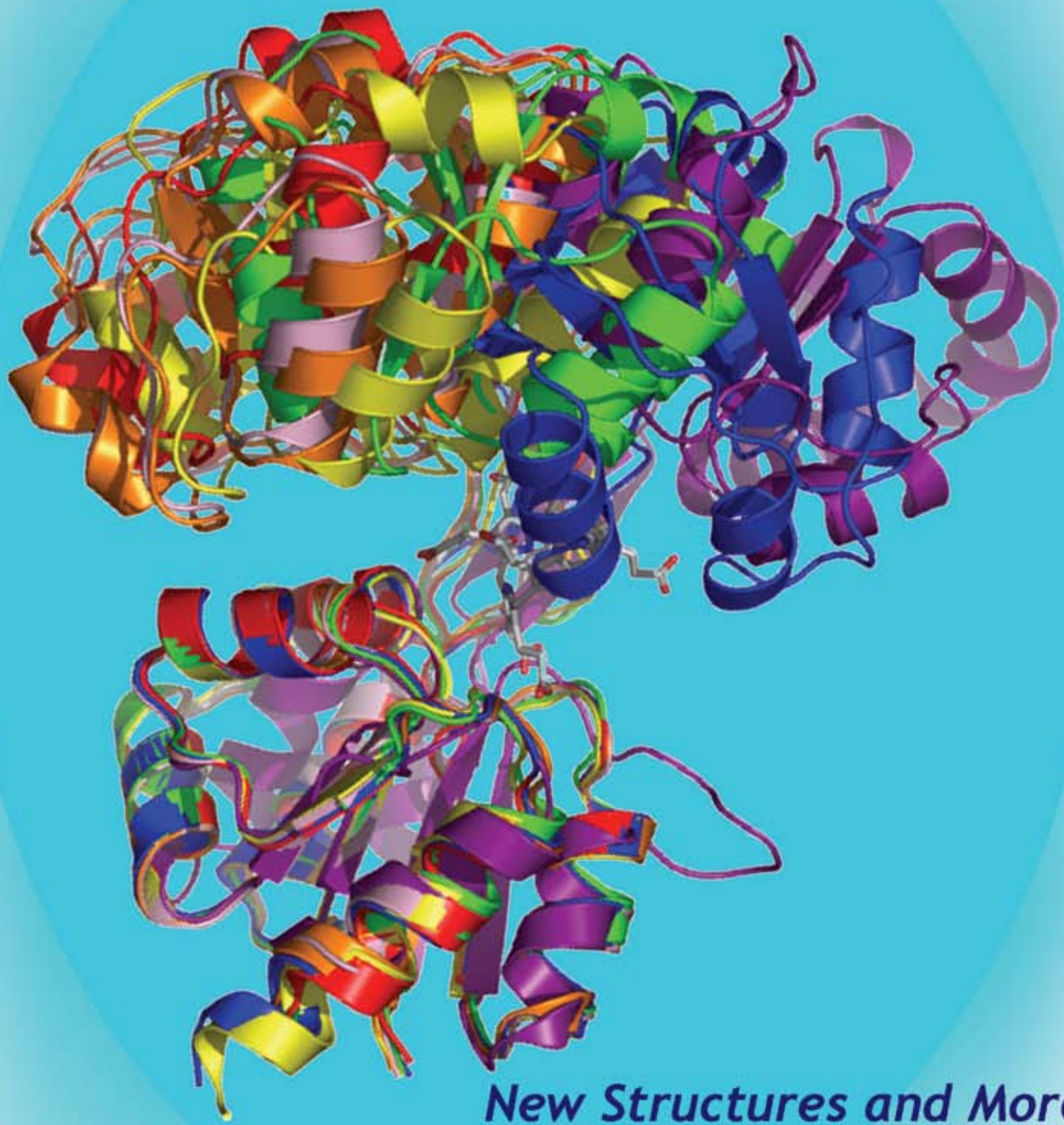
American Crystallographic Association

ACA RefleXions

Number 3
Fall, 2006



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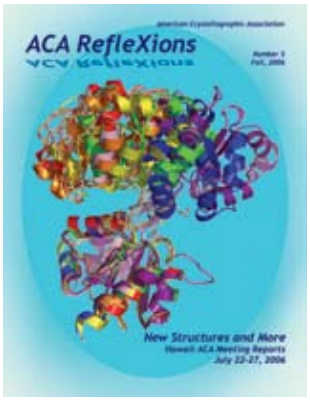
ACA RefleXions

ACA HOME PAGE: www.AmerCrystalAssn.org

Cover: *Image from Heidi Schubert (see p. 15): superposition of 7 uroporphyrinogen III synthase structures.*



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

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THE QUEEN'S AWARDS FOR ENTERPRISE: INTERNATIONAL TRADE 2006

President's Column: Hawaii ACA Meeting a Huge Success

Mahalo (thanks) to all of you who attended, and above all to those who worked hard to make the recently-concluded Hawaii Meeting an outstanding success! The choice of Honolulu as the site of an ACA Meeting was initially a somewhat controversial and risky choice: there were some reservations that it might be too expensive for some members, especially for students and postdocs, and for some vendors and exhibitors (because they have additional expenses such as transportation of hardware). Balanced against those, on the plus side, was the obvious geographical attractiveness of the site, plus the fact that the choice might encourage some scientists from various Pacific Rim countries to attend. The result was, pleasantly, a tremendous success… the Hawaii meeting topped all expectations: it was the second-highest in terms of abstracts and among the highest in terms of attendance in the history of the ACA. Credit must be given to the members of the site-selection committee, who somehow persuaded the hotel management to "bend over backwards" to give special rates to students and postdocs, and who managed to find additional rooms in nearby hotels when it became evident that demand for accommodations was exceeding initial estimates.

Scientifically speaking, the meeting was an outstanding success, with Award Symposia for Helen Berman of Rutgers (Buerger Award), Chuck Majkrzak of NIST (Warren Award), and Carrie Wilmot of Minnesota (Etter Award). These stimulating sessions were coupled with a *Transactions* Symposium on "Smaller Crystals and Larger Molecules with Neutron Diffraction" and pre-meeting Workshops on Synchrotron Image Data, Small Angle Scattering and Computational Methods in Neutron Protein Crystallography. A wide array of scientific sessions on important structural topics, ranging from macromolecular crystallography to small-angle scattering, rounded out the program. There were sessions for all of the broad interests under the ACA umbrella.

Special thanks must go especially to the Program Chair (Judy Kelly), who devoted enormous amounts of energy keeping track of deadlines and designing a workable schedule; the Local Chairs (Charlie Simmons and Karl Seff), who made sure that "on site" arrangements moved along smoothly, and the Program Committe: Simon Billinge, Bryan Chakoumakos, Lachlan Cranswick, Aina Cohen, Chad Haynes, Charles Kissinger, Thomas Koetzle, Jeanette Krause, Paul Langan, Craig Ogata, Allen Oliver and Volker S. Urban who did a terrific job of choosing engaging topics. Thanks is also due the individual chairs of the forty scientific sessions for their selection of interesting speakers. I would also like to thank the various judges of prizes and awards for contributing their time, and above all Marcia Colquhoun, Patricia Coley, Jennifer Curtice and Vanessa Vair for doing the "actual work" involved in running a meeting. The meeting would not have been the success it was without the generosity of the 44 ACA Members who donated a record $8,495 in extra support for student travel in response to an appeal from Bill Duax. Finally, I'd like to thank my fellow ACA Council members for their advice and guidance, especially my predecessor, Louis Delbaere, who was gave an enlightening account of past ACA meetings at the awards dinner.

With that, let me give all of you (participants and exhibitors) one last mahalo for attending. Considering our next meeting, congratulations to Frank Herbstein, the winner of the 2007 Fankuchen Award and to Angelo Gavezzotti, who will receive the 2007 Trueblood Award. They will receive their awards at special symposia organized in their honor at the 2007 meeting in Salt Lake City. Congratulations also to Lisa Randall, who will be presented with the Wood Award at the 2007 meeting (see page 14). See you all in Salt Lake City next year!

Bob Bau

Buerger Award Presented to Helen Berman

The **2006 Martin J. Buerger Award** was presented to **Helen Berman** by ACA President Bob Bau at the Award Symposium organized in her honor at the Hawaii ACA meeting. See page 23 for a report on that symposium. The award recognizes her lifetime work in the pioneering development of information services for the global community of researchers who both produce and use macromolecular structural data. Helen played an influential role in the conception and early development of the Protein Data Bank and pioneered new methodologies in the creation and maintenance of the Nucleic Acid Database. Under her leadership, the Research Collaboratory for Structural Bioinformatics (RCSB) assumed responsibility for the PDB in 1999. Helen is a Board of Governors Professor of Chemistry and Chemical Biology at Rutgers.

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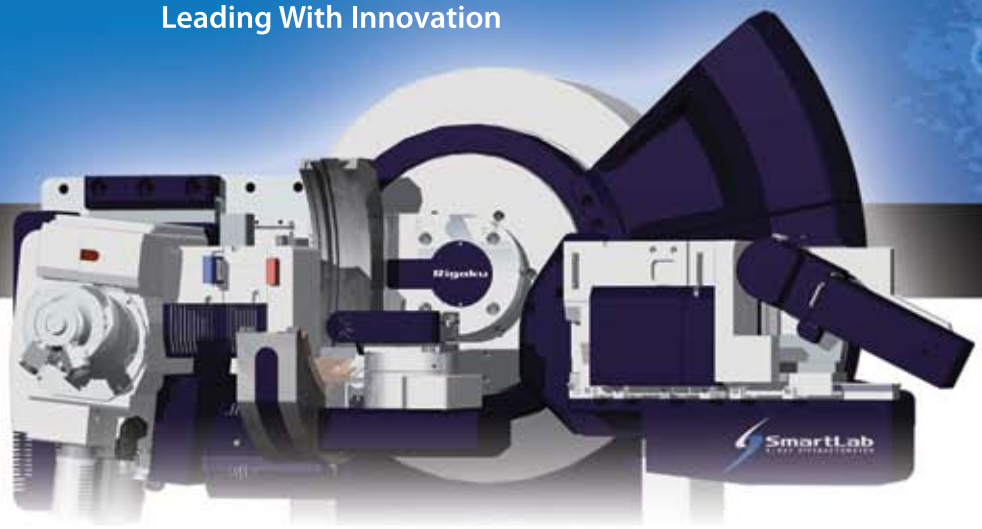

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R&D 100 Awards

2006 Warren Award to Charles Majkrzak

The **Bertran Eugene Warren Award for 2006** was presented by ACA President Bob Bau to **Charles Majkrzak** of the National Institute of Standards and Technology (NIST) at a symposium organized in his honor at the ACA meeting in Hawaii. The award recognizes his seminal contributions to the development of neutron reflectivity and his pioneering work in applying his methods to many challenging problems. In particular, he designed, optimized, and made creative use of supermirror polarizers, integrating them into neutron instruments that attain very low backgrounds and consequently the highest signal-to-noise ratio achieved anywhere.The complete citation is in the summer 2005 issue of the *ACA Newsletter.*

See page 24 for the report on the Warren Award Symposium: ***The Development of Neutron Reflectometry and its Applications to Magnetism, Soft Matter, and Biology.***

Carrie Wilmot Receives the Etter Award

ACA President Bob Bau presented the **2006 Margaret C. Etter Early Career Award** to **Carrie Wilmot** (U. of Minnesota), at a special symposium at the Hawaii ACA meeting (see page 25 for a report on that session). Carrie is a structural biologist who has pioneered exciting new technology that combines macromolecular x-ray crystallography, anaerobic single crystal kinetics and spectroscopy, as well as cryo-capture to identify, stabilize and characterize intermediates in complex oxidation reactions. Her work is exceptional in that she examines biological reactions at the atomic level and develops experimental strategies to prob the complexities of fudamental enzymatic processes. She has recently been named the Director of the Kahlert Structural Biology Laboratory at the University of Minnesota.

Excerpted from the Winter 2005 ACA Newsletter and nomination letters.

Poster Prizes at the 2006 ACA Meeting in Hawaii

Poster judging committees for the prizes were organized and coordinated by Zongchao Jia, Queens U., Ontario.

2006 JCC Poster Prize

The *Journal of Chemical Crystallography* selection committee: **Victor Young** (chair), **Doug Powell, Bruce Noll,** and **Bill Ojala,** chose **M-P164**, a poster by **Christine Beavers**, Univ. of California, Davis: ***Tb_3N @ C_{84} - A Non-IPR isomer of C_{84}*** as the winner of the 2006 JCC Prize.

At left: Christine Beavers with her poster, and at right, Christine receiving the prize from Victor Young. See page 7 for Photo Credit Codes.

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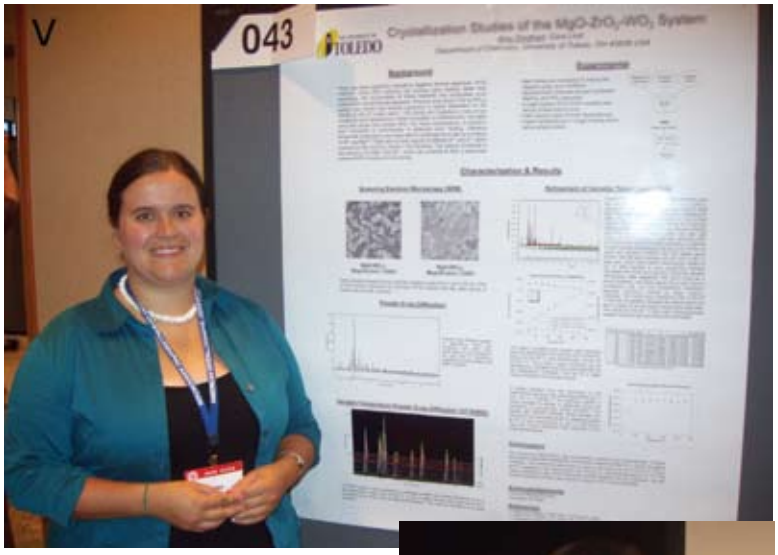


At left above, Teresa De la Mora-Rey with Ed Collins; at right above, Amy Gindhart with her poster S-P043. At right: Justin Chartron with his prize ribbon; below, Nicket Shah.

2006 Pauling Poster Prizes

The Pauling Prize Committee: **Rob McKenna** (chair), **Paul Adams, Vivian Cody, Xinhua Ji, Brian Shilton, Albert Berghuis, Vivian Stojanoff, and George Sheldrick** selected four outstanding posters from the US and one from Canada. The winners were:

Justin Chartron, The Scripps Research Inst., for poster **S-P091**: ***Novel Iron-Sulfur Cluster in Pseudomonas aeroginosa Adenosine Phosphosulfate Reductase*** **(Editor's note: Justin has worked in Dave Stout's lab at Scripps since he was a senior in high school. While interning there as an undergrad he also won an American Physical Sociely prize for best student poster)**;

Nicket Shah, U. Toronto, for **S-P091**: ***Investigating the Catalytic Mechanism of Golgi alpha-mannosidase H: A Possible Target for Cancer Chemotherapy;***

Teresa De la Mora-Rey, U. Minnesota for **S-P043**: ***X-ray Structures of Methylamine Dehydrogenase Reaction Intermediates;***

Amy Gindhart, U. Toledo, for **S-P043**: ***Crystallization Studies of the MgO-ZrO_3-WO_3 System;***

An Honorable Mention went to **Cynthia Sides,** U. Arkansas, for **M-P136**: ***Biophysical Characterization of Collagenase S1 Domain.***

The Canadian Division winner was:

Lisa Pell, (at left), U. Toronto, for poster **S-P097**: ***Mechanism of Hexamerization of gpU, the Tail Terminator Protein from Bacteriophage Lambda.***

Photo of Lisa courtesy of Jeff Deschamps.

Photographs in This Issue of ACA RefleXions

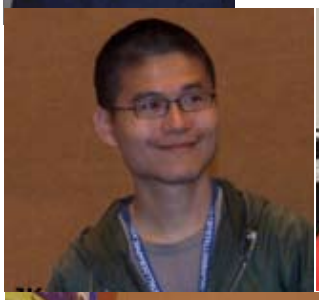
So many people contributed photos for this issues that a code will be used to identify photographers: PF - Paula Fitzgerald; JFA - Judy Flippen-Anderson; JK - Judy Kelly; M - Peter Mueller; JP - Jim Pflugrath; V - Victor Young. Most photos not otherwise identified came from the photo subjects.

Session photographs, pp. 22-49, were taken by student or post-doc attendees at the meeting: Jonathan Cheng, Univ. of Hawaii; Leighton Coates, Los Alamos National Lab; Pierre-Damien Coureux, Brandeis Univ. Stephen D. Drake, Georgetown Univ.; Peter Horanyi, Univ. of Virginia; Sayon Kumalah, Georgetown Univ.; Sergio Martinez-Vargas, Univ. Nacional Autónoma de México; Ekaterina Mironova, A.E. Arbuzov Inst. of Organic and Physical Chemistry, Russia; Nate Schultheiss, Kansas State Univ.; Marvadeen Singh-Wilmot, Univ. of the West Indies, Jamaica; Onome Ugono, Georgetown Univ.; Jiang Yin, Univ. of Alberta, Canada; Minmin Yu, Lawrence Berkeley National Lab; Bin Zhao, Vanderbilt Univ.

2006 IUCr Poster Prize

The IUCr poster judging committee was charged with the unenviable task of choosing one winner from 84 eligible posters, spread over two sessions on Sunday and Monday evenings. The committee, consisting of **Cary Bauer, Elizabeth Goldsmith, Andrej Joachimiak, John Rose, David Rose, Ning Wu** and **Di Xia,** generously committed their time and energy to this process. The number one impression was that the quality of posters was so high that a significant number could be considered at a sufficient level to be award winners. Not having any more specific criteria than the usual categories of science, visual and oral presentations, we chose to take a clue from the sponsor, IUCr, and give additional weight to presentations that included a significant component of technical crystallography – either development of theory or methodology, or unusual application.

After considerable deliberation, the committee chose as the award winner, **Alex Smith**, (at left) U. Illinois, Urbana-Champaign, for his poster **M-P172**: ***Degree-of-freedom-based Methods for Phasing Centrosymmetric Structures from X-ray Diffraction Data***. Members of the committee felt that, in addition to a clever application of triplet analysis to determine phases, the poster was well presented visually, and the presenter was able to use his enthusiasm and knowledge to make the topic understandable to even lowly macromolecular crystallographers.



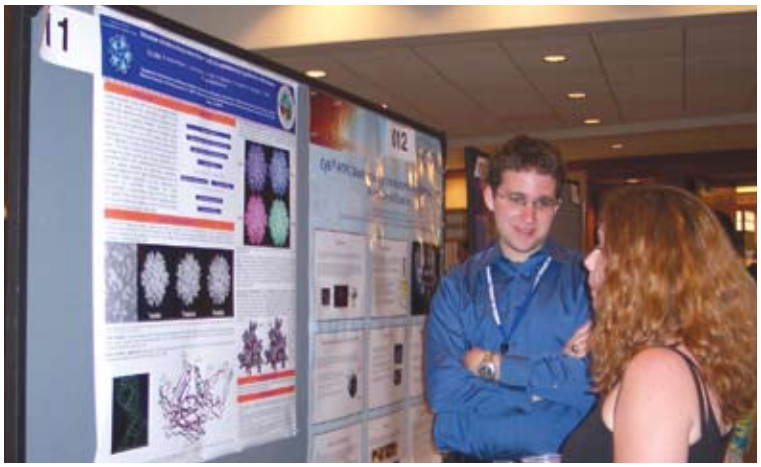
The two very close runners up were: **Shao-Yang Ku** (far left),Hospital for Sick Children and U. Toronto, for **S-P145**: ***Structures of 5-methylthioribose Kinase Phased by ADP-2Ho***, and **Stacy Gates**, U. Toledo, for **M-P112**: ***High-Pressure Diffraction Study of the $A_2M_3O_{12}$ Family***. Both of these presentations were notable for their clarity and organization, in addition to the enthusiasm of the presenters. Congratulations are due to all the poster authors, who provided a very high caliber of science and communication to the meeting. The future of crystallography is, indeed, bright.

