AMERICAN CRYSTALLOGRAPHIC ASSOCIATION

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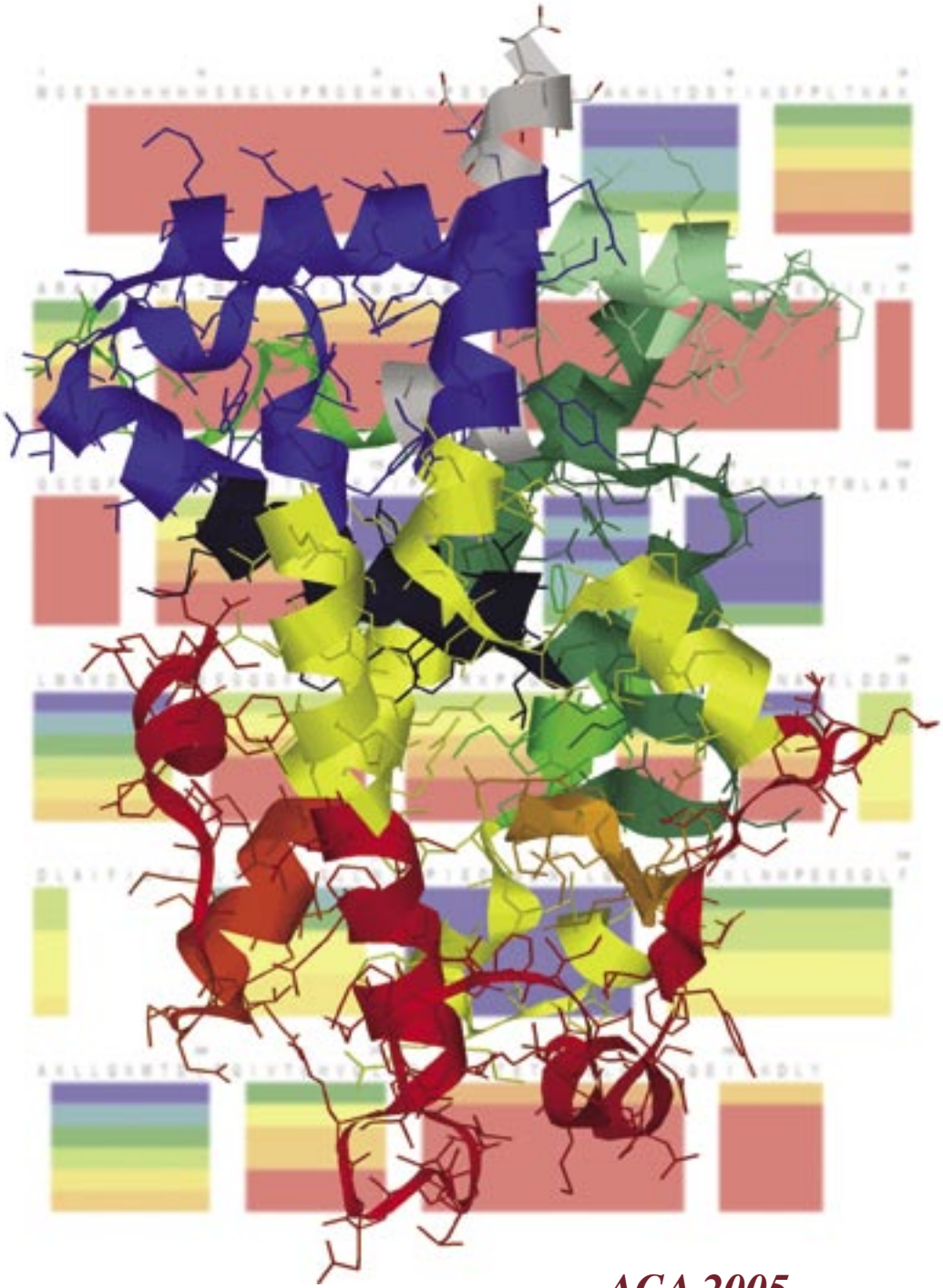

ACA 2005
Transactions Symposium
New Horizons in Structure Based Drug Discovery

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President's Column

The fall ACA Council meeting took place in early November. At this time, Council made a few decisions, based upon input from the membership. First and foremost, many will be pleased to know that a satisfactory venue for the 2006 summer meeting was found. The meeting will be held at the Sheraton Waikiki Hotel in Honolulu, July 22-27, 2005. Council is particularly appreciative of the hard bargaining efforts of S. Narasinga Rao, who negotiated a contract with extremely favorable terms for the ACA. Without his efforts, Hawaii would have been crossed off the list. Thank you, Rao!

Ken Dill, a founder of the "Bridging the Sciences Initiative", presented an overview of the organization and objectives to Council. Ken was eloquent in expressing the reasons for this initiative as well as convincing in his arguments as to why the ACA should participate. In accordance with expressed wishes of ACA members at the Chicago business meeting, Council voted to contribute $4000 for each of two years to the support the coalition, which includes ten national scientific organizations. The coalition hired the Honorable John Porter, a former U. S. Representative from Illinois and former chairmen of the U.S. House Appropriations Subcommittee on Labor during part of the recent five-year NIH budget doubling effort. Mr. Porter will open political doors and advise on all strategies regarding scientific appropriation bills. The ACA Council asked Judy Flippen-Anderson to be the ACA representative to this organization and she has agreed.

Congratulations are in order for Jennifer Swift, the winner of the 2005 Margaret C. Etter Early Career Award. She will be given her award at the presentation of her research in Orlando.

Congratulations are also in order for Bob Bau, who was elected vice president of the ACA and to Lee Groat, the new Canadian representative. It is with warmest regards and considerable regret that we bid farewell to the past president, Ray Davis, and the current Canadian representative, David Rose and thank them for their outstanding service to the ACA. While Ray will continue to be active in the ACA, few people really know about his timely e-mail responses and balanced perspective that he provided on all issues before Council. David Rose will be sorely missed for his wit and his conscientious reporting of Canadian affairs, both to Council and to the quarterly newsletter. Only those of us who have served on the Council with them can truly appreciate their conscientious efforts on behalf of all crystallographers.

As this is my last column, I want to take the time to thank all members of the ACA Council for their hard work. It has been my privilege to work with some very fine people, who have been so generous with their services. In addition to Ray and David, Lisa O'Keefe, as secretary, is burdened with reporting the minutes at each meeting, more than 10 in all including Council's meetings with various groups at the annual ACA meetings. Anyone who has read her detailed minutes knows what an effort this is. Doug Ohlendorf, as treasurer, has the task of keeping the ACA financially solvent. Not only are his quarterly financial reports thorough, but he saves the ACA thousands of dollars annually with his fiscally shrewd suggestions. Our federal government could really use his services! S. Narasinga Rao is the financial officer, who oversees the ACA investment portfolio, the proceeds of which support the ACA awards. Rao is also the best bargainer, bar none, when negotiating contracts for ACA meeting sites. Many a time, he has said his final no to a hotel's last offer, only to have the hotel call him back right before a Council meeting with better terms for the ACA. Bill Duax is the Executive Officer and IUCR President. Bill keeps us in touch with the progress and plight of other crystallographers throughout the world. His enthusiastic quarterly reports are a constant reminder that we all belong to one large community with mutual scientific interests. A huge thank you also goes to Marcia Colquhoun, who has served the ACA for sixteen years as Director of Administrative Services. Marcia, and her cohort Patti Coley, are the heart and soul of the ACA and without them, the ACA would not be the smoothly functioning organization it is today. In addition to Council members, two other people need special acknowledgement – Judy-Flippen Anderson and Connie Chidester who share the quarterly task of reminding the President to write a column and in assembling the interesting and profitable ACA Newsletter. A hearty thanks to all who have made my job easier. And so with all there fine people in place, I am happy to turn over the leadership to Louis Delbaere, who will keep the ACA traditions strong.

The ACA meeting in Orlando is shaping up to be another outstanding meeting. Local chairs Khalil Abboud and Tom Selby have the local arrangements well in hand and Ed Collins is working with the SIGs and the ACA standing committees to produce a scientifically diverse and rich scientific program.

Fran Jurnak

Marcia Colquhoun, Patti Coley and Tammy Colley at the banquet in Chicago

The Protein Structure Initiative: Past, Present, and Future

The **Protein Structure Initiative (PSI)** is a major NIH-sponsored effort in structural genomics. The long-range goal of the PSI is to make the three-dimensional atomic-level structures of most proteins easily obtainable from knowledge of their corresponding DNA sequences. The goal is being pursued by creating a library of structures that systematically samples major protein families, putting many or most new proteins within homology modeling distance of a library member. In order to populate this library, x-ray crystallography and NMR are used to determine three-dimensional structures in an efficient, low-cost way. This mode of high-throughput operation has been visualized as a pipeline for which the input is an expression clone, and the output (at less than 100% efficiency) is a three-dimensional structure. The groups also have elaborate target selection procedures to choose the proteins to be expressed for the pipeline.

In 2000 the National Institute of General Medical Sciences inaugurated the initial or pilot phase of the PSI by making awards to seven centers. Two more were added in 2001. The pilot phase was intended for the development of the comprehensive pipelines that would enable high-throughput structure determination. This pilot phase is coming to a close in the next few months. Applications for the second or production phase of the PSI were due at NIH on 16 October 2004. This seems an appropriate moment to review the progress made by the various consortia during the pilot phase, to assess the benefits of their output, and to anticipate what we may expect from the production phase.

Although the pilot phase was intended primarily for the development of the pipelines and their associated technologies, the PSI consortia together have determined over 800 protein structures since 2000, the vast majority by x-ray methods. Because of the long ramp-up times for the facilities, most of these structures have been done since 1 July 2003. Serious but unpublished comparisons indicate that the quality of these structures closely parallels the quality of PDB depositions as a whole. It seems entirely plausible that in production phase the consortia can each produce (say) 200 structures a year. For the most part the coordinates of these structures have been faithfully deposited in the PDB within six weeks of their completion; in a few cases groups have fallen behind in this process.

A major benefit of the PSI was intended to be the development of procedures, materials, and technologies useful to the scientific community at large. The consortia have invested heavily in this area, and a great deal of progress has been made. Results range from improvements in molecular biological protocols for high-throughput cloning and expression to automation of various crystallographic tasks, such as refinement, and to the introduction or use of robotics for a variety of tasks. The impact of this technical output on those outside the consortia varies widely. Much of the robotics for protein production, purification, and crystallization is too large-scale for an individual laboratory (although not for a biotech company). On the other hand, the systems that sometimes allow a crystal structure – from data collection through map tracing – to be completed in less than 24 hours are becoming available at many synchrotron beamlines, and will spread. Automated map tracing and refinement algorithms are useful for the typical university laboratory.

What can we anticipate from the production phase of the PSI? There are actually two classes of centers being created. Full-scale centers and specialized research centers. The full-scale centers are the direct descendents of the current pilot phase projects. They have 4 goals:

- Develop further the high-throughput pipelines.
- Continue development of technologies and methodologies.
- Determine approximately 200 structures per year.
- Develop new mechanisms of sharing the facilities and materials of the center with others.

The specialized research centers are being created to help surmount the major bottlenecks of the structural genomics pipeline, and they will focus on technology and methodology development. They are being encouraged to deal with challenging classes of proteins that are not currently amenable to high-throughput methods. In particular, the request for applications (RFA) mentions membrane proteins. proteins from human and other higher eukaryotes, and small protein complexes, but other systems may be proposed. By the end of their projects, the specialized centers must demonstrate production and structural determination of significant numbers of proteins in these challenging classes.

In a separate but related program NIGMS has issued an RFA for applications to dramatically improve homology modeling. How useful the PSI library of structures is depends on how well homology modeling works, and progress in this area, at least viewed from the perspective of CASP (Comparative Assessment of Structue Prediction), has been limited in the last few years. A jump start is needed.

It seems to me that there are many important deliverables that the centers will provide to the biomedical community at large. Let me list a few of these.

Structures. New publication methods are being explored so that the thousands of structures determined will be accessible through PubMed searches, bringing them into the realm of most users.

Methods dissemination. Although the methods developed by the various centers are well reported on their websites, and there are functional mechanisms for distributing materials, the fragmented nature of the information has made it less than easy to find and use. In the next generation NIGMS plans a web presence, the PSI Network Knowledge Base. that will integrate many aspects of the centers' output to make it more visible and accessible.

Community participation. The RFA states that "Research center applicants must have plans for activities for participation of the scientific community. For example, centers could designate a limited period of time for the incorporation of special projects from outside scientists into the structural genomics pipeline. Centers could plan for short-term courses and technical workshops for potential users of the pipeline, materials, and PSI results." This requirement is analogous to the rule that synchrotron beamlines must give 25% of their time to general users. I think that this is a vitally important aspect of PSI-2, and one that the community should lobby to strengthen.

3-d BLAST. In a more speculative vein, new software tools are under discussion that, by analogy with BLAST, will bring up on a user's screen 3-d structures of proteins homologous to the one input. Important functional areas will be highlighted on these figures. The preliminary nickname for this application is **Strange**, for **S**tructural **tran**slation of **ge**nes.

In summary, it is my sense that the PSI has made more progress in its first 5 years than almost anyone anticipated, and that the new full-scale centers will be well positioned to determine the ~200 structures per year that the RFA hopes for. There is much to be gained from PSI-2 by the biomedical community as a whole, but careful monitoring will be required to ensure that the dissemination function receives as much attention as the technology function.

Acknowledgements. In order to preserve accuracy some text in this piece has been reworked from NIGMS documents describing the PSI-2 program. The author is a member of the NIGMS advisory committee for the PSI.

Eaton E. Lattman, Johns Hopkins University

Editors Note: More about the PSI can be found at the following NIH website: ***www.nigms.nih.gov/psi/***

Incoming ACA President Louis Delbaere enjoying the opening reception in Chicago with Sue Byram and Wilson Quail.

Robert Bau - New ACA Vice-President

Robert Bau was born in Shanghai, China, in 1944 and grew up in Hong Kong. He received his B.Sc. from the University of Hong Kong in 1964 and did his graduate work in the Chemistry Department at U.C.L.A., receiving his Ph.D. in 1968 under the direction of Herbert Kaesz. Bau was introduced to (small molecule) x-ray crystallography while working in the laboratory of Melvyn Churchill at Harvard, where he accompanied Kaesz from U.C.L.A. on a sabbatical year. He returned to Harvard in 1968-9 for postdoctoral research in the laboratory of Nobel Laureate William Lipscomb, working in protein crystallography as part of the team that solved the structure of aspartate carbamoyltransferase. Following this postdoctoral year, he joined the chemistry faculty at U.S.C., where he has taught for 35 years and now is Professor of Chemistry. Bau has been a fellow of the Alfred P. Sloan Foundation as well as recipient of an NIH Research Career Development Award and the Alexander von Humboldt Senior U.S. Scientist Award. He is also a Fellow of the American Association for the Advancement of Science (AAAS).

Historically, the work of Bau's research group has centered on the study of transition metal hydride complexes and the investigation of unusual modes of metal-hydrogen bonding. Together with his long-time collaborator Thomas Koetzle at Brookhaven National Laboratory, Bau used single-crystal neutron diffraction to examine the structures and bonding in metal hydrides. In particular, Bau's research has demonstrated that hydride ligands can bond to several metal atoms in discreet coordination complexes in a manner similar to that found in binary metal hydrides. In another avenue of research, Bau's group has exploited the sensitivity of neutrons to isotopic substitution to determine the absolute configuration of isotopically substituted molecules.

Bau and his students have been major users and have carried out experiments at many of the neutron scattering centers worldwide, including Argonne, Brookhaven, and Los Alamos in the U.S.A., the ILL and ISIS in Europe, and JAERI in Japan. Recently, Bau's group has been exploring the potential of making the neutron diffraction technique more accessible to protein crystallographers. In this work they are demonstrating that, with the advent of a new generation of sensitive neutron detectors developed by various groups around the world, in favorable cases it is now possible to locate the hydrogen atoms in protein structures at atomic resolution.

Bau is the Principal Investigator of the Instrument Development Team (IDT) for the single-crystal diffractometer (Topaz) at the Oak Ridge Spallation Neutron Source (SNS). In addition, he is a member of the IDT for the macromolecular neutron diffractometer (MaNDi) at SNS.

Tom Koetzle

ACA 2004 Election Results

Vice-President
Robert Bau

Canadian Representative to Council
Lee Groat

Standing Committees

Continuing Education
Gloria Borgstahl

Data, Standards, and Computing
Bernhard Rupp

Communications
Annie Heroux

SIGS

Biological Macromolecules
Chair-elect: Craig Ogata
Secretary: Patrick Loll

Fiber Diffraction
Chair-elect: Gerald Stubbs

General Interest
Chair-elect: Bruce Noll
Member-at-Large: Gary Enright

Materials Science
Chair-elect: Lachlan Cranswick
Secretary: Brian Toby

Neutron Scattering
Chair-elect: Paul Langan
Secretary: Thomas Proffen

Powder Diffraction
Chair-elect: Bryan Chakoumakos

Service Crystallography
Chair-elect: Jeanette Krause
Secretary: John Desper

Small Molecules
Chair-elect: Alicia Beatty

Synchrotron Radiation
Chair-elect: Aina Cohen

Young Scientist
Chair-elect: Robert Scavetta
Secretary: Robert Huether

News from Canada. November, 2004

Northern Light Open for Business

The Canadian Light Source in Saskatoon celebrated its official opening on October 30th. Representatives from all levels of government, the media, the university and the scientific community gathered for the event, which generated considerable national and international attention. The following representatives from established synchrotrons came to the opening: Wolfgang Drube - HASYLAB at DESY (Hamburg, Germany), Murray Gibson - APS (Chicago), Steven Dierker – NSLS (Brookhaven, NY), Ben Feinberg – ALS (Lawrence Berkeley National Lab), Jost Goettert - CAMD/LSU (Louisiana), Manuel Rodriguez – ESRF (Grenoble, France). The Canadian Broadcasting Corporation held *The National News* broadcast from the CLS site on the previous evening, and the popular science radio program, *Quirks and Quarks*, also did a special segment on synchrotrons. Further coverage, including audio feeds, can be found through the CLS website, ***www.lightsource.ca.***

The CLS has been generating radiation for almost a year and commissioning of beamlines is well underway. The beam has been operating at 100 mA or better since April for hardware and configuration testing.

BHT Regional Crystallography Meeting

The 13th annual Buffalo-Hamilton-Toronto (BHT) regional crystallography meeting was held in Hamilton on November 5th, 2004. As usual, the morning was devoted to a technical workshop, and this year participants were treated to a double bill on membrane protein crystallization from ***Michael Wiener*** (U. Virginia) and ***Declan Doyle*** (SGC, Oxford). The speakers described the many difficulties and hurdles, along with some useful tips, for those courageous enough to undertake a membrane protein project. The take-home messages that came through were: lots of patience, extreme care for reproducibility, work fast, and "screen, screen, screen". Also, don't just hang your hat on 3-D crystallography, but take advantage of other techniques that can give significant functional information even in the absence of crystals. Despite these difficulties, the speakers presented some remarkable results on several systems, including the TonB transporter and a number of ion channels. Following the workshop talks, Michael and Declan were joined for a panel discussion by local 'membrane-ologists' ***Gil Privé*** (Toronto) and ***Michael Malkowski*** (Buffalo).

Left: Michael Wiener demonstrating the height of a transmembrane helix. Right: Declan Doyle "screen, screen, screen".

In the afternoon, recent results were presented by trainees in several laboratories in the region. These included ***Robert Garces*** (E. Pai laboratory, Toronto) on the circadian clock machinery, a heme oxygenase from *E. Coli* by ***Michael Suits*** (Z. Jia, Queen's), an enthusiastic discussion of the ornithine cyclodeaminase structure from ***Jessica Goodman***, and an interesting dissection of a hairpin ribozyme mechanism from ***Shabnam Alam*** (both with J. Wedekind, Rochester). These were followed by ***Leanne Wybenga-Groot*** on the Eph Receptor regulation (F. Sicheri, Toronto), ***Alex Ghetu*** on the Bcl-6 BTB complex with BCoR (G. Privé, Toronto), FabZ dehydratase by ***Matt Kimber*** (Affinium Pharm. Toronto) and an introduction by ***Alexei Bochkarev*** to the Structural Genomics Consortium in Toronto. Planning for next year's meeting is already underway. The symposium was generously supported by donations from Hampton Research, Nextal, Bruker AXS, Rigaku MSC, VWR/Biogenova, Affinium Pharmaceuticals and the Canadian Institutes for Health Research (CIHR). Several of these supporters had very informative displays and representatives at the meeting.

The Membrane Panel: (l to r) Michael Malkowski , Gil Privé, Declam Doyle, and Michael Wiener.

Afternoon speakers: (l to r), Back: Matt Kimber, Michael Suits, Alexei Bochkarev, Alex Ghetu; Front: Robert Garces, Shabnam Alam, Jessica Goodman, Leanne Wybenga-Groot.

Anyone in the region of Southern Ontario/Western New York is welcome to attend next year's meeting.

David Rose

Position available

Structural Biologist/x-ray crystallographer or a biophysicist/biochemist with interest in crystallography with a Ph.D. or a M.S. with experience to work on an NCI funded research project on rational design of peptide vaccines for melanoma. Send resume and references to: Dr. D. Ghosh, Hauptman-Woodward Institute, 73 High St, Buffalo, NY 14203, ghosh@hwi.buffalo.edu. The Hauptman-Woodward Institute is an Equal Opportunity Employer.

Report from the ACA Continuing Education Committee

During 2004 the Continuing Education Committee was busy performing its required tasks.

For the second year in a row the committee evaluated proposals for travel grants. A total of 65 proposals were evaluated for scientific content and need. The proposals were divided into three groups: macromolecular crystallography (38), materials and methods (12) and small molecule crystallography (15). Each proposal was evaluated for its scientific merits by a member of the committee who specializes in the area of the proposal. In addition, each was evaluated for need based on several criteria. An overall ranking based 75% on the science score and 25% on need was then provided to the Council. The above criteria were agreed upon by last year's committee.

Five workshops were proposed for the 2004 ACA meeting. Four of the workshops were conducted at the Argonne National Laboratory about 30 miles from the Chicago meeting site. Unfortunately the workshop entitled *GM/CA Synchrotrons for the Biologist* was cancelled. The other four were as follows:

MAD/SAD Phasing, Data Collection, Processing and Structure Solution≤ organized by ***Jim Fait*** (Argonne).

Small Molecule Crystallography at ChemMatCARS organized by ***P. James Viccaro*** (University of Chicago) and ***Victor G. Young*** (University of Minnesota). Registration was limited to 50 and was oversubscribed.

A Protein Crystallographic Toolbox: CCP4 Software Suite and PDB Deposition Tools organized by ***Maeri Howard-Eales*** and ***Peter Briggs*** (CCP4), ***Judith Flippen-Anderson*** and ***John Westbrook*** (RCSB Protein Data BAnk).

APS/IPNS Tour organized by ***Dennis Mills*** (APS) and ***Arthur Schultz*** (IPNS).

One of the official charges to this comminttee is to coordinate workshops and educational sessions at ACA meeting. Therefore, the Committee strongly recommends that it co-sponsor any such sessions in the future to ensure proper integration and coordination of similar topics.

Several members of the committee were actively involved in educational activities. ***Marilyn Olmstead*** was a faculty member at the ACA Summer Course held at Indiana University of Pennsylvania July 25-Aug 4. ***Katherine Kantardjieff*** has been and continues to be active promoting educational activities at the USNCCr.

