afonine** (LBNL) along with the workshop organizers described and then demonstrated the computational tools developed so far.

A goal of the “computation tools for neutron protein crystallography” consortium is to provide software that can be immediately deployed to address a computational bottleneck in neutron protein crystallography. This bottleneck, has been identified at Los Alamos where although the PCS neutron beamline (funded by the Office of Biological and Environmental

Research of the US Department of Energy) is now routinely producing a number of data sets through the Los Alamos Neutron Science Center (LANSCE) user program; structures are not being deposited at the same rate. Workshop participants were told that a patch will be made available, hopefully before the end of the year for the program *CNS* that will allow refinement of protein structures using both neutron and x-ray data. The ultimate goal of the consortium is to incorporate the algorithms and strategies being developed and tested in *CNS* to the automated crystallographic program *PHENIX*. *PHENIX* will provide a workbench that structural biologists with a range of experience can use alternatively or simultaneously for x-ray and neutron protein crystallography.

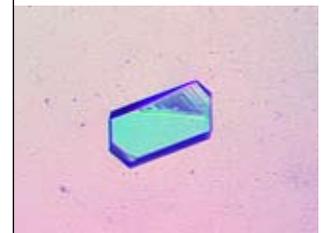
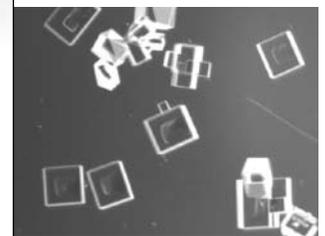
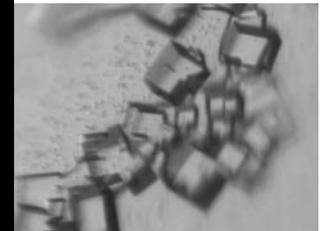
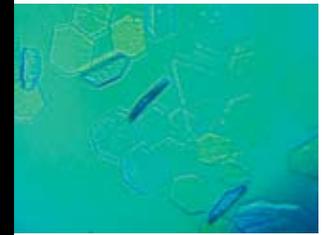
A lively discussion wrapped up the workshop. With deuteration laboratories, (such as the one at LANL and the one run jointly by the Institute Laue Langevin and the European Molecular Biology Laboratory outstation in Grenoble described by **Leighton Coates**), now routinely producing perdeuterated proteins, the attendees highlighted crystallization as an area that requires most attention and development. There were calls to hold this type of workshop regularly and also to make the lecture notes and demonstrations available through a website, perhaps the same website that will be used to distribute software.

Workshop speakers from left to right- Paul Adams, Paul Langan, Bob Bau, Leighton Coates, Nobuo Niimura, Benno Schoenborn, Flora Meilleur



It was decided to hold a methods workshop at the same ACA meeting as a full day *Transactions Symposium* on “*The Future of Neutron Crystallography: Smaller Crystals, Larger (Macro) Molecules*” in order to give those interested in using neutron protein crystallography a comprehensive introduction to the field. The workshop followed a neutron scattering summer school on “*Soft Condensed Matter and Structural Biology*” that was held at LANSCE, 18th through 26th of May 2006, primarily intended for PhD. graduate students and postdoctoral researchers requiring an introduction to the field. A number of students attending the ACA workshop did so after being introduced to the field through the LANSCE summer school. It might be hoped that by organizing a series of regular schools and workshops the neutron protein crystallography community will be greatly strengthened.

Paul Langan



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MICROSYSTEMS

ACA 2006 – Workshop on Management of Synchrotron Image Data imgCIF File System and Beyond

The workshop held on July 22 was attended by 39 participants and began with brief introductory talks in the morning by *R. Sweet, H. Bernstein, G. Bricogne, C. Nielsen, W. Minor, J. Pflugrath, R. Sweet, A. Ashton, J. Westbrook, B. McMahon and T. Proffen*. The rest of the workshop was devoted to lively discussion led in alternation by Sweet and Bernstein, which produced a surprising degree of consensus. Productive discussion continued late into the afternoon, even after formal conclusion of the workshop, despite the lure of the beach just outside the meeting room. The workshop agenda, handouts and pictures are available at www.medshio.org/meetings/ACA_2006_WK02_Report.html.

short introductory talks presenting history and background, were followed by descriptions by investigators with various backgrounds and interests of their own goals or apprehensions about adoption of the imgCIF standard.

The second segment of the meeting was open discussion on a range of topics: Consider the whole flow of information/knowledge in the experiment; where does imgCIF fit? - How does one deal with corrected vs. uncorrected data? - What are the impediments to immediate adoption: can we define a time line? - How should the intellectual property issues relating to compression algorithms



Rear from the left: Graeme Winter, John Huffman, Brian McMahon, Chris Nielsen, Alun Ashton, Thomas Proffen, Ward Smith, Bernhard Rupp, Jeff Deschamps Front from the left: Herb Bernstein, Gerard Bricogne, John Westbrook, Wladek Minor, Bob Sweet



From the left: Joerg Kaercher, Kumar Singh Saikatendu, Peter Turner, Sandor Brockhauser, Jim Pflugrath, Nick Hause

The idea behind the workshop was to organize the adoption of a standard, self-documenting format for diffraction image files. The immediate focus was on adoption of the current imgCIF/CBF standard that has been approved by the IUCr COMCIFS. Eleven

be handled? - What will be the mechanism for an open-source protocol for continuing development of imgCIF? - And finally, we should talk about the dictionary to understand whether to add new items now.

The conclusions and recommendations of the workshop were:

1. This is the right time for more widespread use of imgCIF.

2. Synchrotron sources should start writing imgCIF image files as soon as possible, employing the imgCIF dictionary already adopted by the IUCr Committee on the Maintenance of the CIF Standard (COMCIFS) and published on the web and in International Tables Volume G. Such image files will provide at least as complete and accurate information as the various file headers written now, and will have the added benefit of stimulating further conversion of programs that feed the experimental parameters and of programs that reduce the data. Small teams have been created to start the process by working through one detector/beamline combination at a time.

3. An important step in achieving this goal will be the creation of certified stand-alone conversion programs (“jiffies”) that will convert from imgCIF to the existing standard native file format used for each detector system in the field and from

standard native file formats to imgCIF. This will provide software developers with benchmarks against which to work and allow work with imgCIF to start while conversions of major packages are in progress.

4. The files should include both the corrected and the raw images, with the option of putting both together in the same imgCIF file.

5. Those interested in imgCIF should look for a way to assure continuity in development. Maintenance and development of the dictionary and software library need to be taken up by a consortium where continued interest, and especially, continued funding are assured. There are several possibilities, and some study will be done in the coming year.

6. The items above are the primary "to do list" for the coming year. In addition, it is clear that work is also needed on:

6.1. Identification of a the critical subset of parameters from the imgCIF and mmCIF dictionaries that define "just the image."

6.2. Additions to the dictionary to support derived parameters that may be recalculated and re-refined over time (e.g. beam centers), each variant of which needs to be recorded with a time stamp and other details to identify the history of these parameters.

6.3. The interaction with NeXus to facilitate data management at facilities that will be using NeXus for the overall

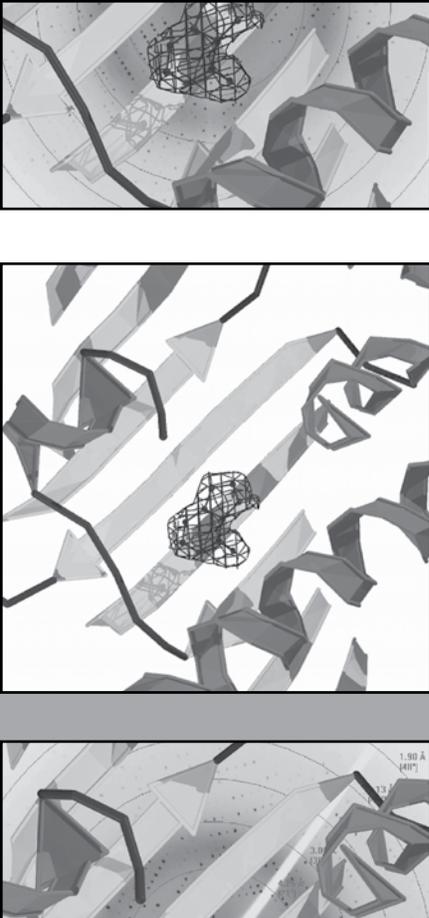
data management but which will be producing imgCIF for PX beamline users to take home.

6.4. Storage of additional data defining the environment within which an experiment has been done such as images of pixels that are blocked by beam stops or otherwise "dead".

While work on these issues is important and helps to explain the need for continued funding discussed in item 5, above, it is our strong belief that our primary focus must be on items 1 through 5, or the base for this other work will not be as firm as it should be.

Partial support was provided by the U.S. Department of Energy under grant ER64212-1027708-0011962, NSF under grant DBI-0610407 and Area Detector Systems Corporation (ADSC). The workshop was run thanks to the help and cooperation of the ACA, the ACA Continuing Education Committee and the ACA Data, Standards, and Computing Committee. The workshop would not have been a success without the hard work of the ACA Buffalo Office and the Hawaii meeting organizing committee. The support, cooperation and encouragement from all these sources are gratefully acknowledged.

Herbert J. Bernstein and Robert M. Sweet





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This year, thanks to the extra generosity of a number of our members and friends we were able to award travel grants to more than 50 young scientists. Following are some of the impressions and experiences at ACA Hawaii.