David Rose, Chair

Charles W. Pemble, Wake Forest U., with **S-P069**: ***Thioesterase domain of human fatty acid synthase: structural insights into chain-length selectivity.***

2006 Oxford Cryosystems Poster Prize

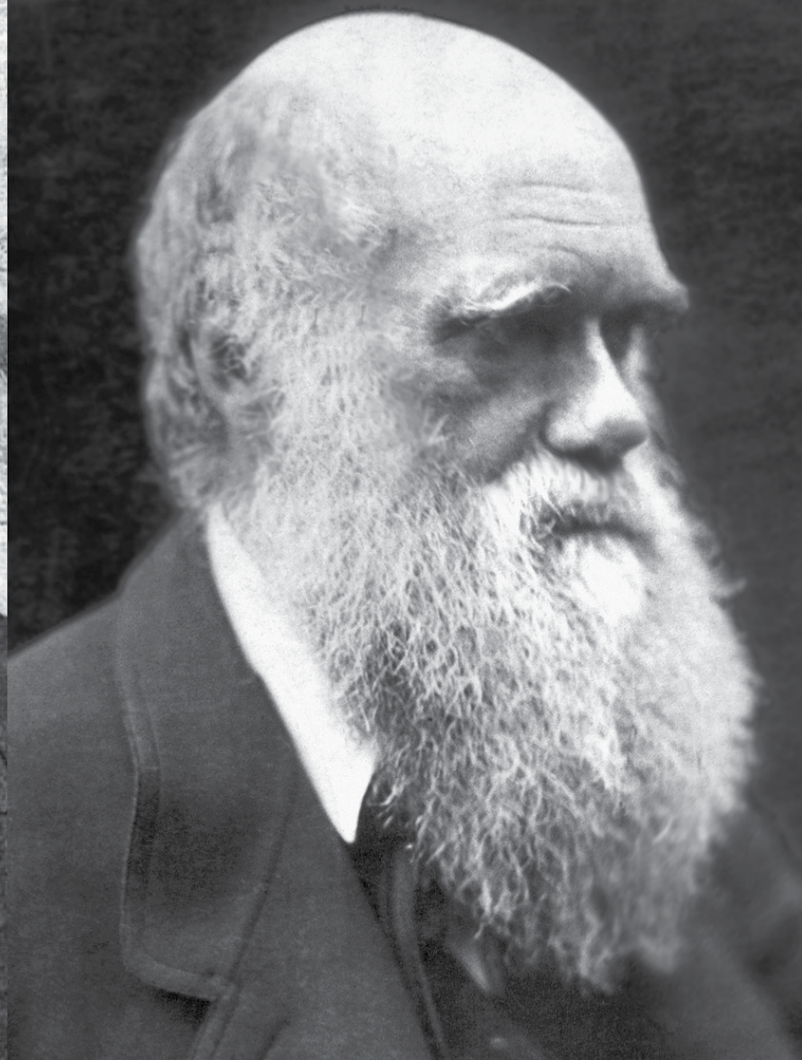
Matt Warkentin, Cornell, shown discussing his poster **T-P047**: ***A New Method for Flash Cooling Crystals*** with B-C Wang, was chosen by the judging committee **Ed Collins** (chair), **B-C Wang, Annie Héroux, Jim Pflugrath, David Garboczi** and **Dan Anderson** to receive the 2006 Oxford Crysystems Poster Prize.



Edward Miller, U. Florida, with his award-winning poster **S-P011**: ***Structure of Adeno-Associated Virus 1 to 8.6 Angstrom Resolution by Cryo-Electron Microscopy.***

RCSB PDB Poster Prize

Zymunt Derewenda chaired the selection committee, and panel members were **Marc Allaire, Charles Weeks, John Badger, Mariusz**, and **Quan Hao**. The posters shown above and at left received 2006 RCSB-PDB Poster Prizes.



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2006 NSSA Prizes

The Neutron Scattering Society of America announced that their **2006 Sustained Research Prize** was awarded to **John Tranquada** at their ACNS meeting in Charles, IL this June. The prize is given to recognize a sustained contribution to a scientific subfield, or subfields, using neutron scattering techniques. Tranquada was cited for his important contributions to the field of high Tc superconductors and for his sustained impact in the field of strongly correlated electron physics. Tranquada and his co-workers conducted many of the critical experiments leading to the discovery of magnetic "stripes" that formed the basis of much of the theoretical work on the relationship of these stripes to superconductivity. John Tranquada is currently the Head of the Neutron Scattering Group at the Department of Energy's Brookhaven National Laboratory (BNL) on Long Island. Among his many activities, he has been heavily involved with designing an instrument providing new capabilities for the forthcoming Spallation Neutron Source at Oak Ridge National Laboratory.

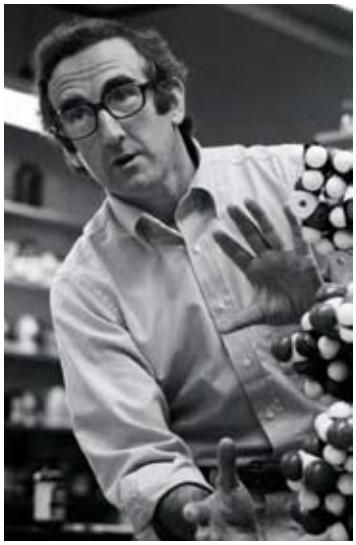
Taner Yildirim, NIST Center for Neutron Research, was awarded the **2006 Science Prize** at the same NSSA meeting in June. This prize is given to recognize a major scientific accomplishment or important scientific contribution within the last 5 years using neutron scattering techniques. Yildirim's study of the important superconductor MgB_2, demonstrated that the high transition temperature is the result of a particularly anharmonic vibration of the atoms that couples strongly to the electronic states in the system, explaining not only the origin of the large value of the superconducting transition temperature, but its pressure dependence as well. Recently Yildirim applied this approach to the problem of hydrogen storage and discovered ways to enhance the uptake of, and the capacity for, hydrogen in a variety of materials including alanates and carbon nanotubes. His results offer the promise of addressing what is widely considered to be the most serious obstacle in the road to a hydrogen-based economy.

Suzanne Velthuis, Secretary, NSSA

Carl Brändén and Dorothy Crowfoot Hodgkin Awards Announced

The Protein Society announced two new awards that will be inaugurated at the 7th European Symposium, May 12-16, 2007, in Stockholm-Uppsala, Sweden. The **Carl Brändén Award**, established by Rigaku Corporation, will be given to an outstanding protein scientist who has also made exceptional contributions in the areas of education and/or service to the science. The **Dorothy Crowfoot Hodgkin Award**, established by Genentech, will be granted in recognition of exceptional contributions in protein science, which profoundly influence our understanding of biology. See **www.proteinsociety.com for more information.**

Brian Matthews to be Editor-in-Chief of Protein Science



The July, 2006 *Protein Society News* announced that **Brian Matthews** will be the next Editor-in-Chief of Protein Science. Mark Hermodson will retire from the post at the end of 2006, but will assist with the transition by serving as an Associate Editor.

Frank Hawthorne Elected to Russian Academy of Sciences

Frank C. Hawthorne, Canada Research Chair in Crystallography and Mineralogy and Distinguished Professor at the Department of Geological Sciences, U. Manitoba, has been elected a Foreign Member of the Russian Academy of Sciences.

Frank has worked extensively on aspects of bond topology of inorganic and mineral structures, and on the role of hydrogen in controlling structural stability and chemical composition. He is well known for espousing the use of spectroscopic and micro-beam analytical techniques in crystallography, particularly where used to derive information on short-range order and chemical variability of light lithophile elements in complex minerals. He has worked extensively on structural relations in borate, sulfate, uranyl, phosphate and aluminofluoride minerals, relating structural connectivity to conditions of crystallization and speciation in nascent aqueous fluids. He is well-known for his work on the crystal chemistry of the amphiboles (a group of rock-forming silicates of great chemical variability), the staurolite-group minerals (important index minerals for metamorphic rocks), the tourmaline-group (and other pegmatite) minerals, and copper-oxysalt minerals. He was first to note the fractal character of oscillatory zoning patterns in minerals, and was involved in the development of high-energy micro-PIXE analysis.

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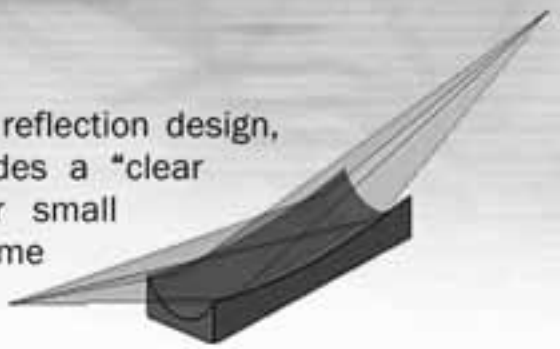

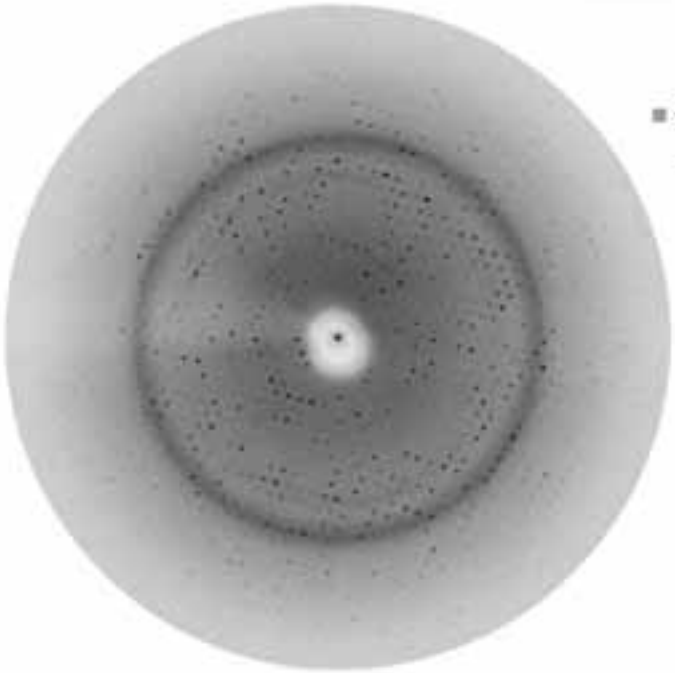

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Data Courtesy of Dr. Andrew GW Leslie
MRC Laboratory of Molecular Biology, Cambridge.

The crystal belongs to space group C222 with cell dimensions a=72.1Å, b=97.4Å, c=191.0Å. Images were collected with an oscillation angle of 0.4°.
The crystal was a thin plate with approximate dimensions 200x75x50 µm³.
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<I>/<sigI> (22.7.-2.43A)	12.1	15
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Call for Patterson Award Nominations

Nominations are solicited for the **2008 A. Lindo Patterson Award**, which will be presented at the annual ACA Meeting in Knoxville, TN. A special symposium will be organized in honor of the recipient and will provide the forum for the Patterson Award Lecture. The Patterson Award, established in 1980, is given every three years *to recognize and encourage outstanding research in the structure of matter by diffraction methods, including significant contributions to the methodology of structure determination and/or innovative application of diffraction methods and/or elucidation of biological, chemical, geological or physical phenomena using new structural information.*

Lindo Patterson's 1934 paper in *Phys. Rev.*: "A Fourier Series Method for the Determination of Components of Interatomic Distances in Crystals," signalled a major step forward in understanding diffraction theory; the Fourier series on F^2, or Patterson function, greatly enabled subsequent structure determination. His section on Fundamental Mathematics in *International Tables, Vol. II* was another important contribution to the community. After working for the government during the war, and then teaching at Bryn Mawr, he moved in 1949 to the Institute for Cancer Research where he worked until his untimely death in 1966. Lindo Patterson was President of ASXRED in 1949 and played an important role in the formation of the ACA in 1950.

Selection committee members are: Frank Fronczek, Paul Langan, George Sheldrick, and Victor Young. Previous winners of the A.L. Patterson Award are: **2005: Alwyn Jones; 2002: Douglas Dorset; 1999: Gerard Bricogne; 1996: Christer E. Nordman; 1993: George Sheldrick; 1990: Michael M. Woolfson; 1987: David and Lieselotte Templeton; 1984: Jerome Karle and Herbert Hauptman; 1981: Wayne A. Hendrickson.**

Please submit nominations to the ACA office in Buffalo (see page 1 for address) no later than May 1, 2007. A nominating letter clearly indicating the accomplishments of the individual is required; additional supporting letters and a *c.v.* for the nominee may be provided but are not required.

Deadline Extended for Etter Early Career Award

The new deadline is November 1, 2006. Nominations should be sent to Marcia Colquhoun **marcia@hwi.buffalo.edu**. For details about the award see the ACA website: **www.AmerCrystalAssn.org**

Apply for ICDD Scholarships Soon!

To encourage promising graduate students to pursue crystallographically oriented research, the International Centre for Diffraction Data has established the **Ludo Frevel Crystallography Scholarship Fund**. 2005 recipients received an award of $2,500. Eight scholorships will be awarded in 2006. See: **www.icdd.com/resources/awards/frevel.htm. NOTE: The Application Deadline is October 31, 2006.**

Art in Crystallography Prize

The Editors are currently accepting entries for the ***Art in Crystallography Prize,*** sponsored by *ACA RefleXions* and the ACA Council. Entries should be sent 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. A photo of the artist would be appreciated but is not required. Winning entries will be posted on the web, and there will also be a display of printed images at the 2007 meeting in Salt Lake City. Prizes will consist of a small monetary award plus a banquet ticket and waiver of registration fees at the meeting. Please contact either of the Editors via email for more details.

AIP Government Fellowships

The American Institute of Physics is accepting applications for an AIP State Department Science Fellowship. Fellows serve one year in Washington, DC with the opportunity to make a personal contribution to U.S. foreign policy while learning how the policy-making process operates. Qualifications include U.S. citizenship; AIP Member Society membership (ACA is a member society); and PhD or equivalent in a physics-related field. Applicants should possess interest or experience in scientific or technical aspects of foreign policy. **Note: the application deadline is Nov. 1st, 2006.** For details on how to apply, please visit **http://www.aip.org/gov/sdf.html** or contact Audrey Leath at **aleath@aip.org**.

New web resource for structures with Z' > 1

Structures with Z' > 1 (*i.e.* more than one molecule in the asymmetric unit) are of intense current interest. As part of an EPSRC funded project, the University of Durham Supramolecular Chemistry Group, run by Jonathan Steed, has developed a web site dedicated to bringing together all the information and publications known about these fascinating systems.

The main feature of the website is an annotated database of structures with Z' > 4, which is updated regularly. Each entry contains the name, chemical formula, journal reference and Cambridge Structural Database (CSD) Refcode (where applicable) in addition to a "Notes" section reporting anything of interest about the packing or composition of the asymmetric unit, as well as links to polymorphs, redeterminations or similar structures. Possible errors in Z' or space group assignment are also highlighted. The structures included in the database are mainly drawn from the CSD; however readers with unpublished high Z' structures are also invited to submit their structures for inclusion in the database. The website also contains a general introduction to the Z' phenomenon as well as a list of useful references concerning all aspects of high Z' structures. For further information please visit **http://www.durham.ac.uk/zprime** or email **zprime@durham.ac.uk**

Kirsty Anderson, University of Durham

Lisa Randall Will Receive the 2007 Wood Award

Lisa Randall, Professor of Theoretical Physics at Harvard University, will receive the **Elizabeth A. Wood Award** at the 2007 ACA Meeting in Salt Lake City next July. The award was established in 1997 to honor the late Betty Wood, (For her obituary and remembrances of Betty see the Spring 2006 *ACA RefleXions,* p 19 and the the article that follows this) Betty was the author of *Crystals and Light*, and *Science From Your Airplane Window.* The Wood Award is given to those who excel in bringing science to the attention of a wider audience.

Lisa's book *Warped Passages: Unraveling the Mysteries of the Universe's Hidden Dimensions,* (HarperCollins Publishers, New York, 2005), has received high praise from critics. Tim Folger, editor of *Best American Science and Nature Writing*, says that *Warped Passages* "gives an engaging and remarkably clear account of how the existence of dimensions beyond the familiar three (or four, if you include time) may resolve a host of cosmic quandaries. The discovery of extra dimensions - and Randall believes there's at least a fair chance that evidence for them might be found within the next few years - would utterly transform our view of the universe."

Lisa was the first tenured woman in the Princeton physics department and the first tenured woman theoretical physicist at MIT and Harvard. She is the winner of an Alfred P. Sloan Foundation Fellowship and a National Science Foundation Young Investigator Award. In 2006, she received the Klopsted Award from the American Society of Physics Teachers and she was featured in *Newsweek's* "Who's Next in 2006" issue. Her research at Harvard concerns the fundamental nature of particles and forces and the relationships among matter's most basic elements. She has worked on a wide variety of models and theories, the most recent of which involve extra dimensions of space. She has also worked on supersymmetry, Standard Model observables, cosmological inflation, baryogenesis, grand unified theories, and aspects of string theory. She has made seminal contributions in all these areas and in autumn, 2004, she was the most cited theoretical physicist of the previous five years.

Elizabeth Wood's Response at the ACA 50th Anniversary Banquet in 2000

Continuing the remembrances of Elizabeth A. Wood,(1912-2006) published in the spring issue of ACA RefleXions, the following is her response in behalf of former presidents which was given at the ACA's 50th Anniversary Banquet July 26, 2000:

First we want to thank the President and her Council for so generously inviting us to be present here. Thanks also for inviting each President to write a letter about "Presidential memories." I understand that Rob Burbank wrote his letter, and then Bill Duax and the Council asked the others to do the same.

As I read through those letters I became aware of two feelings that permeate them. The first is EXCITEMENT. Listen to Charlys Kasper's letter about Dave Harker and John Kasper: "Dave Harker came in a while later and there was great excitement when he saw that John had indeed discovered a possible way out of our impasse." (You have a copy of the rest of this letter.) ***Editor's note: the letters were included in a booklet handed out to banquet attendees. See the summer, 2000 ACA Newsletter, pp 33-45.***

Or Sidney Abrahams where he says, concerning the first meeting at Penn State: "The meeting had an atmosphere of intellectual excitement and confidence that we would meet the challenges of our field."

David Sayre writes "Here I was, looking at a molecule (platinum phthalocyanine) and "seeing" every atom in it! In years the excitement has never worn off."

And, finally, Charles Bugg: "My main impression of crystallography during my brief career is WOW! I feel extremely fortunate to have been in this exciting field during two major revolutions in the field of crystal structure analysis."

The second feeling that permeates those letters is that of COMPANIONSHIP, not only among equal-age participants. X-ray crystallography is such a young science that today's crystallographers have been able to sit at the dinner table with the discoverers of x-ray diffraction in crystals. The Karles' letter speaks of dining with Paul Ewald and Max VonLaue. Max VonLaue, you know, heard Paul Ewald describe x-rays as very short-wavelength electromagnetic radiation. He then wondered whether crystals, described in the 1911 edition of the *Encyclopedia Britannica* as made up of many very small identical units, could act as diffraction gratings for x-rays. He asked his students Friedrich and Knipping to try hitting a crystal with x-rays. It worked and has been working ever since on everything from sodium chloride to complex organic molecules. And the Karles ate dinner with Paul Ewald and Max VonLaue!

That first experiment in x-ray diffraction from a crystal took place in 1912, the year when I was born. (2 minutes for arithmetic)!

The presidents' letters tell especially of companionship in the friendly way in which younger scientists were encouraged. It was Lindo Patterson who invited the Karles to join the table with Paul Ewald and Max VonLaue. In writing of Martin Buerger, Lindo Patterson, David Harker, Jose Donnay, William Zachariasen, and Isidor Fankuchen, the Karles mention that they were very friendly to young people.

Bil Duax remarks "At my first meeting, after my first talk, David Harker spoke a kind word to me. At the time I didn't recognize him and my thesis advisor Norman Baenziger had to tell me that it was the David Harker that I had read about in text books."

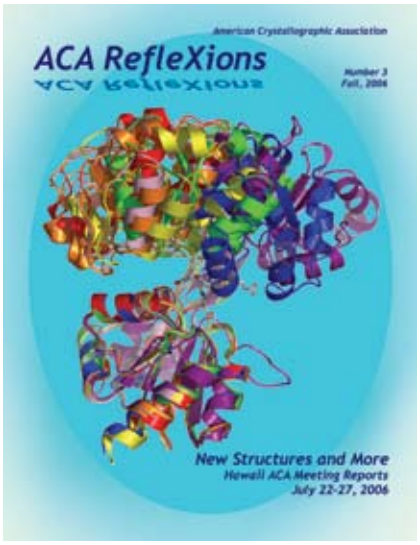
Helen Berman writes "When I gave my first talk I remember how happy I was when Lindo Patterson asked me a question."

David Sayre writes of "the extraordinarily high technical and human quality of this small field of science." Is it a small field? It brings together mineralogists, physicists, mathematicians and biologists. Bill Duax speaks of "the importance of the powerful discipline of crystallography to the infrastructure of science."

So -- I am sure that I am speaking on behalf of the past presidents in hoping that, building on a background of companionship, excitement, and successful advancement, the next 50 years will come somewhere near to approaching the splendid history of the past fifty.

This draft for Betty's talk was supplied by Ann Cooper, a friend, neighbor, and former Bell Labs colleague of Betty Wood. Ann wrote to explain that she found the draft while helping to sort Betty's papers. Ann also wrote, remembering their time as neighbors in the retirement community Applewood Estates, that Betty would often exclaim "I haven't got time!" And this was true, because her days were filled with yoga, French and German conversation groups, play writing and acting, line dancing and recorder playing.