Phil Fanwick

Crystallography Web Watch

I would like to thank ***Sidney Abrahams*** (Southern Oregon University) for contributing to this installment of the Web Watch Column. He would like to draw attention to several sites related to Crystal Engineering news.

www.crystengcomm/crystengcommunity
www.CrystEngComm.org

A special treat for all of us is announced at this site---*Chemical Society Reviews* has just published a special issue (#8 - 2004) on *Current Advances in Crystallography*. Included in this issue are: *Research applications of the Cambridge Structural Database (CSD)* (***Frank H. Allen, Robin Taylor***); *Developments in inorganic crystal engineering* (***Lee Brammer***); *Low temperature single crystal x-ray diffraction: advantages, instrumentation and applications* (***A. E. Goeta, J. A. K. Howard***); *Single-crystal x-ray diffraction studies of photo-induced molecular species* (***Jacqueline M. Cole***); *Polarimetric imaging of crystals*(***Werner Kaminsky, Kacey Claborn, Bart Kahr***); *How to determine structures when single crystals cannot be grown: opportunities for structure determination of molecular materials using powder diffraction data* (***Kenneth D. M. Harris, Eugene Y. Cheung***); *Beyond classical applications of powder diffraction* (***John S. O. Evans, Ivana Radosavljevi Evans***); *Synchrotron and neutron techniques in biological crystallography* (***M. P. Blakeley, M. Cianci, J. R. Helliwell, P. J. Rizkallah***); *High-throughput protein crystallography and drug discovery;* (***Ian Tickle, Andrew Sharff, Mladen Vinkovi, Jeff Yon, Harren Jhoti***).

These sites should also be a reminder to all of us that many journals are conveniently on-line to assist us in our research endeavors. Besides our very popular IUCr site and its excellent journals, a few additional sites are listed here as a reminder:

American Chemical Society ***ubs.acs.org***

Royal Society of Chemistry journals
www.rsc.org/is/journals/current/ctitles.htm

Oldenbourg Electronic Journals
www.oldenbourg.de/verlag/

Elsevier ***www.elsevier.com/wps/find/***

Springer/Kluwer ***www.wkap.nl/***

Nice compilations of crystallographic resources and links covering journals, publishers, databases, programs and much more can be found at:

www.hkl-xray.com/hkl/Links.htm

www-mslmb.niddk.nih.gov/procryst.html

cheminfo.chem.ou.edu/~ahw/groupweb/resources.html

chemistry.library.wisc.edu/instruction/xraycrystallography.htm

Chemistry Biology Information Center ETHZ has put together a nice internet directory of sites and links related to chemistry, biology and crystallography at ***www.infochembio.ethz.ch/links/en/index.html***

Just click on the area of science that tickles your fancy.

Jeanette Krause

Joint CCP4-RCSB PDB Workshop

A joint CCP4-PDB workshop "A Protein Crystallographic Toolbox: the CCP4 Software Suite and RCSB PDB Deposition Tools" was held prior to the ACA annual meeting in Chicago this summer. CCP4 (Collaborative Computational Project No.4) is a UK initiative based at CCLRC Daresbury Laboratory, which provides a suite of programs used for macromolecular structure determination by x-ray crystallography; the RCSB (Research Collaboratory for Structural Bioinformatics) provides and maintains a database of macromolecular structures as part of the worldwide Protein Data Bank (wwPDB). Although this was the third year that CCP4 has held such a workshop, this was the first in collaboration with the RCSB PDB – an obvious step since the majority of protein structures determined with the use of CCP4 software will ultimately be deposited with the Protein Data Bank.

At the workshop: (Back row) Roberto Steiner, Stuart McNicholas, Peter Briggs, Gwyndaf Evans, and Judy Flippen-Anderson (Front row) Paul Emsley, Kyle Burkhardt and Shuchismita Dutta. Martin Noble is pictured below.

The objective of the workshop was not to teach crystallography but rather to show people how to use some of the key programs distributed with the CCP4 package to solve structures, and how to get the best help from the RCSB PDB when they deposit these structures. The workshop was well attended, with over 60 delegates filling the room in the Chicago Hyatt Regency where the conference took place. The attendees varied in their level of experience from graduate students to experienced crystallographers, and had varying levels of familiarity with the software offered by CCP4 and the RCSB PDB.

Because the audience was diverse and the softawre has a broad range of functionality, the attendees were subjected to a fast moving and tightly packed schedule that aimed to give an overview of the software available before focusing in on the practical details. To begin with ***Peter Briggs*** (CCP4) gave an overview of the CCP4 suite that concentrated on the non-crystallographic aspects of the software for both novice and expert users. He was followed by ***Martin Noble*** (Oxford University, UK) who gave an excellent and highly educational tour of the functionality present in CCP4, in itself no easy task. In one of the high points of the workshop he proceeded to give a live demonstration of how to solve two structures in ten minutes.

Shuchismita Dutta (RCSB-PDB) then presented some practical advice on using the pdb_extract suite of programs to make deposition easier, reminding the audience of why the deposition of accurate data is important, and how the software tools provided by the RCSB PDB can help improve the accuracy of the data as well as make the deposition process easier.

Gwyndaf Evans (Diamond Light Source, UK) followed with an overview of using the MOSFLM and SCALA programs for integrating x-ray diffraction images and then reducing and scaling the resulting data, and ***Roberto Steiner*** (University of York, UK) covered refinement with REFMAC5 using a mixture of theory and practical demonstrations. Both speakers covered many practical points and stressed the necessity of collecting good experimental data – if the data is poor then no software can rescue it!

Demonstrations were then given by ***Stuart McNicholas*** and ***Paul Emsley*** (University of York, UK) of projects within CCP4 that are developing a new generation of exciting graphical tools for model building and viewing of molecular models. ***Kyle Burkhardt*** (RCSB PDB) closed with a presentation on how the RCSB PDB validates and annotates deposited structures, giving an enlightening and often humorous account of how the process works. She offered practical advice on making deposition a more successful and more pleasant experience for both the depositor and the annotator.

The workshop wound up with summary points from each of the presentations – particularly useful at the end of a long day when the morning session seemed very distant indeed.

CCP4 and the RCSB PDB were part of the "Data Alley" in the exhibit hall.

The positive feedback provided via the questionnaires suggested that the workshop was very successful, with delegates commenting on "very clear and helpful topics and demonstrations that were very well organized," and how they had been "introduced to many new - and old - programs that I either was not aware of or wasn't aware of their capabilities." Encouraged by these positive comments we are hopeful of running a similar joint workshop at future meetings.

This year's workshop was organized by ***Maeri Howard-Eales*** and ***Peter Briggs*** (for CCP4) and by ***Judy Flippen-Anderson*** and ***John Westbrook*** (for the RCSB PDB), with financial support for the workshop provided by CCLRC (from CCP4 industrial income), the RCSB PDB and by the ACA. The presentations from the workshop can be found online at ***www.ccp4.ac.uk/courses/ACA2004/ACAworkshop04.html.***

Peter Briggs

Scenes from the X-rays Molecules and You Workshop: At the lectures, the afternoon sessions on crystal growing and using the databases, and at the poster session. At the top right: David Goodsell discussing one of the student posters. Along the left side: Alex McPherson lecturing on crystal growing and Tim Herman discussing the SMART team program. On the right: RCSB PDB director Helen Berman discussing database issues with Karen Lipscomb of the CCDC. The workshop speakers are featured in the center of the collage – from left to right: Kathy Kantardjieff (California State, Fullerton), Alex McPherson (UC Irvine), Tim Herman (Minnesota School of Engineering), David Goodsell (Scripps), Karen Lipscomb (CCDC) and Frank Allen (CCDC). Tommie Hata of the Pingry School in New Jersey also spoke but was missing at the time the photo was taken.

X-rays, Molecules and You

It seems difficult to imagine bright-eyed high-school students and their proud teachers discussing structural biology on a summer Sunday morning. Yet this was the scene at the "X-rays, Crystals, Molecules and You" workshop held on July 18th 2004 at the Hyatt Regency Chicago during the ACA's annual meeting. During this workshop, prominent crystallographers and structural biologists introduced high school students and teachers to basic concepts in x-ray crystallography and structural databases to promote interest in structural biology, chemistry, and general science. This workshop generated so much interest that approximately 60 students, teachers, and parents traveled from 18 different states to participate. Several ACA members also attended the lectures. The morning session introduced crystallography concepts, highlighted structural databases, and discussed representational models of structures as teaching tools. Two mini-workshops followed in the afternoon - crystallization for teachers, and modeling and visualization of structures for students.

Judith L. Flippen-Anderson (RCSB PDB) began the morning session with a brief welcome address. ***Katherine Kantardjieff*** (California State University Fullerton) followed by introducing the concepts and procedures involved in the practice of x-ray crystallography. She described how crystals of proteins and other molecules are grown, harvested, and used for data collection. Kantardjieff then discussed how the data collected relate to electron density maps and how these these maps are used to build a model of the structure and generate 3-dimensional coordinates for each atom. She shared her somewhat circuitous route to becoming a crystallographer, and encouraged students and teachers to continue working towards their goals.

The second lecture discussed the data, tools and resources available at the Cambridge Crystallographic Data Center (CCDC; www.ccdc.cam.ac.uk). ***Frank Allen*** (CCDC) explained how crystallography is used to determine the structures of molecules ranging from small metal ions to very large viruses. In all cases this method provides an understanding of the shape, size, dimensions and interactions of the molecule being studied. He then focused on the structures present in the Cambridge Structural Database (CSD), the world repository of small molecule crystal structures and the principle product of the CCDC. He described the different classes of molecules in the CSD and the ways in which the CSD can be used, including predicting where some of these small molecules may bind in an enzyme active site or binding pocket. ***Karen Lipscomb*** (CCDC) then demonstrated some of the tools and resources available at the CCDC by querying the database for the Nobel Prize-winning structures that helped Dorothy Hodgkin win her Nobel prize.

Then ***David Goodsell*** (Scripps Research Institute) discussed how the structural data present in the PDB archives are used for research and education. The growing PDB archive contains the three-dimensional coordinates and related information about biological macromolecules. These structures, including proteins, nucleic acids, and large macromolecular complexes, provide insight into these molecules' roles in fundamental biological processes. Goodsell is also the illustrator and primary author of the RCSB PDB's Molecule of Month educational feature. He presented a historic overview of how the atoms that make up proteins, nucleic acids and other molecules in the PDB have been visually represented by hand drawings, wire-frame, backbones, space-filling models and finally as ribbons. He demonstrated how each representation highlights different aspects and features of molecules.

The final lecture in the morning session was jointly presented by ***Tim Herman*** (Milwaukee School of Engineering) and ***Tommie Hata*** (the Pingry School in Martinsville, NJ). Tim started off by describing how physical models act as "thinking tools" and can make molecular structures "real" for researchers, teachers, and students alike. He briefly described how he uses the 3-D coordinates from the PDB archives to generate physical models of proteins. He also distributed a kit containing a pliable 4-foot tube and colored thumbtacks designed to demonstrate concepts in protein folding and interaction (see ***www.3dmoleculardesigns.com/***). The student-teacher workshops organized by his center to promote an understanding of molecular structure through physical models were discussed. Tommie had attended one of these workshops, after which he involved some of his own students in CBM's "Students Modeling A Research Topic" (SMART) team program. Hata talked about his SMART team's experiences, which included working with research scientists to create a physical model of a class I transcription activation complex.

After lunch, teachers and students participated in different activities. ***Alexander McPherson*** (University of California at Irvine) led the teachers through a hands-on exercise in crystallizing lysozyme. McPherson was awarded the ACA's prestigious Fankuchen Award later in the meeting for his many significant contributions, including his work in crystallization, and the structure determination of various plant viruses, immunoglobulins and other molecules. Meanwhile, Goodsell, Herman, and Lipscomb led the students in various exercises. They explored the RCSB PDB, and located, downloaded and viewed a structure of a DNA-binding protein containing zinc finger domains. The students were challenged to search for and visualize estrogen and testosterone in the CSD within a short time period. They then used the tube kit to model a single zinc finger domain based on what they downloaded and examined from the PDB. The students also explored the exhibitor booths and poster presentations at the ACA meeting. Several students presented posters at the ACA meeting about their own SMART projects.

The workshop provided a great opportunity for students and teachers to learn about crystallography and structural biology alongside expert research scientists.

This workshop was organized by the RCSB Protein Data Bank and co-sponsored by the ACA.

Shuchismita Dutta

ACA 2004 - Travel Awardees

I would like to thank the organizers of the 2004 ACA meeting for giving me the opportunity to attend this valuable scientific meeting and present my work to the international audience in Chicago. The conference gave me a tremendous opportunity to talk with other young scientist as well as with several leading scientists in the crystallography field who have developed many of the crystallographic techniques widely used today. I am glad that I was able to listen to interesting talks and to see many fantastic posters, as well as seeing the latest improvements in the vendor's products. I particularly liked the difficult structures session due to its interesting stories behind the determination of each difficult structure. I focused on lectures related to my research area, particularly hot structures, cool structures, new structures, enzyme evolution and mechanism, atomic resolution protein structures and neutron crystallography. The poster sessions provided me a wonderful opportunity to interact with many interesting people. I was excited in many ways by these lively and interesting discussions and came back not only with wonderful memories but also with ideas and knowledge gained during the conference. Thanks again to the organizers for their efforts and hard work on this well arranged meeting, The Riga/MSC Fun Run and the Brunker/Nonius dinner added a pleasant touch to the meeting.

Lakshmanan Govindasamy

Attending the ACA meeting in Chicago was a refreshing and eye opening experience for me. I am new to the field of crystallography and presenting my research before such a varied scientific audience and being able to explain what I do provided a much needed confidence boost for me. Needless to say, the comments and suggestions from scientists and graduate students alike have been valuable.

The organization and scientific program of the meeting was excellent. Sessions such as "Structural Insights into Transcription", "Membrane Structures" and "Macromolecular Assemblies" were very interesting. A session I particularly enjoyed was the "Topics for Young Scientists" and Dr. Frances Jurnak's talk on "Career Choice: Academia" was truly inspiring. One other session that proved to be really important was "Fresh Approaches to Express and Purify Biomolecules". I have already incorporated a few ideas I got at this session and the results have accelerated my project. Thank you Dr. Studier. The poster sessions were well organized and I enjoyed the opportunity to discuss in-depth research with the scientists. The variety and quantity of posters was incredible. The meeting got people together from different areas of research and was a good exposure to the various aspects of crystallography. There were several chances for social interaction such as the Mentor-Mentee Dinner and the Bruker-AXS dinner at the museum. Overall it was an exciting and valuable experience. My attendance and participation at the meeting was made possible by a generous travel grant from the ACA and the International Union of Crystallography. The meeting was an enriching experience and I would like to convey my sincerest appreciation to the ACA and the IUCr for their generosity.

Ashwini Nadkarni

I would like to thank the ACA for the travel grant and the opportunity to present my work at the annual meeting in Chicago.

I presented a talk on "Kinetic Resolution of Amino Acids in Natural and Modified Gels" in the *Transactions* symposium "Crystals in Supramolecular Chemistry." It was very beneficial to me to hear the comments and suggestions from the symposium participants whose books and articles I have been reading for several years. In addition to that, the topics Dr. Alicia Beatty had chosen for the symposium gave me a comprehensive picture of the achievements and trends in the field of molecular crystals. I also enjoyed the dinner organized for the speakers of our session.

As a graduate student who is about to graduate, I found very interesting the information and job search advice offered in the seminars included in the "Topics for Young Scientists" session. I learned about the advantages that careers in academia and industry might offer. The addition of a job fair to future ACA meetings would be welcome.

Thank you again for the wonderful meeting and for giving me the opportunity to participate in it.

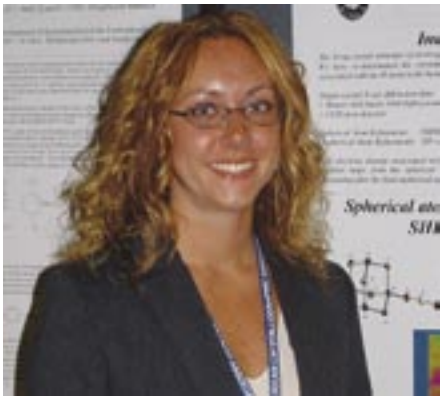
Rositza Petrova

Thanks ACA for spending your dime on me! This is my fourth ACA meeting but the first time I had data ready and was able to apply for your travel awards. The ACA has been great over the past few years. The connections I have made thru the ACA will most likely last a lifetime. I look forward to the meetings every year because I can see colleagues from across the US and beyond. Sometimes we get so caught up in the hallway discussions we miss the session we intended on hearing. I am not suggesting this is always a good idea but when ideas and information are flowing at such a great rate it doesn't matter if you're in a session or at the pub. Generally speaking the science is good all over and all week!

As my scientific training continues so does my interest in science continue to change. My field of study at this point includes primarily proteins and macromolecules. If you had asked me several years ago to sit in on a fiber diffraction session or materials science talk I would have tried to find a way out. However at this years meeting I found myself meandering into all the sessions. Having all the disciplines in one place is good. At first glance I found it too large with too many overlapping sessions. In hind site I find it well done! This year I was able to attend the GRC (Gordon Conference) on diffraction methods the week before the ACA. This meeting was also outstanding and I advise all graduate students to try to attend one.

Having said how good the conference was I want to point out what I consider a downside. With the structural genomics monster knocking on our doors and robotics becoming such a large part of a crystallography lab, I found it strange that only one robotics vendor knew what a pdb file was. Perhaps if they knew the end product we were looking for they might be more useful.

Kent Brown



I would like to thank the ACA for offering me a travel grant that allowed me to attend the national meeting in Chicago. I am grateful for the opportunity to present a poster of my research entitled "Charge density studies of urotropine-N-oxide·formic acid.

This was my first ACA meeting and as I enter my final year of graduate school, I found the meeting very beneficial and informative. The poster sessions allowed me to gain useful tips and encouraging remarks on my research. I was able to interact with crystallographers in a variety of fields which allowed me to learn of available post-doc and job opportunities.

I attended the Small Molecules workshop at the APS at the CHEMMAT-CARS beam-line. I found the lectures to be very helpful for my research, in particular the lecture dedicated to charge density applications.

Cara Nygren

I would like to thank the ACA for providing funding for students like myself to participate in the 2004 ACA meeting in Chicago. Although I have attended other conferences, this was the first ACA meeting I have had the pleasure of attending. I enjoyed the friendly atmosphere of the meeting as fellow researchers were excited to exchange ideas and were eager to discuss their work- past, present, and future. As a poster presenter, I had the opportunity to meet and interact with several remarkable professors from various fields, individuals from industry, and other graduate students who offered both words of wisdom and encouragement as we discussed not only research but also life beyond and outside graduate school. All of the sessions I attended were very interesting and informative. I particularly appreciated the "Topics for Young Scientists" session which targeted graduate students and post docs and provided information about possible future careers in industry and academics and the resources available to us. And, of course, when the sessions and the scheduled events for the meeting ended, I had a wonderful time enjoying only a portion of what Chicago offers visitors. From the art museums, the Navy Pier, and outdoor evening concerts to the variety of restaurants and shopping on Michigan Avenue, the "Windy City" completely blew me away! One afternoon I went to the edge of the city to see the birthplace of American author Ernest Hemingway as well as to tour homes built by Frank Lloyd Wright and step inside his studio. Academically and culturally, the 2004 ACA in Chicago was a wonderful experience!

Cynthia Sides

Thank you very much for the generous travel grant that allowed me to attend the annual ACA meeting in Chicago. As an undergraduate, this was my first attendance at any national chemistry conference.

The opportunity to attend afforded me many chances to see the tremendous work at various institutions. The meeting also served as a guide for narrowing the field of possible graduate schools for my future study.

Being present at the talks of the *Transactions* symposium granted me the amazing chance to hear many prestigious speakers. These outstanding talks made me more enthusiastic about my own research. At the meeting I presented a poster, which permitted me to interact with others who were interested in the same field of study. I received many helpful suggestions on how to further my research.

Once again, thank you very much for the generous travel grant that enriched my time at the Chicago meeting. The experience imparted a wealth of exciting information and memories that I will not soon forget.

Debra J. Salmon

The Chicago ACA meeting was the first big conference I have attended. It was really interesting, informative and motivating. There was so much new and cool information that I sometimes felt overwhelmed but I managed pretty well by taking a lot of notes. The talks that I attended helped me understand more about the process of crystallography as well as how to overcome some of the problems that can be encountered. I also had the opportunity to talk with the people at the CCP4 stand and they were really helpful in explaining some of the mistakes that I was making when I was trying to use their programs. I enjoyed all of the YSSIG session because I think it is never too early to start thinking about scientific careers. Also, it was very useful to hear the concerns and questions of postdocs because, as a student, I do not see the difficulties that they encounter in their jobs and, since I am going to be one at some point in my career, I think it is important to know early what to expect from such a position. I really like the idea of a Young Scientist mixer because it facilitates the networking between upcoming fellow scientists. I wished for a better environment because this year it was held in a big conference room and it did not provide the closeness necessary to interact with each other. I also enjoyed the Mentor-Mentee dinner; it was informal enough that it felt comfortable to approach and talk with the more experienced scientists. Finally, I would like to thank the ACA for granting me a travel award to help me with the expenses of attending such an important meeting.

Teresa De la Mora-Rey

First of all, I would like to thank the ACA for the travel grant that allowed me to attend this important international event.

It was my first ACA meeting and my first time in the USA at all. Attending the 2004 ACA conference in Chicago was a very exciting experience. There was a great variety of topics, a high level of research on display, and ample opportunity to interact with a wide variety of researchers from various parts of the globe.

As a young researcher I had the opportunity to present my work in a poster session and I would like to thank everyone who demonstrated interest in my work; and for the important comments and suggestions. Also, I had the important opportunity to make new contacts and meet possible future research partners. I came back to Brazil full of new ideas and new knowledge. I hope this will be helpful in my future research.

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

Janaina Ferreira

Attending the 2004 ACA meeting in Chicago was a very productive and informative experience that provided a unique opportunity to personally interact with other scientists. Along with an exposure to a broad cross-section of research and techniques, I had the opportunity to discuss the results of my research in detail with several experts in the field. Particularly, I would like to thank Bill Duax, Stephen Sprang, Richard Brennan, Peter Horanyi and Bi-Cheng Wang for their insights. I would also like to thank the ACA, IUCr and other contributors for their generous support of the Travel Grant program that helped make my attendance possible. (*Continued on page 18*)

In retrospect, singling out specific topics is rather difficult since so many of the discussions were thought provoking and informative. The Fankuchen Award Symposium in honor of Alexander McPherson included a diverse, and occasionally colorful series of lectures that were both enjoyable and entertaining. During the *Topics for Young Scientists* section, Francis Jurnak provided helpful, if sobering, insights into the various checkpoints and prerequisites of an academic career path. Learning about advancements in the NIH Protein Structure Initiative was also fascinating as they could potentially change the landscape of structural biology in the not-so-distant future. Additionally, I enjoyed seeing so many of the people that have had a significant impact on the field of x-ray crystallography. Given my very positive experience at the 2004 ACA meeting, I expect next year's conference to be just as personally and professionally gratifying.

Franklin Hays

Attending a meeting with over 1000 participants working in areas closely related to mine has always been of great interest for me. The economical difficulties in Uruguay during the last years have prevented me from attending other big meetings before. This year, after finishing my PhD Thesis, and having interesting research results to present, I was able to apply for an ACA Travel Grant to attend the 2004 ACA Meeting, last July at Chicago.