I am very grateful for the grant to attend the meeting. It was a wonderful opportunity to share my work, meet other scientists and get an update on the frontlines of our field. For me it began with the "Neutron Protein Crystallography" workshop. The workshop and the *Transactions Symposium* clearly showed the progress that is taking place. The new facility at Oak Ridge will allow a broader use of the technique (my crystals might be big enough now) and surely, a better understanding of how hydrogens participate in our lives. It was interesting to see how one can combine refinement procedures of neutron and x-ray diffraction in PHENIX to get a better overall structure. I participated in the "International Macromolecular Crystallographic Advances" session and was happy to see many people from different countries doing crystallography. I only wish some speakers had more time to show their results. For instance, Ziheng Rao could certainly tell us much more about SARS proteins. I can not write about all the presentations I attended, but it is fair to say that structural genomics, macromolecular assemblies, membrane proteins, methodological developments, the posters, inspiring conversations and much more fulfilled my expectations and curiosity. The cordial environment, social events and the amazing island of Oahu (with green turtles appearing every day in front of the hotel) completed this great meeting.

Receiving this award is of grand importance when you come from Brazil or any other country where resources are limited. Science development depends on hard work, funding and collaboration, all of which I could find at the ACA. Thank you very much.

João Alexandre R. G. Barbosa



I was fortunate to be able to participate in the ACA meeting. Throughout the week I was able to listen to and participate in a wide range of relevant topics regarding crystallography.

The conference was well planned and the topics were well organized. As a student though, I would have loved to see one or two workshops tailored toward learning the theory of techniques and methods such as SAXS, neutron scattering etc.

This was my first conference and the experience was invaluable and will undoubtedly help me decide on future directions for my PhD project as well as for my long-term career.

Thank you for the well-organized meeting, which I could not have attended without the generous ACA travel grant

Oliver Baettig

Going to the ACA meeting in Hawaii seemed like an unlikely pipe dream to this starving grad student. I almost fainted when I first looked up the price of plane tickets-I was stuck across an ocean without a paddle. When I learned that I had received a travel grant, I slapped those airline tickets onto a credit card, and eagerly awaited the day that I would attend my first ACA meeting on beautiful Waikiki Beach.



The conference was everything I had imagined only better. Finally I saw the faces of the people I had heard so much about. There were many invigorating talks, and so many people exited about their work. Every day of the conference held its own possibilities of networking, learning and growing as a crystallographer. During my poster session, I shared my work with many interested attendees. It was exhilarating to tell my story and to get feedback from many distinguished people. I am honored to be the winner of the *Journal of Chemical Crystallography's* poster contest.

I am so grateful that the ACA was able to help me attend this meeting. When I first chose to work with Marilyn Olmstead, I sometimes wondered if crystallography was really right for me. The conference provided an answer to that lingering doubt, which was a resounding "Yes!" I now feel like a part of the greater crystallographic community, and it feels like home.

Christine M. Beavers

I would like to thank the ACA for the grant to attend my first ACA meeting. I did enjoy its atmosphere and the wide variety of the topics. I particularly liked the sessions on "Whole-Molecule Disorder", "BioMacromolecular Assemblies", "Large Macromolecular Assemblies", "Difficult Structures" and "Structural Biology in Industry". With several interesting sessions going in parallel it was often hard to decide which one to attend! The evening poster sessions were also of incredible interest, and provided a great opportunity for informal and detailed discussions.



Special thanks to Thomas Earnest and Brian Wimberly for inviting me to speak at the "Large Macromolecular Assemblies" session. I was excited to present my research and to get stimulating comments.

Last but not least, the scuba diving in warm waters of Oahu was just great, especially compared to that in chilly California. It was an exciting experience, and I'm really grateful to the ACA.

Maria Borovinskaya



This year's meeting was a unique experience for me as it was my first international conference. It was a very rewarding and valuable experience to see the varied and interesting research that is going on around the world in the field of crystallography. I was able to exchange ideas with many gifted scientists and gained new perspective and insight into my own research. Special thanks to the ACA for the grant that I enabled me to attend this meeting.

Cory Brooks

I would like express my gratitude for the travel grant, without which my presence at this meeting would have been very hard.

The meeting was very interesting and useful. I am interested in bioinformatics and am just starting in the field with only a computer background so it was very useful to meet people deep into the field of crystallography and biology. As a person who is planning to develop applications for bioinformatics it was interesting to meet and talk with very senior people. This was also my first meeting and the opportunity to present some of my work was a great professional experience for me.



I also hope that our presentation and the applications we have written will be useful. Having this opportunity to meet the people in the field made me realize that the work we do as research assistants is actually used by a lot of people. We presented a new type of encoding binary data (synchrotron images) as text called binUTF. Being able to encode binary files into printable characters could provide the ability to insert binary data along with the metadata, into one easy-to-process XML file.

I am sure I will remember this meeting for the rest of my life not only because it was my first, but also because of all the nice people I met at this wonderful place.

Georgi Darakev

I would like to thank ACA for the travel grant. I signed up for the meeting while at the Carnegie Institute of Washington on a Fellowship. Then at the beginning of the year I moved to the University of Edinburgh in Scotland, so the ACA travel was a crucial factor for my participation at the meeting. Thanks to the Chair of the

Materials SIG, Lachlan Cranswick, and to Judy Kelly, who gave me the opportunity, I also organized and chaired a session on "Non-Ambient Crystallography" sponsored by the Materials SIG that became a conference highlight for me.



We had eight talks on high-pressure high-temperature effects on materials, including experimental, computational and theoretical work. Presenting my work on a high-pressure structure of silane in a poster session, I got to chat not only with other high-pressure scientists but also with people from different scientific fields, mostly biologists working with biomacromolecules, (the subject that has dominated the meeting not leaving a lot of space for material scientists.) I really had a lot of fun participating in the hula dancing competition at the YSIG mixer. One day at 7am, before it was too hot, I participated among others in a fun run organized and sponsored by Rigaku, which was indeed a lot of fun! A party organized by MAR was amazing with very good food, chats with people, and an exquisite ukulele music performance that still stays in my heart after returning to rainy Scotland.

Olga Degtyareva

I wish to thank the ACA for the travel grant to attend the annual meeting. This was my third ACA meeting and once again the experience was thoroughly enjoyable. The main focus of this year's meeting was neutron diffraction and scattering techniques. I found these and other biological topics stimulating and thought provoking. One of the highlights during the meeting was the Neutron Workshop where we heard from Prof. Niimura



about the challenges of growing large crystals for neutron crystallography. The afternoon presentations hosted by Paul Adams covering computational aspects, especially the demonstration of PHENIX, were valuable as I hope to use this software in the near future. As a graduate student in the process of finishing my PhD, meeting interesting scientists at various stages of their careers were a great help in making decisions concerning my own future. I also had the opportunity to give an oral presentation on some of my recent work and had many interested people come up and talk to me about the results. Hawaii was a good choice for such a meeting as it provided the perfect balance of interesting science and breathtaking surroundings – thank you ACA for giving me the chance to attend and participate.

Zoe Fisher



Thank you, thank you, thank you to the ACA! I am sincerely grateful for the travel

grant which allowed me to attend my first ACA meeting. It was a great honor to meet so many of the people I had only read about. I never thought in my wildest dreams that I would have the opportunity to attend a meeting that evoked so many ideas. Many of my unanswered questions about crystallography were answered and so many more questions came up for me to explore. On my return I was exhilarated to continue my project with new found energy. I was impressed by the neutron studies on macromolecular structures that are being conducted at Los Alamos. Leighton Coates gave a really good lecture on the basics of protein crystallography with spallation neutrons. The future potential that neutron diffraction has to offer protein structure studies is incredible. Another aspect of the meeting that drew my attention was how the use of x-ray crystallography in drug discovery can support rational drug design by manipulating functional groups. Kenton Longenecker from Abbott Labs used the crystal structure of DPP-IV to rationally design peptidase-selective inhibitors to help treat type II diabetes. Overall the meeting was a great experience both academically and socially. Many thanks to the organizers for a great meeting and I hope to attend future conferences.

Caroli Genis



I would like to thank the ACA for their generous travel grant, without which I would not have been able to attend the meeting. The meeting was a great reward for finishing my bachelor's degree two months earlier. It was my first visit to Hawaii and my first ACA conference and I had a fantastic time. The sessions were well organized, very informative and presented

in such a fashion that undergraduates could understand them and post-docs would not be bored. I especially enjoyed the presentations in the “Natural Products and Drugs” and “Proteins Involved in Host Immune System and Pathogen Interaction” sessions. I would also like to thank the ACA for the opportunity to present my undergraduate research during the research showcase. It is a great point of pride for me to be able to say that I displayed my work to some of the top minds in crystallography. In addition, I received many helpful suggestions on furthering my studies.

I also took the opportunity to visit the Polynesian Culture Center and I highly recommend it to everyone the next time you visit Hawaii. I knew practically nothing about the Polynesian Islands but after the day I spent at the culture center I almost felt like a native. Thanks again to everyone who made this trip possible!

Larry Grant



It was really great to be at the meeting and I would like to thank the ACA for the grant that made it possible. Although it wasn't my first visit to Hawaii, having been there there for a conference in 2004, it was my first ACA meeting. The venue was truly fantastic with views of the beach, palm trees and the ocean right from the lecture rooms. Fortunately this was not too distracting and I was able to attend many great talks. There were excellent sessions like the ones on "Bio-Macromolecular Assemblies", "Complementary Methods to Macromolecular Crystallography", "Large Macromolecular Assemblies and Membrane Protein Structures". What truly surprised me was the large number of vendor exhibitions and it

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proved very useful to talk to many of the sales representatives and engineers. Furthermore the Mentee/Mentor dinner and the banquet were nice informal settings for talking to some of the giants in the field. I would like to thank the "Difficult Structures" session chairs, Charlie Carter and Tina Izard, for the invitation to speak. All in all it was definitely worth the long trip from the Netherlands; I really enjoyed the meeting and I am grateful to the ACA for their support.