On the Cover: New Structures at the July '06 ACA Meeting



Seven structure superposition of U3S: from **Heidi Schubert.** Heidi solved six new crystal forms of *T. thermophilus* Uroporphyrinogen III Synthase (U3S) generating 10 new independent structures. Her group (Chris Hill laboratory at the University of Utah) had previously solved the human structure, and the RIKEN Structural Genomics/Proteomics Initiative (RSGI) solved two additional structures making 13 structures in all. Only the most dramatically different seven structures are shown in this image. The major difference between structures is that they have just slightly different rotations between their two domains. One of the new structures is a product-bound complex (ligand shown in white). In her talk Heidi used this information to discuss the intricate mechanism of the enzyme.

The tetrapyrrole cofactors support life systems through their essential catalytic functions: Heme (oxidative metabolism and oxygen transport); Chlorophyll (photosynthesis); Siroheme (sulfite and nitrite assimilation); Cobalamin (vitamin B12 - methionine synthesis and methylmalonyl CoA synthesis) and coenzyme F430 (methane production). Their biosynthesis is complicated and requires anywhere from seven to 30 enzymatic reactions involving a variety of catalytic activities including decarboxylation, methylation, metal ion chelation and porphyrin ring oxidation. All five cofactors share their initial four synthetic steps, but at extended points in the pathways cofactor-specific branch points funnel intermediates towards their end product.

The Hill lab has also successfully determined the structure of several tetrapyrrole biosynthetic enzymes in addition to U3S, including human uroporphyrinogen decarboxylase (UroD) and *S. cervisiae* siroheme synthase (Met8p).

(Editor's note: see also the report on the New Structures Session, p. 27)

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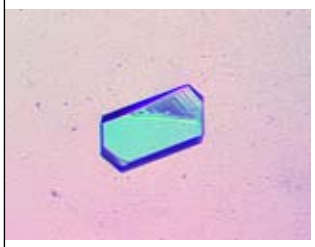

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Evolution / Creationism News from the Editors:

The **ACA Council** has decided that the ACA will join the coalition on "Communicating About Evolution and the Nature of Science." The coalition, coordinated by the ACS in collaboration with the NAS, is made up of about a dozen scientific professional societies. Initially it will conduct a multi-phase research study to provide information that can be used by the participating societies. The objectives of the initiative are: (1) to preempt any dilution of science education in U.S. schools that could potentially result from aggressive efforts to weaken the teaching of evolution or to promote the teaching of Intelligent Design/ Creationism in the science classroom; and (2) to strengthen public support for high-quality science education in U.S. schools.

From *Science*, August 11, 2006: an article on "Public Acceptance of Evolution," by Jon D. Miller of Michigan State U., Eugenie C. Scott of NCSE, and Shinji Okamoto of Kobe U. reviewed the past twenty years of polling in the United States. The authors observe that "After 20 years of public debate, the percentage of U.S. adults accepting the idea of evolution has declined from 45% to 40% and the percentage of adults overtly rejecting evolution declined from 48% to 39%. The percentage of adults who were not sure about evolution increased from 7% in 1985 to 21% in 2005." They also compare the levels of acceptance of evolution in the United States with those in thirty-two European countries and Japan, noting that "Only Turkish adults were less likely to accept the concept of evolution than American adults," and posing the question, "How can we account for this pattern of American reservations about the concept of evolution in the context of broad acceptance in Europe and Japan?" Using a two-group structural equation model, they identifed three relevant factors: the acceptance of fundamentalist religious beliefs, the politicization of science, and the widespread ignorance of biology. "These results should be troubling for science educators at all levels," they warn. "Basic concepts of evolution should be taught in middle school, high school, and college life sciences courses and the growing number of adults who are unsure about these ideas suggests that current science instruction is not effective."

After consultations with representatives of scientific and Christian religious communities, **AAAS** decided to produce a book that could be used by religious educators and others seeking a concise description of the science of evolution and a respectful discussion of the cultural and religious responses to it. *The Evolution Dialogues,* written by Catherine Baker, with input from both scientists and theologians, and edited by James B. Miller, tells why evolution is not a hypothetical idea but rather is the essential framework for modern biology. The book emphasizes the underlying principles of evolution that have continued to stand the test of time: that all species, living and extinct, are related to each other and that the forms of life that populate the Earth have changed over time and continue to change. As the prologue notes, "there are deep misunderstandings about what biological evolution is, what science itself is, and what views people of faith, especially Christians, have applied to their interpretations of the science." With this volume, AAAS seeks to correct some of those misunderstandings." See **www.aaas.org/news/releases/2006/0809evolution.shtml**

Canada: The Summer 2006 issue of *Humanist Perspectives,* which devoted the cover (Brian Alters and Sir William Dawson) and 11 pages to discussing the controversy that arose in the wake of the Social Sciences and Humanities Research Council of Canada's decision not to fund Alters's research project to study the effects of the popularization of "intelligent design" on Canadian students, teachers, parents, administrators, and policymakers. Alters's proposal was rejected, according to a letter from SSHRC, in part because it failed to provide "adequate justification for the assumption ... that the theory of evolution, and not intelligent-design theory, was correct." Hundreds of scientists in Canada and abroad protested what seemed to be SSHRC's crediting "intelligent design" with scientific legitimacy on a par with evolution's. Under pressure, a spokesperson for SSHRC suggested that Alters misunderstood the rejection letter and stated that the rejection of the proposal was not due to SSHRC's having "doubts about the theory of evolution;" subsequently, SSHRC issued a statement acknowledging "the theory of evolution as one of the cornerstones of modern science and of our understanding of the world." But both SSHRC spokespeople and members of the committee that reviewed Alters's proposal were quoted in the press as vaguely expressing doubts about evolution and sympathy for "intelligent design"; these statements have been neither explained nor retracted.

Kansas, from NCSE via the *Washington Post* Associated Press story: With the results of the August 1, 2006, primary election in Kansas, the pendulum swung in favor of the integrity of evolution education. In November 2005, the state board of education voted 6-4 to adopt a set of state science standards that were rewritten, under the tutelage of local "intelligent design" activists, to impugn the scientific status of evolution. Now, no matter who wins in the November general election, two of the members of the board who voted for the standards will be replaced by two new members who have condemned those standards. See also **www.aaas.org/news/releases/2006/0731wichita.shtml/**

Cobb County, Georgia, from NCSE: One result of the Districts 2, 4, & 6 general primary elections for school board candidates is that in the fall all candidates up for election oppose inserting evolution disclaimers in science textbooks. In 2002, the school board voted to require biology textbooks in the Cobb County school district to bear a warning label describing evolution as "a theory, not a fact." A group of local parents filed suit, and in January 2005 a federal district court judge ruled in *Selman v. Cobb County* that the disclaimer was unconstitutional. Following the ruling, the stickers were painstakingly removed, with the aid of putty knives and glue remover, from approximately 34,000 textbooks, during the summer of 2005. Following this, the school board chose to appeal the decision. In May 2006, the appeals court vacated the district court's judgment and remanded the case for further evidential proceedings. The attitudes of the candidates in the present elections suggest that the school board may be willing to settle rather than fight in court.

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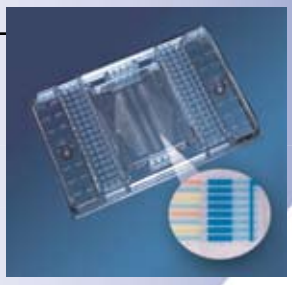

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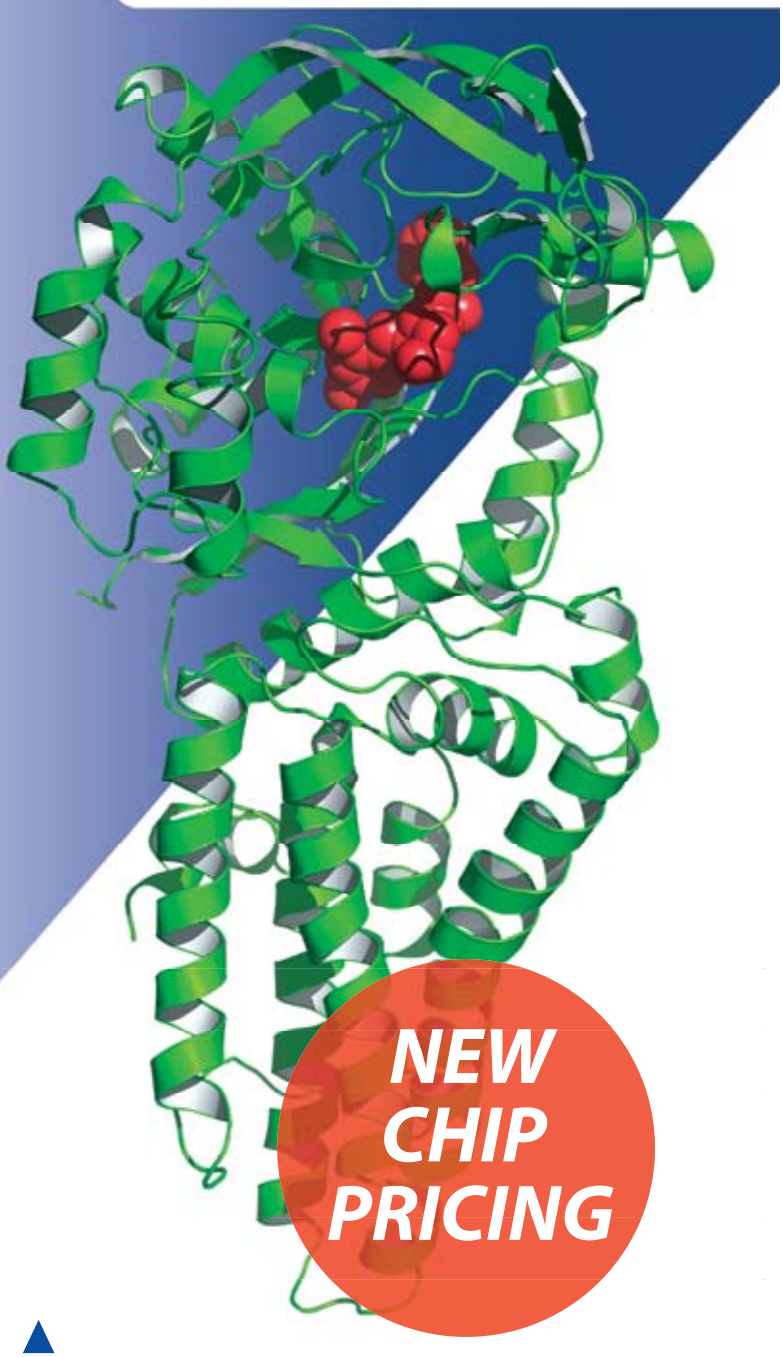

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Highlights of Spring & Summer ACA Council Meetings

The ACA Council met in the spring at ACA headquarters in Buffalo, New York, and then in the summer, meeting several times throughout the annual ACA meeting in Honolulu, Hawaii. Just prior to the start of the annual meeting, there was an all-day council meeting during which ACA business was conducted. On each of the days during the annual meeting, council met with the standing committees and SIG chairs. The standing committees and SIG chairs reported on their activities for the last year and presented their plans for the upcoming year. On the last day of the annual meeting, the session organizers for the 2007 annual meeting met to plan the sessions for the 2007 meeting in Salt Lake City, Utah. Reports from the standing committees and SIG chairs will be posted on the ACA web site.

The 2006 annual meeting in Hawaii was a big success. The meeting attendance was the fourth largest in ACA history, with a total of 963 attendees. Scientifically, the meeting had the second highest number of presentations, with 688 abstracts presented. The very pleasant locale fostered many scientific discussions that lingered well into the evenings.

At council meetings, the business conducted generally includes review of the organization's finances, review of the organization's membership, plans for the annual meetings, the ACA awards, *ACA RefleXions*, the activities and reports from the SIGs and Standing Committees, and other business relevant to the organization. On the financial front, council approved the creation of an *ad hoc* financial review committee to provide oversight and review of the bookkeeping of the ACA accounts at ACA headquarters. This goal of moving to a more centralized accounting system for the ACA that is based at the ACA headquarters in Buffalo, NY, is consistent with the recommendations of the auditors and with the requirements of the IRS. The issue of public policy was discussed and council approved the establishment of an ACA Public Policy Committee to work in collaboration with the AIP Public Policy Committee. Discussed at the council meetings and presented to the membership at the business meeting in Honolulu was the idea of establishing an ACA Fellows program to recognize individuals who have made significant scientific contributions, service to the community, etc. The idea was very well-received by the membership and a motion was approved to set up a committee to explore the creation of the fellows program and to draft a set of guidelines.

The 2007 annual ACA meeting will be held in Salt Lake City, Utah. Two awards will be presented, the Fankuchen Award to Frank Herbstein and the Trueblood Award to Angelo Gavezzotti. Symposia to honor the awardees are being organized.

Lisa Keefe, Secretary

Please note: VISA Alert

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

There is a very useful website maintained by the International Visitors Office of the National Academy of Sciences www7.nationalacademics.org/visas/ that answers most questions pertaining to applications for a visa to attend the ACA meeting in Salt Lake City. It also provides links to State Department websites for further information.

New Name For ACA Website

Please change your bookmarks to our new domain name:

www.AmerCrystalAssn.org

Reminder: Please VOTE!

Please remember to VOTE in ACA Elections! Candidate statements and photos are in the summer ACA RefleXions; the deadline for mailing ballots or electronic voting via the ACA website is November 15th.

From top left: Judith Flippen-Anderson; Judy, Christine Zardecki and Kyle Burkhardt; Carrie Wilmot and Jordi Bella; Next: Charlie Carter, Christine Muchmore and Ethan Merritt; Next: Joe Ferrara and Arwen Pearson; Alan Pinkerton, Howard Einspahr and Frank Fronczek; Bottom left: Rick Bott, David Stout, and David Davies; Gerard Bricogne and Chris Neilson. ***See page 7 for the code identifying contributing photographers.***

By every measure the 2006 ACA Meeting in Hawaii was a huge success. Attendance (963) was among the highest in our history; Montreal, Chicago, and Washington DC were only slightly higher. It was by far the most international of our meetings:25% were non-US crystallographers and 10% of the abstracts were from Pacific Rim Countries. There were 688 presentations, 414 of which were posters. **The *Transactions* Symposium, on "The Future of Neutron Crystallography: Smaller Crystals, Larger (Macro) Molecules"** was a meeting highlight (see page 22), as were the presentations of the **Martin J. Buerger Award** to **Helen Berman**; the **Bertram E. Warren Award** to **Charles Majkrzak**; the **Margaret C. Etter Early Career Award** to **Carrie Wilmot** (pp 3,4) and the Award Symposia organized in their honor (pp 23 - 25). The winter *ACA RefleXions* will carry reports on the workshops, exhibitors, Travel Award winners, and more photos of attendees at various venues.

A great many people contributed to the success of this meeting: Program Chair **Judy Kelly** and Local Co-Chair **Charlie Simmons** are shown at top left. **Karl Seff**, Co-Local Chair, is at left just below them. The registration desk and so many other details were handled by the crew at top right: **Vanessa Vair** (duration-of the meeting assistance); **Jennifer Curtice**, **Patti Coley**, and ACA Director of Administrative Services, **Marcia Colquhoun**. On the right, variously occupying the banquet podium are, from the top: **Charlie Simmons**; ACA President **Bob Bau**; and **Louis Delbaere**, delivering his Past-President Address.

About 205 people went on the excursion at the Polynesian Cultural Center the day after the end of the conference, and **Judy Kelly** and **Charlie Simmons**, at left, were among them.

In back: Arthur Schultz, Tom Koetzle, Leighton Coates; in front: Niburo Niimuro, Lee Brammer, Ray Teller, Bob Bau.

TR.01. Transactions Symposium

In the morning session of the **2006 *Transactions* Symposium, The Future of Neutron Crystallography: Smaller Crystals, Larger (Macro) Molecules,** talks were given by five experts who discussed the present status and future prospects for neutron crystallography.

Robert Bau, USC, led off the symposium with a general overview stressing the unique advantages of neutron diffraction for locating light atoms, including hydrogen, for distinguishing neighboring elements in the periodic table as well as isotopes, especially H and D, and for studying molecular structure. Bau presented some illustrations taken from his own work, for example in locating H atoms with unusual coordination in metal cluster complexes.

Arthur Schultz, ANL, reviewed facilities for time-of-flight Laue single-crystal diffraction at pulsed neutron sources. Existing capabilities such as those at the Argonne Intense Pulsed Neutron Source and the Los Alamos Neutron Science Center in the U.S., and at the ISIS facility in the U.K., will soon be dramatically augmented as facilities come on line at the Oak Ridge Spallation Neutron Source in the U.S. and the Japan Spallation Neutron Source at J-PARC. Single-crystal diffractometers under development at these next-generation spallation sources should allow data collection on much smaller crystals. This is expected to have a major impact, for small-molecule studies and for macromolecular crystallography alike. For SNS, two single-crystal instruments are under development: Topaz for small-molecule work and MaNDi for macromolecular crystallography.

Nobuo Niimura, Ibaraki U., followed Schultz and described the new BIX-P1 diffractometer optimized for macromolecules that is under development at J-PARC in Japan. This instrument promises to have a hundred fold greater flux on sample than the current BIX-type diffractometers installed at the JRR-4 reactor facility.

Lee Brammer, U. Sheffield, reviewed plans for LMX, a Large-Molecule Diffractometer for Supramolecular Chemistry and Biological Structure, which will reside on the new cold neutron target station (TS2) that is under construction at ISIS. Brammer outlined the areas of application envisaged for LMX. These include organometallic chemistry, framework materials, molecular magnetism, fiber diffraction, and protein crystallography.

Leighton Coates concluded the morning session of the symposium. Speaking for himself and his colleagues at the Los Alamos Neutron Science Center, Coates described progress at the Los Alamos Protein Crystallography Station (PCS), which is presently the only instrument in the U.S. that is dedicated to neutron protein crystallography. Results obtained at PCS have demonstrated the power of neutron diffraction for locating H atoms in proteins, even at relatively low resolutions of 2.0 – 2.5 Å. This type of information can be crucial, for example, in elucidating enzyme mechanisms. Several PCS users spoke in the afternoon session of the symposium and described their recent results in more detail.

Tom Koetzle and Ray Teller

Paul Langan, Dean Myles, Chris Dealwis, Wolfram Saenger, Alberto Podjarny and Gerry Bunick.

The afternoon session of the *Transactions* Symposium continued to reflect trends in neutron crystallography by showing how advances in instrumentation and sample preparation methods are pushing the limits of macromolecular structure determination. It was only three years ago that this area was featured in a previous *Transactions* Symposium in Kentucky and the early afternoon scientific presentations clearly demonstrated a large shift in capability. The structures of aldose reductase, xylose isomerase and dihydrofolate reductase presented in this session are some of the largest ever studied by neutron crystallography and they were achieved by using crystals as small as 0.15mm.[3] In the first talk by **Wolfram Saenger**, Free U. of Berlin, it became clear how these exciting results have raised the bar of community expectation.

Wolfram began his talk by illustrating the extraordinary power of neutrons for elucidating the details of hydrogen bonding in cyclodextrins, then explained why neutron diffraction will be his radiation of choice for tackling a much larger problem, the Mn_4Ca architecture in the large membrane bound photosystem II complex. The power of neutron diffraction for visualizing hydrogen atoms in enzymes in order to understand their mechanism was impressively illustrated in the following talks by **Alberto Podjarny**, IGBMC, on aldose reductase and **Gerry Bunick**, U. Tennessee, on xylose isomerase. Alberto and Gerry collected their diffraction

data at LADI and the PCS, respectively. The PCS was also used in determining the structure of dihydrofolate reductase, presented by **Chris Dealwis**, U. Tennessee. However, the emphasis of this study was not on mechanism but rather on understanding the factors responsible for enhanced binding of the anticancer drug methotrexate.

Dean Myles, Oak Ridge National Laboratory, described the MAcromolecular Neutron DIffraction beam line MANDI being planned for the next generation spallation neutron source at ORNL. New beam lines on next generation sources, in combination with deuteration support laboratories being developed at Los Alamos, Oak Ridge and Grenoble, will continue to push neutron macromolecular crystallography towards smaller samples and larger and more complex problems.

In the last talk by **David Langs**, Hauptman-Woodward Inst., the possibility of solving the phase problem from neutron data alone was outlined. The basis of the method is to use the difference between H and D atoms in neutron diffraction to generate isomorphous differences, which in combination with the computational methods pioneered by Herbert Hautpman lead to a direct solution of the phase problem. This approach places neutron diffraction in an equal footing with x-ray diffraction for a complete and independent structure determination.