This participation has strongly marked me for many reasons. It was my first oral presentation at an international meeting (if you were interested in calculating the scattering factor of the laser dot in the screen during my presentation, you will need to add a big thermal motion "B" factor, to account for the hand-shaking produced by my nerves; but it is one particular process where, fortunately, B decreased with time!). I met many of the mentors of the techniques and software programs I usually use (George Sheldrick, Bob Von Dreele, Ton Speck, among many others). I attended the presentations of those teachers that, through their books and articles, have taught me the basic principles and applications of crystallography (Jenny Glusker and Bill Clegg, to mention two). I met other young colleagues with whom, probably in the future, I will develop cooperative work.

Additionally I have learned a couple of lessons about how to proceed in scientific life. Observing the humbleness of the "giants" of modern crystallography, like the people I have mentioned before (and others like Bob Gould or Herbert Hauptman) will help me to act in a more adequate manner when sharing experiences or working with colleagues or students in the future.

I would also like to mention one of the most interesting feelings that I experienced. While attending the Trueblood Award Symposium in honor of Richard E. Marsh, I recalled that, during my MSc. studies, I was "Marshed" by a paper entitled "The perils of Cc revisited", when trying to solve a structure collected as Cc but with true symmetry Fddd.

The only negative thing that I would like to mention is that, in spite of the great efforts of Bill Duax, the presence of Latin American crystallographers was very small in number. I hope we do not belong to the list of "endangered species".

Finally, I would like to explicitly thank the travel award selection committee for the opportunity given to me; Jason Hodges for selecting and guiding me into the "Materials For the 21st Century Session"; Brian H. Toby for his support and suggestions, the organizers of the Mentor-Mentee dinner for helping me to meet very interesting people, and the ACA staff for their help and kindness.

I hope we could meet again in the near future!.

Leopoldo Suescun

I would like to express my gratitude to the organizers of the ACA 2004 meeting in Chicago, for giving me the opportunity to attend this international scientific event and present a poster exhibiting the results of my research. My participation in the meeting would have been absolutely impossible without the travel award which covered most of the expenses of my travel form Poland.

I am especially grateful for the opportunity of attending the Small Molecule Crystallography workshop at ChemMatCARS that preceded the meeting itself. I found the workshop interesting because of the broad variety of topics it covered during the lectures and presentations at the synchrotron station. As for the conference, I really enjoyed the sessions concerning small molecule crystallography, especially the lectures about electron

density analysis and studies of new materials. The poster sessions also proved very interesting and educational to me, especially because a poster presented close to mine covered the topic of twinning in crystals and methods of data detwinning, which always fascinated me. I only regret that I had not enough time to thoroughly read most of the posters.

I also appreciated the opportunity to meet several authorities in the field of crystallography and to discuss some problems presented both at the workshop and later, during the meeting. As a beginner in crystallography I experienced a nice reception and I heard a lot of worthy advice concerning my further education and possibilities for my future scientific career.

Finally I must mention that the possibility of visiting Chicago during the ACA meeting was an advantage, even though not the most important.

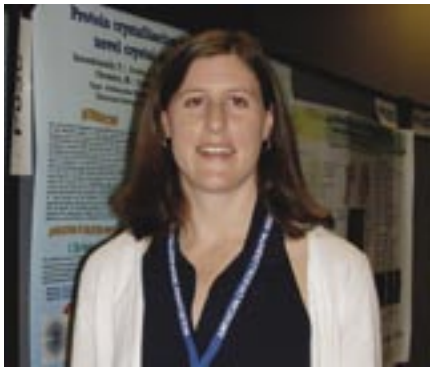
Anna Makal

I would like to thank the ACA, the International Union Crystallography, and all the other donors who so generously contributed towards support for the 2004 ACA meeting. It was with their help that I was able to attend the meeting in Chicago.

This was the first, and currently only, conference that I have attended and it has left me with tremendous memories and experiences. I had an amazing time and found it interesting to see advances within the various fields of crystallography. I particularly enjoyed attending the various talks given at the *Transactions* symposium and find it gratifying that we can share the successes (and failures!) of our research in this way, giving us a great opportunity to learn from one another. At the meeting I presented a poster and was left with helpful suggestions that can benefit me in my future research.

Thank you once again for so generously providing the support which greatly enhanced my stay in Chicago.

Michelle Smith



I am very grateful to the ACA for granting me a travel award to attend the 2004 annual meeting. This was the fourth scientific meeting I attended during graduate school, three of which were ACA meetings. The 2004 annual meeting exceeded every expectation I had based on prior experiences. My hat goes off to the organizers for choosing such a wonderful location. There were fantastic extracurricular activities (I really enjoyed the architectural river tour), and it was easy to meet with colleagues for meals between sessions because there were so many good restaurants nearby. The organizers took care not to schedule sessions with similar focus audiences concurrently; therefore, I did not miss any of the sessions I wanted to attend because of session scheduling conflicts. My favorite session was, as always, the difficult structures session. I find there is a lot to be learned from difficult crystallographic problems, which are not often highlighted in the literature. I thought that the posters were fantastic this year, and the awards well-deserved. In addition, I had many encouraging and beneficial conversations while presenting my own work. I would like to thank the ACA meeting organizers and participants for creating such a fantastic meeting.

Lindsay Odell

The ACA conference in Chicago was important to me for several reasons. First, it was my first attendance at a major scientific meeting and it both inspired me and strengthened my desire to pursue graduate studies and do research. As a recent college graduate, starting a job in CAD software development and then returning to present my work on a molecular surface visualization project was an experience that gave me interesting perspectives on the pros and cons of academic research vs corporate work. Second, as a person coming from a computer science background and being relatively new to the field of crystallography, I found many of the talks and material presented quite challenging but also stimulating. There were also some very accessible and helpful sessions (like those directed towards young scientists), which made me truly regret that I hadn't started attending meetings like the ACA earlier in my life.

I was very intrigued by some of the presentations from the Computational Methods session, like those about model building and completion (the Inverse Kinematics Approach by van den Bedem *et al.*, in particular), and methodology and data mining (Transue *et al.*) In spite of this being my introduction to some of the methods and algorithms used for structure determination, I truly enjoyed seeing computer science applied and interrelated with crystallography. It seemed so much fun that I decided I'd definitely implement some of the ideas presented and try to improve on them.

I was also able to glean a lot of insight from other sessions more related to crystallographic practice as opposed to tool

building, and to learn about the processes and steps that crystallographers apply and the problems they encounter (particularly interesting were the Difficult Structures and Structural Analysis by Hybrid Methods sessions). This helped me get some idea of what areas of crystallographic work could benefit from better software solutions.

In general, there was a lot to learn at this year's ACA – from the lecture sessions, poster presentations, individual discussions, and even from the commercial presentations of new products and techniques. I was most glad to be able to present my contribution to the molecular visualization project in ARCiB Lab at Dowling College and to get comments and feedback from other scientists. Of the people involved in this project, I would like to thank Dr. Herbert Bernstein, who is both a coauthor and my mentor in this work, for his continuous support and encouragement. I also wish to thank the ACA for the travel grant and for giving me this great opportunity. I am looking forward to attending again next year.

Peter N. Zhivkov

I would like to thank the American Crystallographic Association for the generous travel award. This was my first ACA conference and I was very impressed with not only the quality of presenters but also the organization of the overall meeting. I know that many hours went into organizing a meeting of this size, but it paid off and I am grateful to have attended. The neat thing about a meeting like this is the experience of interacting with scientists from all over the world. The opportunity to learn and share ideas with so many leading chemists is so valuable, especially for a young chemist like myself. Once again, thank you for the award and for providing such a great conference.

Nate Schultheiss

My first ACA meeting this past July proved to be very enjoyable. I found the atmosphere surrounding a conference of this size preferable to that of the ACS, where one quickly becomes swamped by the program and resulting inability to attend all the intriguing talks. Likewise, I found the social events more intellectually stimulating and generally less cacophonous; although I am certain that additional beverage tickets and later wake-up calls would have altered things considerably. I always find amusement in the "war-stories" that many in the field have of past structures they battled, and I was happy to be regaled by tales from both new and old friends. It is not common that such encounters are simultaneously entertaining and educational. The lessons learned at this meeting have already benefited my research, and I expect that the new friends I have made will be wonderful audiences and critics of my future endeavours. The ACA has provided me and the other recipients of the student travel grants with fantastic opportunities to see beyond the walls of the research laboratory, and for this I am thankful. I look forward to future meetings.

Jesse Rowsell

I would like to thank the ACA for the travel grant, which helped to defray the costs associated with my attendance at the 2004 ACA conference in Chicago. I enjoyed all of the seminars I attended and especially the one given by Alexander McPherson on the history of crystallography. The Radiation Damage sessions were fascinating and highlighted the point that although much has been learned in this field there is still so much we do not know. I also found the talk by Kim Collins regarding "Ions in the Hoffmeister Series" to be highly interesting and useful in practical terms for protein solubility and crystallization. I had the opportunity to present a poster outlining my research project and was surprised and delighted to receive an IUCr Poster Prize. I would like to thank everyone who showed interest in my research and I appreciate all of their helpful and encouraging comments. Lastly, I really enjoyed my first visit to Chicago and saw enough of that beautiful city to realize that I would like to go back and see more

Rachael Summerfield

I would like to thank the ACA for the travel award that made my visit to Chicago possible. This was my first ACA meeting and I really enjoyed the talks and the impressive number of posters. As a graduate student just starting out, this meeting was very educational and informative and I really

enjoyed meeting experts in the field. The Membrane Structures session was interesting and I particularly enjoyed the talk by Tina Iverson about the structure of cyanobacterial Photosystem II. Also, the talk on proton transfer and the structure of the photosynthetic reaction center was of particular interest as this represented an excellent example of functional and biochemical data backed up by structural data.

There were many sessions that were relevant to my own research, and my favorite session was the Frontiers in Single-Crystal Neutron Diffraction. Talks that stood out for me included the 0.66 Å x-ray structure of aldose reductase. Even at ultra high resolution, only about half of all the hydrogen atoms could be placed. In order to elucidate the protonation state of certain catalytic residues, subsequent neutron studies were carried out. As I am also interested in conducting neutron studeis on deuterated crystals of carbonic anhydrase, it was exciting to meet other scientists that are working on similar problems in other systems.

The evening mixers and poster sessions were great for shop talk and finding out the latest technologies in crystal growth, robotics and data collection and processing. Also, the MAR party at Blue Chicago and Rigaku/MSC party at House of Blues were very entertaining – excellent music and food at both presented great opportunities to meet and socialize with other crystallographers. Overall, the meeting was a stimulating and exciting experience and I look forward to the meeting in Orlando next year.

Suzanne Fisher

Attending the 2004 ACA meeting in Chicago was a great opportunity for me to learn about recent studies and developments in the field of protein crystallography. I was under the impression that talks and poster sessions at the conference are the two main reasons to attend the meeting. However, soon I realized that the coffee breaks, social gatherings and mixer parties were equally important in establishing networking relationships with other attendees and also a great opportunity to meet with experts and known scientists from all over the world.

The talks were not limited to the area of crystallography but also covered some of the concerns that young scientists might have. For instance, how to prepare for academic positions, academic versus industrial positions and preparing CVs, cover letters and interview skills were among the interesting talks that I attended.

I should also mention that the choice of Hyatt Regency Hotel in downtown Chicago was a great idea, since it made visiting the attractive areas of the town very convenient for us.

At the end, I wish to recommend that my fellows attend the 2005 conference in Orlando, which in my opinion would be beneficial to our careers both in the short and long term. And I would like to thank the ACA committee, who provided me with the generous travel award enabling me to attend my first crystallography conference.

Soheila Vaezeslami

A bursary from the ACA allowed me to attend the 2004 meeting in Chicago. It was great experience because I got to meet a lot of people from all over the world who are involved in crystallography. I also had a chance to present my work in a lecture, as I was also lucky enough to receive a 2004 Margaret C. Etter Student Lecturer Award. I talked to other people working in similar areas of research. The sessions I have attended were very good; a highlight for me was "Reticular Synthesis and the Design of New Materials" by Omar Yaghi in the session on materials for the 21st century. The majority of speakers were within their time allocated and their talks were very relevant to the session. Many of workshops were so popular that they were sold out before I arrived. So many sessions and events kept me so busy that I did not get as much free time as I hoped to tour the downtown in Chicago!

I also obtained some useful information about the new developments in x-ray diffractometers and trial versions of new software for crystal structure solution which are available from the commercial market.

I thank the ACA for the travel grant and the committees of ACA for the student lecturer award. Overall it was very impressive, enjoyable and worthwhile.

Zhanhui Yuan

I would like to thank the ACA for the funding to attend the annual ACA meeting in Chicago. This is the second time I have had the pleasure of attending an ACA conference, and I found this one even more rewarding than the first.

I presented a poster at the conference. I really enjoyed the poster session, both for the feedback and challenging questions asked of me, and for the opportunity to learn about the research that others are undertaking. Also, the vast majority of talks I attended were excellent, and the research presented in them left me wanting more.

Additionally, as a graduate student who is planning on finishing my degree in the next year, I had a great chance to meet professors and other experts in the field. This will no doubt aid a great deal in my future job search. Thank you again for your very generous support.

Brock Levin

A big thank you to the ACA for providing me with a travel grant to attend the 2004 meeting in Chicago. This was my first time attending an ACA meeting and my first time visiting Chicago – both were rewarding experiences! As a beginning crystallographer I found a wealth of information at the meeting –including many practical tidbits which more experienced crystallographers take for granted. Meeting other crystallographers was a lot of fun and I particularly enjoyed presenting my poster. I enjoyed attending the Teaching Crystallography session as well as the Macromolecular Crystal Diffraction, New Structures, Difficult Structures and General Interest sessions quite a bit. Although I primarily work in a protein lab, I ventured into the world of small molecules, supramolecular chemistry and small angle scattering to see what that was all about. Looking back at my program from the meeting I see that in addition to all the great stuff I saw, there was so much that I missed! I look forward to attending the ACA again and I thank the ACA for the opportunity to attend this year.

Janel Laidman

I would like to thank the ACA and the IUCr for the incredible opportunity to attend the annual ACA conference in Chicago. It was a tremendous honor to present my research to such an esteemed group of individuals. The highlight of my trip, however, was the sponsored trip to the Advanced Photon Source at Argonne National Labs. The experience has had a profound effect on my perception of work being carried out in the national lab setting and may very well have altered my plans (most pleasantly) for post graduate studies. Thanks so much for this incredible opportunity; without your generous support this trip would not have been possible.

Jason B. Benedict

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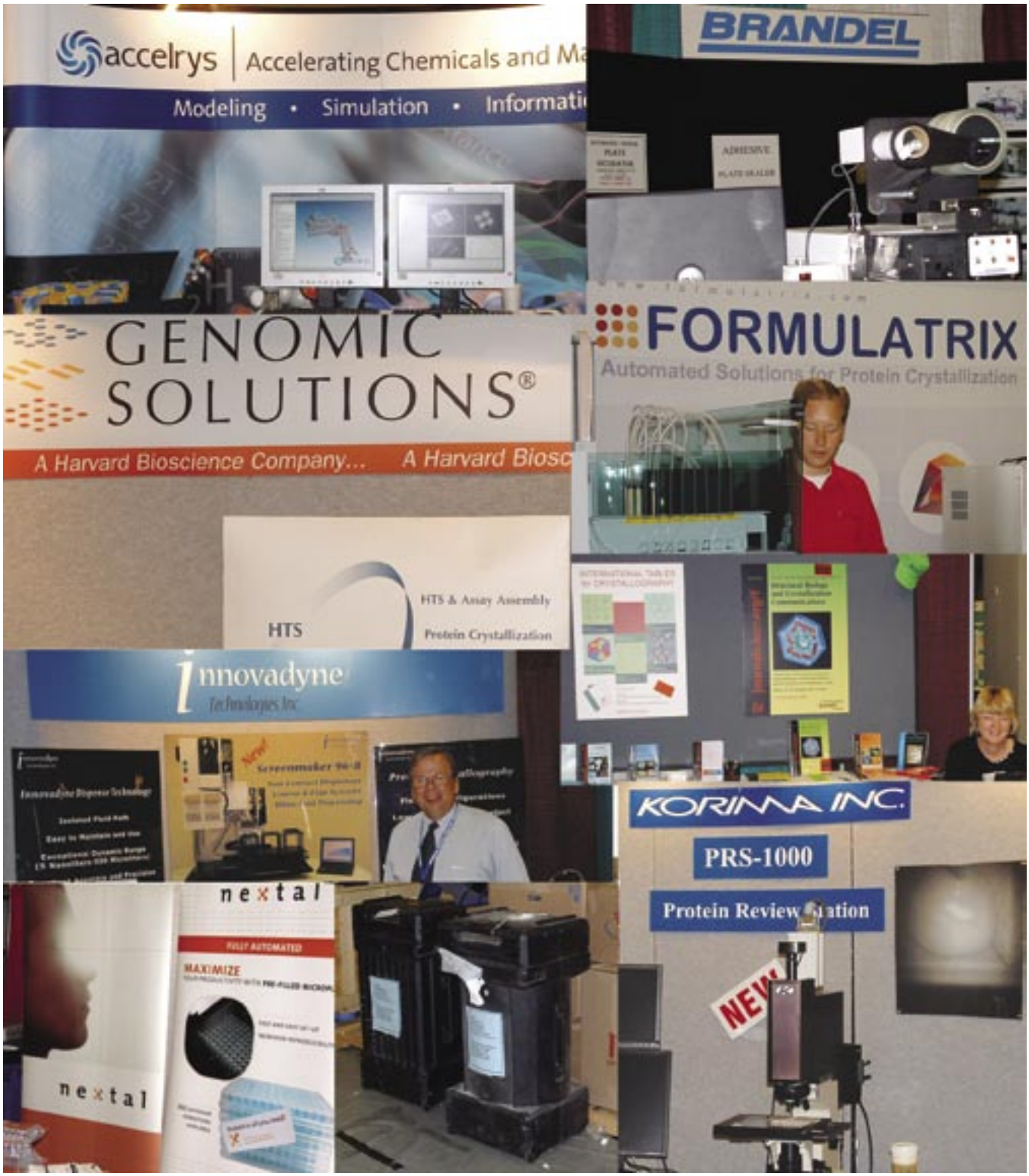

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Paul Janssen Prize

The Paul Janssen Prize in Biotechnology and Medicine was established at the Center for Advanced Biotechnology and Medicine (CABM) at Rutgers Universisy in 1992 to honor the achievements of Dr. Paul Janssen by recognizing outstanding contributions in biomedical research. Janssen, the first recipient, was the founder of Janssen Pharmaceutica Inc. and was a visionary physician and chemist who developed many important drugs that are used extensively in various areas of medicine including mental illness, cardiovascular and gastrointestinal diseases, allergies and infections. Until his untimely death in 2003, Dr. Paul (as he was affectionately known) continued to work vigorously to advance innovation in medical research at the Janssen Research Foundation Center for Molecular Design (CMD) which he founded in 1996 in Belgium. At the CMD, Dr. Paul coordinated the efforts of a multidisciplinary team in developing new anti-AIDS drugs using structure based drug design methods; some of the compounds have shown exceptional promise in clinical trials.

The 2004 Paul Janssen Prize in Advanced Biotechnology and Medicine has been awarded to Wayne A. Hendrickson and Michael G. Rossman.

Left to right: Michael Rossmann, Wayne Hendrickson and Aaron Shatkin (Director of CABM)

Wayne A Hendrickson and Michael G. Rossmann have been selected as the recipients of this year's Paul Janssen Prize for their contributions to solving the phase problem in macromolecular crystallography. The great majority of three-dimensional structures of biological macromolecules determined by x-ray crystallography are now solved by either the multiple anomalous diffraction (MAD) method, p;ioneered by Wayne Hendrickson, or the molecular replacement (MR) method, pioneered by Michael Rossman.

Wayne Hendrickson is University Professor in the Department of Biochemistry and Molecular Biophysics at Columbia University and an Investigator at the Howard Hughes Medical Institute. In addition to developing methods for facilitating experimental structure determination using anomalous scattering, Wayne has also helped to improve the quality of macromolecular structures through developing refinement methods that combine known stereochemical information with x-ray diffraction data. He has solved the structures of many biologically important intracellular molecules and cell-surface protein complexes. These studies have contributed greatly to the understanding of protein recognition involved in cell-cell and pathogen-cell interactions.

Michael Rossmann is the Hanley Distinguished Professor of Bioloigical Sciences at Purdue University. He recognized the p;otential for using non-crystallographic symmetry to help in imaging the structures of complex macromolecular assemblies both with and without internal symmetry. In addition to developing many methods used for solving and analyzing biological structure by x-ray diffraction and cryo-electron microscopy, he has solved structures ranging from metabolic enzymes to entire viruses. Through his comparative analyses of proteins and viruses he has made fundamental contributions to our understanding of protein folding and of molecular and biological evolution.

Both Rossmann and Hendrickson have been highly recognized for their broad contributions to science. Both are members of the National Academy, are recipients of the both the Gairdner International Award and the Aminoff Prize of the Royal Swedish Academy of Sciences. Michael has also received the IUCr's Ewald Prize, the Louisa Gross Horwitz Prize and the Ludwig Darmstaedter Prize. Wayne has been awarded the Arthur H. Compton Award, the Alexander Hallaender Award and was the frist recipient of the ACA's Patterson Award . Both men have been members of the ACA for many many years.

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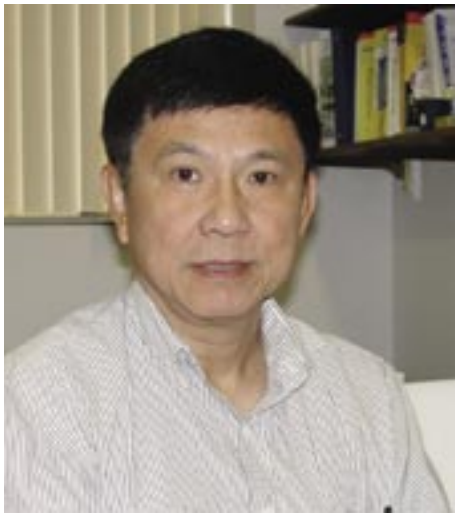
Gregori Aminoff Prize - 2005

The Aminoff Prize is intended to reward a documented, individual contribution in the field of crystallography, including areas concerned with the dynamics of the formation and dissolution of crystal structures. Some preference should be shown for work evincing elegance in the approach to the problem.



The Gregori Aminoff prize for 2005 is awarded to Ho-Kwang Mao, Geophysical Laboratory of the Carnegie Institution, Washington DC, USA, for his pioneering research of solid materials at ultrahigh pressure and temperatures.