Bert Janssen



I wanted again to thank the ACA for a most generous gift. The Honolulu setting created a scenario for imagining and envisioning the amazing field of crystallography. I very much enjoyed the relaxed group of presenters and participants which gave the meeting a casual tone. As a young scientist and new member of the ACA the easy flow of the meeting presented a great opportunity for learning and socializing. Personally the ACA meeting presented a look into an exciting realm of scientific achievements.

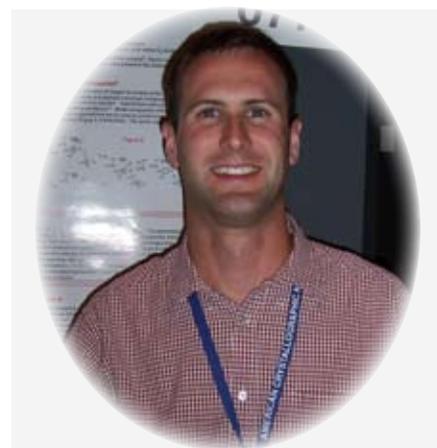
Kent Klemmer



I want to thank the ACA for the travel grant. It was indeed a pleasure to attend a meeting in Hawaii, but also to hear such interesting talks and posters. I was also grateful for the opportunity to present my work and meet with many colleagues who gave advice in planning the next phase of my career. It gave me a chance to meet with various vendors before I begin setting up my new lab. Of particular interest to me were the innovations in crystal cooling and in screening protein fragments for solubility. I also enjoyed the sessions on new structures, macromolecular crystallographic advances, membranes and membrane proteins and the Buerger Award symposium. Listening to Stephen Burley's talk on fragment-based drug discovery I fully understood for the first time what it was and what the implications were for the complexity of the libraries. The "Topics of Interest to Young Scientists" session was excellent and very helpful. It provided a wealth of information on starting out as a young investigator. This was my second ACA meeting and it was an excellent opportunity for catching up on what people are doing, finding

of the people I got to know when working as a PhD student. Needless to say there were several very interesting speakers at the meeting. In particular, the talk by Dmitri Svergun on macromolecular complexes in solution was extremely interesting and in general I am very impressed by recent results on protein dynamics from small-angle x-ray scattering and Cryo-EM. It also made me realize that I should probably be looking in that direction to supplement my results from x-ray crystallography. The poster sessions were also very informative and as usual, they are a great way to pick up good advice and new experimental ideas. The setting for the meeting was amazing and I had some fantastic days in Oahu. It was, however, a bit surreal to come out of the dark rooms after a long session to be faced with bright sunshine and the spectacular view of people either surfing in the ocean or having fun by the hotel pool. While I never got a chance to do any wave surfing or Hula dancing I definitely got a good taste of this great Island. I especially enjoyed the Mai Tai's at the beach bar which were fantastic.

Rene Jorgensen



I would like express my thanks to the ACA for their financial support. Hawaii was fantastic, offering the perfect blend of exciting science against the backdrop of a location equally as refreshing. My favorite sessions were "Membrane Protein Structures" and "Structural Biology in Industry". Both topics were relatively new to me and offered a great deal to learn from. As a graduate student, I enjoyed the YSSIG mixer as well as the mentor/mentee dinner which provided a great forum to meet prominent individuals in both the small molecule and macromolecular fields. More than anything, I enjoyed the opportunity to reunite with old acquaintances as well as make new ones.

Bryan Johnson

I greatly appreciate the ACA travel award. This was my first ACA meeting and also my first time in Hawaii and I truly enjoyed both. It was a pleasure to get a chance to meet fellow crystallographers from a variety of scientific and structural backgrounds. The meeting gave me the opportunity not only to meet some of the people that I only know by name from their publications but also to catch up with some



out about the latest techniques, learning about complimentary techniques such as small angle x-ray scattering, and meeting people in the community. I look forward to attending many future meetings.

Nicole LaRonde-LeBlanc



My experience at the ACA meeting was very positive. Coming from the field of high pressure physics, my knowledge of the crystallographic aspect of my research is not highly developed, and the seminars I attended opened my eyes to a depth and complexity of this field that I had never before realized. I really enjoyed speaking with students and senior scientists with whom I would never normally interact, and it was interesting to think about how principles presented could be applied to my own research.

I had the opportunity to speak at the non-ambient crystallography session, and to reconnect with old friends and make some new contacts in my field. Through my interactions at this session and also at the poster session, I learned of several possibilities for collaboration and a postdoc opportunity, so I am extremely glad to have been able to be present.

Amy Lazicki

As an undergraduate student it was a great honor and a privilege for me to be able to attend the ACA meeting. This being my first scientific conference it truly opened my eyes to the quality and diversity of crystallographic research being performed around the world. This conference was invaluable for me to figure out how and where I would like to continue in the sciences. Sessions on computational methods helped me get a better understanding of the tools used in protein crystallography.



Learning about complementary methods to x-ray crystallography made me understand other techniques that can be used to give valuable information about a protein of interest. The friendly atmosphere made it possible for me to speak to many professors about their research interests and to make lots of friends that I hope will last for the rest of my scientific career. I will never forget the time I spent on Waikiki beach.

James A. Letts



I really appreciate the award that made my trip to the ACA meeting possible. I really enjoyed the meeting there as well as the unforgettable island scenery. I had a chance to present my research project and got useful input from the audience. The meeting also gave me opportunities to discuss my research with the experts in this field. It was a wonderful experience and very fruitful meeting. Thank you all for your efforts to make this meeting successful!

Xuefa Li



It was a great experience to be at the ACA meeting. Compared with other meetings I've attended before, the ACA meeting felt more like a big family reunion due to attendees close research interests and related research fields. You could easily discuss scientific results, share your own research experience, meet some 'old' friends whose names you have seen many times in journal papers but never face to face, and also make new friends. As a student, this may never have come to pass without the generous and extremely helpful travel grant. Thank you very much,

Zhong Li



I would like to express my gratitude for the travel grant. The only other ACA meeting I attended was several years ago, at the start of graduate school, and I was delighted to have the opportunity to give a talk in the membrane protein structures session on an enzyme that consumed most of my graduate career (7 years!). This session was also pertinent to my current research, and I appreciated the stimulating discussions that ensued directly after this

session and later by email.

I found the career advice session interesting and relevant, in particular the talk given by Carrie Wilmot on academic jobs and the talk about the history, success and future of Nextal by Jean-Pascal Viola. Because I gave a talk, I was free to lieisurely browse all the poster sessions, and I enjoyed talking to various presenters. In fact, I ran into a graduate of my current lab who had grown up in Hawaii, and who took me to a local favorite restaurant with real poi. The backdrop of the beach and ocean made for a picture-perfect conference. I got to see old friends from graduate school, the synchrotron, other ACA meetings, and got to meet new friends that I hope to see again at next year.

Raquel Lieberman



I would like to thank the ACA for the financial support that gave me my first opportunity to present at an internationally attended meeting. The poster sessions allowed me to freely discuss my research while learning from the comments and suggestions from other crystallographers. Moreover, the poster sessions allowed me to go into specific details and work through various problems in crystallography with my peers.

While I learned a lot from the various poster sessions, I learned even more from the lectures. In “New Structures” I learned about the most recent biological structures and gained insight into the future of structural biology. “Large Macromolecular Assemblies” explained the challenges of and strategies for determining a multiple protein complex mechanism through crystallography, which could be applied to my own research. Not only did I learn about crystallographic

techniques, but I also learned about the opportunities and difficulties of a career in crystallography during the “Topics of Interest to the Young Scientist” section. Overall, the sessions were informative and helpful for my career.

Once again I would like to thank the ACA for this great opportunity to further my education, to begin networking and to surf the beautiful beaches of Waikiki.

Corey Mandel



I would like to thank the ACA for the generous grant to present my research at my first ACA meeting. I found it to be extremely enjoyable. It was a privilege presenting my research at the poster session and I am honored to have won the Protein Data Bank Prize and to have received honorable mention for both the Pauling and AIP Undergraduate Research Prize. It is highly commendable that the ACA hosts a conference where undergraduates can compete for such prestigious accolades.

I found the talks to be very stimulating. I enjoyed the *Transactions Symposium* on neutron crystallography and found the talk “Protein Crystallography with Spallation Neutrons” on what powerful neutron spallation sources can provide to protein crystallography to be particularly exciting. I was also intrigued by the talks on complementary methods to macromolecular crystallography. I enjoyed hearing Alex McPherson’s talk on AFM and Jack Johnson’s visually stunning talk on virus particle maturation.

Honolulu provided such a beautiful backdrop to the conference. I had a wonderful time waking up each morning for an early swim before talks and catching a quick dip during lunch breaks.

I want to again offer my most sincere

gratitude to the ACA for the travel grant that made my attendance possible. I had a memorable time with the warm Hawaiian sun and warm company. I look forward with much enthusiasm to attending next year’s ACA meeting in Salt Lake City.

Edward Miller



ACA Meetings are always a great events. Many famous scientists not only from the US, but from many other countries present different aspects of crystallography. Such a meeting is the best way to get a clear idea of the current stage of crystallographic development in different areas: new program packages, advances in methods, applications in protein chemistry, medicine, biology and other areas. It is very useful and exiting for crystallographers at all stages of their careers. For young people it is a great opportunity to listen to interesting discussions of leading specialists and to learn about the directions of their future investigations. Discussions about professional education and methods of studying are also important. What is more, such a meeting allows one to make new social contacts, new friends, and decisions about collaborative investigations.