Paul Langan and Alberto Podjarny

AW.01: Martin J. Buerger Award Symposium on Structural Biology from All Angles

The symposium opened with the award presentation to **Helen Berman** by ACA President Robert Bau (see p. 3). Helen then took us on a "Personal Journey Through Crystallographic Space" that began with her early structural research in the 1960s. She detailed her involvement in the grass-roots community action that became the fledgling Protein Data Bank (PDB) at Brookhaven National Laboratory, through the founding and development of the Nucleic Acid Database (NDB), to the transition of the PDB from Brookhaven to the Research Collaboratory for Structural Bioinformatics (RCSB). Her entertaining and informative presentation described how her structural research interests inspired her dream of creating an enabling resource for the structural biology community of macromolecular structure data, and how this vision became a reality.

The other symposium speakers further illustrated Helen's diverse research interests. **Paula Fitzgerald** (Merck) and **John Westbrook** (RCSB PDB) described the development of the macromolecular Crystallographic Information File (mmCIF) dictionary. Paula humorously covered the early trials and tribulations involved in creating the mmCIF dictionary. In 1990, the IUCr formed a working group to expand the CIF dictionary with data items describing macromolecular crystallographic experiments, a group that Helen later joined. At several workshops, versions of the dictionary were presented to the community for review, and then revised based upon feedback. A consensus emerged for a data model in 1994. John followed up by describing how the mmCIF dictionary technology has evolved and has been employed in the data infrastructure of the NDB and PDB databases and other related data resources.

In the next presentation, **Stephen Neidle** (U. of London) described the evolution of his studies on drug-nucleic acid structures over a 30-year period. DNA-binding drugs were already used as cytotoxics, anti-parasitics and anti-bacterials in the 1970s, but little was known about their structures, especially how they actually bound to DNA. He described some of the early work he did in collaboration with Helen on DNA complexed with compounds such as proflavine-dCpG (an intercalation complex with a highly structured water network). The desire to be able to do systematic studies of nucleic acid complexes motivated Helen's development of the NDB as a tool for examining correlations between structures, such as looking at the minor groove in all nucleic acid-drug complexes. He finished up his presentation describing some of his current work on sequence-selective and structure-selective complexes.

Jordi Bella, Bob Bau, Paula Fitzgerald, Helen Berman, Judith Flippen-Anderson, Stephen Burley, Stephen Neidle, Wah Chiu and John Westbrook.

Jordi Bella (U. Manchester) then discussed the challenges of collagen crystallography. In addition to the more common sources (skin, bones, and teeth), collagen has recently been discovered in bacteria and viruses. From 1955-1981, most collagen models were developed using fiber diffraction. The fiber work could not provide detailed descriptions of hydrogen bonding between triplets, what role the water played in the structure, whether the helical symmetry changed along the polymer, or whether there were interruptions in the sequence. As a post doctoral student in Helen's lab, Jordi succeeded in filling in the gaps left by these fiber studies through 'single' crystal studies, and was able to start developing some structural models for hydrogen bonding in collagen structures.

Wah Chiu (Baylor College of Medicine), described efforts to set up an archiving infrastructure for cryo-electron microscopy (cryo-EM) density and structures. As the number of cryo-EM structures continues to increase, there will be a number of challenges involved in archiving the data – similar to the development of the mmCIF dictionary and the NDB and PDB databases. The structures involved are very large, on the order of 2.2 M Daltons, and generate

AW.01: Buerger Symposium, con't gigabytes of data describing millions of atoms. He described the cryo-EM methodologies used to solve three different structures for which data has been collected at three different resolutions: a transmembrane structure with data to 9.5Å, a cryo-EM study of epsilon 15 phage at 7Å, and a 4.2Å map of GroEL that approached a crystallographic map in its structural details.

The session closed with a presentation by **Stephen Burley** (CSO SGX Pharmaceuticals and Chair of the PDB and wwPDB Advisory Committees) on fragment based drug discovery in which he described the SGX approach to developing drug targets for cancer therapeutics. They consider the problem to be a challenge in protein engineering and have developed a procedure that exploits crystallographic screening to detect, visualize and identify small ligands that bind to the target protein. Each ligand that is tested has chemical 'handles' that can potentially bind to the protein. They are soaked into pre-formed crystals and the bound fragment is identified from the shape of the electron density map. He illustrated the success of the procedure with examples of compounds being developed for use against drug resistant mutants such as Gleevec-resistant BCR-ABL.

Judy Flippen-Anderson

Sunil Sinha, Larry Passell, Phillipe Mangin, Sushil Satija, Norm Berk, Mike Kent, Duncan Mcgillivray, Chuck Majkrzak, Hartmut Zabel, Roger Pynn, Susan Kreuger, Jaerk Majewski, Mark Foster, Mike Fitzsimmons. and Julie Borchers.

AW.02: The Warren Award Symposium

The Bertram E. Warren Award Symposium on the ***Development of Neutron Reflectometry and its Applications to Magnetism, Soft Matter and Biology*** was organized by **Julie Borchers** (NIST) and **Brian Toby** (Argonne) to honor **Charles F. Majkrzak** of the NIST Center for Neutron Research (see page 5 for his award presentation and citation).

The talks covered a wide range of fields extending from studies of polymer thin films and magnetic multilayers to biomimetic films, but all 12 showcased the advances and achievements in neutron reflectivity that have occurred in the last decades emphasizing, in particular, the key role that Chuck (as he is known to his many friends and colleagues) has played in many of these activities. As the opening speaker, he touched on the high points of his 25 year career, focusing primarily on the pioneering work he has done in polarized neutron reflectometery. Along with many other valued contributions, this included an extended collaboration with Norm Berk, also at the NIST Center for Neutron Research, on the development of exact methods for phase determination from dynamical specular reflectivity data. By employing different buried reference interfaces, Chuck and Norm were able to solve what had previously been regarded as an intractable problem and demonstrate that specular reflectivity data could be directly inverted to obtain a unique scattering length density profile.

The rest of the morning session was devoted to applications of reflectivity in soft matter and biology. This is an area where the ability to enhance neutron contrast by replacing hydrogen with deuterium makes neutron reflectivity a uniquely sensitive technique for the study of polymeric and biologically relevant films. **Tom Russell** (U. Mass, Amherst) described some intriguing examples of the ordering and orienting of block copolymer nanostructures. **Mark Foster** (U. of Akron) described his recent work with Chuck and others on the investigation of interfacial structure in tethered polymer systems in which it was shown that by combining specular neutron reflectivity with off-specular x-ray reflectivity on the same system it was possible to obtain complementary information about both out-of-plane and in-plane film structure. **Mike Kent** (SANDIA) then reviewed his combined neutron and x-ray reflectivity studies of the binding of diphtheria and other toxins to lipid monolayers after which **Susan Krueger** (NIST) gave a summary of her studies of neutron reflectivity from biological membrane films. Susan emphasized her work with Chuck on the development of instrumentation, sample environment and measurement protocols that extend neutron reflectivity measurements into the 10-8 reflectivity range: a level of sensitivity at which it becomes possible to obtain Angstrom-scale information about membrane structure along the axis perpendicular to the membrane plane. **Jarek Majewski** (Los Alamos) concluded with a review of some of the recent neutron and x-ray studies of bio-membranes that he and his collaborators had done.

AW.02, con't. The afternoon session was devoted to applications in magnetism, reflectivity theory, instrumentation and future directions in neutron reflectivity. Regarding magnetism, **Hartmut Zabel** (Rühr Universität) described how polarized neutron reflectivity could be used to explore magnetic- and spintronic nanostructures. **Mike Fitzsimmons** (Los Alamos) discussed exchange bias in Co/FeF_2 films explaining how the combination of neutron and x-ray reflectivity studies provides a unique insight into the microscopic origin of positive and negative exchange bias in this system. **Phillipe Mangin** (Saclay) then presented some highlights of his studies of the magnetic behavior of rare earth thin films.

Norm Berk (NIST) gave a highly informative summary of his long-standing collaboration with Chuck on the theoretical and practical aspects of phase inversion. A description of an exciting new development on the instrumentation front by **Roger Pynn** (Indiana U.) followed. Neutron reflectivity has thus far been very successful in providing insights into the out-of-plane structures of films but intensity limitations have made it extemely difficult to explore in-plane structures with neutrons. Roger outlined an approach to the study of off- specular scattering in which spin echo is employed to tag each neutron trajectory, thus making it possible to use very wide angle beams and overcome, at least in part, the intensity disadvantage of neutrons. **Sunil Sinha** (U.C. San Diego) concluded the session by reviewing his elegant theoretical and experimental investigations of specular and off-specular scattering both with neutrons and x-rays.

One theme that was apparent throughout the day was the influence Chuck Majkrzak had on these investigations. A number of speakers alluded to the fact that they had started their work on polarized neutron reflectivity only after their visits to NIST to collaborate with him. Another frequent feature which always brought a chuckle was the showing of Chuck Majkrzak's photographs with his trademark checkered shirt by several speakers! The excellent quality of the speakers and of course the informal atmosphere of Hawaii made this symposium a truly memorable affair.

Sushil Satija and Larry Passell

Tom Russell, Chuck Majkrzak, (wearing the trademark checkered shirt), and Mark Foster.

May Tsai, Carrie Wilmot, Eric Brown, S.Zoe Fisher, Thang Chiu and Arwen Pearson.

AW.03: Etter Early Career Award Symposium

The Margaret C. Etter Early Career Award Symposium was sponsored by the YSSIG and the GIG, and organized by Anna Gardberg and Arwen Pearson. It was a special treat for me to preside as the award was given to my postdoctoral mentor, **Carrie Wilmot**, U. Minnesota (see presentation details, p 5). Peggy Etter spent many years at U. Minnesota and **Bill Gleason** (another Minnesotan) gave a brief talk about his personal memories of Peggy. Carrie's award lecture focused on her exciting work in structural enzymology, combining single crystal spectroscopy and x-ray crystallography to gain detailed insight into enzyme catalysis and mechanism.The spirit of the Etter Early Career Award, and the other awards established to honor Peggy's memory, is to encourage and reward young and early career scientists. In that spirit, the first three talks were by graduate students, and the last by a postdoctoral fellow.

S. Zoe Fisher, U. Florida, presented the effects of site-directed mutations on water structure in the active site of human carbonic anhydrase II. She combined crystallography and enzymology to give insights into the role of individual water molecules in shuttling protons out of the active site. **Eric Brown**, U. Iowa, presented a talk combining crystallographic studies of two new ferredoxin structures with computational methods to predict ferredoxin reduction potentials and likely binding modes to partner dioxygenases. **May Tsai**, U. Toronto, then told us about her work on the adenylosuccinate lyase family of enzymes. Using a mutant she was able to obtain a substrate complex that revealed the residues involved in substrate binding and catalysis. The final talk was by **Thang Chiu**, NIDDK, NIH. Thang presented the results of his research on protein folding. He studied a 35 amino acid fragment of villin which folds extremely fast. His detailed experiments revealed the role that individual residues played as the fragment folded and he also reported mutations that resulted in ultra-fast folding.

Arwen Pearson

SP.01: The Undergraduate Research Showcase

Greg Ferrence, Katsuo Katagiri, Meg Fasulo, Kathy Kantardjieff, and Marilyn Olmstead.

Katherine Kantardjieff, speaking about the state of education in crystallography, stated that she has seen more interest in crystallography by students at Cal State U., Fullerton over the past few years. However, generally there are fewer people going into the field and it is becoming even more rare to find crystallography in the curriculum before graduate school. According to her surveys, the introductions to crystallography usually found in physical chemistry texts have been removed in the newest editions. Hence there is less exposure and consequently less interest in the field by new students. Even students who do become interested study crystallography for a comparatively short amount of time. Many biology and chemistry students that use crystallographic analysis end up treating it as a "black-box." They put their samples in and take the results from the computer as golden. If they understood the process of crystallography: how x-rays diffract off different atoms and how to read the patterns generated, they would be better equipped to deal with incorrect structure identifications which arise often from today's software. The audience was obviously sympathetic to these ideas, and some complained about the ineptitude of their graduate students and even of some professional crystallographers. Gregory Ferrence commented that his students have caught obviously incorrect structures in professional crystallographic publications. To address these problems, Katherine and her colleagues are proposing inclusion of crystallography in more texts even down to the junior high level. They have already seen new releases of introductory chemistry texts including crystallography, so it looks like things are moving in the right direction.

Gregory Ferrence, Illinois State U., dealt with remote access to crystallographic analysis. Through a network of schools that have instruments, students in locations without such hardware can use the instruments remotely. The students prepare and send out the crystal samples, and once the samples are in place they can control the experiment and analysis through the internet. This allows for more students to access the necessary tools, and will hopefully lead to more competent crystallographers in the future.

Meg Fasulo, Kansas State U.,(on the right) was presented with the AIP Undergraduate Research Prize by Katerine Kantardjieff. Meg gave an impressive talk on co-crystals. Co-crystallization is a method of changing the solubility and thermal stability of a particular substance, without changing its chemical action. For example a pharmaceutical drug can be made shelf-stable and easily delivered upon administration by making it into a co-crystal. A hydrogen atom on one end of the drug is hydrogen bonded to a ligand. She compared this to creating a salt out of the drug in question, where a hydrogen is replaced by a metal or a radical that acts like a metal. While creating a salt can also change solubility and thermal stability, in her study it also changed the chemical effect in about 46% of the cases, while a co-crystal only changed the chemical effect in about 5% of the cases. The talk focused on how to better create and identify co-crystals by using different ligands to form them.

Kazuo Katagiri, an undergraduate from Boston College, gave a very detailed analysis of range docking programs. These programs help to visualize how a drug will dock to a host receptor or how different ligands and proteins fit together. Each program has its advantages for particular applications, and Kazuo explored which program is best for each.

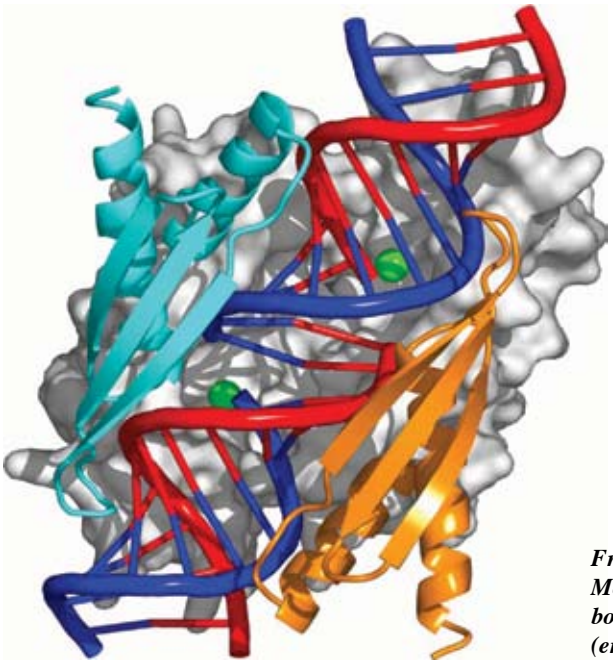
Jeremy Kowalczyk (an AIP student reporter)

Photos courtesy of Laurel Reitfort.

1.01: New Structures:

Chris Jurgenson, David Garboczi, Stephan Ginell, Heidi L. Schubert, Tommi White, Xinhua Ji, Bomina Yu, Uhn Soo Cho.

A diverse range of topics was covered, starting with **Shaodong Dai** (National Jewish Medical and Research Center, Denver) who described the steps in the reduction of the thioredoxin active site disulfide by the 4Fe-4S cluster of ferredoxin/thioredoxin reductase. Complexes of the enzyme with either ferredoxin or thioredoxin revealed details of the reactions that together use reducing equivalents produced through photosynthesis to reduce the disulfide of thioredoxin. **Heidi Schubert** (U.Utah) described the flexibility of uroporphyrinogen III synthase alone and in complex with product and how flexibility relates to its cyclization of a linear tetrapyrrole, a required step for making heme (***see On the Cover, p. 15***). **Xinhua Ji** (National Cancer Institute) described studies on the RNase III of bacteria, which is an excellent model for the mammalian Dicer, that plays a key role in the mechanism of RNA interference. He demonstrated that two metal ions are involved in cleaving double-stranded RNA (***see image***).



Tommi White (U.Missouri-Columbia) described the proline dehydrogenase from *Thermus thermophilus* that is involved in converting proline to glutamate and that generates reactive oxygen species in a proline-dependent manner. Interestingly, in humans this enzyme is coded at the mapped location for some mutations that lead to increased susceptibility for schizophrenia. **Chris Jurgenson** (Cornell) provided insight into the function of the octameric thiamin biosynthetic enzyme Thi4. **Bomina Yu** (Columbia U.) presented structures of the DNA/RNA repair enzyme AlkB complexed with nucleotide substrates and products. **Uhn Soo Cho** (U. Washington) showed how the PhoQ sensor operates by binding to at least three metal ions to neutralize the charged area on PhoQ, enabling membrane binding. The significant dimer interface change in metal-free conditions suggests that a conformational change may be involved in the signaling process. **Jeremiah Joseph** (Scripps) summarized the structural genomics of the SARS virus and the unexpectedly high number of unique protein folds that have been revealed. **Alex Wlodawe**r (NCI) ended the session with his description of the fascinating domain-swapped anti-viral protein griffithsin. Its dimeric organization of lectin domains seem to be central to its picomolar activity against HIV.

David Garboczi and Steve Ginell

From Xinhua Ji: Ribonuclease III (RNaseIII), a symmetric dicing machine. Members of the RNase III family are double-stranded (ds) RNA-specific endoribonucleases, characterized by a signature motif in their endonuclease domains (endoNDs) and a 2-nucleotide (nt) 3' overhang in their products. While Dicer is currently the focus of intense interest, bacterial RNase III serves as a paradigm for the entire family. The bacterial enzyme functions as a dimer; each subunit contains an endoND and a dsRNA-binding domain (dsRBD). The highly symmetric structure of an RNase III-product complex (Gan et al., Cell 124, (2006), 355-366) reveals that the dimerization of the two endoNDs is essential for the formation of two RNA cleavage sites precisely arranged to produce the characteristic 2-nt 3' overhang of dsRNA products. The two endoNDs are shown as molecular surface; the two dsRBDs are illustrated as ribbon diagrams (helices as spirals, ß-strands as arrows, and loops as pipes) and colored in cyan and orange, respectively. The Mg^{+2} ions are indicated with green spheres; the two RNA strands are shown as tubes in blue and red, respectively.

Photo courtesy of Laurel Reitfort.

1.02: Computational Methods: Macromolecular Structure Solution and Refinement

This session was intended to present the latest and most exciting new developments in the area of macromolecular structure determination methods. Of special interest were methods designed to increase automation in high-throughput environments.

Charles Weeks, Nicholas Furnham, Ralf Grosse-Kunstleve, Pavel Afonine, Min Yao, Ethan Merritt, Serge Cohen.

Ethan Merritt (U. Washington) gave an outstandingly clear overview of the TLSMD algorithm. In recent years TLS (Translation-Libration-Screw) refinement of macromolecules has become increasingly popular. For this, the macromolecules under refinement have to be subdivided into TLS groups. Determining the optimal grouping manually is often difficult and time consuming. TLSMD is designed to automate this task. TLS groups obtained via TLSMD often lower R-factors and help in the analysis of large scale motions and the analysis of local flexibility.

Nicholas Furnham (Cambridge, UK) presented his work on RAPPER which automates exploration of conformational space. Given a preliminary starting model (e.g. a molecular replacement model), RAPPER is used in combination with a refinement program to iteratively rebuild and refine the model. The rebuilding procedure includes systematic sampling of conformational space using a combination of grid searches and a rotamer library. RAPPER has proven particularly useful for the modeling of low resolution structures via ensembles.

The emphasis of **Charles Weeks'** (Hauptman Woodward MRI) presentation was the adaption of the BnP program system to a grid computing environment. BnP includes procedures for data normalization, direct-methods substructure solution, phase refinement and solvent flattening. The substructure solution step is parallelized using grid computing technology. A web-based portal is available to make BnP accessible from anywhere on the Internet without requiring local installation.

Min Yao (Hokkaido U., Japan) presented another approach to automated rebuilding and refinement. The LAFIRE (Local-correlation-coefficient-based Automatic FItting for REfinement) program completes partial models and rebuilds fragments with a poor match to the electron density. The rebuilding algorithms take information from the Ramachandran plot into account. In addition, side chains of selected amino acids are automatically flipped based on an analysis of B-factors. The building and rebuilding algorithms are fully integrated with refinement programs.

Serge Cohen (NKI, The Netherlands) introduced new developments of the popular ARP/wARP package for automatic model building. ARP/wARP builds atomic protein models given an electron density map and sequence information. Mature model building algorithms include main chain building, assignment of polypeptides to the given sequence, use of NCS information if available, and building of side chains. These capabilities are enhanced by novel empirical likelihood estimates, post-processing with a multi-layer neural network, and a new loop building feature. In combination with a new development version of the REFMAC refinement program ARP/wARP is capable of building models that could not be solved automatically before.