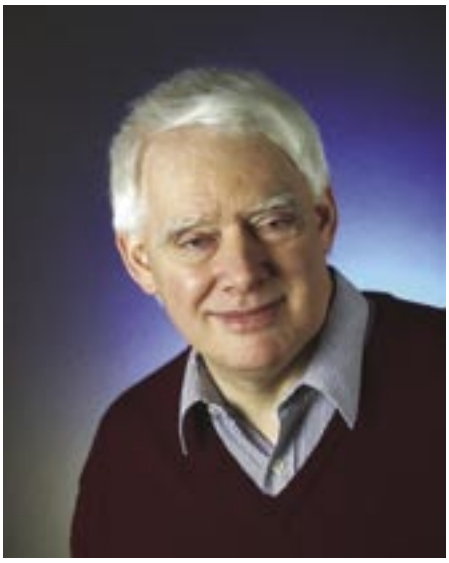
Ho-Kwang Mao (Dave) is director of the High-Pressure Collaborative Access Team (HPCAT) at the Advanced Photon Source in Argonne, Il. He supervises the HPCAT sector, which the Carnegie Instituion manages, and where much of the institution's high-pressure research is conducted. He is one of the pioneers in the development and use of diamond anvil cells. Over the years he has improved on both the diamond anvil cell and measurement instrumentation that reveals the properties of materials as they undergo extreme conditions. He has made many important discoveries about the chemical, structural, and other physical characteristics of matter along the way.

Mao also explores what happens to elements in planetary cores. He is looking at defining thermodynamic, elastic, and vibrational parameters of elements such as iron and hydrogen at core conditions. This work is important to basic research and for understanding seismological phenomena.

2004 Max Perutz Prize of the European Crystallographic Association

In 2004 the European Crystallograhic Associations's ECA prize was renamed to be the Max Perutz Prize. The European Crystallographic Association has awarded the first Max Perutz Prize (2004) to George Sheldrick.

George Sheldrick has made seminal contributions to the development of direct methods and helped to transfer the methodology into a straightforward procedure for solving small molecule structures. He has made significant contributions to structural chemistry and has published well over 700 publications in leading international, peer-reviewed journals. In recent years, his work has also become very important in biological crystallography, in the areas of structure solution based on anomalous phasing and in the refinement of protein structures at atomic resolution.



His program SHELX, which is constantly evolving, has underpinned the automation of chemical x-ray crystallography in the past three decades has become a routine tool for physical and organic chemists. SHELX is the most comprehensive, reliable, and useful program for the determination and refinement of crystal structures from diffraction data. SHELX is the most cited software in crystallography and its continual use is in fact part of the foundation on which the remarkable success of our discipline rests: a large proportion of the several hundred thousands crystal structures that have been determined owe their 'existence' to SHELX. The wealth of information available in the Cambridge Structural Database rests firmly on structures determined using his software. The free availability of the SHELX programs to the academic community has been especially important, setting a standard for others to follow. In the past fifteen years, George has focused his research on the problems of macromolecular structure determination. He has pioneered the use of direct methods for large molecules containing many atoms when atomic resolution data is available, building on the ideas of dual space refinement to provide an easy-to-use powerful phasing package in the program SHELXD. This has proved that size alone is not an insurmountable barrier when modern computing resources are exploited. This has fostered a new attitude in macromolecular crystallography by showing that with proper treatment even the biggest macromolecular structures can be refined to a level that is not very far from what has been traditionally reserved for small molecules. However, the most frequent application of SHELXD is in locating the anomalous scatterers in protein structures, a prerequisite to structure solution using anomalous phasing. His accompanying program SHELXE takes the process one step further, rapidly calculating the phases required to produce an electron density map and using a novel density modification procedure to resolve the phase ambiguity for SIR or SAD data.

George Sheldrick is head of Department for Chemistry at the University of Göttingen. He is an excellent and dedicated teacher. His graduate students and young colleagues carry on his research traditions, and they can be found in many European laboratories. He also contributes to many workshops and training courses throughout Europe. His lucid lectures, and his deep understanding of crystallography delight students and other participants.

George Sheldrick's contributions to crystallography have previously been recognized by many international awards including the 1993 ACA Patterson Award.

David Blow (1931-2004) - A Remberance

I was very fortunate to have pursued my doctoral studies under the direction of David Blow. Having heard of his untimely passing in June, and reading the many obituaries* written recently outlining his scientific achievements I felt compelled to share a few memories from the perspective of one of his former graduate students. Specifically I wanted to share the unique training environment David provided for myself and other graduate students that were part of his laboratory.

I first met David at the IUCr meeting in Hamburg in 1984. Having not yet completed my MSc degree in small molecule crystallography, and wanting to move to the world of macromolecular structure determination for my doctoral studies, I spoke with him about the possibility of joining his lab. I had been impressed with his outstanding work in the development of macromolecular phasing techniques, his work on the structure of chymotrypsin, which contributed significantly to understanding the catalytic mechanism of serine proteases in general, as well as his more recent work on structural studies of tyrosyl-tRNA synthetase. Our meeting left me with a strong impression of David as an excellent teacher and mentor and he encouraged me to join his group at Blackett Laboratory, Imperial College of Science and Technology in London. I could not have picked a better lab to pursue my doctoral studies!

David was a very committed scientist who inspired many of us by the enormous passion and the enthusiasm he showed for his work. He was deeply committed to his students, not only striving to provide them with excellent training opportunities, but also creating an environment rich in learning and scientific interaction. His laboratory was endowed with highly skilled and committed postdocs and research associates possessing a wide range of skills in structural biology from important software developments such as the CCP4 suite of crystallographic software, still widely used by crystallographers around the world today, to the development of equipment used in crystallization (work in David's lab ultimately led to the development of the IMPAX microbatch crystallization robot). Needless to say, being submerged in such an eclectic environment, built and supported by David, provided outstanding learning opportunities for a young gradate student such as myself.

Furthermore, David strove to instill in all of his students a spirit of collaboration and a strong attitude of working together as a team. David's early insight in the importance of creating such collaborative skills in his students have proven to be extremely important in today's multidisciplinary world , particularly within biotech and pharmaceutical companies where crystallographers are constantly required to work within multidisciplinary teams. Although as PhD students we all managed our own projects, strong group interactions helped maximize our opportunities to learn from each other. Group meetings were always productive forums focused on methods to solve difficult issues. Morning coffee and afternoon tea times in our so-called "Interaction Room" also provided opportunities for stimulating conversations on the nuances of aspects of data processing, refinement and model building, not to mention critical discussions on new structures from recent journal articles which littered the coffee table.

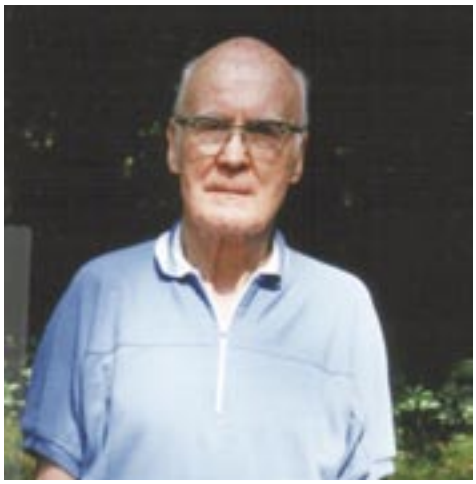
A most vivid memory of my initial months at Imperial College, and an outstanding example of David's commitment to his students, included the first time I went to the synchrotron facility at Daresbury. Despite his extremely busy schedule, David took time to accompany us.. I'm certain however that he saw these opportunities as welcome escapes from the more mundane paperwork tasks and thus an opportunity to do "real" science. During this trip, he instilled upon us the importance of working together during synchrotron runs. If your data was not being collected it did not mean that you went to sleep and waited for "your turn". Rather your function was to provide as much assistance as possible to the person whose data was being collected in order to guarantee everyone a highly successful data trip. In addition, emphasis was placed on pursuing the highest quality data. For example, great pains were taken to ensure that the conditions for maximal quality data were achieved; time was spent fine tuning the configurations of data collection instruments in order to obtain the best data possible with the lowest noise levels. Also emphasis was placed on knowing your crystal morphology and using it to your advantage. Although many of these techniques are not used today (now we tend to shoot first and think later), I believe that the emphasis David placed on learning these fundamentals ultimately made us better crystallographers and gave us a more thorough understanding of the science. Furthermore, these values have provided me with a fundamental basis for critical thinking and an appreciation for the importance of detail in pursuing the best of possible results.

The lasting impact David had on his graduate students was perhaps most strongly felt and expressed when, in the summer of 2001, he celebrated his 70th birthday in Devon where he and his wife Mavis had retired. He organized and invited all his former graduate students and their families to a truly memorable two day reunion. Virtually all his surviving graduate students were in attendance (only Paul Sigler, David's first PhD student, who sadly, had passed away only a short while before our reunion, was not in attendance). We had a wonderful opportunity to visit with David and Mavis and to enjoy each others company. Sadly, for many of us, this was the last time we would see David. Unforgettable to me, during this wonderful visit, were the accolades that were shared amongst us, of David's contribution to moulding each of our careers as scientists and teachers. Although he is no longer with us, the spirit of scientific endeavor, enquiry and enthusiasm that he instilled in us during these formative years of our careers will remain with us for the rest of our careers.

Alice Vrielink

* see the fall ACA *Newsletter* for on such obituary

Leroy E. Alexander (1910 - 2004)



In June L.E. Alexander passed away in his 94th year. Leroy retired in 1976 from the Mellon Institute of Carnegie-Mellon University in Pittsburgh, Pennsylvania, as Professor of Chemistry, and Senior Fellow. To obtain his academic education he had a difficult road to follow. After high school he obtained his teacher's certificate and was teaching in one-room rural schools by the age of eighteen. By alternating teaching and college studies he was able to earn a bachelor's degree at the State Teacher's College in River Falls, Wisconsin, in 1937. During his teaching years he organized a school band and taught the students how to play all the instuments. He supported himself during graduate study by playing clarinet and saxophone in dance bands, and was awarded a Ph.D. in physical chemistry from the University of Minnesota in 1943. After working at the General Electric Laboratories in Pittsfield, Massachusetts, Leroy was offered a position in the Department of Chemical Physics at the Mellon Institute of Industrial Research in Pittsburgh. He headed up the x-ray diffraction section and became an authority in this field. Together with Harold P. Klug he wrote the classic "X-ray Diffraction Procedures" (Wiley,1954). This book can still be found in many x-ray diffraction laboratories around the world, because it is written in a clear and instructive way. With Gordon S. Smith he published a number of influential papers on the geometry of single-crystal x-ray diffractometry. His second book "X-ray Diffraction Methods in Polymer Science" (Wiley, 1969) was also a success, and for quite some years was the only book on this subject. He was ACA secretary 1958 to 1960.

In the early sixties Leroy was on sabbathical at the Delft University of Technology in The Netherlands, where he worked with his long time friend the late Peter de Wolff. While at Delft he collected material for his book on diffraction methods in polymer science. Those fifteen months in the Netherlands were a wonderful time for the Alexanders. While he was working on his second book, Leroy started a project to study chain folding in polymers, in particular of polyamides. This subject was a source of controversy and played an important role in the phenomenological description of the deformation of polymers. The study resulted in a series of papers on the structural determination of nylon cyclic oligomers. Together with Roger Pettersen and Earl Baker he worked on the synthesis and the structures of chlorophyll-related compounds.

With his great knowledge of x-ray diffraction and talent for writing well-styled and clearly formulated texts, he was a source of inspiration for all those who had the privilege to work with him. Leroy was a great friend and colleague to many people from different countries and backgrounds. He had a broad range of interests; playing music was one of his great pleasures. He was an optimistic and religious man, respected as well as admired by those who knew him. In his work he was strongly supported by his beloved wife Eleanor, who for many years transcribed books into braille. She died several years ago and Leroy is survived by his daughters Kathryn and Karen, and two grandchildren.

Maurits Northolt

Howard F. McMurdie (1905-2004)

Howard F. McMurdie – known as Mac to his friends and colleagues – was an exemplar of good living. Blessed with excellent health, a loving family, and many close colleagues, Mac was active and productive to the very end. It is therefore with the deepest regret that we report the death of Howard F. McMurdie at age 99 ½ of pneumonia only a few months before an anticipated 100 year birthday celebration. Although Mac officially retired from the National Bureau of Standards (NBS) in 1966, he continued to work as a consultant in crystallography until 2003. During his "real retirement" party at National Institute of Standards and Technology (NIST) in April 2003, he was awarded a special certificate of appreciation "for his significant contributions to the Materials Science and Engineering Laboratory of NIST during the past 75 years." The certificate noted that McMurdie's "research interests encompassed areas such as measurements of phase equilibria and reference powder x-ray patterns, characterization of solid-state materials, compilation and evaluation of data for phase equilibria diagrams, and for the Powder Diffraction File."

Howard McMurdie was born on February 5, 1905 in Kalamazoo, Michigan, and graduated from Northwestern University in Evanston, Illinois. He went to work for what was then called the National Bureau of Standards on April 2, 1928. In the early 1930s he was sent to Riverside, California to test the cement that was to be used in the construction of Boulder (now Hoover) Dam. After returning to NBS he was assigned to the Petrographic Laboratory. His study of Portland cement was the start of what evolved into a lifetime interest in phase diagrams. In those early days, McMurdie also pursued the use of x-ray powder diffraction for phase analysis of solids. These activities paved the way for him to become Chief of the Crystallographic Section. Mac was a beloved chief. He had confidence in his people, encouraged

them to pursue independent research , and supported their work. As Section Chief and as a researcher, McMurdie contributed significantly to many areas of research throughout his 75 years at NIST/NBS. McMurdie considered three areas as especially important, and he had been closely related to two of them for the 38 years following his formal "retirement" in 1966.

His first area of interest centered on the production of Powder Diffraction patterns and NBS's productive association with the International Centre for Diffraction Data (ICDD). In 1953, he established an ICDD Research Associateship in the Crystallographic Section at NBS/NIST. For more than 30 years, this Associateship, under his guidance and leadership, prepared a broad set of important, accurate, and widely used experimental powder diffraction patterns. He also served as an editor of the Powder Diffraction File (PDF) and continued to edit patterns until age 98. His work with the ICDD was recognized by two honors. In 1984, he became a Distinguished Scientist of the ICDD. In the late 1990's, ICDD set up a biannual award – the McMurdie Award to honor his contributions to the organization and to the Powder Diffraction File. His second area of interest focused on refractory oxides. It was through research in this area that he established a relationship with the American Ceramic Society (ACerS) and started the publication of the series, *Phase Diagrams for Ceramists*. After his retirement, Mac continued to be an editor for the phase diagrams until age 98. In materials science, these diagrams have long been used in the development of new materials and processing of important ceramics. The third area in which he had a keen interest was initiated in the Crystallography Section and involves the study of materials at high pressure. His vision together with the ingenious work of a group of world-class scientists at NIST/NBS led to the development of the diamond anvil cell (DAC), of the high pressure single-crystal diffraction technique utilizing the DAC, and of an optical ruby fluorescence method to measure very high pressure in the DAC. This work earned NBS/NIST a stellar international reputation in the field of high-pressure science and technology. Several key papers resulting from this long-term research effort are now widely regarded as key milestones in the evolution of high-pressure science.

Over the years Mac served as a paradigm of how to live with his emphasis on balance, diversity, and moderation in all things. Not only was he a dedicated and hard-working scientist, he was also a thoughtful and generous person who was well-liked. To balance his scientific work, he developed a broad spectrum of interests including cooking, reading, travel, photography, computing, opera and Gothic architecture. He was a gourmet cook and prepared dinner at his home every Wednesday evening for his extended family (3 children, 6 grandchildren and 5 great grandchildren). Often, he would invite friends to his home for wine and cheese or even a meal and conclude the evening with a glass of fine wine or Rebel Yell, his favorite bourbon-style whiskey. He derived great pleasure from the social interaction with us in our periodic luncheons sometimes held in one of his favorite local restaurants. Clearly Mac will be missed enormously, but he will not be forgotten. He will live on in his work and in our collective fond memories!

Alan Mighell, Gasper Piermarini and Winnie Wong-Ng

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Where are We Going, and Where Have We Been?

Alex and ACA President Fran Jurnak at the awards symposium

Let me being by saying that I am indeed grateful and humbled by this honor, particularly so because it comes from my many colleagues in crystallography for whom I have so much respect. I thank you sincerely.

Now, I know there will be some in the audience who will say, "McPherson, humble? That will be the day!" But this is in fact the day. I am indeed humbled, and I ask who among you would not be so by the names of the previous recipients of the Fankuchen award. To name just a few,

Michael Rossmann, from whom I arm wrestled a PhD. degree in times long past, my professor and mentor. David Harker, the greatest x-ray crystallographer since Bragg. Lyle Jensen, my role model as a young crystallographer. Jenny Glusker, whose books taught me x-ray crystallography, Dorothy Hodgkin, the veritable earth mother of protein crystallography.

Well, enough for humility, let's press on to science. I thought it might be appropriate for me, at the beginning of this session on crystallization to review the past and preface the future, and along the way provide context by calling attention to some of the things we have learned along the way.

I'd like to begin by reviewing as concisely as possible what I consider to be the milestones in the development of crystallization research, and that begins more than 150 years ago in Germany with the discovery by Hunefeld that the protein hemoglobin could be crystallized. He accomplished this by simply squeezing the blood of certain worms and small fishes onto microscope slides and letting them slowly dry. This simple demonstration had two profound implications, which, unfortunately, went largely unappreciated for many years. First, they showed that proteins could be crystallized, like salts and other conventional molecules, by evaporation, by dehydration, the physical basis of most of the techniques that are in use today for the crystallization of macromolecules. Second, he clearly showed that proteins, of which hemoglobin was a recognized representative, must be a distinct chemical and physical entity with a unique three-dimensional structure. Of course, at this time the real nature of crystals was still somewhat obscure, thus it is not, perhaps, so odd that the significance of the experiments was missed. Finally, we must score hemoglobin with one more first; it was both the first animal protein, and the first protein of any kind to be crystallized.

The crystallization of hemoglobin was repeated and reported numerous times in the succeeding years, but it was not until Osborne in the late 19th century took note of the phenomenon and sought to apply it to plant proteins, that the significance of protein crystallization attracted notice. Osborne was the first to realize that the crystallization of a protein provided a means of separating it from accompanying proteins and other molecules in its parent tissue or organism. It was a purification tool, and in many ways the most efficient known for proteins, because when successful, it also demonstrated the fact of its success. A crystalline material was taken by chemists to be a pure material. The crystal was the gold standard of homogeneity. For the next sixty years it remained so, and it continued over that time to be the premier purification procedure in biochemistry. Osborne succeed in growing crystals of a wide variety of plant seed proteins, many of which provided some of the earliest samples of crystals for x-ray diffraction analysis.

Osborne's work was particularly significant for another reason, it introduced the use of salt concentration and temperature to control the solubility of proteins, and it demonstrated that manipulation of these parameters were effective in promoting the crystallization of proteins. Osborne was also the first to report the use of alcohol to precipitate and crystallize proteins. Through his experiments, Osborne may be said to be the father of protein crystallization, for he developed many of the methods that we still use today.

In 1898, Hopkins and Pinkus, followed shortly thereafter by Hoffmeister, the great chemist, crystallized albumin from chicken eggs. Thus, ovalbumin became the second animal protein to be crystallized. This was also significant because crystallization of ovalbumin was induced by altering the pH of the protein solution in the presence of high concentrations of sodium chloride. Thus another of the tools that we depend so heavily upon today, pH change, was identified.

Early in the 20th century, the true giant of the field of protein crystallization made an appearance, and this was J.B. Sumner at the Agricultural Experiment Station of Cornell University. Seeking to show that enzymes were in fact protein molecules, which had unique chemical compositions and three-dimensional structures, Sumner attempted to crystallize the enzyme urease. This enzyme was known to be abundant in the lowly jackbean (Canavalis ensiformis), a close relative of our lima bean. While unsuccessful in his initial attempts with urease, in 1919 he did publish the crystallization of Concanavalin A (our first lectin crystals) and Concanavalin B. Sumner, of course knew the biochemical function of neither of these proteins, simply naming them after the plant source. Concanavalin B, however, we now know to be the enzyme chitinase. Thus, ironically, Sumner had in fact succeeded in crystallizing the first enzyme; he had accomplished his original goal but neither he nor any other realized it. And so, fortunately for us all, Sumner proceeded in his quest, and along the way provided us with many of the conditions,

reagents, and methods that we use today in protein crystallization. He used dialysis against very low ionic strength, variation of pH and temperature, the introduction of organic solvents, a greater variety of salts, and he introduced new methods for the extraction of proteins from tissues.

It was in 1926 that Sumner succeeded in growing crystals of urease and making his demonstration know to the world. Later he would be awarded the Nobel Prize along with Northrup, the other giant of protein crystallization. In the meantime, however, an event of truly monumental importance occurred involving the crystallization of a protein. This was the crystallization by Abel and his colleagues of the hormone insulin. The importance of this is difficult to overestimate, because it provided in demonstrably pure form the single most important protein drug, arguably the most important drug of any kind, of the 20th century. It had enormous impact on medicine, and was directly responsible for saving countless lives. Sometimes overlooked, but nonetheless worthy of note, is that the use of metal ions (Zinc in this case) to promote protein crystallization was introduced, again a technique of continuing value today.

Beginning in the 1930s, Northrop, and his almost equally illustrious technician Moses Kunitz, proceeded to crystallize the enzymes of the pancreas and thereby confirm Sumner's earlier argument and evidence. From their work we were given, along with additional crystallization techniques and insights into the problem, crystals of trypsin and trypsinogen, chymotrypsin and chymotrypsinogen, pepsin, pepsinogen, ribonuclease, and deoxyribonuclease. Although, even up until this time, the crystallization of proteins was appreciated mainly as an excellent means of purifying proteins and demonstrating their purity, the successes of Northrup had profound consequences for the newly emerging field of x-ray crystallography. These protein crystals from the pancreas, along with hemoglobin, myoglobin, and lysozyme provided the majority of those samples used in the initial x-ray diffraction studies. The first protein crystallographers didn't have to be proficient biochemists as they do today; Sumner and Northrup had taken care of that.

The year 1935 may probably be taken as the year of the advent of modern protein crystallography, and when protein crystallization assumed a new role as a source of samples for x-ray diffractionists. Bernal, Crowfoot, and Fankuchen began that year their studies of pepsin, insulin, and other proteins. Indeed, Fankuchen may also be considered the progenitor of virus crystallographers, for it was he who began the x-ray study of tobacco mosaic virus, the first virus ever crystallized, by Stanley, that same year, 1935. In 1937 Abraham and Robinson crystallized lysozyme, the protein that has served over many years as the model protein for crystallization studies, and the protein which has revealed to us so much of the physics and chemistry of protein crystallization. The new importance of protein crystallization, and the new enthusiasm for its development was perhaps best summed up in a Royal Society paper in 1942 by Bailey titled *The Growth of Large Protein Crystals*. The new day had dawned.

A decade of successes in protein crystallography followed the determination of the first protein structures of myoglobin and hemoglobin by Kendrew and Perutz and their colleagues beginning in 1959, along with the award of more Nobel prizes to x-ray diffractionists. The structures of the crystals grown first by Sumner and Northrup, ribonuclease, trypsin, pepsin, and the others became known. Gradually, however, an awareness came upon the field that the backlog of protein crystals from the past hundred years was dwindling, was becoming exhausted, that it might soon be time to find new sources for diffraction studies. This was a new fact of scientific life, and the reason protein crystallization began to again be granted the respect and appreciation that had been lost in the wake of so many successes.

Some watershed events, in some cases as much philosophical as physical, occurred in the 1970s. Transfer RNA was crystallized and solved. It was no longer protein but now macromolecular crystallography. The first virus crystals were solved, no longer just macromolecules but assemblies and particles. Two new developments emerged. From the transfer RNA experience it became apparent that whoever could obtain the raw material to grow the crystals were competitive. Producing the molecule, purifying and crystallizing it, that was the name of the game. And that, curiously, is essentially the same set of circumstances that we find ourselves in today. The second concept to take hold was within the broader community of biological scientists, and that was an appreciation of the keystone role that X-ray crystallography had assumed in biochemistry and molecular biology. Indeed, macromolecular crystallography was totally transforming those fields.