The ACA grant gave me the chance to attend such a meeting. My trip was both cognitive and exciting (Honolulu is really the paradise on earth)! I attended “Whole-Molecule Disorder”, “Undergraduate Research Showcase”, “New Structures”, “Natural Products and Drugs” and many other sessions with great pleasure. The atmosphere for the discussions and questions after the talks was warm, friendly and informative. I felt that all the sessions and social activities were organized very carefully and on a high level. I am very grateful to the ACA (cont'd on page 48)



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for such a marvelous chance to attend the 2006 meeting. Sweet memories about the conference and the beautiful landscapes of Hawaii will always be fresh in my mind.

Ekaterina Mironova



Many thanks to the ACA for their financial support. This was the second ACA meeting I attended and I found the lectures and poster sessions to be quite stimulating. *Although I must admit, I kept hearing the beach calling out my name.* The meeting provided an excellent opportunity for me to meet and interact with other crystallographers from all levels of experience. While at the meeting, I had the chance to attend both the YSSIG Mixer and the Mentor/Mentee Dinner where I met several people, including a mentor, *Carol Brock*, that I interacted with several years ago by email, but had never met in person. I especially enjoyed the poster session which allowed me to present my data and get very insightful feedback from others. It also provided a perfect opportunity to learn about research in other labs and to interact with students and post-docs from a variety of scientific backgrounds. A few of my favorite sessions were "Structural Biology from All Angles", "Remote Data Collection", "Difficult Structures", and the "Topics of Interest for Young Scientists", and especially the Buerger Award and the Etter Early Career Award lectures. Above all, I thank the ACA for the opportunity to meet and interact with those *giants* of crystallography, those *gurus* who write all the books and programs we use everyday, those Nobel Prize winners, and those *people* who inspire us everyday.

Nicholas Noinaj



Supported by a travel award from the ACA I was able to attend a wonderful scientific festival on beautiful Waikiki beach. Everything was fantastic. It was a great pleasure to see and to discuss fellow scientists' work on structures from small organics to large proteins to huge complexes such as the ribosome and fatty acid synthase and from crystal structures of protein and protein complexes to cryo-EM reconstruction and cryo-EM tomography structures of bacterial viruses. I was also very grateful to see the advances in all kinds of techniques, from protein crystallization and cryo-crystallography to newly developed algorithms and software. The meeting attracted such a large variety of scientists that I was able to learn both theories for developing new methods and applications of structural biology in all kinds of drug design. At the posters or on the beach we had pleasant conversations and made friends with other young scientists from both academia and industry. It was great to discuss and enjoy each other's work and definitely a golden opportunity to receive other people's suggestions, to learn new things, to broaden our minds, and to appreciate all kinds of beautiful work being done in different fields. We also had opportunities to exchange thoughts with the exhibitors about new and developing products and techniques that have been and will be facilitating our research. It was a great experience and I am already looking forward the next year in Utah.

Jinhau Pan

My experience at this year's ACA meeting was as exciting and rewarding as ever. Besides going to the scientific sessions, I also visited the poster sessions and the product shows, met many fellow



scientists and had very stimulating conversations. I had the honor of giving an oral presentation of my research on cytochrome oxidase during the "Membrane Protein Structures" session. Like almost everyone else, this was my first ever visit to Hawaii. I got to experience the spirit of Aloha, enjoy the beach and sunshine, play beach-volleyball with a bunch of local youngsters, and to take a tour of the Polynesian Cultural Center. I sincerely thank the ACA for the generous travel grant to help make this trip possible. I am sure the memory will last a lifetime.

Ling Qin



I would like to thank the ACA for their generous support. As an undergraduate, the meeting was a great opportunity for me to present my work on "The Reaction of PMM/PGM: Structural Insights Into a Simple Processive Enzyme." to many of the experts in my field of research. This experience allowed me to gain a better understanding of the dedication it takes to be a successful graduate student and the opportunities available to MA and PhD students. (Con't on page 50)



Top Row: Mark Arbing, Simon Jenni, Elena Kovaleva, Elisabette Sabini, Thang chiu. Between first and sescond row: Teresa de la Mora. Second row: Bret Dillard, Arewn Pearson, Peter Horanyi, Heather Pinkett, Bryan Johnson. Third ow Katherine Page, Emma-Karin Millers, Carrie Wilmot, Rebecca Hoeft. Bottom row: Yulia Servyugina, Jim Carey, Michael Suits, Bomina Yu.

The Mentee/Mentor dinner and the YSSIG Mixer gave me the chance to meet a wide variety of people from diverse backgrounds. I also particularly liked the sessions on “Cool Structures” and the “Undergraduate Research Showcase.” It was very refreshing to talk with researchers about their undergraduate experiences and the life decisions that led them to choose the field of crystallography.

Overall, I had a wonderful time at this meeting and I am extremely grateful to have been selected as a travel award recipient.

Andrew Schramm



with discussions on crystallographic education policies, offered valuable advice on curriculum development in crystallography at both the undergraduate and postgraduate level. I also enjoyed the sessions on the use of neutron sources in crystallography since this took me to the cutting edge. However more than anything else I benefited tremendously from the many discussions I had with the people I aspire to follow, the experienced professional crystallographers. I am particularly grateful to Franck Fronczek for his mentorship before, during and after this meeting. I chatted with the authors of the books I learn from and the developers of the software I use. What a rewarding experience! To have been afforded two individual tutorial sessions with George Sheldrick, learning how to model disorder and attack specific problems I was having with structure refinement. What a wonderful privilege! I shared some of the work we have been doing through my poster entitled “X-ray Crystallography at the University of the West Indies (UWI), Jamaica: Structures of Novel Metal Complexes and the H-Bonding Interactions Featured in Them” and was very encouraged by the comments and advice I received, so much so that the organizers had to turn the lights off in order to get us out at the end of the session. I now feel that through the ACA I am a part of an entire network of crystallographers who are willing to support young people like me from developing countries like Jamaica who strive to become professional crystallographers. Congratulations and thanks to the ACA! Aloha and Mahalo,

Marvadeen Singh-Wilmot



I am grateful for the travel award to attend the meeting. Highlights included: swimming and snorkeling in the ocean, indulging in fresh seafood, and of course presentations by world-class scientists. I primarily attended the "Crystal Engineering and Supramolecular Chemistry: From Assembly to Structure and Function" sessions in which industrial and academic researchers from all over the world presented their latest and most exciting results. I would like to personally thank the organizers of the crystal engineering session for allowing me to present my graduate research to an audience of scientific role-models.

Nate Schultheiss

I would like to thank the ACA for their generous support. The meeting provided me precious opportunities to attend talks, visit posters, and meet with expert scientists. The organizers did a wonderful job. The programs and location of the meeting were wonderful. I attended and enjoyed many of the sessions, particularly the “Management of Synchrotron Image Data: imgCIF File System and Beyond”, “New Structures”, “Difficult Structures”, and “Membrane Proteins Structures”

as well as the “Topics of Interest to the Young Scientist” which provided valuable information to graduate students and post-docs to help them prepare for their future careers. Also, I enjoyed the discussions as well as feedback during my poster presentation. Another exciting thing was to be able to meet many friends and colleagues at the meeting to learn of their work and plans.

Ke Shi



The ACA meeting was a rewarding experience for me and I appreciate the travel grant that helped with my expenses. From the oral and poster sessions to the exhibitions, social events and the many informal discussions that were held, the aloha spirit of Hawaii was all around and created an atmosphere suitable for learning and networking. I found sessions such as “Whole Molecule Disorders” and “Difficult Organic Organometallic Structures” helpful for common problems associated with structure solution and for those of us in academia; sessions like “Undergraduate Research Showcase”,



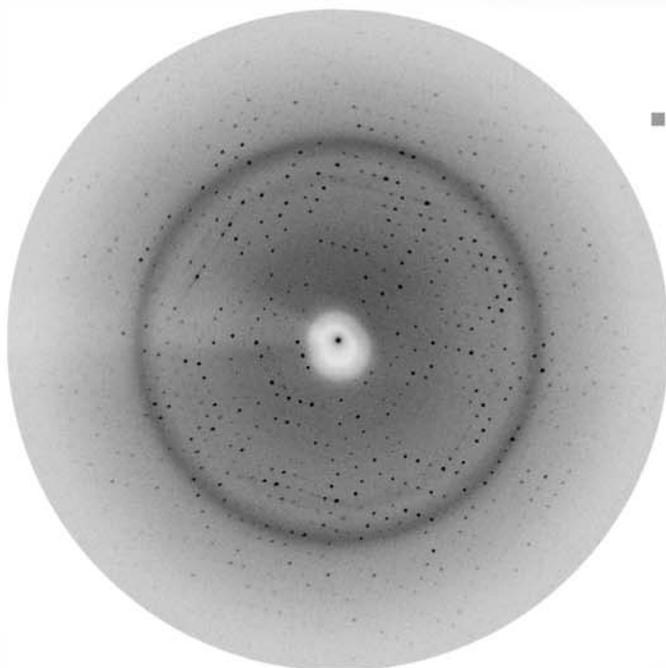
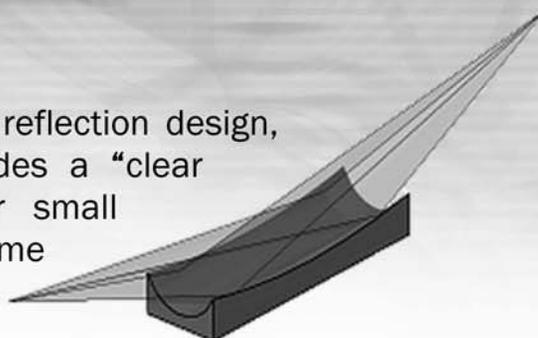
(Con't on page 52)

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The crystal belongs to space group C222 with cell dimensions $a=72.1\text{\AA}$, $b=97.4\text{\AA}$, $c=191.0\text{\AA}$. Images were collected with an oscillation angle of 0.4° . The crystal was a thin plate with approximate dimensions $200 \times 75 \times 50 \mu\text{m}^3$. The generator was a Rigaku RuH3R running at 50kV, 100mA (300 μm focus) and the data were collected on a Mar345 image plate detector.