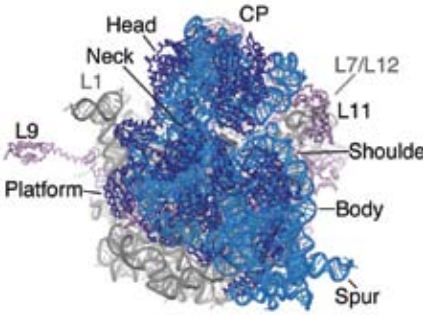
Pavel Afonine (Lawrence Berkeley National Lab) gave an overview of the current state of the phenix.refine program, which is under active development as the structure refinement component of the Phenix project, a collaboration of five groups in the US and the UK. Phenix.refine achieves a high degree of automation through a tight integration of all key components required for a refinement engine. Supported are simulated annealing, TLS, grouped B-factor, and rigid body refinement along with individual coordinate and B-factor refinement. Combined x-ray and neutron refinement is under development.

Ralf Grosse-Kunstleve and Tom Terwilliger

1.03: Large Macromolecular Assemblies

Brian Wimberley, Maria Borovinskaya, Patricia Grob, Timm Maier, David Bushnell, Simon Jenni, Thomas Earnest, John Miao.

Maria Borovinskaya (LBNL and UC-Berkeley) began with the crystal structure of the intact *Escherichia coli* ribosome at a resolution of 3.5 Å. The significant improvement in resolution over earlier whole-ribosome structures allowed a much more precise definition of the proteins and of the functionally important subunit interface region.



The structure of intact Escherichia coli 70S ribosome at 3.5 Å resolution. View from the solvent side of the small subunit. 16S rRNA and proteins in the small subunit are light blue and dark blue, respectively. 23S rRNA and in the large subunit are gray and magenta, respectively. Reprinted from B.S. Schuwirth, M.A. Borovinskaya, C.W. Hau, W. Zhang, A. Vila-Sanjurjo, J.M. Holton, J.H.D. Cate, Science, (2005) 310, 827-834, with permission from Science © 2005.

In addition, comparison of the two ribosomes in the asymmetric unit (comprising almost 5 MDa) suggested how a rotation of the head of the small subunit may help move the transfer RNA and messenger RNA substrates through the subunit interface, a process known as translocation. A conserved RNA feature of the small subunit was proposed to act as a barrier or gate during translocation. She also discussed recent structures of the ribosome bound to spectinomycin and a few aminoglycosides, which are inhibitors of translocation. The spectinomycin structure supported the proposal that this antibiotic blocks translocation by freezing the small subunit head in a particular orientation, while the aminoglycosides were found to bind in two sites, one previously described on the small subunit, and an interesting new site on the large subunit.

RNA synthesis requires RNA polymerase II, which has varying numbers of subunits in various organisms. The structure of the twelve-subunit (~0.5 Mdalton) RNA polymerase II from yeast was presented by **David Bushnell** (Stanford), revealing the basis for a nucleotide entry that is significantly different from that of single subunit enzymes. The size and complexity of this enzyme, along with its relatively low abundance in the cell, have made this a challenging project. Studies of this complex in a number of functional states are proceeding.

The application of new computational methods to analyze conformational variation in large complexes which have been imaged by cryo-EM was described by **Patricia Grob** (UC-Berkeley). This approach uses covariance information from 3D reconstructions and variance maps. For human TFIID concerted domain motions were seen that reshaped the DNA-binding cavity. Human RNA polymerase II moves in a more complicated manner that is being interpreted using the crystallographic information available.

Simon Jenni and **Timm Maier** (ETH - Zurich) presented crystal structures of large assemblies that perform the *de novo* synthesis of fatty acids. Most prokaryotes have a type II fatty acid synthesis system in which each of the steps of fatty acid synthesis is catalyzed by a distinct and small enzyme. In contrast, in mammals and in fungi, homologs of these small prokaryotic enzymes are concatenated into just one or two polypeptide chains that aggregate to form a single large assembly known as fatty acid synthase (FAS). Despite their nearly identical functions, these fungal and mammalian type I FASs are surprisingly different in architecture. The fungal FAS is a 2.6 MDa $\alpha 6\beta 6$ assembly, while the mammalian FAS is a 540 kDa $\alpha 2$ dimer. The new crystal structures reveal that the fungal assembly is a stout 260 x 230 Å barrel with two reaction chambers, each containing three sets of active sites separated by distances up to 130 Å. In contrast, the mammalian FAS is X-shaped, with overall dimensions of 210 x 180 x 90 Å. Despite the moderate resolution of these structures, Simon and Timm were able to place all but one of the catalytic domains in electron density, using previously determined structures of homologous type II enzymes. Also unassigned in both structures (due to disorder) is the acyl carrier protein (ACP) domain, which is covalently attached to the growing fatty acid. These results have important implications for the design of experiments to probe reaction mechanisms, which must involve large movements of the ACP domains and the reaction chamber of the mammalian FAS.

Brian Wimberly (on right) presenting Simon Jenni with a Margaret C. Etter Student Lecturer Award.

The use of coherent x-ray imaging coupled with the oversampling of the speckle pattern produced when non-periodic targets are illuminated with coherent radiation was discussed by **John Miao** (UCLA). He described the underlying theory of this method, which derives from the work of David Sayre in the 1950's, and presented examples of the way the method is used to image objects at high-resolution. An extension of the method offers an approach to investigating the subcellular localization of multi-protein complexes in cells at 5-10 nm resolution and in cells too thick for cryo-EM. The potential use of fourth-generation light sources to study non-crystallizable molecules was discussed as a future possible source of structural information, and this idea generated a great amount of discussion among the attendees and speakers.

Thomas Earnest and Brian Wimberly

1.04 Membrane Proteins

In recent years, the membrane protein structure session has proven to be one of the most exciting, and this year's collection of speakers was the best yet. The talks covered technical advances, structural complexities, transient membrane protein complexes, and a number of beautiful, large, complex membrane protein structures.

David Shultis, Heather Pinkett, Hartmut Luecke, Ling Qin, David Stout, Susan Buchanan, Marc Allaire, Raquel Lieberman, Susanna Tornroth-Horsefield, Lothar Esser, and Pia Wadsten.

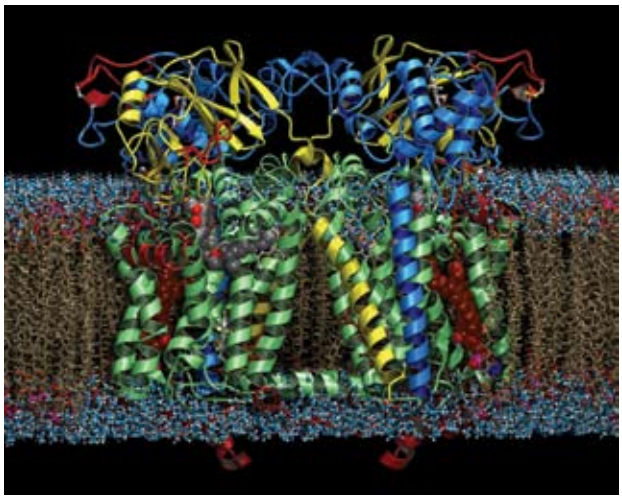
The first half of the session focused on membrane protein transporters. **Susanna Tornroth-Horsefield** opened the session with her presentation on the structure of a plant aquaporin, one of the first eukaryotic membrane proteins to be produced heterologously (in *Pichia pastoris*) for structural studies. Comparison of the aquaporin SoPIP2:1 in closed and open conformations shows how pH, phosphorylation, and Ca^{2+} may regulate the passage of water. Susanna's colleague, **Pia Wadsten**, gave an interesting talk about the use of bicontinuous lipid systems for membrane protein crystallization. While the lipidic cubic phase imposes technical difficulties due to its high viscosity, Pia presented data showing that a 'sponge' phase (analogous to a melted cubic phase) is more fluid, can be used in hanging drop crystallization trials, and contains larger aqueous pores. This technique may be useful for crystallizing membrane proteins with large hydrophilic domains, *e.g.* photosynthetic reaction center crystals from *Rhodobacter sphaeroides* diffracted to 2.1Å.

Talks by **David Shultis** and **Marc Allaire** described transient membrane protein complexes between (related) outer membrane transporters for vitamin B_{12} and iron chelates and an inner membrane protein, TonB, that transduces energy required for transport of the small molecules. In both cases, a periplasmic portion of TonB was co-crystallized with the outer membrane transporter and bound substrate. Each transporter contains a sequence of 5 residues near its N-terminus that adopts a beta strand conformation in the presence of TonB, using a strand pairing mechanism to extend an existing TonB beta sheet. These structures lay the foundation for understanding this complicated transport process involving the entire cell envelope.

Heather Pinkett ended the transport half of the session with a new high resolution bacterial ABC transporter structure. Her protein comes from *Haemophilus influenzae*, and is thought to transport heme. It will be interesting to learn more about this protein and how heme is transported. A poster by **Christopher Reyes, T-P201**, described two structures of MsbA, a multidrug efflux ABC transporter, in the presence of ADP-Vanadate and (substrate) LPS, and in complex with a clinical multidrug resistance modulator. From all of these structures, it's becoming clearer how hydrolysis of ATP is coupled to substrate transport.

In the second half of the session, **Raquel Lieberman** talked about her method for producing well ordered crystals of particulate methane monooxygenase, a complex trimeric membrane protein structure that functions to convert methane to methanol. While the structure itself is fascinating, Raquel chose to describe her unusual methods for obtaining good crystals. In particular, the batch of protein mattered, as did using undecyl maltoside instead of the more common dodecyl maltoside. She also found that only aged PEG solutions produced good crystals, and her best crystals were obtained from phase-separated drops. Unusual methods, but it's hard to argue about a 300 kDa complex that diffracts to 2.8Å. Similarly, **David Stout** told us about experiments to improve bacterial transhydrogenase crystals, with the important message that care must be taken to obtain fully functional material. Choice of detergent and placement of histidine tags are important parameters too.

Hartmut Luecke described a sensory rhodopsin structure from *Anabaena* at 1.9Å resolution. His group has also determined the structure of its soluble transducer, which is tetrameric and is thought to interact with a single copy of the 7-TM sensory rhodopsin. **Lin Qin** described the 2.1Å structure of a 2-subunit bacterial cytochrome oxidase (catalytic core) and determined a number of lipid binding sites which appear to be conserved among cytochrome oxidases from a variety of sources. Finally, **Lothar Esser** described the 2.4Å structure of a four-subunit bacterial bc1 complex (although no density is observed for subunit four). The asymmetric unit is very large, containing three dimers each of cytochrome b, cytochrome c1, and the iron sulphur protein. Density was observed for inhibitors, lipids, and detergent molecules. Although bacterial respiratory enzymes have proven more difficult to crystallize than their more complicated mitochondrial cousins, they offer unique views of the simplest way to establish the proton gradient necessary for ATP synthesis.



From Lothar Esser: The crystal structure of Rhodobacter Sphaeroides bc1 embedded in a modeled lipid bilayer. The surrounding membrane was computer generated; the membrane protein was placed into it, and overlapping lipids were removed.

1.04: Membrane Proteins, con't. From expressing enough functional protein, to purifying in the best detergents, and encouraging well ordered crystals to grow, membrane proteins and their complexes present some of the biggest challenges in protein crystallography. The progress made in determining membrane protein structures continues to amaze and inspire us.

Susan Buchanan

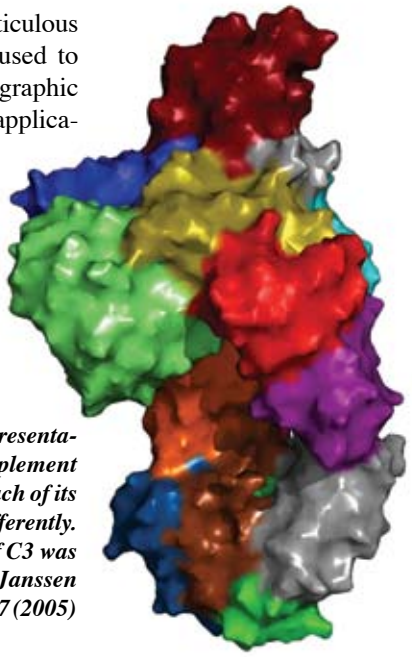
1.05: Difficult Structures

Tina Izard, Charlie Carter, Bert Janssen, Gerard Bricogne, Zbyszek Dauter, Poul Nissen, Wim Hol.

Zbyszek Dauter opened with the provocative title: "How to Make the Structure Difficult," identifying four degrees of difficulty. "The most difficult structures are those that are never solved. There are very, very hard structures, those requiring novel solutions to new problems." He cited Perutz's solution of the hemoglobin structure as the most difficult of these. "Then, there are those hard structures that require a modicum of thought to arrive at a solution. Finally, there are all the rest, the vast majority of structures solved almost without thinking." Dauter proceeded to give examples from his own experience of how we often litter our path with speed bumps that we might well avoid. First of these examples was mis-indexing, and especially the choice of an incorrect centroid for the detector face. This common mistake can hide behind perfectly fine statistics, until one discovers that the structure is more stubborn than it ought to be. In this same cautionary tale, he had mistakenly chosen the wrong space group, and reinforced this choice by keeping Friedel mates separate in order to extract the anomalous signal. The error here was hidden by the fact that the polar space group, $P4_3$, permitted a shift along c* without an alarming increase in R_{merge}. Other examples involved missing a large real cell in a crystal with near-crystallographic translation symmetry that reduced the intensities of two-thirds of the reflections, and a case where new scanning software had inadvertently reversed the hand of the indexing, giving an enantiomeric electron density in which the ß-carbon atoms poked out in the wrong directions.

Gerard Bricogne presented significant advances in the BUSTER refinement program. BUSTER v 1.0 implemented much of the maximum likelihood paradigm envisioned in his fundamental papers, but because it was interfaced to the TNT minimizer, there were important details left to be developed. These included much of the formulation of derivatives and elliptical likelihoods that were to make BUSTER into a superior refinement program, and not simply a program for calculating optimal electron density maps at a given state of the model. Many of the deficiencies in v 1.0 have now been corrected and tested. These include a new algorithm for scaling the model to the data, new parameterization of rigid bodies, improved geometric regularization with new, NOE-like restraints, and derivatives based on the full variance/covariance matrices, new occupancy refinement, and a new implementation of the user interface. Bricogne described in some detail work done by Meindert Lamish on the *E. coli* polymerase III, including the spectacular improvement in the rate of convergence, as well as the final statistics. This splendid structure was presented by John Kuryian at the ASBMB meeting in April, a presentation in which Kuryian spoke of the significant new detail brought out in the structure by the BUSTER refinements.

Bert Janssen next described a lovely new structure of complement component C3 from the humoral immune defense system. Key to the success of this difficult structure was a meticulous pruning of the masks used to impose non- crystallographic symmetry and repeated applications of PHASER.



Accessible surface representation of human complement component C3 with each of its 13 domains colored differently. The x-ray structure of C3 was initially published by Janssen et al. in Nature, Vol. 437 (2005) 505-511.

Wim Hol summarized many difficulties from his experience with the RNA editing proteins from trypanosomal plastids and from Vibrio cholera. Solutions to an idiosyncratic array of problems encountered in such a comprehensive program, including cross-linking crystals, aggressive processing of minor Se sites, extreme care in controlling the crystallization pH, and mutation of the molecular surface. Perhaps his most important message was the imagination and persistence necessary to find the best-diffracting crystals. He made such efforts seem almost second nature, though they require the most nimble-witted and ingenious co-workers.

Poul Nissen followed with descriptions of problems associated with solving representatives of the energy-coupled Ca^{++} pump from sarcoplasmic reticulum, a membrane protein.

(cont'd on page 34)

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1.05: Difficult Structures, cont'd. Poul stressed the necessity of finding the appropriate detergent and of paying close attention to vapor phase equilibria involving glycerol in the drop containing the protein. The crystals were thin plates, and necessitated careful design of the mounting loops to avoid distortion and loss of resolution. The crystals were cooled first to an ambient temperature above freezing before cryocooling, in order to preserve the crystals' inherent 2.5 Å resolution. SIRAS phases had to be blurred by a B-factor of 100 before they could be successfully merged with SAD phases. Finally, Nissen stressed the usefulness of isomorphous difference Fourier maps during model building in identifying structural changes and problem areas.

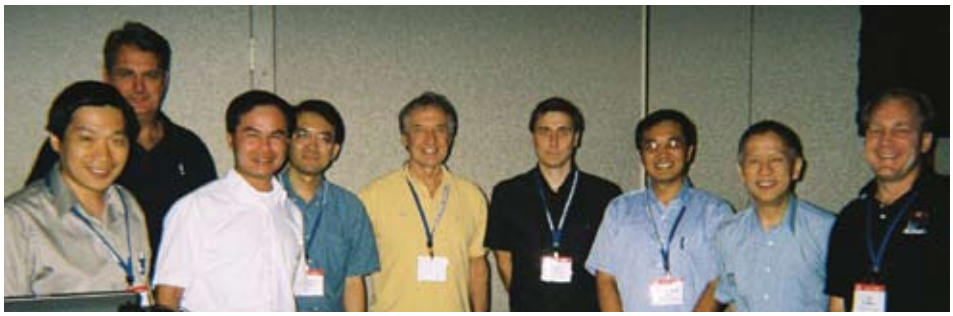
The final talk of the afternoon was given by **Michael Sawaya** on a severe example of diffraction anisotropy. He centered his talk around pseudo-precession photographs, which several other authors also used in their presentations. The problem he addressed was to balance the loss of data in the low resolution directions against the corruption due to scaling the data in the high-resolution directions. The solution he described had an appealing logic to it, and was instructive to follow.

As Dauter pointed out in his opening remarks, "difficult structures" continue to provide the staging ground for advances in our field, so this session remains a perennial favorite.

Charlie Carter and Tina Izard

1.06: Proteins Involved in Host Immune System and Pathogen Interactions

The NIH focus on biological warfare, the sequencing of bacterial genomes and the recent increase in the rate at which structures are determined has resulted in a wealth of information about host:pathogen interactions. In this session, a small cross section of this explosion was presented. **Ian Wilson** began the session with a description of how the host recognizes pathogen-associated molecular patterns. CD1 proteins bind to lipids and derivatives that are not present in host membranes. The difficulties associated with crystallizing a lipid binding protein with a single ligand bound were described. **David Davies** thanked Ian for an excellent introduction and followed by describing another component of the host innate immune system, Toll-like receptor 3. This leucine-rich repeat (LRR) protein binds to dsRNA, and early studies suggest that the ligand does not bind in the horseshoe as previously described for other LRR proteins. **Jia-Huai Wang** showed the structure of Dscam, a component of insect innate immune systems, that also appears to play an important role in the neurophysiology of the fly. **Jim Sacchettini** fought back for the pathogens by describing the *Mycobacterium tuberculosis* structural biology consortium and their recent successes. He finished by inviting everyone to help with this critical world health problem. Four excellent posters were picked for short oral presentations. **Hongmin Li** began with a description of a ternary complex of T cell receptor (TCR), class I



Peter Sun, Jim Sacchatini, Sean Juo, Chung-I Chang, Ian Wilson, Rene Jorgensen, Hongmin Li, Jia-Huai Wang, and Ed Collins.

MHC and superantigen. Unexpected superantigen binding to the TCR alpha chains were implicated in the structures. **Chung-I Chang** described the structure of trachela cytotoxin, another trigger of insect innate immune system. **Rene Jorgensen** made excellent strides into the enzymatic mechanism of action of a mono-ADP-ribosylating toxin from *Pseudomonas* trapping structures in various phases of action. **Sean Juo** described the structure of a decoy protein from cytomegalovirus, m157, which keeps CMV-infected cells from being recognized for killing by natural killer cells of the immune system. The structures suggest that the protein binds NK inhibitory receptors in a manner different from how they normally bind class I MHC.