Some other more recent and perhaps better remembered events and developments deserve mention for their great impact on the field of macromolecular crystallization. These include the development of synchrotron radiation, high speed computers, area detectors, and automated procedures. These reduced the number of crystals required for structure determination and the size of crystals, and opened up whole new areas for the development of phasing techniques. Perhaps the greatest development, however, the one that propelled the field forward, was the invention of recombinant DNA technology and the ability to produce proteins of very low abundance in large quantities for crystallization. This is what opened up the biochemical world to x-ray crystallography, and in a sense, converted a generation of crystallographers into a generation of molecular biologists. And finally, something that escapes the attention of many. That was the development and commercial availability of crystallization screening kits. These simple expedients have had a profound effect on our science, for they have opened up x-ray crystallography to the biochemists, molecular biologists, and enzymologists who previously could only look on and hope.

The last twenty years have seen an explosion of research into the crystallization of proteins, nucleic acids, viruses, and macromolecular complexes of all kinds. We have seen the application of a host of physical techniques and approaches once reserved

for the science of conventional molecule crystallization, or developed as a response to the unique properties of macromolecular crystals. These have included interferometry, atomic force microscopy, light scattering, x-ray topography, low angle scattering, and a host of other methods. At the same time, much research of an empirical nature, trial and error, often more practical in nature has complemented the more analytical approaches. Without doubt, over the past twenty years we have learned better how to grow protein crystals. Our successes mount by the day, and we now ask if there are any macromolecules that cannot be crystallized if we search hard enough, or tinker long enough. But in addition to growing more and better crystals, we may also ask what, in a physical–chemical sense, has been learned from all of this. I contend that we have learned a great deal indeed about macromolecular crystals, their character, how they grow, why they grow, and how to grow them better. Let me here present just a few examples to illustrate.

We have learned that the growth of protein crystals proceeds according to the same mechanisms as do conventional crystals (screw dislocations, two-dimensional nuclei formation, normal growth). At the same time we now know that the unique properties of biological macromolecules in aqueous solution permit some unexpected phenomena not otherwise seen (e.g. three dimensional nucleation). We now know that the major differences between the growth of protein crystals and conventional crystals are fundamentally due to slower kinetics (as much as three orders of magnitude). We have learned that protein crystals tolerate much higher rates of impurity incorporation and a far wider variety of impurities. The defect densities of macromolecular crystals are far higher than for conventional crystals by as much as 10^6. We now have quantitative measures for many protein and virus crystals of critical nuclear sizes, surface free energy α, and the kinetic coefficient β, critical thermodynamic and kinetic parameters. There is mounting evidence that protein crystallization shares many of the properties of colloid crystal growth: water is of crucial importance, and the liquid protein phase is a relevant consideration. Finally, we now know that the second virial coefficient of potential mother liquors, obtained from light scattering, is a valuable predictor of successful crystallization conditions.

That there are remaining problems there can be no doubt. Many of the questions that remain are familiar to most of us, but it may nevertheless be instructive to simply identify them and give them explicit form. Among these are the refolding of proteins from inclusion bodies as well as improving the expression of otherwise soluble molecules, and of course, the expression and solubilization of lipophilic and membrane proteins. We must begin by understanding the problem cases and their sources: why some proteins will not crystallize (aggregation, dynamics, microheterogeneity). We need to devise better procedures and approaches for seeding, and the use of surfaces for the promotion of nucleation. The development of new reagents for protein crystallization (precipitants, detergents, chaotrops, osmolites, additives) remains a continuing quest. Crystal handling and manipulation, *in situ* data collection, development of reliable, universal cryogens, understanding annealing, and the consequences of crystal defects require attention as well. We must learn to make a more intelligent selection of crystallization trial conditions and screens, to use combined human and artificial intelligence in place of random screens and sparse matrices. Systematic genetic modification of proteins for crystallization (mutation, truncation, domains, chimeric proteins) requires developing a rationale. This, I feel, could be the most propitious and potentially profitable area available to us. It is an area where we should encourage research and the development of new ideas. The protein truly is the most important parameter in protein crystallization. With the advent and success of the Structure Genomics Initiative, we further have the possibility of compiling databases from large-scale screening, data mining, and prediction of crystallization conditions from physical-chemical properties.

Finally, we may ask, what do we still need to learn that might help? A few ideas. Can we make any correlations whatever between any physical-chemical property of proteins and how they might best be crystallized? What reagents, detergents or additives work best with which classes of proteins? Knowing what interactions and forces stabilize lattices and which destabilize is essential for genetically engineering enhanced crystallization probability. How does nucleation occur? What promotes nucleation, and can we identify the means to encourage nucleation? How can we more intelligently and efficiently genetically engineer proteins to crystallize? How can we increase the size of microcrystals to make them useful for analysis? These are the questions currently at the forefront of our field, and there is much optimism that they may soon be answered.

The Fankuchen award is based very much on teaching as well as research, and I would like to comment briefly on what I consider to be a salient function of the scientist, teaching.

All of us have heard at one time or another the old saying that, "those who can, do; those who can't, teach," and of course the corollary, to which there may be some truth, that "those who can do neither, become deans and vice chancellors."

But I reject those sentiments, they are not true. I believe that those who can do best, teach best. I would like to offer a different thought. In his lovely eulogy to his own mentor Meg Greenfield, George Will paraphrased Henry Brooks Adams in saying that " A teacher gains a sort of immortality, in that it can never be known where his influence ends".

So, my fellow teachers, on those cold, bitter, gray February mornings when you stumble into class and look upon that desolate sea of faces, hollow eyed, slack jawed, noses pierced, baseball caps on backwards, purporting to seek wisdom, but really a warm place to sleep, remember those words, because they may be the only thing you have to sustain you.

Thank you.

Alexander McPherson

ACA Summer School in Small Molecule Crystallography (2004).

The Course was held July 25 through August 4, 2004 on the campus of Indiana University of Pennsylvania (IUP), Indiana, PA. There were 19 attendees and 15 teaching faculty, including two representatives from Bruker-Nonius and two from Rigaku. A questionnaire indicated that the Course was very successful.

The Attendees: Back row (from left): Alan Berezov (U Penn), Amanda Ritter (Proctor & Gamble), Daniel de Lill (GWU), Mark Frisch (GWU), Indunil Nishantha (OSU), Eric Yearly (U Toledo), James Golen (UMass Dartmouth), Noel Gunning (GWU). Middle row: Xiulian Du (U Penn), Gianella Facchin (Montevideo), Janeira Ferreira (Sao Carlos, Brazil), Anna Kelley (Rice), Cristina Hofmann-Cruz (Rice), Ines Eluen (Montevideo). Front row: Gabriel Taylor (IUP), Alecio Pimenta (Sao Carlos, Brazil), Nelson Garces (WVU), Douglas Ogrin (Rice).

Faculty: Standing (from left): Robert Stewart (CMU), Wim Klooster (ANSTO, Sydney), Jenny Glusker (Fox Chase CC), David Duchamp (Pharmacia), Hamilton Napolitano (U. Goias, Brazil), Charles Lake (IUP), John Woolcock (IUP), Marilyn Olmstead (UC Davis). Kneeling: Curt Haltiwanger (Bruker Axs), Bryan Craven (IUP). Absent: Robert Blessing (HWI), Steven Geib (Pitt).

The attendees were all from academia except one from a corporate lab. There were seven women and twelve men. Twelve full scholarships were awarded consisting of tuition, student housing and two meals a day. These scholars included four graduate students from Latin America who also received travel assistance, thanks to the support of the US National Committee for Crystallography and an initiative from Marilyn Olmstead.

The instruction consisted of 25 lectures that emphasized the basics of x-ray crystallography using both powder and single crystal methods. Three lectures were given each morning. A special evening lecture was presented by Jenny Glusker on the history of crystallography. In addition, there were 7 tutorial sessions on practical topics such as radiation safety, the use of crystallographic data bases and the use of modern software packages such as SHELX, SAINT (single crystal) and Gsas, Crysfire (powder). These were backed by sessions in which all attendees had individual computers. Almost one-on-one tutoring was available for problem-solving and symmetry recognition.

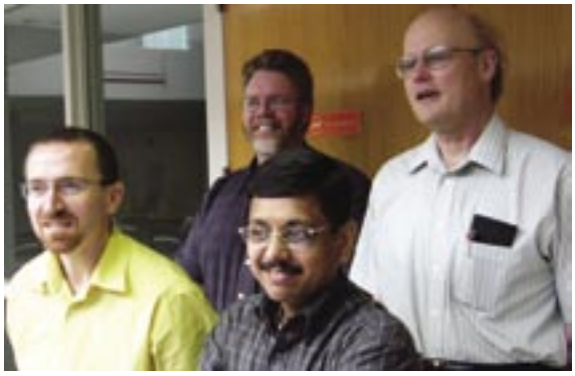
Several of the attendees brought single crystal or powder samples which were used for x-ray data collection and structure analysis. For this work, attendees were divided into groups of 3 or 4. The instruments available were a Bruker-Nonius CAD4 at IUP and a modern APEX with CCD detector which was located in Steve Geib's lab at the University of Pittsburgh but was electronically linked to the x-ray lab at IUP. On the Sunday of the Course, everyone visited Steve's lab and then went on a sight-seeing tour in Pittsburgh. Powder data were collected using a Bruker-Nonius D8 diffractometer and a Miniflex diffractometer that was on loan from Rigaku. All four instruments were operational throughout the Course. On the final morning of the Course, representatives of the 6 working groups gave brief presentations on the results they had obtained.

The organizers received questionnaires from all attendees which in many cases were supplemented by essay-length commentary with valuable suggestions for 2005. Their remarks were generally very positive. Their input will be circulated as we consult with the faculty regarding future plans.

The organizers are very grateful for direct financial support for the 2004 Course from sponsors and from tuition charges. This amounted to almost $14,000. There was a net carry-over of $90. The Course sponsors consisted of the ACA, the USNCCr, the Pittsburgh Diffraction Society, IUP, Rigaku and Bruker-Nonius.

In addition, there was critically important support not recorded on the balance sheet. IUP was most generous in providing air-conditioned lecture facilities with audio-visual aids, and also the two

vans that were used for airport shuttling. The Departments of Physics and Computer Science provided computing facilities. The four representatives from Bruker-Nonius and Rigaku were greatly appreciated for their contributions to the tutoring sessions. The International Centre for Diffraction Data and the Cambridge Crystallographic Data Centre provided the most recent versions of their data bases



Faculty - The powder experts: At back: Thomas McNulty (Rigaku), James Kaduk (BP Corp) Front: Kurt Erlacher (Bruker Axs), Nattamai Bhuvanesh (Texas A&M).

Finally, the faculty provided a wealth of expertise with great generosity and enthusiasm. Many received no remuneration, while others received only their hotel room expenses. They represented a broad spectrum of the ACA membership and included three former ACA presidents. The most junior faculty member was Prof Hamilton Napolitano who attended the 2003 Course as a graduate student from the University of Sao Paulo at Sao Carlos, Brazil.

Bryan Craven and Charles Lake

ACA Macromolecular Crystallography Summer School: 2004 Session

Attendees of the 2004 ACA summer course on macromolecular crystallography

The American Crystallographic Association helped sponsor the 2004 session of the ACA Macromolecular Crystallography Summer School. The school was held at Illinois Institute of Technology and at the Advanced Photon Source at Argonne National Laboratory from 5 July through 17 July 2004. Fourteen students attended; twelve were from the US, and two from Canada. Several applicants from non-North American institutions were unable to attend because of financial constraints or visa difficulties. The students were mostly graduate students from major US and Canadian universities, but there were several postdocs and two faculty members; one employee of a US government lab participated.

The school consisted of: lectures on the fundamentals of crystallography, macromolecular crystallographic realities, and closely related topics; seminars on current research in structural biology; a tour of the conventional small-molecule and macromolecular crystallographic facilities at the University of Illinois Chicago; chemical-laboratory sessions, mostly associated with protein crystallization; computer-laboratory sessions, at which students learned to visualize reciprocal space and goniometry, process diffraction data, and familiarize themselves with phasing and refinement software; extended visits to the macromolecular crystallographic beamlines at the Advanced Photon Source (APS), at which students learned the techniques of synchrotron data collection and collected data on protein crystals that they themselves had grown earlier in the school or in their home laboratories; and opportunities for group tours of Chicago and surroundings.

The faculty for the school was drawn for the most part from the rich crystallographic community of Chicagoland. Among those giving lectures were: ***Jim Kaduk*** (BP), ***Grant Bunker, Andrew Howard, Timothy Morrison, Thomas Irving . Dragutin Knezic*** and ***Alfred Lee*** (IIT), ***Chuck Campana*** (Bruker AXS), ***Jim Pflugrath*** (Rigaku MSC), ***Tristan Fiedler*** (U.Miami / Cold Spring Harbor), Jim Fait (SER-CAT /U.Georgia), and ***Ed Westbrook*** (Molecular Biology Consortium).

Among those giving seminars or lecture-demonstrations or assisting in the laboratories were: ***Andrew Mesecar, Bernie Santarsiero***, and ***Constance Jeffery*** (UIC), ***Wayne Anderson*** and ***Pamela Focia*** (Northwestern University Medical School), ***Phoebe Rice*** (University of Chicago), ***Scott Lovell*** (deCode Genetics, Inc), ***Albert Fu*** (U. Georgia), ***Christopher Dankulich*** and ***Bingyi Yao*** (Proterion, Inc.).

Many staff members of the APS Collaborative Access Teams (CATs) worked

long hours to help the students use their beamlines in a safe and effective manner. Some of these CATs provided beamtime as part of the APS's General User Program; others provided beamtime directly from their own allocations. The CATs participating in the school were: DND, NE, BioCARS, IMCA, SBC, and SER. Every student collected or actively observed data collection on at least two beamlines, and many worked at three or more.

Some students brought their own crystallographic projects from their home laboratories, and everyone grew crystals of lysozyme and thaumatin at the school. There was no shortage of samples to test. The students came in with a wide range of crystallographic experience, from near-neophytes to students who had already solved protein structures, but by the end every student had been exposed to a wide variety of theoretical constructs, approaches, experiemental methods, and structural realities.

Most students lived in the IIT dorms while they were taking the course, but the three local students commuted. The students took advantage of Chicago's appeal as a tourism spot, and several stayed in Chicago after the school to attend at least part of the ACA Annual Meeting.

Financing for the school was derived from ACA funds, from tuition and fees paid by the students or their sponsoring institutions, and from contributions from several equipment manufacturers and pharmaceutical companies. Several companies made in-kind contributions as well. The school could not have succeeded without these generous contributions, nor could it have succeeded without the hard work of the lecturers, lab managers, and beamline scientists who made the organizers' job a pleasurable one. None of the lecturers received any compensation for their contributions. Even the living expenses of the faculty were for the most part uncompensated. Therefore the expenses were modest relative to the value received by the students.

The organizers of the 2004 Macromolecular Summer School look forward to the opportunity to offer a similar program in July 2005 as well. Watch for further information at ***acaschool.iit.edu/***.

Andy Howard

2005 Margaret Etter Early Career Award

The Council has selected ***Jennifer Swift*** (Georgetown University) as the 2005 Etter Early Career Winner. Jennifer is a Clare Boothe Luce Assistant Professor at Georgetown. Research in her lab is directed toward gaining a more detailed understanding of the mechanisms by which molecular crystals nucleate and grow. Most of the projects in this research area are quite interdisciplinary - meaning students will be expected to gain experience in at least a few different areas of chemistry including x-ray crystallography, atomic force microscopy (AFM), organic synthesis, and computational modeling. Arwen Pearson and Jeanette Krause will organize the Etter session at the Orlando Meeting in May of 2005.

RCSB Protein Data Bank Update

There are currently more than 28,000 structures in the PDB archive. As of October 1, 2004, approximately 4,128 structures have been deposited in the PDB archive during 2004. Of the structures received, 77% were deposited with a "hold until publication" release status; 13% with a "release immediately" status; and 10% with a specific release date. 83% of these entries were the result of x-ray crystallographic experiments; 14% were determined by NMR methods.

The RCSB Protein Data Bank (RCSB PDB) has continued to develop resources for data deposition and data query during 2004. Tools to ease data deposition include Ligand Depot and pdb_extract. Ligand Depot (***ligand-depot.rutgers.edu***) is a data warehouse that integrates databases, services, and tools related to small molecules bound to macromolecules. The initial release focuses on providing chemical and structural information for ligands that are found as part of the structures deposited in the PDB archives. pdb_extract takes information about data processing, heavy atom phasing, molecular replacement, density modification, and final structure refinement from the output files produced by many x-ray crystallographic applications. The program merges these data into a macromolecular Crystallographic Information File (mmCIF) data file that can be used with ADIT to perform validation and to add any additional information for PDB deposition. pdb_extract has been integrated into the CCP4 Program Suite (version 5). It is available from the RCSB PDB as a web server and it can be downloaded in binary or source form for use on personal workstations. (***deposit.pdb.org/mmcif/PDB_EXTRACT/***).

As part of data distribution services the re-engineered RCSB PDB website and database is now available for public beta test (***pdbbeta.rcsb.org***). This site was developed using feedback derived from the RCSB PDB help desk, conference attendance, focus groups and other personal interactions between the users of the PDB and RCSB staff. The new system has been designed using an Enterprise Java framework and is based on a three-tier model; an underlying database, a presentation layer, and a middle tier connecting them. The underlying database consists of curated mmCIF files resulting from the data uniformity project, which will allow improved query access to the unified data. The beta test site is available at ***pdbbeta.rcsb.org/pdb*** alongside the current production site. Both sites are updated regularly. The RCSB welcomes ongoing community testing and feedback sent to ***betafeedback@rcsb.org***.

Currently the entire contents of the PDB archives including structure files, structure factor files, NMR constraints and some contributed software and resources may be obtained on CD ROM or on DVD. Beginning in 2005 the full January release will be issued on DVDs and quarterly updates will be released on CDs.

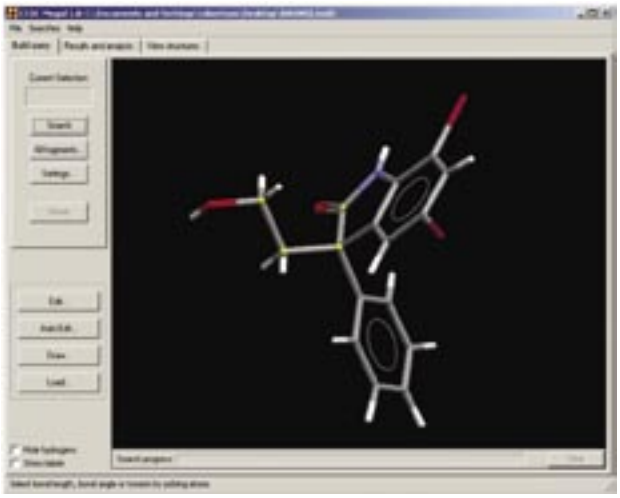
Weekly news about these resources and about other developments is available from the RCSB PDB home page at ***www.pdb.org/***.

Christine Zardecki and Elizabeth Walker

Mogul - Easy Retrieval of Molecular Geometry from the Cambridge Structural Database (CSD)

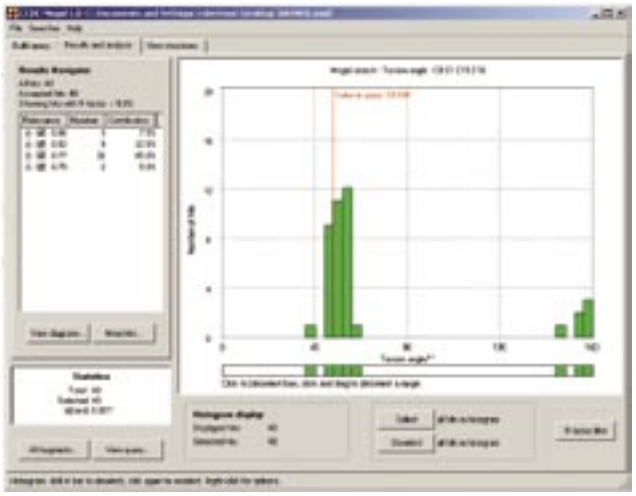
The CSD contains a wealth of experimental information on molecular geometries. However, accessing this information by means of conventional substructure searching can be time consuming. In consequence, these valuable data have been underutilized. To remedy this situation the CCDC have developed a new program for the automated retrieval of molecular geometry data from the CSD, *Mogul*.

Mogul provides easy access to information on the preferred values of bond lengths, valence angles and acyclic torsion angles. The program uses a system of keys to encode the chemical environments of fragments (bonds, valence angles and acyclic torsion angles) in CSD structures. Use of a search tree indexed on these key values then enables the distribution matching any given query fragment to be retrieved, without the need for graph-based atom-by-atom matching. The search tree, together with a novel similarity calculation, also allows the retrieval of similar

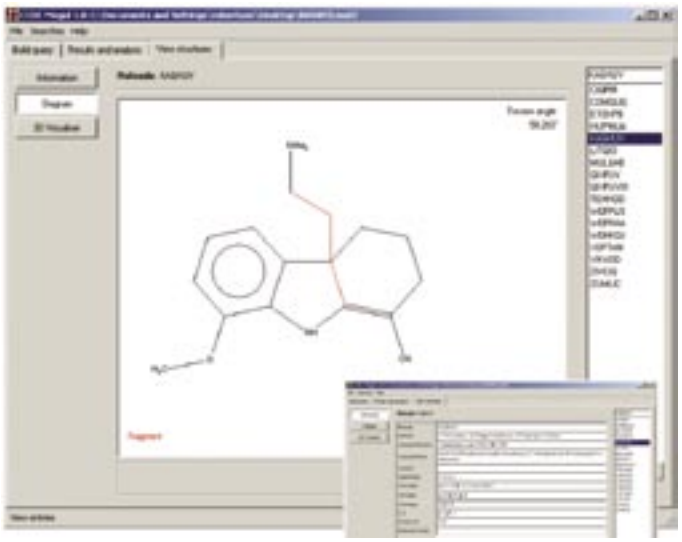


geometric features ranked according to a relevance score.

Histograms and summary statistics for retrieved CSD distributions are displayed interactively and the CSD structures that contribute to a histogram can be viewed. Searches can also be run automatically *via* an instructions file, thus providing a way of integrating *Mogul* with client applications.



Validation experiments indicate that, with rare exceptions, search results afford precise and unbiased estimates of molecular geometrical preferences (see: "Retrieval of Crystallographically-Derived Molecular Geometry Information" Ian J. Bruno, *J. Chem. Inf. Comput. Sci, submitted*).



Mogul has many potential applications including:

- validating the geometries of libraries of modelled molecules or of newly determined crystal structures
- assisting structure solution from low-resolution (e.g. powder diffraction) x-ray data.

Mogul is now available as part of the CSD System, for further information please contact: ***admin@ccdc.cam.ac.uk*** or visit the CCDC website: ***www.ccdc.cam.ac.uk/products/knowledge_bases/mogul/***

Gary Battle

Reminder: Art in Crystallography Prize

In our fall issue, the Editors announced a new competition open to all ACA members: ***Art in Crystallography***, sponsored by the *Newsletter* and the ACA Council. Entries are being accepted in the form of images emailed to either of the Editors (***conniechidester@earthlink.net or flippen@rcsb.rutgers.edu***). Each entry should be accompanied by a paragraph explaining the science and the method of producing the image. We would appreciate receiving a photo of the artist as well. Prizes will consist of a small monetary award and a banquet ticket and waiver of registration fees at the annual meeting. Of course we hope that the **GLORY** garnered by the winners will be an additional incentive. The winning entries will be posted on the web, and displayed at the ACA Meeting. We will also feature some of the images in the *Newsletter* from time to time. Judging will be by a panel appointed by the Editors; please let us know if you are interested in being a judge.