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

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I would like to thank the ACA for the generous travel award. At the meeting I was able to listen to some tremendous talks by people from research groups all over the world. I particularly enjoyed the supramolecular symposium that will aid me in my own research. I presented a poster at the meeting and received valuable feedback that could benefit me in my future research. The travel award not only enabled me to attend the meeting, but to also experience the beautiful and diverse city of Honolulu, and the island Oahu itself. Thank you for the support that was provided to me.

Michelle Smith



great deal of what to do and what not to do when presenting my work.

I had a poster for in which I presented work we have done on CIF validation. I had an interesting discussion with Brian McMahon about the next steps we need to take. Ralf Grosse-Kunstleve also took part in the discussion. On the next day I started working on something based on these discussions. Also, an interesting experience I had was that a woman who stopped by our poster noticed my name and asked me about my nationality. When I said I am from Bulgaria, she said that one of her assistants is also Bulgarian. That was really fascinating considering that Bulgaria has a little less than 8 million people.

My impression from an organizational point of view is that the ACA really had everything under control. I noticed some problems with the wireless internet access, but that was not a serious problem at all.

Georgi Todorov



I had a really great time at the meeting. The most important thing was how well developed the small molecule program was. I think the talk by Prof Fujita was really outstanding. Just from the size of his assemblies, you could think he did not even belong in the "small molecule" symposium. However, all the lectures were really outstanding, and the poster sessions were very informative. I am very thankful for the experience I got to have in Hawaii, and consider myself privileged to have met so many outstanding scientists.

Tony Sokolov

The ACA meeting in Honolulu blended many things that make this young scientist happy: exposure to great scientific discoveries and techniques, as well as the beach, water sports, beautiful weather and scenery! At first glance, being in Hawaii, one would expect that a young person like myself would spend most of his time away from the meeting--actually, while I did spend lots of time at the beach, taking tours around the island, and relaxing, I spent just as much time at the

meeting itself. This year's ACA had many great talks and posters about all things crystallographically related so that it was a pleasure to attend this conference. Being from Toronto, the cost of the flight would have been prohibitive had I not received a travel award. Thank you the for the travel grant and for a great conference!

Peter J Stogios



I wish to thank the ACA for the grant that brought me to a meeting with very interesting people from all over the world. The was my second crystallographic meeting and it was a very good experience not only because of the location, but also because of the people that I met there. Everyone I talked to seemed so friendly and happy. This second meeting proved to me that crystallographers really enjoy what they do and really love to get together and talk about it.

Since I am still an undergraduate most of the experience I gathered was personal. The presentations I attended taught me a



Thank you very much for the travel award. I really appreciated the opportunity to attend the ACA meeting this year.

I am in a virology program and became interested in structural biology as a way to address interesting questions that many techniques used in classical virology labs could not answer. I have used macromolecular crystallography to help elucidate the cell entry pathway of rotavirus. I realize this is only a small part of what the field of crystallography has to offer so I viewed this meeting as a way to immerse myself in the field. I was also drawn to this meeting because of an increased focus on alternative methods such as SAXS and AFM. Using these

complimentary methods in conjunction with more traditional x-ray crystallography allows even more interesting questions to be answered. The grant made this meeting affordable enough to convince my advisor that it was worth sending me. I was able to get exposure to many new facets of crystallography and to other methods that will help expand the scope of my future research. I likely would not have had this opportunity without the travel award. Thanks again for this great opportunity.

Josh Yoder



Many thanks to ACA for the grant to attend this important and eye-opening international conference. I am also grateful to have presented a talk in the structural genomics session for which I received many nice suggestions and comments even days after my talk. Thanks to my supervisor for valuable advice and to my labmates for their help. Although I attended quite a few other scientific meetings before but this was my first ACA meeting and it was a wonderful experience.

I was able to find something interesting every morning and afternoon. Sometimes, I even wished I could split myself to sit in two sessions at the same time. I enjoyed very much learning about recent studies and new technologies from many fantastic talks and posters. The evening programs of the YSSIG mixer, mentor-mentee dinner and the awards banquet were very inspiring. The vendor exhibitions provided a lot of resources as well.

This meeting also gave me a great opportunity to meet my mentors and colleagues from my former two labs, some of whom I had not seen for years. It

exciting to catch up on the news. I have very beautiful memories from this ACA meeting in Hawaii. Thank you all again!

Minmin Yu



This was my third ACA meeting, but my first as an actual crystallographer. As a non-crystallographic graduate student in a crystallography lab I had gone to Buffalo in 1999 and Chicago in 2004, more as a voyeur than an actual participant. Now that I'm actually doing crystallography, attending the meeting was an entirely different experience. It was great. I could have conversations with people and sympathize appropriately with their tales of synchrotron trips, whereas before I was just kind of faking it. I could commiserate with the "scooped" as only other structural biologists can. I could talk to vendors without just feigning interest to get to the chocolate and free t-shirts. (Though, sadly, I never got my hands on a beach towel.) This year, I even had work to present and was given the opportunity to present it in a lecture session. I was horrifyingly nervous, of course, but it was still really exciting! I thought it was great that more talks were given by postdocs this year. It helps us to be proud of our work and accomplishments. This is a good thing because normally we're just frustrated! This was the first conference of any kind that I have been to where I thought that the people that I met would be with me for years to come. They would be my future colleagues, collaborators, competitors, business associates, and friends. It was nice to feel like part of a real community, and I'd like to thank the ACA for making it possible for me. See you next year!

Bomina Yu



When I was notified that I was selected to give an Etter lecture I was surprised and pleased to present our work on the use of ultra high energy for experimental phasing in front of such panel of experts. To be honest I was also very pleased to visit Hawaii. After spending days working on the data and preparing my talk (scheduled for the last day) while following all the other interesting sessions I finally presented our team work in an exciting session with a large audience. This was my first talk in English. The whole radiation damage session was tough and challenging with a lot of excitement, which was a sign of strong interest. The work I presented covered our work on the potential use of ultra high energy in protein crystallography to minimize radiation damage. High resolution data collected at 55 keV (0.2 Å) allowed building a complete model using only one wavelength via the SAD procedure for the first time. I also presented similar data recorded at medium energy (12 KeV) which showed clear signs of radiation damage while the ultra high energy data were absolutely "clean", with no sign of radiation damage. Both crystals used for the comparison diffracted to 1.25 Å resolution, were grown under the same condition and were the same size.

Jean Jaconic

The ACA conference in Honolulu was as enjoyable an experience as one can have at a conference. Obviously, the location was unparalleled, and the experience of just being in the city with all of its attendant sights and sounds was a once in a lifetime opportunity. I thoroughly enjoyed the time

I was able to get away and see the amazing scenery and culture that are prevalent throughout that area.



The conference itself was invaluable as well. This was my second ACA meeting (2004 in Chicago) and compared to many other conferences I have attended, the organization and support were excellent.

I was honored to receive a Margaret C. Etter Student Lecturer Award from the Small Angle Scattering SIG that afforded me the opportunity to present a talk rather than a poster, which at this point in my education was invaluable. As a PhD candidate writing my dissertations as I enter the final months of my studies, the input I received from the individuals in attendance at my session greatly influenced the focus of my final months as a student. The perspectives and suggestions I received have dramatically helped as I wrap up some of the final modeling work that will make up a large part of my dissertation.

I am very grateful to the ACA, Volker Urban, the SIG, and my advisor Dale W. Schaefer (U of Cincinnati) for the nomination and receipt of the Student Lecturer Award. Your kindness and support will always be fondly remembered.