Ed Collins and Peter Sun

Contributors to This Issue

Christer Aakeröy, Dan Anderson, Eddy Arnold, Bob Bau, Maria Borovinskaya, Jim Britten, Susan Buchanan, Chris Cahill, Branton Campbell, Charlie Carter, Vivian Cody, Ed Collins, Ann Cooper, Bob Cudney, Valentina Degryareva, Olga Degtyareva, Louis Delbaere, Jeff Deschamps, Bill Duax, Thomas Earnest, Lothar Esser, Paul Fenter, Greg Ferrence, Paula Fitzgerald, Frank Fronczek, David Garboczi, Steve Ginell, Ana González, Ralf Grosse-Kunstleve, Alla Gustchina, Frank Hawthorne, Peter Horanyi, Lynne Howell, Tina Izard, Bert Janssen, Xinhua Ji, Zongchao Jia, Jack Johnson, Katherine Kantardjieff, Lisa Keefe, Judy Kelly, Herb Klei, Tom Koetzle, John Konnert, Jeremy Kowalczyk, David Londono, Joe Luft, Mike McDonough, Alex McPherson, Peter Mueller, Ann Mulichak, Larry Passell, Arwen Pearson, Alan Pinkerton, Jim Pflugrath, Thomas Proffen, Andrew Prongay, Laurel Reitfort, David Rose, Alec Sandy, Amy Sarjeant, Sushil Satrija, Heidi Schubert, Karl Seff, Nick Silvaggi, Charlie Simmons, Ward Smith, Peter Sun, Yuh-Ju Sun, Bob Sweet, Ray Teller, Tom Terwilliger, Hiro Tsruta, Volker Urban, Suzanne Velthuis, Brian Wimberley, Victor Young, Christine Zardecki, Elizabeth Zhurova.

Bostjan Kobe, Mariusz Jaskolski, Chwan-Deng Hsiao, Marta Martinez-Julvez, Zihe Rao, Maria Nyblom, Pedro Matias, Xiao-Dong Su, Joao Barbosa, Zongchao Jia.

1.07: International Macromolecular Advances

Presentations were drawn from the contributed abstracts; the speakers were from nine countries on five continents and many of the talks described the results of international collaborations.

There were descriptions of high-throughput functional genomics programs in Canada (**Zongchao Jia**), Brazil (**Joao Barbosa**), and Australia (**Bostjan Kobe**). Barbosa described high throughput analysis of a protein with a new fold but unknown function. Kobe's group is focused on structures related to plant disease resistance, and Jia discussed a new conformation for Calmodulin in a complex with calcieurin. **Xiao-Dong Su** (China) described a medium-sized, high-efficiency, low-cost platform of structural genomics studies. The structure of a gigantic all helical ferritin (iron binding protein) from a hyperthermophilic archaeon that encapsulates up to 17 Fe(II) ions per monomer was described by **Pedro Matias** (Portugal). The structure of a bifunctional L-asparaginase from plants is being studied to determine details of its mechanism of action. The study is expected to contribute to a better understanding of how asparaginases can be used as drugs against leukemia (**Marius Jaskolski**, Poland). **Maria Nyblom** (Sweden) described techniques for purifying solublizing and analyzing membrane proteins. The structure of a human DNA binding protein complexed with a 16 base pair duplex containing a promoter sequence that provided new insight into the winged helix/forkhead class of DNA binding proteins was presented by **David Hsiao** (Taiwan). The mechanism of cofactor binding to flavodoxin inferred from a comparrison of apo and halo forms of the enzyme was described by **Marta Martinez–Julvez** (Spain) with only 24 hours advanced notice that she would be speaking. Martinez-Juliez put together her power-point presentation overnight.

Zihe Rao, the newly appointed President of Tinghua University, Beijing, said he was pleased to return to an ACA meeting after 23 years. He has been directing major research laboratories in Beijing and tried to summarize what he had been doing for the past 23 years with an emphasis on his critically important work on the SARS virus.

Bill Duax

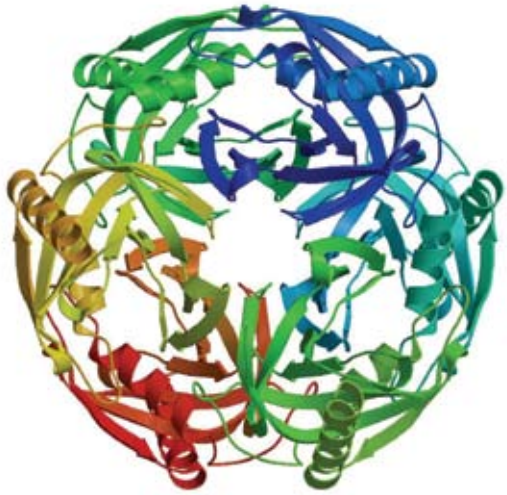
BIO-MAC Posters:

An impressive number and range of posters related to biomacro molecules – 248 out of the 414 total – were presented. As these posters were visited, this traditional English rhyme came to mind: "something old, something new, something borrowed, something blue, and a silver sixpence in your shoe", which is used to note what a bride might bring to her wedding to ensure a happy marriage. Apparently, the spirit behind this rhyme can also be applied to ensure vibrant poster sessions. Old was represented by HIV-1 protease: **S-P197** ***Molecular Dynamics reveals the Binding Conformation of HIV Protease with the MAC4A Binding Domain of GAG*** by **Philip Martin** *et al.* and **T-P030** ***Structural Insights into the Evolution of Drug Resistance in HIV-1 Protease*** by **Holly Heaslet** *et al.* New was represented by these and more novel structures: **T-P070** ***Crystal Structure of the Human TRPV2 Channel Ankyrin Repeat Domain*** by **Clare McCleverty** *et al.* and **T-P100** ***Structure of Homolog of F420-0: Glutamyl Ligase from Archaeoglobus filgidus Reveals a Novel Fold*** by **Bogi Nocek** *et al.* Borrowed folds and catalytic mechanisms were also abundant: **T-P068** ***Crystal Structure of SO1698 Protein from Shewanella oneidensis, a putative Aspartic Endopeptidase*** by **Jerzy Osipiuk** *et al.*, **T-P076** ***Crystal Structure of a S. aureus Pathogenicity Island Protein, EAR*** by **Ramachandraiah Gosu** *et al.*, **T-P081** ***Crystal Structure of Imidazolonepropionase from Argobacterium tumefaciens at 1.87 Å Resolution*** by **Rajiv Tyagi** *et al.*, and **T-P114** ***Structure of a Novel Acyltransferase*** by **Rick Bott** *et al.* Even blue was represented by multi-copper laccase from the blue oxidase family of enzymes: **T-P082** ***Crystallization and Preliminary X-ray Analysis of the Laccase from Coriolopsis gallica*** by **Eugenio De la Mora** *et al.* As far as the sixpence in the shoe (a symbol of future prosperity) is concerned, you'll just have to use your imagination. A summary of conversations with several presenters follows. It is far from comprehensive and was certainly limited more by time than interest.

Two posters, which described novel structures that emphasize the importance of iron as a cofactor in enzyme catalyzed oxidation reactions, highlighted work on two different enzyme classifications: non-heme Fe(II) and heme dioxygenases. In **T-P048**, **Arwen Pearson** et al. revealed a prokaryotic cytochrome P460 that possesses a novel c-type cytochrome fold comprised predominantly of ß-sheet. The structure confirms earlier biochemical reports that the heme is covalently attached to the protein through two cysteine residues and a unique heme meso-carbon crosslink to a lysine residue.**T-P078** by **Yang Zhang** *et al.* described the structures of two dioxygenase enzymes involved in one of the first tryptophan-based quinolate biosynthetic pathways found in prokaryotes. One of the dioxygenases, tryptophan dioxygenase, is a heme-containing **cont'd p. 36**

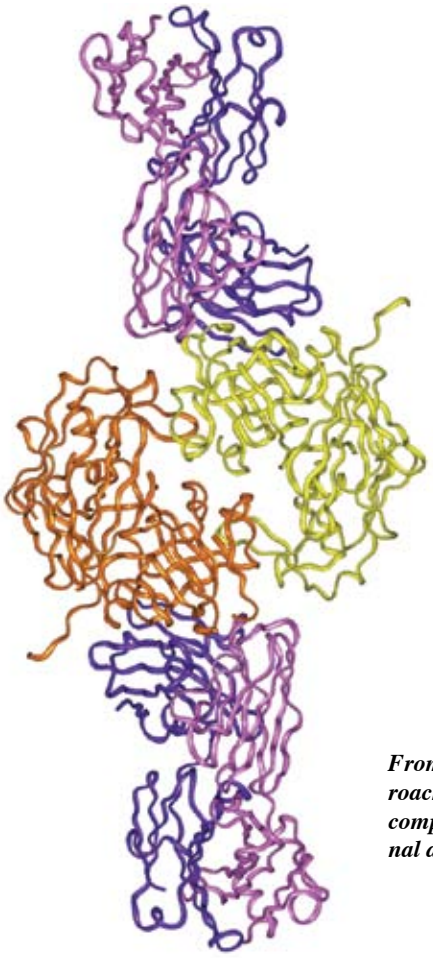
Bio-Mac Posters, cont'd: enzyme that catalyzes the first step to form N-formylkynurenine. The other, 3-hydroxyanthranilate-3,4-dioxygenase, is a non-heme Fe(II) dependent dioxygenase that catalyses the oxidative ring opening of 3-hydroxyanthranilate.

Inorganic pyrophosphatases (PPases) catalyze the conversion of pyrophosphate (PPi) to orthophosphate (Pi). Many biological processes – from amino acid activation to nucleic acid polymerization – produce PPi as a byproduct. Therefore, PPases are critical enzymes in all organisms because clearing PPi from the cytosol maintains the overall cellular equilibrium in favor of biosynthesis. **T-P062** by **Yuh-Ju Sun** *et al*. dealt with the crystal structure and kinetics of the inorganic pyrophosphatase from *Helicobacter pylori* (HpPPase). The structures of both the unliganded and PPi-bound forms of HpPPase were determined. Consistent with the association observed in solution, a hexamer was also observed in the crystal structure. Comparison of the *H. pylori* enzyme with other PPases indicated that, while the overall structures are very similar, there are differences in flexible loops in the vicinity of the active site that may be important for catalysis.



From Yuh-Ju Sun: the architecture of hexameric HpPPase is that it is composed of two trimers. This work is described in a paper accepted by Proteins: Structure, Function, and Bioinformatics: "Kinetic and structural properties of inorganic pyrophosphatase from the pathogenic bacterium Helicobacter pylori."

Evolution of drug resistance in HIV-1 protease was the subject of **T-P030** by **Holly Heaslet** *et al*. In studies designed to understand the structural determinants of substrate preference in wild-type and drug-resistant protease variants, structural and kinetic analyses showed how the mutations involved changed the way the enzyme interacts with the TL-3 inhibitor. In the case of the 6X variant, the changes were quite dramatic, introducing conformational asymmetry in both the enzyme and bound inhibitor. This work could prove to be valuable in the design of new HIV-1 protease inhibitors.



In **T-P083**, the structure of the hypothetical protein TM1727 presented by **Mahendra Madegowda** *et al*. of the NYSGRC provides an interesting example of using structural information to help assign enzymatic function. The enzyme, which has no homologues in the PDB based on primary sequence, has 15 structural homologues. Based on the structure, which clearly shows the bound NADP cofactor, and its structural similarity to the prephenate dehydrogenase, TM1727 is proposed to be a NADP-dependent dehydrogenase.

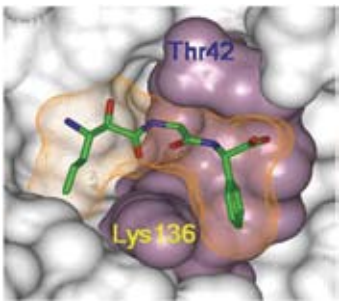
Last, but certainly not least, as presented in **S-P193**, **Alla Gustchina** *et al*. showed the crystal structure of the potent cockroach allergen Bla g 2 in complex with the Fab fragment of the monoclonal antibody 7C11. Bla g 2, an aspartic protease with marginal activity, can induce sensitization (i.e. undesired production of IgE antibodies) at exposure levels much lower than other common indoor allergens. In the structure of the allergen-antibody complex, two antibody molecules interact with an allergen dimer that is stabilized by the formation of a four-helical bundle comprised of two α-helices from each allergen monomer. This novel dimerization mode is attributed to the presence of a unique disulfide bridge connecting two helices within each Bla g 2 monomer. The structure of the complex defines the epitope for the mAb 7C11, which was shown to inhibit Bla g 2 binding to IgE. Mutagenesis of the epitope will specify the residues involved in IgE binding. This work may lead to the development of engineered allergens with lower IgE reactivity, which still elicit T-cell response, and thereby reduce the adverse side effects of specific immunotherapy.

Nick Silvaggi, Mike McDonough, and Herb Klei

From Alla Gustchina: A dimer of the cockroach allergen Bla g 2 (orange and yellow) complexed to Fab' fragments of the monoclonal antibody 7C11 (two shades of purple).

Posters on Structure and Function of Macromolecules

S-P163 (**Andrew Prongay** and colleagues) provided an interesting example of how structural data can provide insight into the design of novel inhibitors using data from the native and S139A mutant of apo-HCV. The native structure showed that the ligand binding pocket was shallow, making it difficult to model inhibitor binding. These data also revealed a disorder in K136 near the binding pocket. Results from the inhibitor complex with a ketoamide peptide with 10-fold increased binding showed a C-clamp interaction that stabilized the conformation of K136.



Pocket S1' (residues Q41, G137, S138, S139: mauve surface) Pocket S2' (residues Q41, T42, R109, K136: mauve surface) P1' & P2' optimized; A P1' ketoamide glycine and a P2' phenylglycine combine with the P1 side chain to form a "C-clamp" around Lys 136. This clamp stabilizes an ordered conformation of the side chain, which is disordered in the unliganded protein. The presence of these moieties improves the inhibition constant 10-fold.

S-P171 (**John Domsic** and coworkers) reported the mechanism for azide inhibition of human manganese SuperOxide Dismutase. Data for Mn-SOD bound with azide at 2.3Å resolution revealed the azide interacts with F34 and Mn. These data support spectral data that showed 3-fluorotyrosine at position 34 inhibited azide binding., The importance of ion pair networks and salt bridges were shown in **S-P175** (**Kam-Bo Wong** and coworkers) who compared the structures of acylphosphatase obtained from thermophililic and mesophilic sources. These data show that the ion pair network observed in the thermophilic structure is absent in the mesophilic enzyme. Mutational studies highlighted the role of the salt bridge formed between Arg20 and Gly91 of the thermophilic enzyme in the structure of the catalytically more active G91A mutant that has lost the salt bridge without affecting the active site of the structure. **S-P181** (**Milagros Medina** and coworkers) reported a penta mutant of ferredoxin-$NADP^+$/H reductase.The data for the mutant enzyme shows an increased affinity for NAD^+ and revealed a change in the conformation of loop 261-265 that contained most of the mutations. The new loop conformation resembles that observed in the $NADP^+$ complex. These results suggest that the conformational change can better accommodate the cofactor.

Vivian Cody

Herb Klei, Brian Kelley, Michele McTigue, Kenton Longenecker, Qiang Zhao, Nanhua Yao, Jack Gougoutas, and Paula Fitzgerald.

4.01: Structural Biology in Industry

This very well-attended session was sponsored by the Industrial SIG. Attendees were rewarded with six first-rate presentations. The session showcased the use of crystallography in commercial settings on several different levels: 1) spectrum from big pharma to small biotechs, 2) macromolecules (proteins and nucleic acids) and small molecules, and 3) structure-based drug design and methods development.

Jack Gougoutas presented work done at Bristol-Myers Squibb on hypersalts. The diverse ways in which nature is able pack these compounds into crystalline solids was illustrated through numerous examples. The use of graph theory to systematically describe chemical connectivity was outlined. A key point is that compounds with very similar graphs can crystallize in remarkably different ways.

Michele McTigue from Pfizer presented several x-ray crystal structures of the kinase associated with one of the vascular endothelial growth factor receptors (VEGFR2 kinase). VEGFR2 is linked to unwanted angiogenesis which plays a fundamental role in the pathophysiology of cancer and ocular diseases. Two conformations of the activation loop were identified from the crystal structures of inhibitor complexes: 1) An "open" conformation in which the beginning DFG segment of the activation loop has the phenylalanine in the "in" conformation and the remainder of the activation loop is disordered and 2) in which the entire activation loop is disordered and the DFG is in the "DFG-out" orientation. Mike described the iterative structure-based drug design process employed to transform unselective inhibitors that bound to the disordered open conformations to selective inhibitors that bound to the DFG-out conformation and were suitable for clinical study. **Nanhua Yao** presented work done at Valeant Pharmaceuticals on the RNA-dependent RNA polymerase NS5B from hepatitis C virus. The sheer number of patients affected by this pathogen, both current and projected, and the issues associated with current therapies demonstrated the magnitude of this medical need. An x-ray crystallographic study of two novel series of NS5B inhibitors identified by high-throughput screening revealed two different binding sites associated with different mechanisms of action. One analog, which binds near the center of polymerase close to the catalytic site, interferes with the primer binding. The other analog, which binds within a narrow cleft in the thumb domain on the surface, is an allosteric inhibitor. It locks the polymerase conformation and perturbs fluctuation within polymerase subdomains. How the crystal structures were used to elucidate the structure-activity relationships was also covered.

Herb Klei and Paula Fitzgerald

Murli Manghnani, Valentina Degtyareva, Olga Degtyareva, Eugene Gregoryanz, Chrystele Sanloup, Michael Ruf, Wayne Pearson, Colin Glass, Amy Lazicki.

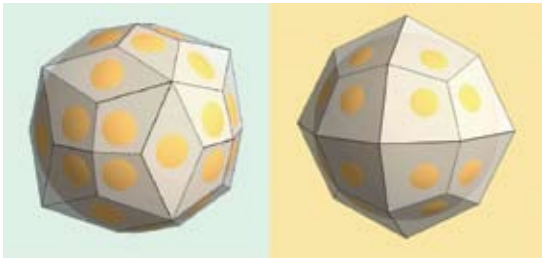
5.01: Non-Ambient Crystallography

The session focused on the high pressure and high temperature effects on crystal structure of various materials, including pure elements, deep-earth minerals, ionic compounds and complex molecules. It included experimental, computational and theoretical work as well as technique development. **Eugene Gregoryanz** (U. Edinburgh, UK) opened the session by presenting recent x-ray diffraction data on high-pressure behavior of elemental nitrogen, including its non-molecular phases.

Colin Glass (PhD student at ETH Zurich) extended the discussion of complex structures in elements and compounds at high pressures by presenting a recently developed method for prediction of crystal structures, based on an evolutionary algorithm merged with *ab-initio* total-energy calculations. **Murli Manghnani** (U. Hawaii) closed the first half of the session by presenting *in-situ* diffraction and Raman studies of B_4C.

Valentina Degtyareva (Inst. of Solid State Physics, Russia) continued by discussing complex structures in pure elements occurring at high pressures, such as in lithium, and also in binary alloys, offering a theoretical model that explains the occurrence of such complex structures in simple systems.

Below, from Valentina Degtyareva: (unpublished), Brillouin zones for γ-brass Cu_5Zn_8 and Li-cM6 with the inscribed Fermi spheres. Construction is performed by the program BRIZ (Smirnova I.S. and Degtyareva V.F., The Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka). Crystal structure data are taken from Pearson W.B. A Handbook of Lattice Spacings and Structures of Metals Vol. 2 (New York: Pergamon Press, 1967) and Hanfland M. et al., Nature 408, 174 (2000).



Chrystele Sanloup (U. Pierre *et* Marie Curie, Paris) introduced us to the long-standing "missing xenon" problem: the deficiency of xenon compared to other rare gases in the atmosphere, and presented a possible solution to this problem based on her studies of Xe reactivity with silica at high pressures. **Amy Lazicki** (U. California - Davis and LLNL) reported her experimental and computational studies on ionic Li_3N and Li_2O, concluding with a systematic interpretation of high-pressure behavior of all alkali chalcogenides.

The last talks of the session focused on single-crystal diffraction studies. **Wayne Person** (US Naval Academy, Annapolis) reported on the high pressure molecular structure of RDX, an explosive material used for military applications. **Michael Ruf** (Bruker AXS Inc.) concluded by outlining the latest developments in single-crystal data collection strategies for high-pressure experiments with CCD detector systems. Discussions continued at the poster session later in the evening.

Olga Degtyareva

Bill Ojala, Bill Gleason, Paula Garcia-Reynaldos, Chuck Strauss, Debbie Stean, Charlotte Stean, Judy Neiswander, Carole and Victor Young.

9.02 Bio-Molecular Assemblies

Youli Li, William Heller, Jack Johnson, Michel Koch, Hiro Tsuruta, Volker Urban, Dmitri Svergun, David Tiede.

This session, sponsored by the small angle scattering SIG, showcased recent methodological developments and cutting-edge high resolution structural studies of biological macromolecular assemblies by primarily non-crystalline diffraction and scattering methods. **Dmitri Svergun** (EMBL-Hamburg) reviewed the impressive array of computational techniques his group has developed for studies of proteins and assemblies by solution x-ray and neutron scattering. He discussed *ab initio* shape and domain structure determination at moderate resolution, rigid body refinement for assembling a quaternary structure from component structures, and neutron contrast variation for protein-nucleic acid complex studies. The application examples highlighted the important role of these techniques in bringing subcomponent crystal structures into the context of functional assemblies in solution and inspired potential future studies.