This has come about partly because of the ***Web Watch*** column contributed to the spring *Newsletter*. The Communications Committee found an interesting website: the UK Center for Materials Science, which had just sponsored an Art in Science Competition this September. Their winners are at ***www.materials.ac.uk/photocomp/***. An article in *Science* (Vol. 305, pp 1903) described their "2004 Visualization Challenge" . Winners can be seen at ***www.sciencemag.org/sciext/vis2004*** Crystallographers have a history of interest in art as demonstrated by our occasional art exhibits at meetings and by the Art with Small Molecules contests formerly sponsored by the Small Molecule SIG (the cover of the fall 2000 *Newsletter* featured the winners). So, please send us your images by email at any time. It would be fun to conclude the first competition in time for the spring ACA Meeting, though time is short for that.

Index of Advertisers

Database Challenges in Biology, September 10, 2004

Data resources for the biological sciences are acquiring vast amounts of experimentally derived data. The ever increasing complexity of these data presents challenges to those that develop and manage them. A symposium entitled "Database Challenges in Biology" sponsored by the RCSB PDB was held at the Center for Advanced Research in Biotechnology on Friday, September 10, 2004. This workshop brought together experts in biological data management who described how they organize these data resources in ways that enable scientists to derive new knowledge about structure and function. The meeting highlighted many of the challenges facing biological database resources that include the increasing rate of data acquisition and complexity, database integration, data validation and data mining. In attendance were nearly 100 scientists from various academic and research institutions and a number of government-funding program officers.

Symposium speakers - from left to right: John Johnson, Wah Chiu, Mark Ellisman, Helen Berman, John Markley, Stephen Bryant and Cathy Wu

After a welcome and brief introduction by ***Gary Gilliland***, (RCSB PDB and CARB), ***Mark Ellisman*** (University of California, San Diego) began the presentations with his lecture entitled "Multi-scale Imaging and Databasing of the Nervous System with Advanced Cyberinfrastructure." This lecture focused on data acquisition and analysis issues associated with nervous system data, and provided an overview of several aspects of the Biomedical Informatics Research Network (BIRN, ***www.nbirn.net/***). Next ***Wah Chiu*** (Baylor College of Medicine) lectured on the "Database for Cryo Electron Microscopy." He described his activities that center around the use of electron crystallography and cryomicroscopy to determine the three-dimensional structure of macromolecular assemblies. His presentation included a description of The National Center for Macromolecular Imaging (***ncmi.bcm.tmc.edu***) which is an extensive network of collaborative projects, many of which are focused on structural investigation targets that may be critical for use in developing drugs for healthcare. The next presentation by ***John Johnson*** (Scripps) was entitled "**VI**rus **P**article **E**xplore**R** (VIPER): a Database of Standardized Atom Coordinates for Icosahedral Viruses and Derived Description of Subunit Interactions." This presentation highlighted a web-based resource that deals with icosahedral virus structures (***mmtsb.scripps.edu/viper/***). The structural data has been put into a uniform format that allows viewing and analyzing the complete capsid structure. Novel tools have been developed that help users explore and analyze the data.

In the afternoon ***John Markley*** (University of Wisconsin) presented a lecture entitled "Data Management in the Laboratory: User Facilities and Research on Small and Large Scales." The facilities involved include the National Magnetic Resonance Facility (***www.nmrfam.wisc.edu/***) at Madison and the BioMagResBank (***www.bmrb.wisc.edu***). His lecture described the issues associated with the complex data associated with NMR structure determinations, from sample preparation to data analysis and an approach for capturing these data. ***Stephen Bryant*** (National Center for Biotechnology Information) (NCBI, ***www.ncbi.nlm.nih.gov/***) then lectured on the "Conserved Domain Database: A Protein Family Database." His presentation included a description of the novel tools for visualizing and analyzing structural similarities and also illustrated how the structural data is integrated with the functional annotation data and reference information that is generated and maintained by NCBI. Next ***Cathy Wu*** (Georgetown University Medical Center) presented a talk entitled "PIR Integrated Bioinformatics for Functional Genomics and Proteomics." She described the current state of the Protein Information Resource (PIR, ***pir.georgetown.edu/pirwww/***) and how this resource is now involved in UniProt (Universal Protein Resource, ***www.pir.uniprot.org/***), a joint effort by PIR, the European Bioinformatics Institute (EBI) and the Swiss Institute of Bioinformatics to consolidate protein sequence information from diverse sources. The final presentation of the day entitled "The Protein Data Bank: An Integrated Resource for Structural Biology" was given by ***Helen Berman*** (Rutgers University and the RCSB PDB). Her presentation gave a historical perspective of the PDB (***www.pdb.org***) and its current status and future challenges. She capped the day by highlighting many of the issues and advances associated with international efforts to insure a single archive for the structural data.

The diversity and challenges of the database activities described by the speakers made this a memorable event.

Gary Gilliland

ACA Elections - 2005

Call for Nominations

The ACA nominating committee is starting the process of selecting candidates for the 2005 elections. The positions to be filled are Vice-President, Secretary, and one member for each of the ACA Standing Committees: Continuing Education, Data, Standards and Computing and Communications.

Suggestions are welcome and can be sent to any member of the nominating committee:

Kathy Kantardjieff (Chair) kkantardjieff@fullerton.edu

Ray Davis: redavis@mail.utexas.edu

Wayne Anderson: wf-anderson@northwestern.edu

Dodson Fest, September 2004

There was great celebrating in York, England from September 10-12, when colleagues and friends from around the world gathered to celebrate the careers of ***Eleanor*** and ***Guy Dodson.*** The Dodson are known far and wide for the quality of their science, and for having contributed enormously to the building of a scientific community devoted to collaboration and education.

Eleanor came to the University of York in 1976. She obtained a degree in mathematics from the University of Melbourne, Australia, and followed that with a post at the University of Oxford, working with Dorothy Hodgkin on the structure of insulin. The underlying theme of Eleanor's career has been development of methods for crystallographic structure determination and refinement. She has been a main contributor to the Collaborative Computing Project in Protein Crystallography (CCP4) for all of its 25 years of existence, and I know of many a graduate student who was able to solve their first structure following the excellent advice Eleanor is always willing to dispense on the CCP4 mailing list.

In 1998, Eleanor was awarded the ACA's Pankuchen Memorial Award, for "developing and implementing major computational techniques for macromolecular crystallography and for teaching countless student how to use the resultant programs." In 2001 she received an Honorary Doctorate at the University of Uppsala, and in 2003 she became the first woman at the University of York to be elected Fellow of the Royal Society.

Guy was born in New Zealand, and obtained his PhD in Auckland. He joined the Hodgkin lab at Oxford in 1962, where he contributed greatly to the determination of the structure of insulin. In 1976, he moved to the University of York, and over the years he helped build a diverse Structural Biology Laboratory, which currently has around 80 staff. Guy's research has covered a broad range of biological problems, using crystallography to study proteins such as insulin and hemoglobin, and enzymes including bacterial ribonucleases, lipases, amylases and penicillin acylase.

In 1993, Guy was appointed Head of Protein Structure at the National Institute of Medical Research, Mill Hill, where he developed a second Structural Biology group. Being a man of enormous enegy and vision, Guy has simultaneously held both the York and Mill Hill positions since 1993. In 1991 Guy was

Top row: Philip, Thomas and Vicky Dodson (three of the four Dodson children), Guy Dodson, Keith Wilson, Brian Matthews. Next row: Steve Gamblin, Johan Turkenburg, Gideon Davies. Lorna Wilson (Keith Wilson's wife). Phil Evans, Janet Smith, Guy Dodson. Third row.: Eleanor Dodson, Tom Blundell, Ted Baker, Judith Howard. Fourth row: Guy Dodson, Carol Evans (Phil Evans' wife), Margaret Isaacs (Neil Isaacs' wife) Photos courtesy of Paula Fitzgerald.

awarded the Kratos Medal of the Royal Society of Chemistry, and in 1994 he was elected Fellow of the Royal Society.

It is a true tribute to how dearly loved Guy and Eleanor are in the scientific community that people traveled from far and wide to attend the Symposium. Of course there were many participants from Britain and Europe, and quite a number from the United States, but quite a few people came from as far away as New Zealand, India, and Singapore.

The symposium opened on Friday afternoon with a keynote address by ***Tom Blundell***. Tom set the theme of science in the context of friendship that was followed by all of the other speakers, and like all of them, he filled his talk with priceless photos of Guy and Eleanor from over the years. This first session, devoted to Insulin: Then and Now, was followed by sessions on Cell Processes, Crystallographic Developments, Structural Genomics, Protein Dynamics, Low to High Resolution and Hot!!.

The centerpiece of the meeting was the banquet Saturday evening, held at the National Railway Museum in York. Both the opening cocktail session and the banquet itself where held in halls containing historic railway cars, and the guests were free to wander and explore. After a bibulous meal, we were treated to a very funny tribute/roast by ***John Cutfield***, followed by touching talks by Guy and Eleanor themselves.

The meeting ended on Sunday as you would expect a Dodson event to end, with an invitation to the entire meeting to drop by the Dodson's home for an impromptu Sunday brunch and cook-out. I've been lucky enough to have attended many such spontaneous gatherings at that wonderful home, and it was perfectly fitting that this symposium in tribute to two such well-loved scientists should end just that way.

Paula Fitzgerald

Crystallography in Venezuela – Intensive Course on Advances in Single Crystal X-ray Diffraction

An intensive course on *Advances in Single Crystal X-ray Diffraction* took place from 18 to 22 of October at *Centro de Química*, *Instituto Venezolano de Investigaciones Científicas* (IVIC) in Altos de Pipe, Estado Miranda, Venezuela. This course was organized as part of the activities of the *Laboratorio Nacional de Difracción de Rayos-X* (LNDR-X), funded by FONACIT-Venezuela, with additional support from IVIC, Universidad de Los Andes (ULA), CSIC, Spain and Rigaku-MSC. More than 80 undergraduate, graduate students, and young researchers from Venezuelan universities and research centers and from Universidad Industrial de Santander (UIS, Bucaramanga, Colombia) participated in the course. Lectures on the basic concepts of symmetry, diffraction, structure solution and refinement were followed by advanced topics related to area detectors, instrument developments, structural databases, and applications to macromolecules, among others.

Fernando Lahoz (CSIC, Zaragoza), ***Martín Martínez-Ripoll*** (CSIC, Madrid), and ***Joe Ferrara*** (Rigaku-MSC) were the invited instructors along with ***Reinaldo Atencio*** and ***Rodolfo Vargas*** (LNDR-X, IVIC), ***Miguel Delgado*** and ***Graciela Díaz de Delgado*** (LNDR-X, ULA), and ***Juan Murgich*** (Centro de Química, IVIC). On the last day, ***Fernando Lahoz*** presented examples of how crystallography can help understand and rationalize chemical reactivity. ***Martín Martinez-Ripoll*** presented an overview of the use of structural databases, in particular the Cambridge Structural Database. The final lecture was delivered by ***Bill Duax***, President of the IUCr. He summarized the activities of the IUCr and the ACA, in particular the possibility of country membership in the ACA for Latin American countries. The LNDR-X will provide the funds to start Venezuela's membership in the ACA. Afterwards, he delivered an inspiring lecture on Nobel Prize recipients for work related to crystallography. He stressed the importance of collaborative research and the fact that many women have contributed significantly to the development of crystallography. A quick head count of the attendance to the course indicated a high percentage of young women. The course also received coverage on national TV. In addition to details about this activity, the relevance of international partnerships to address current challenges in structural science was emphasized.

Crystallography in Venezuela will certainly be boosted by the recent acquisition of an area detector for the single crystal diffractometer at IVIC. Plans are underway for the purchase of a single crystal diffractometer with area detector for ULA. An advanced course dedicated to powder diffraction will be conducted next year at the LNDR-X site in Puerto Ordaz, a city in southeast of Venezuela home to most of the mining resources and industries of the country. It is hoped that this course will expan to neighboring countries in South America and The Caribbean.

Reinaldo Atencio, Miguel Delgado and Graciela Díaz de Delgado

SARX Meeting, Cordoba, Argentina, November 2004

Over 150 people attended SARX 4, 80 km outside Cordoba, Argentina. The program of 30 plenary lectures, 20 oral contributions, and 120 posters covered a wide range of x-ray diffraction and x-ray fluorescence instrumentation and applied research. Six Latin American and five European countries were represented along with two people from Japan and one from South Africa. The majority of the attendees were from Argentina (53) and Brazil (46).

The meeting had three official languages: English, Spanish, and Portuguese. The participants were urged to provide English language abstracts, posters and slides for oral presentations. 34% of the abstracts were bilingual, 50% English only, and 16% Spanish or Portuguese. Half of the invited talks and a few of the contributions selected for oral presentation were given in English, but 90% had English text slides, making it possible for English speakers to follow. Over half of the posters were in English and the presenters were happy to discuss their work in English.

Over half of the presentations concerned x-ray fluorescence and total reflection x-ray fluorescence. The other half was distributed among single crystal, powder, small angle scattering, electron probe microanalysis, particle induced x-ray emission, and a few other techniques. These techniques are vitally important to technological advances and development in Latin America at this time. The applications described included determination of the metal and mineral content of samples to foster more profitable mining, and studies of clay swelling which are of immediate relevance to oil drilling but also of potential importance to management of catastrophic landslides. When you see the thousands of people living in ultra low income housing in the steep hills surrounding Latin American's large cities, you can appreciate the potential significance of this. There were talks and posters covering measurement of pollutants in rivers in Mexico and Brazil, as well as the accumulation of toxic elements in soil, honey, animals, and man. Particularly interesting were studies comparing metal content in the teeth of contemporary miners, fishermen, and patients with renal disease, and samples from different prehistoric populations. There was a detailed report on the analysis of iron content and formulation in bread samples to determine whether they meet government standards.

Daniel Vega described a very challenging single crystal study of a mixed E/Z steroidal pre-gestational agent with eight independent molecules in the P1 cell. Each of the eight sites has different ratios of the E/Z components. Two individual single crystals studied were found to have different overall E/Z ratios (1.7 and 2.0). Both ratios were larger than what that found for the entire sample. Another interesting presentation concerned the growth in volume of scientific publications coming from Spain, Portugal, and Latin American countries. There has been a doubling of their share of the language scientific literature beginning in 1995 to a current 3%.

Very lucid presentations on advances in x-ray fluorescence instrumentation and applications including detection of lead in human bone and brain were presented by ***Peter Wobrauschek*** and ***Christine Streli*** (Austria). They conducted a workshop, which they will also be presenting at the next Denver Diffraction conference. Wobrauschek and Strelis are struggling to maintain access to ESRF and have run a workshop entitled "New research with old instruments".

I was asked to identify the two best posters in the section on single crystals, powder, and SAX applications. At least half of the 25 posters were of such high quality that selection of just two was difficult. The best posters involved combinations of two or more techniques applied to more than one crystal form of a material or a series of related materials. Four ACA awards were presented to the authors of the best student posters (complimentary membership, waiver of registration to an ACA Meeting, and a copy of the ACA *Transactions* of their choice).

The award winners were: *X-Ray Diffraction Analysis of Clay Swelling in Aqueous Solutions*, ***Cintia L. G. Amorim***, Ricardo T. Lopes, Regina C. Barroso, João C. Queiroz, Carlos A. Pérez; *Modificaciones Estructurales de Formiato de Praseodimio en Función de la Temperatura*, ***Martín E. Saleta***, Dina Tobia, Daniel R. Vega, Griselda Polla, Hilda Lanza, Andrés Goeta; *Computer Simulation of X-Ray Diffraction Measurements of Surface Stresses with Strong Gradient*, S. A. Filippov, ***J. T. Assis***, V. I. Monine; and *Hydration Water and Crystal Structure in Lanthanide Malonates*, ***G. Echeverría***, G. Punte, E. V. Brusau, J.C. Pedregosa, G. E. Nard.

Bill Duax

Southwest Macromolecular Symposium, Houston, May 22-24, 2004

The first Southwest Macromolecular Symposium was organized in 1990 by ***Edgar Meyer*** (Texas A&M). Continuing the traditionhe started, the 15th Annual Southwest Macromolecular Symposium took place Oct 22 - 24, 2004 at The Marriott Woodlands Waterway Hotel and Convention Center just north of Houston. Close to 100 participants and 10 major vendors were in attendance. On Saturday there were four sessions of scientific presentations covering Structural Biology of Infectious Diseases, Cryo-EM and Structural Methods, and General Structure and Function of Macromolecules. On Saturday night ***Wayne Hendrickson***(Columbia University) gave an outstanding keynote address on the *Triumphs and Challenges of Protein Crystallography*. Sunday's sessions featured oral presentations by the two winners of the poster competition, a vendor session on technological advances, and an open forum on the ideal computational workbench for protein crystallography. The event finished with a world-class, Texas-style barbeque lunch and a promise to return next year for an even bigger crystallography gathering.

(continued on next page)

SWMS XV – 2004: a) Saturday session; b) Poster Award winners and their supervisors (Hong Zhang and Xuejun Zhang (UT Southwestern), Chair Kurt Krause, John Bruning and Yousif Shamoo (Rice University); c) Joe Ferrara and Paul Swepston (MSC – Rigaku, sponsors of SWMS); d) keynote speaker Wayne Hendrickson; e) Bob Fox and Yousif Shamoo; f) David Bouchard and Rose Marie Ndiaye (Nextal); g) Eva Blanpied and Matt Benning (Bruker-AXS); and h) Mike Holcomb and Sue Duncan (MSC-Rigaku) made sure everyone had fun at the Sunday picnic (photos by Marv Hackert).

Saturday Sessions:

Structural Biology of Infectious Diseases - chair ***Kurt Krause*** (University of Houston). ***Sangita Sinha*** (UT Southwestern) spoke on Rv1900c, a *Mycobacterium tuberculosis* nucleotidyl cyclase, composed of an N-terminal α/β-hydrolase domain and a C-terminal cyclase homology domain (CHD). CHD structures with and without an ATP analog were presented and indicate that two of the residues required by mammalian adenylyl cyclases (mAC) are unimportant for Rv1900c activity. A model of half-of-sites reactivity that may be general to CHDs was presented. ***Chad Brautigam*** (UT Southwestern), brought us up to date on their Treponemal structural genomics project that focuses on lipoproteins. ***Hye-Jeong Yeo*** (University of Houston) described her inspiring progress on the structural elucidation of the *Haemophilus influenzae* Hia autotransporter.

Cryo EM and Structure Methods – chair ***Yousif Shamoo*** (Rice University). ***Wen Jian*** (Baylor College of Medicine) described recent advances in cryo-EM followed by ***Chris Colbert*** on the use of combined NMR and x-ray diffraction methods as complementary structural methods to study an oxidoreductase. ***Bob Fox*** (UTMB Galveston) concluded the session with an update on progress at the CAMD beamline and showed how upgrades are increasing the scope of the beamline's functionality for both MAD and higher flux experiments.

Structure Function- I. ***Vince Licata*** (LSU) presented a series of wonderful SAX studies on whether TAQ polymerase exists in a compact or in an extended structure when bound to DNA. The high resolution SAX studies showed TAQ exists as an extended structure in solution and exhibited the power of SAX studies. ***Marilyn Yoder*** (UMKC) spoke on her structure-function studies of phosphatidylinositol transfer proteins (PITP) and provided an evolutionary model for the development of these common enzymes. ***Mischa Machius*** (UT Southwestern) presented a study of the decarboxylase/dehydrogenase component of the human branched-chain alpha-keto acid dehydrogenase complex that regulates the accessibility of its active site by a conserved phosphorylation loop.

Structure Function - II - chair ***Hong Zhang*** (UT Southwestern). ***Christopher Booth*** (Baylor College of Medicine) spoke on the EM structures of the hexadecameric mammalian chaperonin TCP-1 Ring Complex (CCT/TriC). Both the open, nucleotide-free form, and the closed, ADP-AlF_3 bound form of CCT/TriC were characterized at ~15Å resolution. While the closed form of CCT/TriC complex resembles that observed in the crystal structure, docking of TriC subunit structure to the open form CCT requires a large hinge motion between the equatorial and intermediate domains. Such nucleotide binding induced domain motion suggests a mechanism for the closing and opening of the chaperon chamber. Next ***David Lodowski*** (UT Austin) reported the complex structure of G-protein coupled receptor kinase 2 (GRK2) and $G_{\beta\gamma}$, as well the structure of GRK2 alone. The GRK2 contains three domains – the RGS homology (RH), protein kinase, and PH domains. While the PH domain is shown to make primary contact with $G_{\beta\gamma}$, recent mutagenesis and modeling studies have indicated that the RGS homology domain of GRK2 interacts with G_{α} using an interface entirely different from that previously characterized for RGS4. ***Bornali Chakravarty*** (Baylor College of Medicine) concluded the Saturday sessions with her crystal structure of the thioesterase (TE) domain of human fatty acid synthase (FAS) determined at 2.6Å resolution. FAS TE contains two subdomains: an α/β hydrolase-like and a four-helical bundle subdomains. A hydrophobic groove located at the interface of two subdomains is proposed as the palmitoyl acyl substrate binding site while a catalytic triad consisting of Ser2308, His 2481 and Asp2338 was also identified.

Sunday Sessions:

Poster session winners ***John Bruning*** (Rice University) and ***Xuejun Zhang*** (UT Southwestern) opened the Sunday morning session. John spoke on complexes of human PCNA bound to peptides derived from DNA polymerase and flap endonuclease-1 proteins, while Xuejun described how the function of a hypothetical protein from *S. aureus* was determined from the serendipitous discovery of a bound methoinine as its structure was solved.

A panel of computational experts was assembled to discuss and pass on advice on what hardware and software combinations are now preferred for protein crystallography. ***Mitch Miller*** (SSRL), ***Joe Ferrara*** (Rigaku-MSC), and ***Yousif Shamoo*** (Rice) along with active input from the audience responded to questions from session chair, ***Kurt Krause***. A consensus recommendation emerged for a PC/Linux combination, although ***Bob Fox*** (UTMB Galveston) suggested that a Mac-based OSX structure laboratory was now another viable option.

The final session featured a couple of presentations by some of the industrial exhibitors. ***Eric Reese*** (MicroCal) presented recent advances and applications of isothermal titration calorimetry, and ***Angela Criswell*** (MSC-Rigaku) described new crystal ranking software.

At the conclusion of the morning sessions, the participants retired to a nearby park for Texas BBQ, refreshments and discussions of all things crystallographic (and non-crystallographic).

Marv Hackert and Kurt Krause

Contributors to this issue

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2004 NSLS Annual Users Meeting, May 17-20, 2004

Nearly 400 participants came together to attend the 2004 National Synchrotron Light Source (NSLS) Annual Users Meeting at Brookhaven National Laboratory (BNL). The meeting consisted of the main meeting and four workshops. ***Sue Wirick*** received the UEC Community Service Award. ***DArio Arena, Mehmet Aslantas, Alexei Grigoriev, Marianna Kissel, Meghan Ruppel and Xianqin Wang*** were presented poster prizes.