Ryan Justice

Participating in the 2006 ACA meeting was clearly a highlight in my scientific career! Through the generous support from the ACA, I could embark on the long journey from the other side of the world to the beautiful islands of Hawaii. We had started to crystallize the fungal fatty acid synthase some years ago and this was my first opportunity to present our work to a broad international audience. I was delighted and honored to have been

selected for an Etter Student Lecturer Award and I would like to thank the Macromolecular SIG, as well as Brian Wimberly and Thomas Earnest who chaired our session. I really appreciated having the chance to meet again with the instructors of the famous x-ray course at CSHL, who taught me so much a few



years ago. The number of excellent talks and posters was impressive, and I still remember many interesting conversations we had during the poster sessions. We all got caught by the Hawaiian spirit, the people, the landscape, the music and the dances, that made the stay in Honolulu an unforgettable experience,

Simon Jenni



I would like to thank the ACA for the opportunity to present my work at my first crystallographic conference and I enjoyed it thoroughly. The location was beautiful and it was wonderful just to be in this environment. The conference was very well-organized and there many interesting evening activities such as the YSSIG mixer, the mentor/mentee dinner, and the awards banquet where it was easy to meet and communicate in an informal atmosphere. I met many professionals working in the areas closely related to mine. Everyone was open for discussions and sharing of experiences. This was also the first time I presented my results as an oral talk and

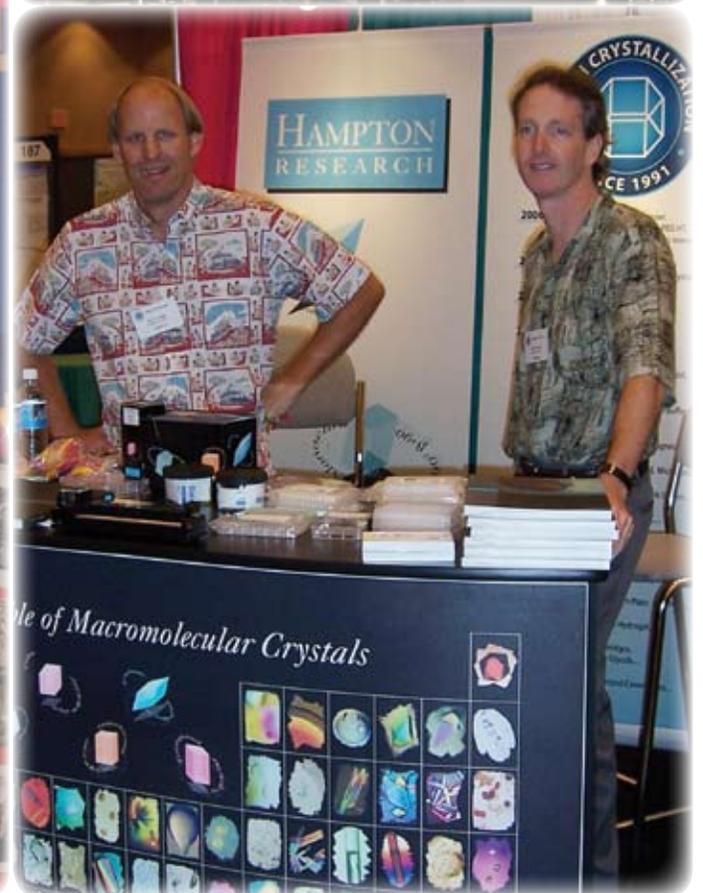
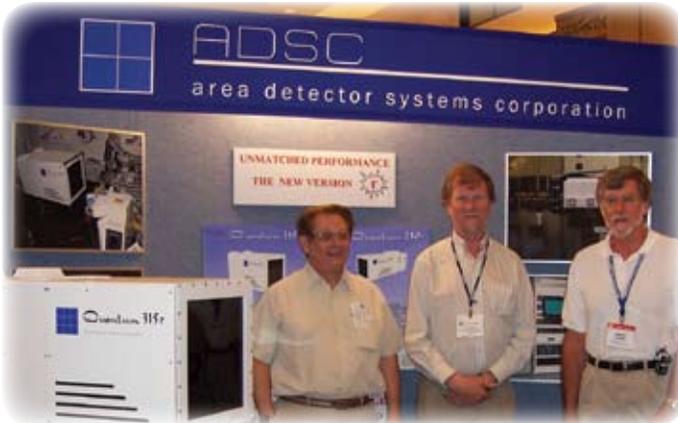
I found the audience to be very friendly and encouraging. I was greatly honored to receive an Etter Student Lecturer Award. In terms of science, this meeting was tremendous. I was able to meet leading luminaries in crystallography of whom I knew since the very beginning of my studies. The poster sessions covered a broad range of topics and were beneficial and informative. Many thanks to the ACA for the travel grant that allowed me to gain many rewarding and motivating experiences.

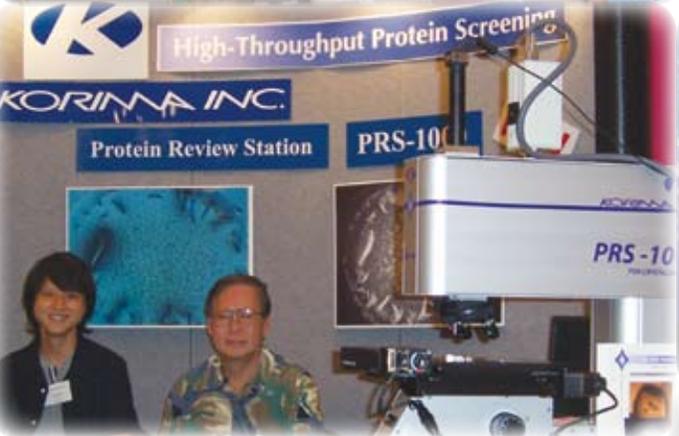
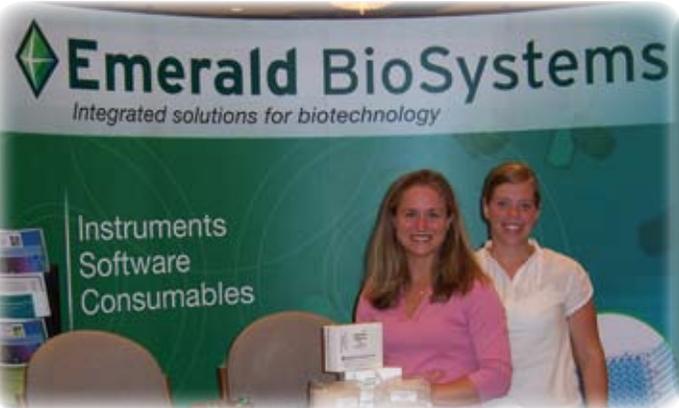
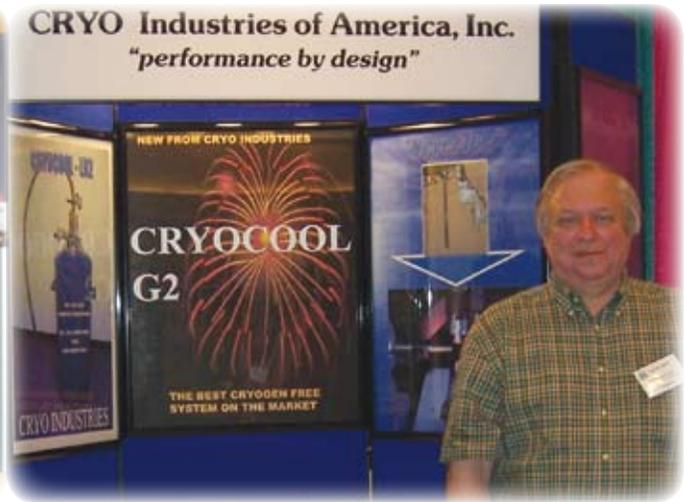
Yulia Servyugina



I am very glad to have had the opportunity to attend the meeting. As a graduate student I learned a lot. The GISAS workshop and sessions on scattering technologies highlighted work in this area. It is really a pleasure to know the excellent work of other scientists. I met Dr. Sinha, one of the smartest scientists in the world, and I had a very constructive discussion about my future work with my old friends, Dr. Lee and Dr. Jarek. I must thank the ACA for the travel grant and for being selected to receive an "Etter award".

Peng Wang









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J.D. Bernal: A Life in Science and Politics

Andrew Brown has compiled an excellent biography, subtitled *Sage of Science*, of the brilliant crystallographer, J. Desmond Bernal (1901-1971) (the nickname Sage was acquired at Cambridge, according to Perutz, "because he knew everything, from physics to the history of art"). There have been other accounts of Bernal's colorful life, including his own unpublished *Microcosm*, but this is the first attempt to portray the immense range of his scientific and political



energies, interwoven with glimpses of his unconventional domestic life. Twenty-five years after the publication of Bernal's most influential book, *The Social Function of Science* (London, Routledge, 1939), Charles P. Snow contributed a perceptive personal portrait, emphasizing Bernal's bravery and imagination, to *The Science of Science* (ed. M. Goldsmith & A. Mackay, Souvenir Press, 1964).

Dorothy Hodgkin composed a beautiful, affectionate, authoritative and detailed appreciation (*Biogr. Mem. Fellows R. Soc.*, 26, 17-84, 1980) of her friend Bernal's early life and subsequent career. She included Lord Mountbatten's admiring memories of Bernal's pertinent scientific advice for the 1944 Normandy invasion. More recently, Brenda Swann and Francis Aprahamian edited a collection of 15 essays, *JD Bernal* (London: Verso, 1999), predominantly on Sage's international peace campaigning and other political activities, but including a useful chronology of events in Sage's life.

Andrew Brown has now produced a comprehensive and scholarly, but very readable biography (Oxford: University Press, 2005) based on five year's research into Bernal's papers and war reports and from information derived from many of his family, friends and colleagues. Brown's approach is broadly chronological. However, some of the 22 chapters are topic-based. Thus, a chapter on the *Physical Basis of Life* covers the emergence of molecular biology, while another on Peace brokering puts the anti-nuclear-bomb campaigns of the 50s and 60s in context.

Bernal was perhaps the most international of crystallographers. He was one of the scientists credited with ensuring that the new UN organization should include an S for Scientific (UNESCO). The *Social Function of Science* not only dealt in immense detail with the organization of science education and research in the UK, but also embraced a survey of science across the world. His proposals were both visionary and controversial at the time. As early as 1930, Bernal was involved with Ewald on committees on abstracting, nomenclature and tabulation of space groups. More generally, early recognition of the problems of dissemination and retrieval amid the information explosion led to far-reaching proposals for what would ultimately be an international institute for scientific publication and information abstraction. The suggestion that new structures should be logged was made in 1948, but it was not until 1970 that Olga Kennard could dedicate the first two volumes of the CCDC's *Molecular Structures and*

Dimension to Bernal. His familiarity with post-1945 Schools of Crystallography in Britain and the Commonwealth is shown in Chapter 17 of *Fifty Years of X-ray Diffraction* (ed. P.P. Ewald, Utrecht, IUCr 1962). Having been one of those involved in the 1946 decision to set up the IUCr, he became President in 1963 until incapacitated by his second tragic stroke in 1965.