David Tiede (Argonne) described his recent studies on nucleic acid structure and dynamics by x-ray diffraction fingerprinting, one of the new high angle scattering techniques in biology made possible by advanced synchrotron facilities. Using A-tract polyA-polyT DNA as an example, he demonstrated that solution x-ray scattering recorded at sub-nanometer resolution is highly sensitive to minute differences in secondary structure. It also provides an effective experimental approach to quantitatively evaluating MD simulations in solutions *in-situ*.

William Heller (Oak Ridge) presented an overview of several studies where the combination of small-angle scattering and modeling methods provided insights into the structure and function of macromolecular complexes. The examples included a study of the solution conformation of vitronectin; a study of calcium-induced structural changes in phosphorylase kinase; investigations of the activation of protein kinase A; and a study of the interaction of the methionine repressor protein MetJ with three different target DNA sequences.

Jack Johnson (Scripps) discussed the kinetics of quaternary conformation change during the maturation of bacteriophage HK97. It was shown that the combination of time-resolved x-ray scattering results with those from crystallographic and cryoEM studies revealed the highly concerted structural change in the initial and final maturation stages. Spontaneous self-catalytic cross-linking was shown to be a critical step in transforming cooperatively the maturation intermediate to the matured form in the final stage of its morphologic transformation.

At right, from Jack Johnson: A montage of four morphological forms of the bacteriophage HK97 capsid superimposed on the single crystal data (right) used to determine their structures and the solution scattering data (left) used to follow the transitions between forms. The earth is shown in the center to emphasize that bacteriophage constitute a significant fraction of the terrestrial biomass.

Michel Koch (EMBL-Hamburg) presented a comprehensive review of small angle scattering techniques in structural studies of crystalline and non-crystalline biological systems. He covered a number of important topics ranging from the fundamental scattering process and electron density contrast to several applications in foods and pharmaceuticals. Among them, he reminded us of the unique ability of solution scattering techniques to visualize interaction potentials and counter-ion clouds around proteins and nucleic acids. The importance of conducting non-crystalline diffraction studies free from the constraints of the crystallographic lattice was demonstrated by a set of bacteriorhodopsin studies.

Youli Li (UC Santa Barbara) reported an extensive set of x-ray scattering studies on nanotube structures formed by microtubule-spermine and microtubule-lipid complexes, illustrating a remarkably intriguing array of unusual macromolecular assemblies under certain conditions. The former complex undergoes a novel transition from a normal tubular structure to a columnar phase of inverted tubules where the internal protein faces are positioned outside. The presence of lipid induces completely different microtubule assemblies such as beads (lipid vesicles) on a rod (microtubule) structure and a multi-shell tubular structure with a tubulin-lipid bilayer-tubulin radial profile.

Volker Urban (Oak Ridge) reported the latest facility developments at the Center for Structural Molecular Biology (CSMB) for biological neutron scattering studies at HFIR and SNS. The HFIR Bio-SANS instrument will become available in 2007 and will be dedicated to the analysis of the structure, function and dynamics of complex biological systems. The CSMB support of this facility will include additional biophysical characterization, x-ray scattering infrastructure, advanced comptational tools for neutron analysis and modeling, and operation of a Bio-Deuteration Laboratory for *in vivo* production of H/D labeled macromolecules.

Hiro Tsruta and Volker Urban

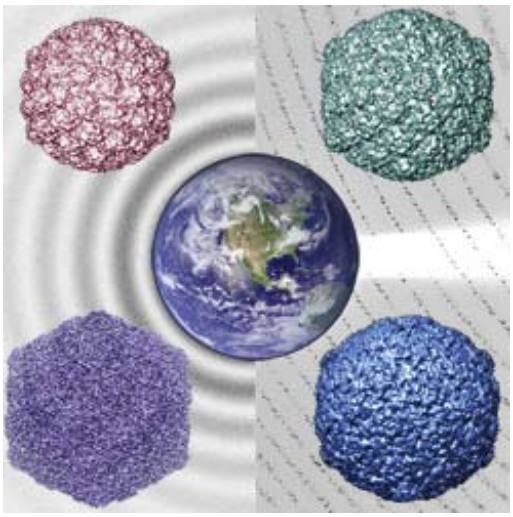


Figure by Lu Gan, reprinted from: Wikoff, W. R., Conway, J. F., Tang, J., Lee, K. K., Gan, L., Cheng, N., Duda, R. L., Hendrix, R. W., Steven, A. C., and Johnson, J. E. 2006. J. Struct. Biol. 153:300-6, © 2006, with permission from Elsevier.

David Londono, Brian Landes, Norbert Stribeck, Ryan Justice, PappannanThiyagarajan, Elena Loizou, Volker Urban, Alexander Boeker, A. Mahendrasingam.

9.03 Polymer Science and Technology

This session provided a comprehensive overview of the use of small angle scattering in conjunction with complementary techniques in the characterization of polymeric materials. It showcased everything that is exciting about this field: sophisticated methods of analysis; insightful methods of data collection; the use of multiple techniques; the dramatic effect of external fields; and the ongoing transformation from traditional polymer science to nanoscience.

Norbert Stribeck, (U. Hamburg, Germany), presented results from advanced Fourier-transform methods as used in the analysis of synchrotron radiation data from semicrystalline polymer parts during nanostructure evolution resulting from crystallization and melting, as well as the spatial variation of structure within a part. **Brian Landes**, (Dow Chemical), presented wide and small angle x-ray scattering data from ethylene based copolymers collected *in-situ* during tensile testing. This method of testing offers a viable alternative to standard tensile test methods, which are not always good indicators of product performance. Methods for reduction of large amounts of data resulting from *in-situ* deformation experiments were also reviewed. **Arumugam Mahendrasingam** (Keele U., UK), presented results from an *in-situ* study of strain-induced crystallization in the biodegradable polymer poly(lactic acid) during fast uniaxial deformation. Fast crystallization rates for this polymer, as studied *in-situ* at the ESRF synchrotron, are similar to those rates which had been observed for PET by the same method.

Alexander Böker (U. Bayreuth in Germany) summarized his results on electric field induced orientation of diblock copolymer microdomains in concentrated solutions as studied by synchrotron SAXS and other techniques. Macrodomain formation occurs by either rotation of microdomains or by nucleation and growth. The effect of several variables on the kinetics of macrodomain formation was investigated.

P. Thiyagarajan (Argonne) discussed the phase behavior of nanoparticle/diblock copolymer composites. Their research focused on developing techniques to organize nanoparticles in 2D arrays by using self-assembled copolymers as templates. Their method involves the synthesis of nanoparticles covalently attached to a polymer that can selectively sequester into one domain of diblock copolymers. He presented evidence showing that nanoparticles preferentially sequestered in one of the domains lead to an increase in the interfacial curvature and hence the nanostructure of the composite. This effect was proposed to be responsible for the observed properties, and will be important in developing applications for these materials. Subsequently, **Elena Loizou**, (Louisiana State U.) working at the NIST Center for Neutron Research, gave an excellent talk on the shear-induced structural response of polyethylene oxide-clay nanocomposite hydrogels, exploring the structural changes that occur at various length scales in response to a shear field by means of rheology, small angle neutron scattering and microscopy. The effects observed are thought to be relevant to future applications.

Finally, **Ryan Justice** (Air Force Res. Lab, WPAFB, OH), an Etter Student Lecturer, presented a method to obtain simplified models for hierarchical structures based on disks, rods, and tubes. This engaged the audience in discussion about proposed alternative approximation methods based on the series expansions of the form factor from these shapes.

Ryan Justice, at right, accepting an Etter Student Lecturer Award from Volker Urban.

David Londono and Volker Urban

Christer Aakeroy's group. Christer Aakeroy, Nate Schultheiss, Katie Schultheiss, Benjamin Scott, Michelle Smith, Meg Fasulo, and Yasmin Patell.

From top left: Crowd scene; Bob Bau and Margaret Churchill; Next: Håkon Hope; Jeff Deschamps and David Kelly; Jenny Glusker and Gerry Bunick; From bottom left: Kahil Abboud; George Sheldrick; Sue Byram, above, and Amy Katz, bottom right.

See page 7 for code identifying contributing photographers.

10.01: Applications of Crystal Growth and Low Temperature Techniques

Amy Sarjeant, Ilia Guzei, Allison Dobson, Bruce Noll, Donna Smith, Carly Anderson, Alan Pinkerton, and George Sheldrick. Photo courtesy of Amy Sarjeant.

Despite the specific title, this session encompassed a variety of interesting crystallographic techniques from handling sensitive materials to data collection and processing routines to final publication. We accomplished our goal: to foster the passing-on of knowledge from the "old-school" crystallography set to a younger generation now taking up the science. To that end, well-seasoned speakers presented their material alongside graduate and undergraduate students.

Donna Smith (Los Alamos National Lab) began the session with an informative talk about the challenges of working with radioactive materials. She described several of the procedures in place at LANL for working with various "hot" materials. Two of the session's younger speakers then followed: **Maxime Siegler** (U. Kentucky) and **Carly Anderson** (Berry College, GA). Max's discussion of the polymorphic system $[Ni(H_2O)_6]$ $(NO_3)_2 \cdot 2H_2O$ which is given to an unusual series of reversible phase transitions highlighted the usefulness of variable temperature data collections. A complete understanding of the interrelationship of the phases was achieved via coupling multiple datasets collected at various temperatures with DSC data. Max had shown subtle differences in the hydrogen bonding scheme of his material led to the various ordered and disordered, and even commensurately modulated structures of this phase system. **Carly Anderson** provided us with an undergraduate's perspective on an interesting quirk of crystallography in her enlightening presentation about α–nitro-*trans*-stilbene. Her investigations into this disordered system demonstrated that a careful inspection of the data can sometimes lead to unexpected results. In this case, the structure was found to be disordered. Carly considered both C2/c and Cc as possible spacegroups. Initially, the lower R-factor given by the Cc refinement appeared as the best choice; however, upon further review, the geometrical parameters given under C2/c proved more reasonable once a suitable disorder model was discovered. Despite the slightly higher R-factor Carly determined this was the better structural model, demonstrating that the devil is often in the details!

Bruce Noll's (Notre Dame) presentation "[Fe(TPfP)(1-MeIm)(NO)], provided a beautiful demonstration of his theory that unexpected results come from unusual circumstances. Collecting room temperature data on a routine crystal after turning off his cold stream for the weekend led Bruce to discover a series of twinned, ordered, and disordered structures ultimately collected over a range of different temperatures. These multiple datasets yielded valuable information about the conformational relationship between the NO and MeIm groups bound to the iron center of the porphyrin. A second crystal, subjected to the same rigors as the first showed no phase changes or signs of twinning. It was only the serendipitous combination of a "bad" crystal and a non-routine room temperature data collection that provided for exceptional results for a seemingly unassuming sample.

George Sheldrick (U. Göttingen) took to the podium in front of a packed house to discuss his scaling and absorption correction techniques for small molecule and macromolecular area detector data. Real-life examples were presented, illustrating the vaious problems endemic to scaling and correction programs and solutions for them. George also presented the program TWINABS as a complement to SADABS for the scaling and correction of twinned and multiplet samples. Again, real-life examples were shown to demonstrate the functionality of these algorithms.

In another technical talk, **Alan Pinkerton** (U. Toledo) demonstrated the combination of theoretical methods and structural information to describe electron density and related properties for very low temperature or high pressure structures. Alan used Density Functional Theory to achieve a good estimation of intra- and intermolecular bond critical points in the electron density as per various descriptors for the pentaerythritol system.

And then for something completely different. **Allison Dobson** (Georgia Southern U.) told of her success in teaching small molecule crystallography to undergraduates. Despite numerous challenges: limited lab space; students fearful of physical chemistry; and untrained research students, Allison's various techniques allow her students practical and theoretical experience. She showed how her programmed course of study has yielded fruitful results. Students have grown their own crystals, solved structures and published the results of their work.

What better way to end a session on crystallographic techniques than with a talk concerning methods used to prepare data for publication. **Ilia Guzei** (U. Wisconsin) described programs useful for creating and perfecting CIF files and demonstrated their use. He highlighted the IUCr program publCIF which allows easy and more user-friendly editing of CIF files. Additionally, the publCIF publication wizard helps to prepare the CIF file for publication in *Acta Cryst. C* or *E*. ModiCIFer, a program that Ilia developed, allows for easy creation of a checkCIF-acceptable file which can then be edited in publCIF.

Amy Sarjeant

10.03: Supramolecular Chemistry

This symposium featured an impressive and particularly international line-up of nineteen speakers from seven nations. Despite the potential competition from more beach-based activities, the symposium was very well attended from beginning to end, which goes to show that good science can prevail even in the face of Mai Tais, surfing and the occasional late-night Luau.

Dedong Wu, Christer Aakeröy, Joel Bernstein, and Joseph Lauher.

The sessions were arranged around three broad themes. The first session, **Intermolecular Forces, Crystal Growth, and Polymorphism**, provided a suitable foundation for what was to follow. **Andrew Beasley** described how diffuse scattering methods can be used to elucidate disorder arising from the internal flexibility of molecules in polymorphic systems. **Joe Lauher** described an elegant method for identification and classification of hydrogen-bonded networks and **Michal Sabat** examined the structural role of a hierarchy of intermolecular interactions. **Joel Bernstein, Dedong Wu, Kraig Wheeler,** and **Christer Aakeröy** then discussed fundamental and applied aspects of molecular co-crystals.

Christer Aakeröy, Kraig Wheeler and Michael Sabat.

The second session, **Directed Assembly of Organic and Hybrid Architectures**, was primarily geared toward the construction and function of coordination polymers. In particular, **Susumu Kitagawa** demonstrated that crystalline materials can indeed be dynamic and highly flexible systems suitable for storage and guest recognition. **Michaele Hardie, Jesus Valdes-Martinez, Guy Orpen, Eric Bosch**, and **Hilary Jenkins** subsequently covered various aspects of ligand design, synthetic coordination chemistry, and supramolecular assembly. It is very encouraging that practitioners in this field continue to make significant progress despite the considerable challenges inherent in crystal engineering.

Jesus Valdes-Martinez, Eric Bosch, Michaele Hardie, Guy Orpen, and Hilary Jenkins.

The highlight of the symposium (and arguably of the whole meeting) was **Makoto Fujita's** plenary lecture on chemistry within confined spaces. He demonstrated that his carefully assembled metal-containing capsules are capable of facilitating an extraordinary array of synthetic transformations with amazing regio- and stereo selectivity. Furthermore, the ability to create nano-sized "droplets" of fluorine within a solid cage is a remarkable achievement. The remainder of the third session, **Function and Reactivity of 'Engineered' Materials**, provided additional evidence that the distance between synthetic supramolecular architectures and function is getting shorter and shorter. **Travis Holman** and **Nate Schultheiss** presented work on host-guest chemistry, **Tony Sokolov** showed how co-crystallization strategies can afford new semiconductors, and **Jane Li** and **Matthew Peterson** gave an important industrial perspective on co-crystals and pharmaceutical applications.

Jane Li, Matt Peterson, Nat Schultheiss, Travis Holman, and Tony Sokolov.

Finally, the audience provided insightful questions and considerable enthusiasm. Supramolecular chemistry continues to involve scientists with very diverse interests.

Christer Aakeröy

View of Honolulu from a hotel lanai.

11.01 Radiation Damage and Macromolecular Crystallography

Nobutaka Shimizu, Zbyszek Otwinowski, Rob Thorne, Leif Hanson, Eddie Snell and Jean Jakoncic.

Eddie Snell (Hauptman-Woodward Med. Res. Inst.) opened the well-attended Radiation Damage session with a description of the experimental setup and calibration procedures used to locate and monitor changes in temperature in macromolecular crystals by thermal imaging. He then explained how this method could be applied to obtain a quantitative estimate of the temperature increase in crystals in intense x-ray beams; although protein crystals could not be directly used for this study, glass beads of different diameters provided a good experimental model. In the worst case scenario (using a 1mm bead) a temperature increase of 22° K was observed when exposing the sample to the beam while in a cooling gas stream. These initial results suggest that crystal heating does not rise to the glass transition temperature. Whether it provides enough thermal energy to mobilize free radicals is still open to some debate, but this seems unlikely with a well aligned cryostream and a typical macromolecular crystal sample.

Leif Hanson (U.Toledo) presented a comparison of the x-ray induced diffraction decay of crystals cooled to 15 and 100°K with a Pinkerton Device open flow, and conventional nitrogen cryostream, respectively. Although plots of $I/\sigma I$ against beam exposure for increasingly damaged crystals showed a negative slope at all temperatures, the slope was 33% less for the crystals cooled to 15°K. Leif explained these results by decreased mobility of OH radicals at 55°K. Since the cost of running the He cryocooler is not dramatically more than with nitrogen cryocoolers, he concluded that the routine use of open He flow devices on macromolecular beamlines would be well justified. **Robert Thorne** (Cornell) (speaking for Jan Kmetko) described an experiment to quantify the global effects of radiation damage for different protein samples treated with different concentration of heavy atom salts. They found that the increase of the Wilson temperature factor per absorbed dose remained roughly constant regardless of the mass-energy absorption coefficient and the protein studied. This implies that mitigation effects from scavengers or temperature reduction will be limited to about a factor of 2. **Nabutaka Shimizu**, (SPring-8), presented recent results of a systematic study comparing the effects of radiation damage over a large range of x-ray energies (6.5 to 33 keV) for tetragonal lysozyme crystals. The exposure time at each energy was corrected for incident beam intensity and detector response. Under these controlled conditions, no significantly large difference in radiation damage per dose received by the crystal at different energies was observed; *i.e.*, optimizing dose in a crystal is critical at any x-ray energy to obtain accurate structures. **Jean Jakoncic** (National Synchrotron Light Source at BNL) showed that both single or multiwavelength anomalous phasing experiments at the holmium K edge at the NSLS X17B1 and ESRF ID15B high energy beamlines (~ 55 keV) produced high quality electron density maps. He argued that data collection at ultra-high energies can slow down the onset of radiation damage, based on the comparison between these data and other data collected at 12 keV.

The last speaker, **Zbyszek Otwinowski** (U.Texas SW Med. Ctr.) started by examining the decay in different forms of lysozyme crystals with attention to the variation in the structure factor amplitudes and damage to specific sites. He showed that the presence of NO_3 in the crystallization buffer had a protective effect on monoclinic lysozyme, preventing reduction of disulfide bridges, and went on to emphasize the importance of modeling radiation damage in reciprocal space. He illustrated these with some examples where data quality improved dramatically after applying radiation damage corrections at the scaling stage, showing that this approach is worth pursuing despite the difficulties in choosing the correct damage model for the general case.

Ana González

Peter Horanyi, Jean-Pascale Viola, Leif Hanson, Carrie Wilmot, Bob Bau, and Doug Ohlendorf.

12.01: Topics of Interest to the Young Scientist

The YSSIG session began with an overview of the academic life of a crystallographer. **Doug Ohlendorf** (U. Minnesota) discussed the necessary steps in the academic interview process. He showed how to prepare for the interview as well as how to learn from those events that do not work out for the best. **Carrie Wilmot** (U. Minnesota) talked about the essentials of setting up a new lab. She emphasized the responsibilities of being a Principal Investigator. **Leif Hanson** (U. Toledo) gave great advice about the attitude the young scientist must have about science. He recommended keeping a childhood mindset and being perpetually open to new things as the best way to advance in any scientific field.

ACA President **Robert Bau**, (USC) gave a brief overview of the organization's past and present and explained how the ACA is related to other scientific organizations in physics and chemistry. Photographs of ACA members were used to illustrate our history.

The highlight of the session was a success story by Jean-Pascale Viola, the founder of NEXTAL, now Qiagen-NEXTAL. Jean-Pascale showed that a business or finance degree is not required to start a profitable company. In his case both intellectual property and the ways he used patents drove the business.

Peter Horanyi

13.02: Whole-Molecule Disorder

L to r: Carolyn Brock, Yulia Sevryugina, Brahama D. Sharma, Peter Mueller, Gary Enright, John Desper, Håkon Hope, Peter Zawalij and Chuck Campana. Session photo and photo of Yulia Sevryugina by Peter Mueller.

This session focused on a crystallographic phenomenon that has been observed by many but described only very rarely and not usually with this term: *Whole Molecule Disorder* (WMD). A crystal structure is always a spatial average, the representation of all molecules in the crystal by just one unit cell. If not all unit cells in the crystal are perfectly identical, this description of the structure is problematic. One of the easier problems of this kind is simple static disorder, where a part of the molecule possesses two almost equally preferred orientations. In the spatial average this situation results in two sets of coordinates for the atoms in question. When all atoms in the unit cell, the whole molecule so to speak, are found in two distinct orientations in the crystal and a symmetry operator in form of a 3 x 3 matrix can be found to transform one orientation into the other, we have ourselves a twin. If this symmetry operator can be applied to the unit cell in a way that the transformed crystal lattice perfectly overlaps with the original one, we speak about a merohedral or pseudo-merohedral twin. (No overlap between original and transformed lattice means the twin is non-merohedral. Supposing a molecule crystallizes in two distinct orientations without a simple symmetry operator that transforms between them? For example when the second orientation is a different rotamer of the same molecule or another enantiomer? When the ratio between the two is precisely 1:1, the situation may be described as a unit cell with doubled volume and two molecules per asymmetric unit. But if the ratio is not 1:1 then we can use the term WMD.