The main meeting: In his welcoming remarks, ***Lawrence Shapiro*** described the continuing excellence in NSLS Research, exemplified by the 2003 Nobel Prize in Chemistry awarded to Roderick MacKinnon. ***Steve Dierker***, NSLS'chair, gave a flavor of the diversity and quality of science that continues at NSLS saying: "The NSLS has a well-deserved reputation for outstanding productivity."

Chris Jacobsen described the multiple applications of x-ray and infrared imaging techniques, such as spectromicroscopy, trace element detection, phase contrast, tomography, and lensless imaging via diffraction. ***Mark Croft*** talked about his research on strain fields in macroscopic materials, in which he uses an energy dispersive x-ray diffraction method. ***Simon Billinge*** presented his work on the structures of complex materials that display order on the nanoscale, using the rapid acquisition pair distribution function technique. ***John Hill*** discussed the advantages of using soft x-ray scattering to probe the behavior and arrangement of electrons in transition metal oxides. ***Lois Pollack*** described a new technique to observe the folding of RNA using small angle x-ray scattering. ***Yvonne Akpalu*** described her work to understand the complex structure of Ethylene/Olefin copolymers, and develop chemical microstructure-morphology-property relations for the materials.

The workshops: "Better Ways to See the Light (Advanced Detectors for Synchrotron Radiation)" was organized by ***Peter Siddons and Gianlurgi De Geronimo. Gareth Derbyshire*** talked about detector developments for synchrotron radiation in Europe. ***Oswald Siegmund*** presented interesting developments in microchannel electron multiplier device technology. ***Gabriella Carini*** spoke about a new integrated circuit for coplanar-grid detector readout". ***Chris Ryan*** reported on the development of a new technique for real-time spectral deconvolution of energy-resolving detector data. ***Kent Irwin*** brought the participants up to date on the cryogenic microbolometer x-ray detectors devices. ***Ke Zhang*** described the development and application of multi-element analyzer systems based on synthetic multilayer optical elements. Then, ***Ed Westbrook*** talked about silicon pixel array detectors for protein crystallography. ***Tae Joo Shin*** told us about his work towards using 2-D position-sensitive proportional counters for x-ray speckle experiments and ***Mark Rivers*** talked about the software solutions he has developed for interfacing area detectors, in particular CCD devices, to data acquisition systems based on the EPICS framework. The take home message from this workshop is that further detector developments are essential to a full utilization of powerful synchrotron facilities.

At the workshop "Anatomy of a Virus", from left to right, Front row: Michael Chapman, Wayne Hendrickson, David Stuart, John Johnson, Donald Caspar, Michael Rossmann, Denis Leclerc, Philip Dormitzer, Huilin Li, Stacy Benson; Back row: Paul Freimuth, Marc Allaire, Dieter Schneider.

Marc Allaire and ***Paul Freimuth*** organized "Anatomy of a Virus" that brought together prominent experts in the field of Structural Virology. ***Don Caspar*** gave a historical perspective on the important factors that were required for the success and birth of structural studies of viral capsids. ***Denis Leclerc*** then reported on his progress on the assembly of nucleocapsid-like particles of Hepatitis C virus. ***Michael Chapman*** presented on structural studies of a gene therapy vector, the Adeno-associated Virus. ***Huilin Li*** talked about the genomic RNA packaging in the Vesicular Stomatitis Virus revealed by single particle cryo-electron microscopy. ***Stacy Benson*** followed and reported on their structural studies of the major coat protein of PRD1. ***Michael Rossmann*** described the use of both electron microscopy and crystallograhy to construct detailed atomic models of large complexes in order to understand their extraordinary dynamic character, such as the entire base plate complex of bacteriophage T4. ***Philip Dormitzer*** described the structural rearrangements during Rotavirus cell entry. ***Wayne Hendrickson*** described the structural biology of HIV attachment and entry into cells. ***David Stuart*** presented his extensive work on the x-ray crystal structure analysis of the entire 66 MDa bacteriophage PRD1 which contains approximately 2000 protein subunits from 18 different protein species including integral membrane proteins associated with an internal lipid bilayer. ***John Johnson*** closed the workshop with a lively talk about structure-based studies of auto-catalytic chemistry in virus particles.

"Grazing Incidence Small-Angle X-ray Scattering (GISAXS)" was organized by ***Ben Ocko*** and ***Detlef Smilgies***. Detlef opened with the history and applications of GISAXS. ***Sunil Sinha*** talked on the underlying scattering theory associated with GISAXS with a focus on the Distorted Wave Born Approximation. ***Ian Robinson*** presented on coherent GISAXS investigations of granular micro-structures in thin metal films and speckle patterns. ***Hartmut Metzger*** presented a review on combined GISAXS and GID studies of semiconducting nanostructures, so called quantum dots. ***Alain Gibaud*** reported on time resolved GISAXS *in-situ* studies of surfactant templated silica thin films. ***Thomas Russell*** spole on the assembly of nanoparticles at the interface of two immiscible fluids. ***Christine Papadakis*** described the inner structure of lamellar di-

block copolymer thin films. ***Matthew Misner*** presented on real time studies of block copolymer thin films. ***Phong Du*** gave an overview of GISAXS studies on silica nanostructures and ***Oleg Gang*** talked on liquid films on nano-sculptured surfaces. ***Gilles Renaud*** described work on real-time *in-situ* investigations of the morphology, organization, and internal structure of growing metal nanoparticles on oxide surfaces in ultra-high vacuum. ***Jin Wang*** spoke about the kinetics of nanocomposites obtained from both SAXS and GISAXS.

"Pharmaceutical Applications of Synchrotron Radiation" was organized by ***Peter Stephens, Raj G. Suryanarayarian***, and ***Evgenyi Shalaev*** who gave an overview of the drug development cycle. ***Peter Stephens*** discussed the differences between laboratory and synchrotron x-ray sources, first from the standpoints of source properties and later in terms of access issues. ***Bill David*** emphasized the value of detailed structural crystallography. ***Kenneth Shankland*** discussed the importance of various steps taken in experimental design and data collection to ensure the accurate solution of structures. ***Mike Pikal*** talked about the degradation of pharmaceutical compounds such as freeze-dried proteins in the form of glassy solids. ***Evgenyi Shalaev*** spoke on the nature of the disordered states, i.e., amorphous state and crystalline mesophases of pharmaceutically relevant solids. ***Raj Suryanarayanan*** discussed x-ray measurements of the degree of crystallinity of pharmaceuticals, especially from the standpoint of monitoring physical instability of products that are prepared as non-crystalline phases. ***Satyendra Kumar*** discussed model systems related to the issue of delivering water-insoluble drugs. ***Heinz Amenitsch*** talked on the use of simultaneous small- and wide-angle x-ray scattering to study nanostructural features of relevant solids.

Peter Takacs and ***Steve Hulbert*** organized "Advanced Optical Systems and Metrology for High Power and Coherent Beamlines". ***Chris Jacobsen*** gave a summary of capabilities of various groups around the world to produce small spot sizes from present sources of coherent x-rays. ***John S. Taylor*** discussed the development of diffraction-limited multilayer-coated optics for normal incidence extreme ultraviolet lithography systems. ***Phil Stahl*** gave an overview of future space telescope missions and the technology that will be required to build large, lightweight mirrors and structures. ***Don Golini*** spoke on a new surface finishing technique that looks quite promising for the production of spherical and aspherical surfaces. ***Ken Evans-Lutterodt*** discussed refractive optics for focusing x-ray beams to small spot sizes and the optimum elliptical hole shape with an e-beam writer. ***Peter Takacs*** discussed metrology issues related to the Long Trace Profiler. ***Wayne McKinney*** spoke on issues that are driving the direction of synchrotron radiation metrology. ***Gene Ice*** gave a description of Kirkpatrick-Baez (KB) mirror nanofocusing systems. ***Riccardo Signorato and Daniel Hausermann*** presented jointly on the fabrication and use of modular piezoelectric bimorph mirrors as adaptive optics.

"Applications of Synchrotron Based Methods to Hydrogen Storage Materials" was organized by ***Wolfgang Caliebe*** and ***Trevor Tyson***. ***Doon Gibbs*** emphasized the importance of the Hydrogen Energy Project (production, storage, utilization) as one of the missions of the Department of Energy. ***John Petrovic*** described the targets for automotive research over the next 15 years. ***James Reilly*** presented several ways to create nano-composite metal-hydrides, and their properties. ***Zafar Iqbal*** talked about the different ways to synthesize single-wall nanotubes and ways to functionalize them. ***Tom Vogt*** emphasized the importance of characterizing these materials for better understanding of their storage and release mechanisms. ***Alexander Ignatov*** talked about the x-ray absorption studies of hydrogen storage materials, their strengths and limitations. ***Yan Gao*** presented the first powder-diffraction data of the re-hydrogenation process measured with high time-resolution. ***Najeh Jisrawi*** discussed synchrotron XRD studies of hydrogen absorption in metallic multilayers and nano-particles.

Cecilia Sanchez-Hanke and ***Peter Sutter*** organized "Nano-probes for Nanoscience." ***Bob Hwang*** gave an overview talk on the status of the Center for Functional Nanomaterial at BNL. ***Harald Ade*** presented an extensive review of his work on characterization of polymers using soft x-ray transmission microscopy. ***Chris Jacobsen*** gave a review of x-ray microscopy using zone-plates and talked about diffraction imaging. ***Cev Noyan*** presented a study of strain in SiGe crystals grown on Si crystals. ***Barry Lai*** talked about the applications of micro-fluoresence and x-ray absorption near edge spectroscopy to life science problems. ***Ken Evans-Lutterodt*** gave an overview of the microdiffraction project at the X13B beamline at the NSLS to perform sub-micron x-ray micro-diffraction and imaging. ***Rudolph Tromp*** gave a broad overview of the history, current state-of-the-art, and the future possibilities of low-energy electron / photoelectron microscopy (LEEM/PEEM). ***Stefan Heun*** presented the capability and results from the X-PEEM instrument located at Synchrotrone Trieste. ***Jun Feng*** spoke on the design of the PEEM3 project which will have a spatial resolution down to 5 nm, almost an order of magnitude better than the PEEMs currently operating at various synchrotron facilities.

A hands-on crystallization workshop organized by ***Naomi Chayen*** and ***Vivian Stojanoff*** focused on Membrane Proteins. ***Naomi Chayen*** discussed several different crystallization techniques developed for soluble proteins and the modifications necessary for crystallization of membrane proteins. ***Peter Nollert*** presented on the difficulties of membrane protein crystallization and ***Petra Fromme*** talked about the importance of the phase diagram to the crystallization of PhotoSystem (PSI and PSII). Vapour diffusion methods with focus on seeding techniques were discussed by ***Marie-Claude Marchand*** and the Counter Diffusion method was introduced by ***Ana Merlo***. The workshop was designed to allow participants to experience the crystallization of photo system I and bacteriorhodopsin.

A bright future: NSLS-II: Steve Dierker stressed that the NSLS, designed 30 years ago and the only remaining second-generation DOE light source, is now performing at the limits of its capabilities. ***Pedro Montano*** acknowledged this, referring to the NSLS as the "workhorse" of the DOE light sources. Dierker, Montano and Chaudhari repeated the need and excitement for NSLS-II, the proposed third-generation light source that would replace the NSLS. "I think NSLS-II is necessary," Montano said. "A huge number of scientists in the Northeast would benefit from it." The NSLS-II is needed to broaden and enrich their research.

Marc Allaire

CSHL 2004 X-ray Methods in Structural Biology

The annual X-*ray Methods in Structural Biology* course was held for the 17th time at Cold Spring Harbor Laboratory in October 2004. This well-regarded course, funded by a training grant from NIH, teaches the fundamentals of macromolecular x-ray structure determination from both the theoretical and practical viewpoints. This year, the 16 participants were outnumbered by the course instructors during the 16 day workshop. All the participants grew crystals of several different representative proteins and solved the crystal structure of orthorhombic hen egg white lysozyme by several methods.

The theoretical lectures were anchored by ***Alex McPherson*** (U California, Irvine) who covered basic crystallography and crystal growth. ***William Furey*** (VA Medical Center and U Pittsburgh) covered many aspects of solving the phase problem including Patterson maps, MIR, MAD, and NCS. ***Jim Pflugrath*** (Rigaku/MSC) covered cryocrystallography and x-ray diffraction data collection. ***Gary Gilliland*** (CARB/NIST/UMBI) covered databases, structural genomics, and crystal seeding along with managing the ever changing schedule. ***Morten Kjeldgaard*** (Aarhus U) helped with computer graphics, ***Randy Read*** (U Cambridge) with molecular replacement and maximum likelihood, ***Tom Terwilliger*** (LANL) with phasing and automated map fitting, ***Tassos Perrakis*** (NKI) with automated map fitting and refinement, ***Dale Tronrud*** (U Oregon) with the theoretical aspects of refinement, ***Paul Adams*** (LBNL) with phasing and refinement, ***Zbigniew Dauter*** (NCI) with data collection, ***Wayne Hendrickson*** (Columbia) with theory of the MAD method as well as practical advice, ***Jane and Dave Richardson*** (Duke) with validation methods, ***Gerard Kleywegt*** (Uppsala) with even more validation methods and an admonishment to the course instructors to deposit structure factors. A student from last year's course, ***Scott Strobel*** (Yale), presented a lecture on his recent successful crystallographic studies entitled *RNA crystallography: Structure of a self-splicing intron reaction intermediate*.

The course was hosted by ***Leemor Joshua-Tor*** and ***Rui-Ming Xu*** of Cold Spring Harbor Laboratory. In addition ***Robert Sweet*** and his colleagues ***Anand Saxena, Alex Soares and Grace Shea-McCarthy*** of Brookhaven National Laboratory contributed immensely during the 2 days of synchrotron beamtime used by the course participants. ***Irina Persikova and Kyle Burkhardt*** from the RCSB Protein Data Bank were on hand to demonstrate the steps of a structure-determination deposition.

Despite the long hours of the course, the students and instructors ere rested enough at the end to dance on the Plimpton seminar room table and break it. Applications for the 2005 Course to be held October 10th through 25th will be accepted until July 1th, 2005. For more information see ***www.cshl.edu***.

Left to right, front: Calvin Yip, Qun Wan, Mihwa Lee, Kelly-Ane Wilson, Neelamegam Sivakumar, Yinan Wei; middle: Jesse Cochrane, Jane Richardson, Anastasia Mylona, Toshimitsu Kawate, Alex McPherson, Louidmila Loukachevitch, Irina Persikova, Gary Gilliland; and back: Natalia Beglova, Oki K. Dzivenu, Jim Pflugrath, Jennifer Litowski, Bill Furey, Jill Dombrauckas, Dave Richardson, Dale Tronrud, Tomislav Kamenski, Morton Kjeldgaard, Gale Rhodes, Wayne Hendrickson.

Jim Pflugrath

Future Meetings

JANUARY 2005

17-19 **Protein Crystallography in Drug Discovery.** Dedicated to structural genomics & proteomics. South San Francisco, CA **www.protcrystconf.co**

MAY 2005

19-29 **Evolving Methods in Macromolecular Crystallography,** 37th crystallography course, Erice, Italy. **www.crystalerice.org/futuremeet.htm**

24-28 2nd International Conference on Photo-Induced Transition, U. of Rennes1, France. Contact: gmcm-pipt@listes.univ-rennes1.fr, **www.gmcm.univ-rennes1.fr/pipt/**

MAY / JUNE 2005

28-2 **ACA Annual Meeting, ACA 2005, Walt Disney World Swan Hotel, Orlando, FL. www.xray.chem.ufl.edu/aca2005/index.htm Local Chairs: Khalil Abboud, abboud@chem.ufl.edu, and Tom Selby, tselby@mail.ucf.edu; Program Chair: Ed Collins, edward_collins@med.unc.edu.**

AUGUST 2005

18-23 **IUCr Computing School** (prior to IUCr Congress in Florence), in Siena, Italy.

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

JUNE 2006

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

JULY 2006

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

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.

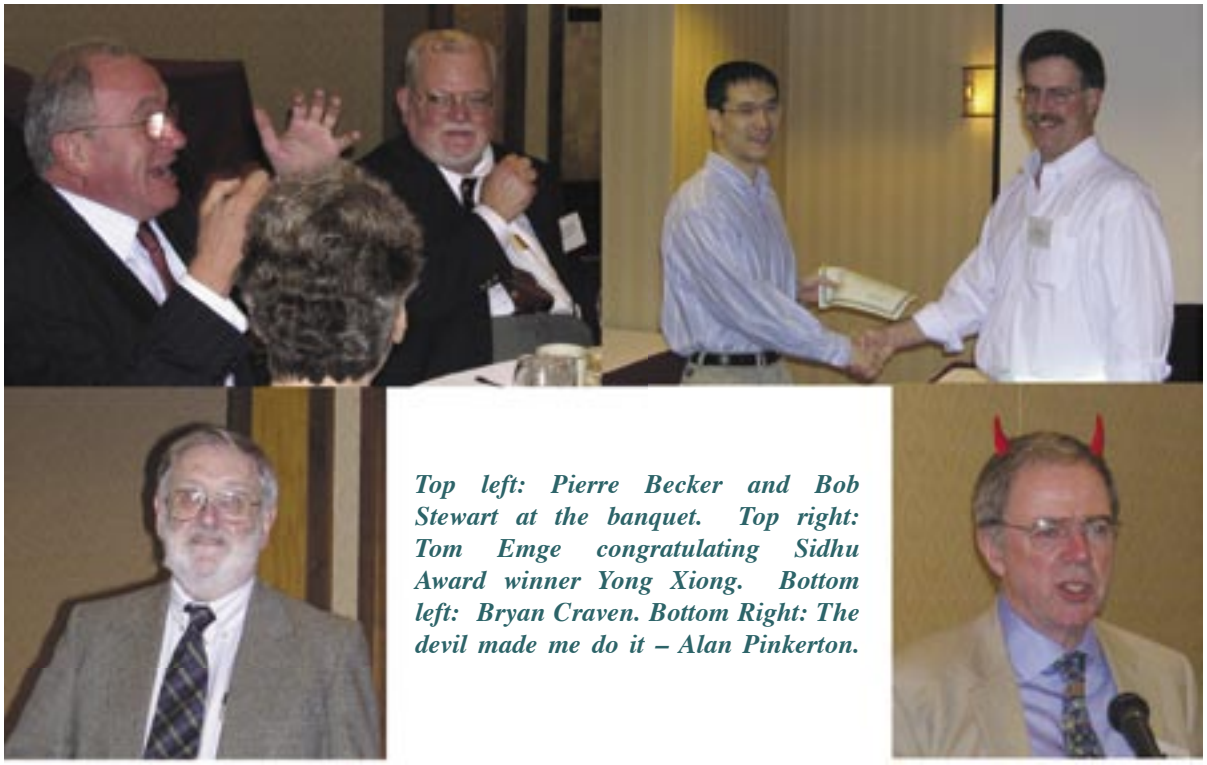
62nd Pittsburgh Diffraction Conference

The 62nd Pittsburgh Diffraction Conference commenced on October 28, 2004 at the University of Pittsburgh Holiday Inn with a welcome to the participants by President ***Tom Emge***. The conference was well attended, with participants from as far afield as Australia, Britain, France and Italy.

One of the highlights at each PDS conference is the presentation of the *Sidhu* and *Chung Soo Yoo Awards*. The Sidhu Award recognizes the outstanding contributions of an early career scientist. This year's Sidhu Awardee, ***Yong Xiong***, highlighted his findings of enzymatic CCA addition to tRNA and the mechanism by which the ATP or CTP molecule is recognized while GTP and UTP are not.

Wim Klooster, who traveled the furthest to present, gave an overview of the development of the Australian neutron source due to be operational in 2005. The opening day concluded with a presentation by ***Jason Hodges*** detailing the development of a third generation neutron powder diffractometer to be installed at the Spallation Neutron Source at Oak Ridge National Laboratory.

The second day was dedicated to ***Robert Stewart*** in honor of his pioneering work in the fundamentals of crystallography. He presented an overview of his own career showing the breadth of studies he has undertaken over the years. This symposium boasted a large number of international participants with researchers from France (***Pierre Becker*** and ***Claude Lecomte***), Italy (***Riccardo Destro***), Britain (***Lee Brammer***) and Canada (***Yvon Le Page***) all giving excellent presentations of their work and the influence that ***Bob Stewart*** had on it.



Top left: Pierre Becker and Bob Stewart at the banquet. Top right: Tom Emge congratulating Sidhu Award winner Yong Xiong. Bottom left: Bryan Craven. Bottom Right: The devil made me do it – Alan Pinkerton.

The Chung Soo Yoo Award is presented to the graduate student with the best poster. ***Eric Yearly*** from the University of Toledo was the deserving recipient for his charge density analysis of diethylstilbestrol.

The meeting consisted of four symposia. The opening session, chaired by ***Leif Hanson***, detailed progress and advances in neutron diffraction. The first speakers, ***Paul Langan*** and ***Dean Myles*** discussed techniques to aid macromolecular crystallographers in locating elusive and reactively important hydrogen atoms. In particular the deuteration of samples, which enhances analysis by neutron diffraction, was widely discussed. The late afternoon session consisted of three talks that discussed advances in new technologies for measurement of neutron diffraction data. ***Chick Wilson*** pointed out the importance of increasing the detector coverage to decrease collection time and obtain useful data that had been previously missed with older detector configurations.

Bryan Craven (IUP) discussed two morphologies that uracil can adopt and their studies in resolving the problem. ***Riccardo Destro*** introduced the topic of magnetoresistance with the work his group has done examining the magnetic properties and structural changes of materials. ***Pierre Becker*** followed with a strong theoretical discussion on pseudo-atomic decomposition models. He gave supporting evidence for his theories by comparison with experimental data. This technique may have significant implications for future drug design based on the understanding of the drug/receptor charge surface. ***Claude Lecomte*** continued with a presentation regarding charge density studies of guest molecules when interacting with host molecules and how their charge surfaces are affected by such interactions. ***Lee Brammer*** concluded the morning with a lively discussion on the study of electrostatic potentials of halide containing compounds and how they can be used to predict C-X..N, C-X..O or even M-X'..X-C interactions and be useful as supramolecular synthons.

The afternoon opened with ***Tom Emge*** presenting a missive from ***Lyle Jensen*** regarding his interactions with Bob. This led immediately into ***Bob Stewart*** presenting a overview of the last forty years of his career. There was an amazing variety of work covered, which surprised even some of his colleagues. ***Yvon Le Page*** reported on a set of computer-based database tools and expert systems that will enable crystallographers to correlate and investigate crystal structures with a view to performing molecular calculations to predict, for example, the surface chemistry of adsorbed molecules. ***Jerry Gibbs*** detailed the theoretical predictions of bond critical points in minerals and showed the high correlation between the theoretical and experimental data. Continuing with the prediction theme, ***Lisa Zhurova*** discussed how charge density studies can highlight the probable activity of "energetic" (explosive) materials. The day was rounded out by an energetic discussion by Ned Seeman on the various ways DNA can be manipulated to systematically design large scale structures.