Several visits to the USSR in the early 1930s made a strong impression on Sage, although his irrevocable position on religion and politics had been established earlier. His first adult visit to the US was curtailed by the outbreak of World War II in 1939. Post-1945, many of Sage's visits to the USSR, Eastern Europe (several of whose scientific academies awarded him Membership), China and India included both scientific lectures and peace campaigning. He met Khrushchev, Mao Zedong and Nehru, gave a demonstration to Churchill, and participated in committee meetings in the White House, the Kremlin and 10 Downing Street. His experience of less developed countries began with laborious and uncomfortable war-time travel for Mountbatten but thereafter he made many lengthy tours to countries with emerging economies to advise on the development of each nation's science. His expertise across chemistry, physics, mathematics, biology and structural materials made him a valuable and inexpensive science consultant and also enabled him to indulge his wider intellectual interests with visits to historic sites and museums.

X-ray crystallographers of a certain age will be especially conscious that Bernal rejected W.H. Bragg's spectrometer, then in vogue at the Royal Institution in the 20s, in favor of Polanyi's rotating-crystal photographic method. He made the laborious calculations, first for Bragg and rotation angles and then for reciprocal-lattice coordinates, to facilitate the construction of indexing charts. (Incidentally, Polanyi, by this time at Manchester, was in the late 30s to disagree with Bernal both about his advocacy of the central direction of science and about life in Russia.) Bernal then designed what became the Pye (later Unicam) universal x-ray photogoniometer, widely used from the 30s to the 50s.

Perhaps Bernal's greatest scientific contribution was to nurture a clutch of Nobel Prizewinners in the development of molecular biology. Brown notes that with Bernal's prolific writing, this Renaissance man changed the course of science and initiated much systematic discussion and some action about what we now call science policy and the integration of science with society.

Outstanding intellects often display surprising discrepancies in behavior and judgment. Against much evidence, Bernal remained uncritical of Stalinist Russia (he accepted a Lenin Peace Prize in 1953) and continued to support Lysenko. He also lived what might euphemistically be described as a Bohemian lifestyle. With regard to personal achievement in scientific research, some would feel that he dissipated too much of his admittedly enormous energy in committee meetings or, indeed, in just too many activities. Thus, perhaps, was lacking the long-term obsession within a single field (though he returned to liquid structure, for example, quite late in his research career) that might have led to a Nobel Prize, whether in science or for peace. Brown neither ignores nor dwells on these matters unduly. He has produced a fascinating 470-page biography that does justice to the rich life of an inspirational and imaginative scientist and an ebullient, influential and wide-ranging character.

Derry W. Jones - Bradford University, England



July 21-26, 2007

Salt Palace Convention Center
Salt Lake City Utah

Deadlines:

Abstracts: March 1, 2007

Advance Registration: June 1, 2007

Hotel Reservations: June 13, 2007

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Program Chair

Jill Trewhella

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Workshops

Full Day - SHELX – Refinement of Twins/Disorder and Phasing with SHELX, C,D,E

Part 1: Refinement of Disordered, Twinned and High-Resolution Structures (Small and Macromolecules). **Part 2:** Experimental Phasing of Macromolecules.

Speakers: George Sheldrick -Regine Herbst-Irmer - Peter Müller -Thomas R. Schneider -Ton Spek

Half Day -Standards for Publication of Macromolecular NMR Structures

Award Symposia

Kenneth N. Trueblood Award in honor of Angelo Gavezzotti
Isidor Fankuchen Award in honor of Frank Herbstein
Margaret C. Etter Early Career Award in honor of Cora Lind



Transactions Symposium

Diffuse Scattering for the Masses: Local Structural Correlations in Molecular, Macromolecular, and Inorganic Crystals

Speakers: Ross Angel -Simon Billinge - James Britten - Branton J. Campbell - Donald Caspar, - Friedrich Frey - Lars Meinhold - George N. Phillips - Lee Robertson - Stephan Rosenkranz, T. Richard Welberry

Microsymposia - Organized by SIGs**Biological Macromolecules****New Structures****Strategies for Crystallization Challenged Macromolecules****Experimental Phasing with Longer Wavelength X-rays****New Membrane Protein Structures****Informatics in Structural Biology****Function from Structure**

*Speakers: Janet Thornton - Doug Brutlag - Sung-Hou Kim - Osnat Herzberg-
Aled Edwards - Alfonso Valencia,*

Computational Methods**Large and Difficult Structures**

Speaker Venki Ramakrishnan

Industrial**Impact of Crystallography in Industry**

Speakers: Barry Finzel - John Barker - Ping Chen - Giovanna Scapin

Materials Science**Non-Ambient Crystallography****Mineralogy and Crystallography: Real Crystals, Extreme Conditions**

Speakers: Bryan Chakoumakos - Lee Groat - George Lager - Ron Peterson

Neutron**Neutron Macromolecular Crystallography**

Speaker: Julian C.-H. Chen

Powder Diffraction**SDPD (Structure Determination from Powder Diffraction): Getting Better and Better!**

*Speakers: Abraham Clearfield - Carmelo Giacovazzo - Chris Gilmore - William I.F. David - Jason P. Hodges - James Kaduk
- Peter W. Stephens - Robert Von-Dreele - Matthew Peterson*

Small Angle Scattering**USAXS/USANS**

Speakers: Dale Schaefer - Paul Butler - Govindarajan Muralidharan - Andrew Allen

Characterization of Surfaces and Interfaces

Speakers: Changyong Park - Randall E. Winans

X-ray Imaging and Resonant Scattering**Small Molecules****Important Science from Small Molecule Structures**

Speakers: Bruce Foxman - Joel Miller - Chick Wilson, Univ. of Glasgow, Scotland

Tricks of the Trade: Interpretation of Structural Results

Speakers: Larry Falvello - Anthony Spek - Phillip Fanwick - Victor Young

Supramolecular Chemistry

Speakers: Christer Aakeröy - Len Barbour - Silas Blackstock - Kenneth Doxsee - Bruce Bart Kahr - John MacDonald

Cool Structures**Young Scientist****FLYS – Fun Lectures for Young Scientists****Undergraduate Research Showcase**

Joint Symposia

**General Interest I and II
Advances in Data Collection
Detectors**

Speakers: Mark Tate - Gerard Bricogne

Biomacromolecular Assemblies and Biomembranes

Speakers: B.T. Nixon - J.K. Krueger - H.W. Huang - J.G. Grossmann - S. Krueger - J. Lipfert

Time and Field Dependent Responses in Scattering Experiments

Speakers: Wim Pyckhout-Hintzen - Charles Dewhurst - Tom Mason - Matthew Kramer - Jim Richardson - Jon Hanson

Structural Mechanisms of Infectious Disease

Energy Storage and Conversion

Nanostructures

Micro-Crystals, Micro-Beams, and Multiple Crystals

Teaching Gadgets and Educational Tools

Speakers: Wally Cordes - Jenny Glusker - Henk Schenk

Radiation Damage

Exhibit Show 2007

An exhibition of the latest instruments and techniques for sample isolation, purifications and preparation; crystal growth and data collection, computer software for data storage, retrieval analysis, graphics systems, databases, and books, journals and other materials essential to modern crystallographers is scheduled to begin on the evening of Saturday, July 21 in conjunction with the Opening Reception. The 2007 Show will run through Wednesday, July 25. The Advertising and Exhibits Div. of the American Inst. of Physics is managing the show. For further information contact Bob Finnegan, AIP, 2 Huntington Quadrangle, Suite 1NO1, Melville, NY 11747, rfinneg@aip.org, ph. (516) 576-2433; fax (516) 576-2481.

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[Register online at www.AmerCrystalAssn.org](http://www.AmerCrystalAssn.org)



Little Cotton Wood Canyon (Photo by Eric Schramm)

Registration fees

| Fee | Advance (before June 1) | Late (after June 1) |
|----------------------------------|------------------------------------|--------------------------------|
| Regular Member | \$390 | \$585 |
| Retired Member | \$156 | \$234 |
| Post doc Member | \$195 | \$293 |
| Student Member | \$156 | \$234 |
| Nonmember* | \$585 | \$878 |
| Post doc Nonmember* | \$293 | \$439 |
| Student Nonmember* | \$234 | \$351 |
| Guest** | \$ 50 | \$ 50 |
| SHELX Workshop – full day | \$110 (60 students) | |
| SHELX Workshop – half day | \$70 (40 students) | |

| | |
|-----------------------------|-----------------------------|
| Mentor/Mentee Dinner | |
| Mentor | \$30 |
| Mentee | \$20 |
| Banquet | \$55 (\$25 students) |

* The nonmember registration fee includes a complimentary membership to the Association for 2007. Those registering as nonmember post docs or nonmember students must include documentation of this status with registration form.

**Guest registration includes Opening Reception, Exhibit Show and Get Together on Sunday morning.

Register on-line or download forms to register by fax or by mail.