Bi-Cheng Wang and ***John Chrzas*** began the third day of the conference with a talk on the development of the SER-CAT beamline at the APS and how they are working towards improving user access, interface and range of experiments at Sector 22. ***Greg Petsko*** followed with a lively, animated presentation of proteins and their vibrational behavior in their primary role as catalysts. Through the use of movies, ***Andy Mesecar*** detailed how we should think about developing a systematic approach to understanding protein or enzyme catalytic steps. This included a discussion on how form and function within enzymes and proteins only allow certain reactions to occur, a theme that was reinforced later in the day. ***Keith Moffat*** showed his technique of singular value decomposition - based on the analysis of a wide variety of proteins - to provide researchers with a framework to analyze and determine the locations within proteins which influence the catalytic reactions they perform. ***Wah-keat Lee*** delighted the audience with movies of an ant feeding and the respiration of an insect in his discussion on the uses of phase-enhanced radiography at the APS.

Afternoon talks focused on synchrotrons, particularly hardware, with ***Qun Shen*** presenting on the development of the optics systems at CHESS. Multi-layer monochromators and zone plates for beam focusing were included in his talk. Continuing the synchrotron optics theme, ***Donald Bilderback*** discussed the development of monocapillary optics and the utility and advantages of these simple, yet effective devices. ***Jonathan Lang, Ulrich Lienert*** and ***Daniel Hausermann*** completed the conference with further presentations on developments at the APS. The range of options available to users at synchrotron sources is being expanded very rapidly and this was well displayed in the final three presentations.

The conference was very well attended, with a large international participation. The breadth of research being carried out in crystallography today was eminently displayed ranging from synchrotron development to theoretical analysis of problems to furthering our understanding of biological function.

Allen Oliver

USNCCr Report - November 2004

Back row: Frank Fronczek, Ray Davis, Ken Downing, Jim Kaduk (Vice-Chair), Fran Jurnak, Ron Stenkamp, Jon Clardy (Chair), Kathy Kantardjieff, Doug Ohlendorf, Joel Brock (Secretary/Treasurer), and Peter Vekilov. Front Row: Phil Bourne, Brian Toby, Cheryl Klein Stevens, and Peter Kuhn. Missing from the photo: Marilyn Olmstead, John Parise, Matt Redinbo, Ned Seeman, Bill Duax and Han-min Zuo.

The US National Committee for Crystallography (USNCCr) met on November 13 at the National Academies Keck builiding in Washington, DC. The main topics on the agenda included the election of new members, a report on the recent International Union of Crystallography (IUCr) Executive Committee meeting, a report on the developing program for the IUCr Congress in Florence in August, 2005, a discussion of the process for selecting the U.S. delegates to the IUCr Congress, and setting up the travel grant program for graduate students and post-docs for the IUCr Congress.

Results of USNCCr elections **-** New Members (2005-2007)

Julia Chan - Louisiana State University

Peter Kuhn - The Scripps Research Institute

Miriam Rossi - Vassar College

Ron Stenkamp - University of Washington

The USNCCr is currently seeking nominations for the position of vice-chair of the Committee and for delegates to the IUCr Congress in Florence. Suggestions should be sent to ***Joel Brock (jdb20@cornell.edu***).

The USNCCr is also currently seeking nominations for four committee members for the 2006-2008 term. Suggestions may be sent to any member of the Nominating Committee.

Frank Fronczek (ffroncz@lsu.edu)

Katherine Kantardjieff (kkantardjieff@fullerton.edu)

Matthew Redinbo (redinbo@unc.edu)

Brian Toby (brian.toby@nist.gov)

XX IUCr Congress

Both the 2nd circular and the program for the IUCr Congress are now available on the IUCr web site (***www.iucr.org/***) as well as in issue 12#3 of the *IUCr Newsletter*.

The USNCCr will be awarding travel grants to students and post-docs for attendance at the IUCr Congress in Florence in August, 2005. The application deadline is April 30th. Details will be posted on the USNCCr website www7.nationalacademies.org/USNC-IUCr and are also listed in this Newsletter on page 68.

About the Committee

The USNCCr represents US crystallographers in the IUCr through the National Academies' (NAS) National Research Council (NRC). It promotes the advancement of the science of crystallography in the US and throughout the world. Crystallography is a key tool for a variety of fields in biological and physical sciences. The USNCCr brings together a broad spectrum of crystallographers from diverse fields. The IUCr is a member union of the International Council for Science (ICS)

By representing the broad US crystallographic community, the USNCCr also serves a unique role in bringing together crystallographers with a wide range of perspectives. This role is increasingly important for maintaining a high level of professionalism in a community that spans several disciplines and professional societies and that needs communication and coordination internationally.

Functions - The Committee's primary functions are:

1. To inform crystallographers in the US concerning the activities of the IUCr and to advise the President of the NAS on matters pertaining to US participation in the IUCr.

2. To nominate to the NRC persons to represent the US as delegates to the General Assemblies of the IUCr and other meetings sponsored by the Union. and to provide information and guidance for such delegates.

3. To plan and sponsor scientific meetings in the US in consonance with the objectives of the IUCr.

4. To perform such other duties as are required of national committees of adhering countries under the statutes of the IUCr.

5. To take any other action directed toward the benefit and advancement of the science of crystallography.

Projects and Activities

- Delegation to IUCr Congress
- Resolutions for IUCr General Assembly
- Nominations for IUCr Commissions and Committees

USNCCr Standing Subcommittees

- Nominating Subcommittee for Members and Officers
- Interdisciplinary Subcommittee

USNCCr Ad hoc Subcommittees

- Crystallographic Databases
- Crystallographic Education
- Research Resources and Facilities
- Research and Travel Supports

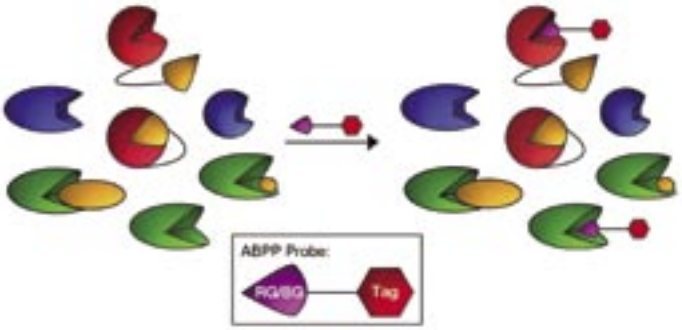
Collaborations and Joint Activities with other US National Committees and International Groups:

- Exploring the use of Collaboratories or Virtual Laboratories for research and education
- Enabling new opportunities for collaborations and access to research resources
- Fostering communications through activities such as the Inter-American Workshop on the Use of Synchrotron Radiation for Research.

Joel Brock

New Horizons in Structure Based Drug Discovery - ACA Transactions Symposium - Orlando - 2005

Structure -based rational design of specific ligand and protein activities is one of the grand challenges in research at the biology-chemistry interface. This transitional symposium will present a new set of cutting-edge tools that not only greatly empower the design work, but also help target new and novel protein functions. Two of the Symposium speakers kindly provided a graphical sneak peak at their research. The cover illustration was provided by *Pat Weber* (ExSAR): Hydrogen/Deuterium exchange experiments conducted in solution reveal global conformational changes that accompany ligand binding. The molecule has been colored according to the observed H/D exchange. The background shows a plot of the time-dependent changes in H/D exchange along the sequence of the protein. Blue and red regions indicate slow and fast exchange, respectively. Because structural changes that forms the basis for molecular signaling may be masked by crystal contacts, characterization of molecules in solution by H/D exchange provides an important structural biology tool for drug design.



The above image was provided by ***Ben Cravatt*** (Scripps Research Institute): General strategy for activity-based protein profiling (ABPP), where proteomes are treated with chemical probes that label active enzymes, but not enzymes inhibited by intra- or inter-molecular regulators (orange) or that lacking complementary binding sites (blue). (RG = reactive group, BG = binding group, Tag = biotin and/or fluorophore).

ACA Summer Course in Small Molecule Crystallography, 2005

This course will be offered June 5 through June 15, 2005 at the Indiana University of Pennsylvania, in the town of Indiana located about 80 miles east of Pittsburgh. Each day there will be three lectures in the morning on single crystal and powder diffraction methods, followed by afternoon and evening workshops for problem solving, data analysis and crystal structure determination. The curriculum will emphasize the basics in X-ray crystallography. Attendees are expected to have completed at least undergraduate courses in chemistry, physics and mathematics. No prior experience of X-ray crystallography will be assumed, but attendees are advised to read in advance *"Crystal Structure Analysis: A Primer"*, by Jenny P. Glusker and Kenneth N. Trueblood, Oxford Univ. Press (1985).

The organizers aim for a total of 25 attendees, who in past years have come from academia (students and faculty), government and corporate institutions, both in the U.S. and from abroad. There will be at least 12 experienced teaching faculty. Tuition will be $250 (or $750 for applicants from corporate labs). Student apartment housing at IUP (including breakfast and lunch) is available for a total of about $400. Approximately 12 graduate student scholarships will be offered. These will consist of a waiver of tuition and living costs. The scholarships will be awarded based on the student's (1) scientific ability, (2) expected benefits from the course and (3) skills in English. We encourage applications from Latin America.

Instruments available will be two Bruker-Nonius single crystal diffractometers (a CAD4 at IUP and a modern APEX instrument with CCD detector located at the University of Pittsburgh which will be electronically linked to the x-ray lab at IUP). Also available at IUP will be a Bruker-Nonius D8 powder diffractometer and a Miniflex powder diffractometer on loan from Rigaku. There will be individual computers for each attendee. Facilities will include access to the Cambridge structural data base and the ICDD powder diffraction data base.

The Course registration form can be obtained from the ACA web site at ***www.hwi.buffalo.edu/ACA.*** Completed forms must be received before April 1, 2003 by Prof. Bryan Craven, Chemistry Department, Indiana University of Pennsylvania, Indiana, PA 15705, USA or electronically by Prof Lake at ***lake@iup.edu.*** Further information will be updated on the web site or can be obtained from ***craven@icubed.com***.

We shall observe the basic policy of nondiscrimination and affirm the rights of scientists throughout the world to adhere or to associate with international scientific activity without restrictions based on nationality, race, color, age, religion, political philosophy, ethnic origin, citizenship, language, or sex, in accordance with the Statutes of the International Council of Scientific Unions. At this Course, no barriers will exist which would prevent the participation of *bona fide* scientists.

Bryan Craven and Charles H. Lake, Organizers.

ACA Summer Course in Macromolecular Crystallography, 2005

The Illinois Institute of Technology (IIT) announces that plans are underway for the third ACA-sponsored Summer School in Macromolecular Crystallography at IIT and the Advanced Photon Source (APS), Argonne National Laboratory. The Summer School will be held from Sunday 10 July 2005 through Saturday 23 July 2005. The Summer School will feature lectures, laboratory exercises in crystallization and software use, and data collection on conventional sources and at several macromolecular crystallographic beamlines at the APS. Lecturers from several prestigious Chicago-area universities and research laboratories, as well as visiting lecturers from elsewhere, will participate in the school. Students will be invited to bring protein crystals for synchrotron data collection, and will participate actively in exploring new crystallization efforts and structure determinations. Food and lodging will be available at IIT, and the cost will be modest -- roughly $900 plus food. Limited scholarships will be available. For further information contact Andy Howard at howard@iit.edu or examine the Summer School website, acaschool.iit.edu.

Andy Howard

Call for Nominations for the 2006 Margaret Etter Early Career Award

The Margaret C. Etter Early Career Award recognizes outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career. The award was established to honor the memory of Margaret C. Etter (1943-1992), who was a major contributor to the field of organic solid-state chemistry. Her work emphasized the use of hydrogen bonds and co-crystals. In addition to a large body of experimental work she was the major force in devising a set of rules known as graph sets to describe hydrogen bonds, revealing similarities between structures without being tied up in the crystallographic details. Her experience teaching at an undergraduate institution and in working in both an industrial and academic setting gave her an unusually broad perspective from which to mentor students. She had a love for people, for science, and especially for people who do science. The award consists of a monetary award of 1,000 dollars and a plaque. The winner will present a lecture at the 2006 ACA Meeting.

Scientists involved in crystallographic research in the broadest sense will be eligible for the award. At the time of the closing date for nominations, nominees must must have begun their first independent (not postdoctoral) position within the past 6 years (not including career breaks). Nominations must include a nomination letter clearly indicating their accomplishments since beginning their independent career and an assessment of their future potential. Additional supporting letters and a c.v. may be provided but are not required. Self-nominations are not permitted. Nominees may be employed in academia (including service crystallography), in industry or in government laboratories.

Deadline for submission: March 1, 2005

(send to ***marcia@hwi.buffalo.edu***)

Buerger

Rudolf Allmann
Blake Industries Inc.
Abraham Clearfield
A W Cordes
Karl F Fischer
Judith C Gallucci
Gary L Gilliland
Theodor Hahn
Joseph Xiaomin Ho
Heinz Jagodzinski
L H Jensen
Judith A Kelly
James R Knox
Rudolph K Kullnig
Alan D Mighell
George M Sheldrick
Clara B Shoemaker
Carla Slebodnick
William C Stallings
Hugo Steinfink
Robert M Sweet
Thomas C Terwilliger
Thomas Webb
Elizabeth A Wood
Shu-Cheng Yu

Etter

Paul W Baures
J Michael Bennett
Helen M Berman
Joel Bernstein
Blake Industries Inc
Lee Brammer
Doyle Britton
Carolyn P Brock
William R Busing
Martin Caffrey
Connie Chidester
Abraham Clearfield
A W Cordes
Paula M D Fitzgerald
Mark D Hollingsworth
Jeanette A Krause
Mariusz Krawiec
Samuel Larsen
James H Loehlin
Bruce C Noll
Virginia B Pett
James C Phillips
Stephen B Robie
Frank J Rotella
Timothy J Rydel
F Raymond Salemme
Carl H Schwalbe
Leonard J Soltzberg
William C Stallings
Thomas C Terwilliger
Brian H Toby
Patricia Weber
Scott R Wilson
Fred C Wireko
Alexandre FT Yokochi
Victor G Young

Fankuchen

Helen M Berman
Blake Industries Inc.
Bruce W Brown
Donald L D Caspar
Connie Chidester
Abraham Clearfield
Thomas J Emge
Gary L Gilliland
Joseph Xiaomin Ho
L H Jensen
Hellmut J Juretschke
J Lawrence Katz
Alan D Mighell
Frank Milillo
Masashi Miyano
James F Pletcher
Michael G Rossmann
Timothy J Rydel
Clara B Shoemaker
William C Stallings
Hugo Steinfink
James M.Stewart
Robert M Sweet
Thomas C Terwilliger
Dale E Tronrud
Thomas Webb
Winnie Wong-Ng
Elizabeth A Wood

Patterson

Andrew J Allen
Helen M Berman
Connie Chidester
Abraham Clearfield
A W Cordes
Bryan M Craven
Howard M Einspahr
Paula M D Fitzgerald
Gary L Gilliland
Jenny Glusker
Philip W Hemily
L H Jensen
James R Knox
Allen C Larson
P Galen Lenhert
Richard E Marsh
Paulus Moore
Bruce C Noll
C E Nordman
Sean Parkin
Erich F Paulus
Edward Prince
Michael G Rossmann
W Robert Scheidt
Nadrian C Seeman
George M Sheldrick
Clara B Shoemaker
William C Stallings
Hugo Steinfink
Robert Stewart
Boris Strokopytov
Marianna K Strumpel
Robert M Sweet
David H Templeton
Thomas C Terwilliger
Dick Van der Helm
Norman M Walter
Thomas Webb
Elizabeth A Wood

Pauling

Paul W Baures
Helen M Berman
Lee Brammer
Martin Caffrey
Joseph C Calabrese
Connie Chidester
Abraham Clearfield
A W Cordes
David E Cox
David R Davies
Robert Degeilh
Drake S Eggleston
Paula M D Fitzgerald
Frank R Fronczek
Judith C Gallucci
Philip W Hemily
Joseph Xiaomin Ho
Hakon Hope
Thomas D Hurley
Hellmut J Juretschke
Daniel R Knighton
James R Knox
Boris Kodess
Jeanette A Krause
Emil B Lobkovsky
Richard E Marsh
Mark Mashuta
Ethan A Merritt
Bruce C Noll
Sean Parkin
Virginia B Pett
C E Pfluger
Frank J Rotella
Timothy J Rydel
George M Sheldrick
Clara B Shoemaker
William C Stallings
Hugo Steinfink
Edwin D Stevens
Robert M Sweet
Thomas C Terwilliger
Diana R Tomchick
Joseph E Wedekind
Roxy B Wilson
D L Worcester

Student Travel

Robert Bau
Paul W. Baures
Helen M Berman
Jeffrey T Bolin
Roger M Burnett
Paul Butler
Martin Caffrey
Connie Chidester
Abraham Clearfield
A W Cordes
Drake S Eggleston
Ulrich Englich
Frank R Fronczek
Judith C Gallucci
Gary L Gilliland
Jane F Griffin
John Richard Helliwell
Joseph Xiaomin Ho
Donald Huddler
Daniel R Knighton
Boris Kodess
Jeanette A Krause

Roger A Lalancette
Catherine L Lawson
Emil B Lobkovsky
Patrick J Loll
Karen Magnus
Ethan A Merritt
Cory Momany
William H Ojala
Helen C Pace
Sean Parkin
A Alan Pinkerton
Marc Lee Pusey
Phil Rudolf
Timothy J Rydel
Giovanna Scapin
George M Sheldrick
Carla Slebodnick
Edward Snell
William C Stallings
Boguslaw Stec
Göran Svensson
Thomas C Terwilliger
Diana R Tomchick
Trixie Wagner
Thomas Webb
Winnie Wong-Ng

Supper

Abraham Clearfield
Carol P Huber
Daniel R Knighton
James R Knox
Masashi Miyano
Sean Parkin
William C Stallings
Thomas C Terwilliger

Trueblood

Helen M Berman
Joel Bernstein
Lee Brammer
Doyle Britton
Donald L D Caspar
Connie Chidester
Abraham Clearfield
A W Cordes
Charles L Coulter
Bryan M Craven
David J Duchamp
J L Flippen-Anderson
Frank R Fronczek
Judith C Gallucci
Gary L Gilliland
Jenny Glusker
Elihu Goldish
Sydney R Hall
Kenneth I Hardcastle
Joseph Xiaomin Ho
Hakon Hope
Carol P Huber
Jeanette A Krause
Allen C Larson
Richard E Marsh
Ethan A Merritt
Bruce C Noll
Marilyn M.Olmstead
Dieter Schwarzenbach
George M Sheldrick
Clara B Shoemaker
William C Stallings
Robert M Sweet
Thomas C Terwilliger
Dale E Tronrud
Ivan Vorontsov
Thomas Webb
Elizabeth A Wood

Warren

Blake Industries Inc.
Abraham Clearfield
John M Cowley
David E Cox
Takeshi Egami
Heinz Jagodzinski
Boris Kodess
A C Lawson
Leonard Muldawer
Richard J Nelmes
Clara B Shoemaker
Lester A Siegel
Robert M Sweet
Thomas C Terwilliger
Thomas Webb
Michael K Wilkinson
Elizabeth A Wood

Wood

S C Abrahams
Lawrence S Bartell
Helen M Berman
Robinson D Burbank
Connie Chidester
Abraham Clearfield
Ann S Cooper
Melinda M Dixon
J. L Flippen-Anderson
Ethan A Merritt
Bruce C Noll
Timothy J Rydel
Clara B Shoemaker
William C Stallings
Thomas C Terwilliger
Norman M Walter
Elizabeth A Wood

Latin American Initiative

Michael Becker
Paul Butler
Martin Caffrey
Abraham Clearfield
William L Duax
David J Duchamp
J. L Flippen-Anderson
Sean Parkin
Clara B Shoemaker
William C Stallings
Robert M Sweet
David H Templeton
Thomas C Terwilliger
Dale E Tronrud

AIP Congressional Fellowship

Paul Butler
Abraham Clearfield
Thomas C Terwilliger

In Memory of

Helen M Berman
(Walter Hamilton)

Joseph A Stanko
(Theron S Piper)

Undesignated

Bruce Hammond Bailey
John D Barnes
Adele L Boskey
Richard G Brennan
Paul Butler
Martin Caffrey
Christopher L Cahill
Abraham Clearfield
Klaus Fleischmann
Richard D Gilardi
Douglas M Ho
Carroll K Johnson
Steven Jordan
Thomas Laube
James W Pflugrath
Timothy J Rydel
Leroy W Schroeder
Arthur J Schultz
James L Smith
Hugo Steinfink
Robert M Stroud
Jeanne Stuckey

JUST ANNOUNCED!

ACA 2006

July 22- 27, 2006

Sheraton Waikiki

Honolulu, Hawaii

And don't forget...

2005 Dues are Due

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Jeffrey Travel Award: Call for Applications

A fund established in memory of George A. Jeffrey will be used to assist an outstanding student to attend the XX Congress of the IUCr to be held in August 2005 in Florence. Applications are invited worldwide. These must be from graduate students in good standing at the time of the Congress.

Applications must include: A one-page letter explaining the student's background and any special circumstances in support of the application. Letters of recommendation from the student's mentor and from one other person familiar with the student's crystallographic abilities and background. The mentor should state the expected date for the student's graduation. A one-page biographical sketch of the student. Copies of any reprints, preprints or abstracts in which the student is an author. An abstract with the student as first author, which has been submitted for the program of the Florence Congress. The student's e-mail address.

The original and two copies of the application (in English) should be mailed to ***B. Craven, Chemistry Dept., Indiana University of Pennsylvania, Indiana, PA 15705, USA.*** Applications must be received no later than April 27, 2005. They will be judged by B. Craven, H. Berman (Rutgers U.) and R. Stewart (Carnegie-Mellon U.). The important criteria will be the scientific excellence of the student's research, the student's financial need and the student's proficiency in English, the official language of the Congress. The Jeffrey Award will cover at least the student's registration fee and the cost of student housing.

Structure Determination by X-Ray Crystallography

Ladd, Mark F.C., Palmer, Rex A., Fourth Illustrated Edition, 2003, hardcover and softcover, SBN: 0-306-47454-9, Kluwer Academic/Plenum Publishers. This edition contains several new chapters and the remainder of the book has been subjected to a very thorough revision and up-dating; computer programs have been supplied with it (on CD) for the purposes of study and problem solving. The earlier editions were very popular and well received: C A Beevers (Foreword, 2nd Edition): ***"…….It is a very straightforward and thorough guide to every aspect of the subject……."*** A M Glazer (Foreword, 4th Edition): ***"……. This Fourth Edition is a substantial and scholarly work that deserves to be on the shelves of anyone wishing to determine crystal structures……."***

International Tables for Crystallography Volume G

Volume G, *Definition and exchange of crystallographic data*, is the latest addition to the International Tables for Crystallography series from the IUCr. It will be available in the spring of 2005 from Springer (hardback, ~550 pp., ISBN1-4020-3138-6, ***www.iucr.org/iucr-top/comm/commit/volg.html***). Edited by S.R. Hall and B. McMahon, this volume describes the standard data exchange and archival file format (the Crystallographic Information File, or CIF) used throughout crystallography. It will be an essential guide and reference for programmers writing crystallographic software and for data managers handling crystal-structure information. It will provide in-depth information vital for small-molecule, inorganic and macromolecular crystallographers, mineralogists, chemists, materials scientists, solid-state physicists and others who wish to record or use the results of a single-crystal or powder diffraction experiments. It will provide the detailed data ontology necessary for data managers in other fields to design interoperable computer applications and databases. An accompanying CD-ROM will contain the dictionaries in machine-readable form as well as a collection of libraries and utility programs.

We are grateful for the support of our corporate members, many of whom took part in the vendor exhibition at the ACA meeting in Chicaco (see pages 24-29). Corporate members not exhibiting in Chicago:

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