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[Questions: aca@hwi.buffalo.edu](mailto:aca@hwi.buffalo.edu)

Symposium and Workshop on Charge Density and Time Resolved X-Ray Studies, MIT, February 10-11, 2007



The motto of the 2007 Bruker/MIT Symposium is going to be **Extreme Diffraction Data – the Cutting Edge of Structure Determination** with a focus on Charge Density Calculations and Time Resolved X-Ray Diffraction Studies in chemical and biological crystallography. Even though these fields are not brand-spanking new, they are clearly on the rise and major developments are to be expected within the next few years. Until very recently, only a few “extremists” were using these techniques, but lately the interest within the community has been growing. It seems fair to predict that within a decade or so these methods will be more or less commonplace, but right now, only very few people know how to use them. The upcoming Bruker/MIT symposium is meant to introduce a somewhat broader audience than just the “usual suspects” to these fascinating aspects of x-ray diffraction.

The lineup of speakers for both the workshop and the symposium is truly spectacular: **Philip Coppens** (SUNY Buffalo), author of the book “X-Ray Charge Densities and Chemical Bonding” (Oxford University Press, 1997), is one of the world’s foremost experts on charge density calculations as well as on time-resolved studies. In addition, two other world experts on charge density, **Tibor Koritsanszky** (Middle Tennessee State) and **Anatoliy Volko** (SUNY Buffalo), will be teaching at the workshop. Both Koritsanszky and Volko are among the authors of the program XD, which will be the basis of the workshop. Other speakers include **Christopher Cummins** (MIT), **Gregory Petsko** (Brandeis), and **Dietmar Stalke** (University of Göttingen), as well as **Roger Durst** (Bruker-AXS).

More information about the symposium, as well as an online registration form can be found at web.mit.edu/x-ray/bmit07.html. Registration will be open until a few days before the meeting.



Seventh Canadian Powder Diffraction Workshop, Trois-Rivières, Québec: 16th to 18th of May, 2007

The next workshop, including a one day on Total Scattering/PDF analysis, will be chaired by **Jacques Huot**. A powder workshop was held in 2005 at Trois-Rivières, where the university’s Pavillon Ringuet building was found to be an excellent venue; the workshop lecture theatre and computer facility are combined into a single room. Registration costs are still to be finalized, but we hope the student costs for the three day workshop will not exceed Cdn \$150. The costs will include a traditional “Maple Bush” Quebec dinner on the Thursday night. The workshop webpage is at www.cins.ca/cpdw/

As in the 2006 CPDW workshop, the first two days will focus on powder diffraction and the use of the GSAS Rietveld analysis

software. Lecturers and tutorial instructors are **Bob Von Dreele** (Argonne National Lab) co-author with **Allen C. Larson** of the GSAS software, **Angus Wilkinson** (Georgia Tech); **Ian Swainson** and **Lachlan Cranswick** (Canadian National Research Council). The third and final day will be on Total Scattering/Pair Distribution Function analysis with **Thomas Proffen** (Los Alamos National Lab) as lecturer and tutorial instructor.

Based on comments from the previous 2006 workshop, lectures have been modified with increased emphasis on fundamentals. This includes new lectures “Introduction to Powder Diffraction and Powder Diffraction Hardware” by **Angus Wilkinson** and “Introduction to the Basics of Crystallography” by **Ian Swainson**. The Synchrotron and Neutron Experiments lectures have been merged into a single talk. We look forward to seeing participants keen on learning, or on refreshing their learning, on powder diffraction.

The XVIII International Conference on the Chemistry of the Organic Solid State (ICCOSS XVIII), Universidad de Los Andes in Mérida, Venezuela, July 8 to 13, 2007.



This meeting follows the tradition started by Gerhard Schmidt and George Adler in 1968 at Brookhaven, which has continued through the years in Jerusalem (1993), Matsuyama (1995), Stony Brook (1997), Cambridge (1999), Mainz (2001), Sydney (2003), and Los Angeles 2005. This will be the first time it will take place in South America. For this occasion, a “School on Materials Applications of the Organic Solid State” (SMAOSS) will be conducted the week prior to ICCOSS-XVIII (July 1 to 6, 2007). The Conference and School Topics include:

Reactions in crystals: photochemical, thermal, high energy radiation - Crystallization phenomena: crystal growth, biomineralization, habit control - Theory and modeling - Crystal engineering and supramolecular interactions - Metal organic frameworks - Polymorphism and phase transitions - Functional crystals: magnetic, metallic semiconductors, photonic, etc. - Crystal dynamics - Polymers - Molecular machines - Nanocrystals - 2D Crystals: self-assembled monolayers - Pharmaceutical solids.

Support from the IUCr, ICDD, and other organizations is expected in order to help graduate students and young scientists attend the school and conference. The oral and poster presentations at the ICCOSS will be published in the *Conference Proceedings* in a special volume of *Molecular Crystals and Liquid Crystals*.

For more information: Graciela Díaz de Delgado, Laboratorio de Cristalografía, Facultad de Ciencias, Universidad de Los Andes, Mérida, Venezuela diaz@ula.ve, icco18@ula.ve, and www.ula.ve/eventos/icco18.

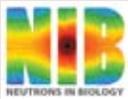
APRIL 2007

- 2-6  **Latin American Workshop on Applications of Powder Diffraction** and satellite workshop on **Methods of Powder Diffraction**, Laboratorio Nacional de Luz Sin-crotron, Campinas, Brazil. Invited speakers include Simon Billinge, Bob Von Dreele, Carmelo Giacovazzo, Peter Stephens, Brian Toby www.inls.br

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.crystallalice.org

JULY 2007

- 11-13  **Neutrons in Biology**, Oxfordshire, UK www.isis.rl.ac.uk/conferences/nib2007/

- 21-26  **ACA Annual Meeting, ACA 2007**, Salt Lake City See pages 60-62

AUGUST 2007

- 13-17  **9th International Conference on Biology and Synchrotron Radiation**, Manchester, England. www.bsr.2007.com

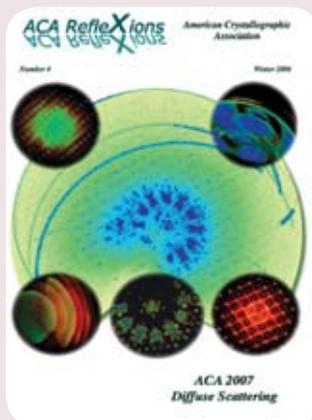
- 22-27  **ECM-24** Marrakech, Morocco. www.ecm24.org

NOVEMBER 2007

- 4-7  **AsCA - Asian Crystallographic Association Meeting, Taipei, Taiwan R.O.C.** www.asca2007.tw/index.html

MAY 2008

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

What's on the Cover:


The topic of the *Transactions Symposium* at ACA 2007 in Salt Lake City is Diffuse Scattering. The images chosen for the cover of this issue of *Reflexions* are snapshots of reciprocal space volumes, including some beautiful examples of diffuse scattering. Lower left: reciprocal space for a polycrystalline solid (Niewczas, Britten). Upper right: Texture in multilayered Cu/Ag sheets (Embury, Britten). Upper left: diffuse scattering from stacking disorder in a Ru complex (Siebert, Wadepohl). Lower right: Diffuse scattering in OF2Xe(NCCH3) single crystal (Schrobiglen, Bilir, Britten). Background and Lower middle images: hexagonal diffuse scattering from partially ordered stacks of hexanaphthylbenzene (Harrington, McGlinchey, Britten). The data contributors are Walter Siebert and Herbert Wadepohl (Universität Heidelberg) and Marek Niewczas, David Embury, Gary Schrobiglen, Vural Bilir (visiting student), Laura Harrington (McMaster University), and Michael McGlinchey (University College Dublin). The software used to display the 3D data was MAX3D (Weiguang Guan, Jim Britten).

Contributors to this issue:

Oliver Baettig, Joao Barbosa, Bob Bau, Christine Beavers, Herbert Bernsetin, Marina Borovinskaya, Jim Britten, Joel Brock, Marc Brodsky, Cory Brooks, Charlie Carter, Aina Cohen, Bryan Craven, Georgi Darakev, Olga Degtyareva, Louis Delbaere, Graciela Diaz Delgado, Jeff Deschamps, Gian Felcher, Zoe Fisher, Caroli Genis, Larry Grant, Lee Groat, Marv Hackert, Martha Heil, Andy Howard, Jean Jaconcic, Simon Jenni, Derry Jones, Ryan Justice, Jim Kaduk, Charles Lake, Paul Langan, Jeff Milton, Peter Mueller, Allen Oliver, Graciela Punte, Mark Saper, Andrew Schramm, Nate Schultheiss, Yulia Servyugina, Andrea Sharpe, Ke Shi, Marvadeen Singh-Wilmot, Michelle Smith, Edward Snell, Tony Sokolov, Peter Stogios, Robert Sweet, Georgi Todorov, Peng Wang, Ellen Weiss, Josh Yoder, Minimum Yu, Bomina Yu and Branton Campbell for the diffuse scattering image used as the backdrop to the pages acknowledging contributions to ACA funds.

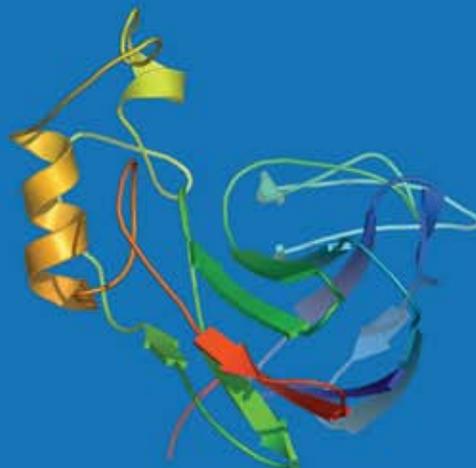
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