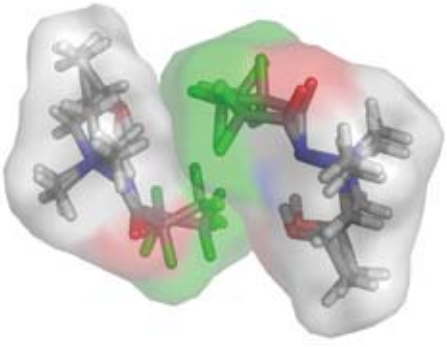
Håkon Hope (UC Davis) opened the session with a thorough review of the history of fully disordered molecules and pointed out that there was no reason WMD should not happen, though he cautioned that other effects should be ruled out before splitting every atomic site in a structure. **Chuck Campana** (Bruker AXS), one of the foremost experts on structure refinement, described how to recognize WMD during structure refinement and how it should be treated. Using three examples he explained which restraints to use, how to keep the refinement stable and how to make sense of confusing looking residual electron density. **Peter Mueller** (MIT) gave a brief overview of prerequisites for WMD: a molecule must have more than one possible orientation that fits in the same envelope and the charge distribution on the surface of the envelope should not be very different for the various orientations. He pointed out that in his experience typical occupancies for the main component are between 0.75 and 0.95 and that for molecules containing only light atoms, WMD can be missed very easily. When molecules contain only one heavy atom, residual electron density corresponding to the second component of this heavy atom can be mistaken for Fourier truncation or absorption artefacts. He noted that valuable information can be contained in the space between Bragg reflections in the form of diffuse scattering.

Yulia Sevryugina (SUNY Albany) received an **Etter Student Lecturer Award** for her work on penta-tert-butyl-corannulene and corannulene. She reported several difficult structures, some of which suffered from WMD.

In four short presentations, **Peter Zawalij** (U. Maryland), **Carolyn Brock** (U. Kentucky), **John Desper** (Kansas State U.) and **Gary Enright** (NRC, Ottawa, Canada) gave examples of structures with WMD from their structure determinations. In the final talk, **Brahama D. Sharma** reminded the audience that "disorder may be a misnomer," that lack of order is not compatible with crystallinity and that other effects also need to be considered.

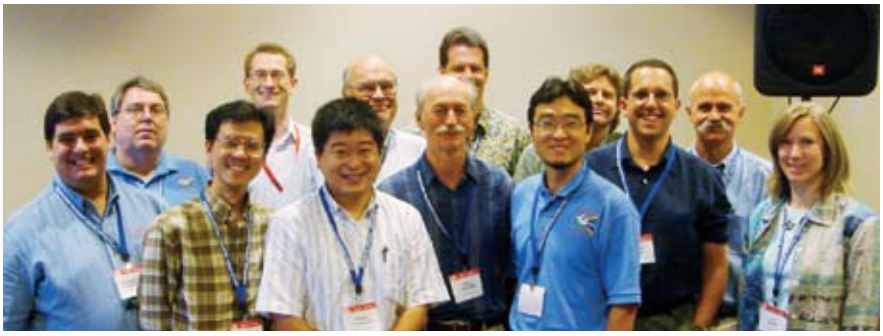
The high level of similarity in the speaker's experiences was echoed by many in the audience in discussions throughout the session. It is clear that WMD is a real phenomenon.

Peter Mueller



From Peter Mueller: two molecules showing WMD. Both components of the disorder fit into the same envelope (drawn as semi-transparent surface) with roughly the same charge distribution on the surface of the envelope.

13.07: Remote Data Collection



Greg Ferrence, John Rose, Xiang (Sean) Ouyang, Jörg Kärcher, Masaki Yamamoto, John Huffman, Dieter Schneider, David Smith, Zhongmin Jin, Mike Soltis, Graeme Winter, Bob Sweet, Lisa Keefe.

Greg Ferrence, and **Xiang (Sean) Ouyang**, Cal State Fullerton (CSUF), described STaR-BURSTT-CIC (Science Teaching and Research Brings Undergraduate Research Strengths Through Technology - CyberInstrumentation Consortium - **www.StaRBURSTT.org**). The Consortium provides remote access to instrumentation and an intellectual network in crystallography to Primarily Undergraduate Institutions (PUIs) particularly as they pertain to crystallography. They illustrated remote data collection at CSUF using open-port software such as iLinc and LogMeIn for remote data collection.

John Huffman (Indiana U.) described the Common Instrument Middleware Architecture (CIMA **www.iumsc.indiana.edu**) project, aimed at "Grid enabling" instruments as real-time data sources. The CIMA Crystallography Portal allows remote monitoring of instruments and provides remote data-processing capability. Huffman described how the "data capacitor" system assures long-term data integrity using distributed university-maintained resources. **Michael Soltis**, Stanford SSRL, (**http://smb.slac.stanford.edu/**) illustrated remote data collection using the SSRL Automated Mounting (SAM) system at the macromolecular crystallography beam lines at SSRL (video of the crystal mounter at **http://smb.slac.stanford.edu/public/facilities/hardware/SAM/SAM_M.m1v**). The SAM system is often employed by remote users who can access up to 288 samples after an assistant at the beamline has loaded up the dewar. Crystal screening software and a web-interfaced screening-system database stores information about the samples in the cassettes and uploads this information to the beamline software.

Graeme Winter (Daresbury Lab, UK) and **Sandor Brockhauser** (EMBL, Grenoble, France) described components of the remote data (e-HTPX) and data-collection automation (DNA) projects being executed by a broadly based European and partly US consortium. Winter explained how the intelligent hub of DNA knits together otherwise independent component programs to give a self-reliant and nearly independent data-collection system. Brockhauser showed the construction and operation of a MiniKappa Goniometer Head which, with its software STAC, offers routine crystal re-orientation and fast data collection sweeps without stability problems. See **www.e-htpx.ac.uk, www.embl-grenoble.fr/groups/instr/mk2videos.html** and **www.dna.ac.uk**. **Dieter Schneider** (Brookhaven Biology) provided a history of their group's remote data systems starting with the 1998 remote web tools and culminating in the current highly integrated system, incorporating an experiment-tracking database, beamline control, and specimen automounters. He emphasized the effort at the NSLS to provide a fluid interplay between dipole beam lines, where users may screen specimens for quality, and ID lines where they may measure final data. Schneider described the needs for and implementation of rapid access, flexible scheduling, facilities with one look and feel, redundant automounters, loop and crystal centering, and database support.

Masaki Yamamoto (RIKEN Spring-8, Japan) described the automated beamline operation at the Spring-8 Structural Genomics Beamlines (**www.spring8.or.jp/wkg/BL26B1/instrument/lang-en/INS-0000000386**). Constructed for high throughput protein crystallography, the system uses the sample changer robot SPACE (Spring-8 Precise Automatic Cryo-sample Exchanger), which has been in continuous operation at BL26B2 since October 2003. SPACE uses a duel threaded polyacetal sample pin to ensure $<10\mu$m positional reproducibility of the crystal. Their web-based software allows crystal screening to occur with a daytime rate of 10 min/sample.

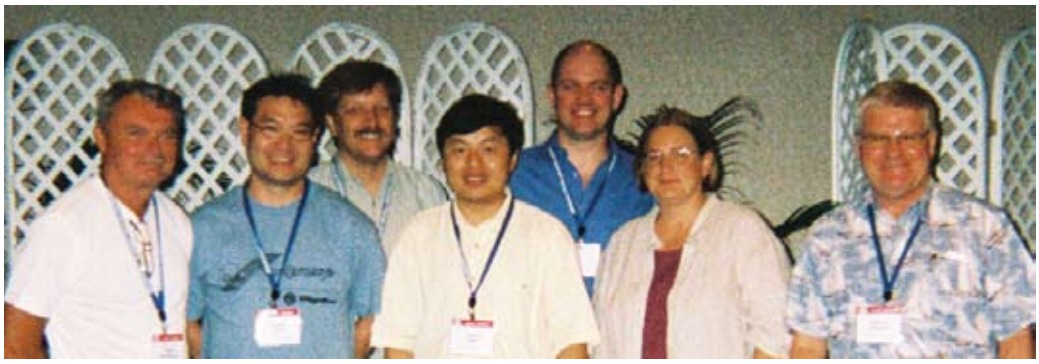
John Rose and **Zhongmin Jin** (U. Georgia) described the sample-to-structure automation process helping to meet demands for remote access to the Southeast Regional Collaborative Access Team beamlines at the APS (**www.ser-cat.org**). They have developed local software to handle the local experiment in ways similar to other stations. In addition, their SGXPro system automates structure solution. They have developed a three-screen remote user workstation that nicely mirrors the on-site experience. This is finding increasing application for their user community, all of whom live hundreds of miles from the APS.

Lisa Keefe (IMCA) introduced the high-throughput macromolecular crystallography data collection taking place at Industrial Macromolecular Crystallography Association beamlines at the APS (IMCA-CAT **www.imca.aps.anl.gov**). Their robotics (Rigaku ACTOR) provides a sample capacity of 60 crystals on the ID beamline and 180 crystals on the BM beamline and enables rapid sample mounting, autocentering, screening, tracking, sorting, and ranking. **Jörg Kärcher** (Bruker AXS) described solutions for remote data collection for single-crystal and powder diffraction available from Bruker. This included showing their screening software, the BRUNO robotics, and their motorzied goniometer head which work in concert to load and center specimens.

David Smith (SGX Pharmaceuticals, Inc.) (**www.sgxcat.com**), described the "mail-in crystallography" process at SGX-CAT, Argonne, the longest running and most successful remote system in the world. In 2005, 9000 crystals were screened and 4200 datasets were collected using highly automated and remote controlled screening and collection processes, including protocols for data collection, centering of loops, removal of surface ice, scoring of crystal quality, processing of data, and updating of the database.

Bob Sweet and Greg Ferrence

13.08: Complementrary Methods to Macromolecular Crystallography



Alex McPherson, Joshua Sakon, Bill Royer, Quan Ho, Andrew Stewart, Clare Peters-Libiu, and Jack Johnson.

Mechanistic biology is frequently confronted with an experimental paradox. High resolution structures are required to develop a chemical description of macromolecular interactions, but the processes themselves are dynamic and often not concerted. Chemists and molecular biologists have been successful in generating homogeneous components and entire complex systems that are amenable to crystallization and high resolution analysis. If the dynamics of the systems are small, time resolved studies could be performed in the context of the crystal lattice. If the dynamic features of the biological reactions are large and not homogeneous, the motility must be studied in solution with techniques that do not demand a uniform ensemble of molecules. This session addressed techniques in which atomic models are "brought to life." The goal was to understand better the dynamic processes associated with biological function.

Alex McPherson (UC, Irvine) began with an introduction to atomic force microscopy and its use to investigate everything from crystal growth to the release of RNA from virus particles. The method provides nm resolution in the vertical direction of the scan and 2-3 nm resolution in the plane of the scan. AFM provides a detailed surface view of the objects investigated and it can be performed in solution. **Quan Ho** (Cornell) discussed the use of small angle x-ray scattering to determine molecular envelopes of macromolecules and the application of these envelopes for determining crystallographic phases. To do this the known envelope must be properly positioned and oriented in the crystal lattice. Programs developed for this purpose were discussed. **Bill Royer** (U. Massachusetts) discussed time-resolved crystallography of hemoglobin, providing nano second time resolution and atomic spatial resolution of transitions that occur in the molecule as it loses its ligand and moves from the R to T state. The method requires a system that will repeatedly undergo the transformation in the crystal lattice and one that can be triggered by a laser. Single-bunch x-ray data were collected with a limited Laue approach at a specific time interval after activation. A number of patterns must be collected at each interval to create a reasonably complete data set. The results of the study are interpreted by difference Fourier analysis allowing the motions of the molecule to be clearly observed.

Andrew Stewart, Stony Brook U., provided a progress report on the development of the x-ray microscope. Significant progress has been made in this project initiated originally by David Sayre who remains deeply involved. While the current resolution is approximately 5 nanometers, the ability to penetrate cellular samples much thicker than those used for conventional electron microscopy make this an exciting technique that may provide exceptional 3-dimensional detail in the near future.

Clare Peters-Libeu (Gladstone Inst., UCSF) presented a model for the human apolipoprotein E.DPPC obtained from crystallographic analysis of Bragg reflections and diffuse scattering as well as from small angle x-ray scattering data. Their model conforms to a spheroid shape in contrast to the disc shape that has been generally accepted to date. The data presented also allowed the modeling of the conformational change that occurs in the LDL-receptor binding region of apoE when it binds to DPPC.

Joshua Sakon (U. of Arkansas) described multiple methods to characterize the transition of the collagen binding domain (CBD) of collagenase from the alpha to beta form. Questions arose regarding the effect of calcium binding on CBD and whether differences in the two crystalline forms (without and with calcium) was due to crystallization or if it was biologically relevant. Employing NMR, light scattering, size exclusion chromatography and thermal scanning calorimetry, Sakon and his colleagues were able to demonstrate that the changes observed in the crystal also occurred in solution. **Jack Johnson** (Scripps Research Inst.) finished the session by describing a 17Å resolution asymmetric cryoEM reconstruction of the bacteriophage P22. High resolution x-ray models of the tail spike proteins were readily fitted into the cryoEM density confirming the validity of the reconstruction. The structure showed clear density for the dsDNA packaged in a solenoid configuration and suggested that a dodecameric structure associated with DNA entry may be a sensor for when the virus particle is full of DNA.

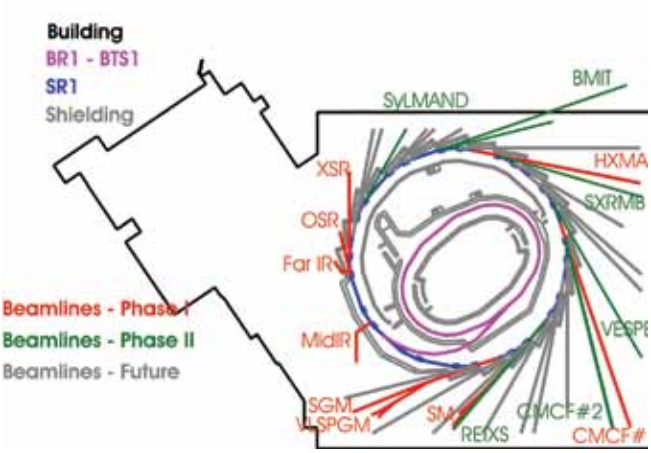
Overall this lively session demonstrated the strength of multifaceted approaches to the determination of macromolecular structure and dynamics.

Jack Johnson and Alex McPherson

Photo courtesy of Laurel Reitfort.

13.10: Canadian Light Source Symposium

The first light from the Canadian Light Source (CLS) 2.9GeV storage ring was detected in a diagnostic beamline on 12/9/03, and beamline commissioning began in January 2004. Papers with CLS data have now been published. Pawel Grochulski was an instigator for this session, which focused on the diffraction studies being undertaken and planned for the CLS, and the design and capabilities of the supporting beamlines.



Louis Delbaere started with an interesting historical account involving a lot of dirty laundry, and then described the protein crystallography undulator beamline (CMCF1), which is suitable for microcrystal and MAD studies. He indicated that it will be accepting research proposals early in 2007. **Ernst Bergmann** described CMCF2, a high throughput macromolecular facility with a novel high throughput peer review system, and an innovative data management system. **Brian Shilton** taught us how SAXS can be used for determining models of protein shapes in solution, before and after ligand binding, as well as crystal packing effects. Technical details were supplemented in each talk with some very nice structural studies. Three of Canada's younger researchers, **Andy Lovering**, **Desiree Fong**, and **Alex Ghetu**, also gave excellent presentations on their protein and protein complex systems. The CMCF beamlines will be busy.

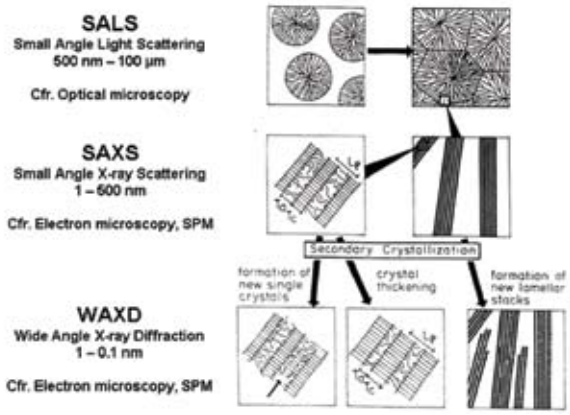
A review of the the materials and chemical crystallography projects underway at the CLS followed. **Serge Desgreniers** told us about a high energy diffraction setup for extreme environments at the end of the EXAFS (HXMA) beamline. He showed amazing images of oxygen as it went through phase transitions as the pressure and temperature increased, ending up in a metallic state! **Stefan Kycia** outlined the plans for the Brockhouse Sector for hard x-ray materials scattering and diffraction experiments, to be located beside the BMIT imaging facility. It incorporates an undulator and a wiggler in one straight section, as well as a bending magnet line. Micro and anomalous single crystal scattering, high resolution and extreme condition XRD, SAXS/WAXS, inelastic scattering, and reciprocal space mapping are all on the books.

We are all excited about the future of the CLS and how it will enhance our research efforts. Everyone is welcome to participate.

Lynne Howell and Jim Britten

Session 13.11: Combined Techniques in Materials Science

The first speaker, **Bart Goderis** (Belgium) discussed the complexity of polymer crystallization. It is necessary to distinguish structures at the various length-scales ranging from local crystal structure that coexists with amorphous layers to the larger scale crystallite size. A combination of wide angle x-ray scattering, small angle x-ray scattering, and small angle light scattering is used.The figure outlines the various experimental tools used to distinguish polymer morphologies at different length scales.



From Bart Godaris, Combined techniques applied to studying polymer crystallization.

R. Aravinda Narayanan (U.S.) continued on this theme by discussing changes to polymer mechanical properties by the addition of alumina nanoparticles as probed with both small angle x-ray scattering and x-ray photon correlation spectroscopy. **Bob He** (U.S.) provided a different perspective on the combined use of x-ray diffraction and Raman spectroscopy as non-destructive combinatorial probes, particularly for pharmaceutical applications. The microstructure of self-assembled amyloid peptides, such as those responsible for Alzheimers and related diseases, was discussed by **Sai Venkatesh Pingali** (U.S.) in particular focusing on the role of hydrophobicity/hydrophilicity on controlling ribbon size. **Peng Wang** (U.S.) an **Etter Student Lecturer Award** winner discussed his work concerning the characterization of epoxy-silane films being developed as anti-corrosion coatings using x-ray and neutron reflectivity. The use of fluctuation x-ray microscopy as a novel approach to probe medium range order in non-crystalline systems was discussed by **Lixin Fang** (U.S.) in particular focusing in on covalent networks and soft matter. **Qun Shen** (U.S.) showed that it is possible to distinguish orbital ordering from cooperative Jahn-Teller distortions through the use of three-beam diffraction and resonant scattering, and discussed the application of error correction algorithms to phasing near-field coherent x-ray diffraction data, in particular, for the special case of multiply-twinned lead microcrystalline particles. Poster **T-P007** by **Paul Fenter** (U.S.) discussed the ability to observe the distribution of elementary steps on single crystal surfaces using novel x-ray reflection interface microscopy and to determine their height using phase contrast.

Alec Sandy and Paul Fenter

13.12: Metal-Organic Hybrids- Crystal Engineering.

Pingyun Feng, Dwight Sweigart, Travis Holman, Chris Cahill, Seth Cohen, Sayon Kumalah, Jing Li.

The intent of this session was to highlight the inorganic components of hybrid materials and focus on ionic and covalent interactions as contributors to extended topologies. **Chris Cahill** led with a talk on f-metal containing hybrids that emphasized the tendency of Ln elements to polymerize into higher dimensional secondary building units when forming metal-organic frameworks (MOFs) or coordination polymers. In contrast, uranium tends to form polynuclear clusters which assemble into extended topologies. **Seth Cohen** (UC-San Diego) spoke on heterometallic metal-organic framework materials prepared using a metallo-ligand precursors. Specifically, the use of highly chromophoric metal centers as 'nodes' has resulted in compounds possessing enhanced thermal stability, spectroscopic behavior and anion exchange properties.

The organizers were able to obtain additional funding enabling **Dwight Sweigart** (Brown) to attend the meeting and present his work using π-bonded organometallic quinonoid complexes to direct assembly of higher dimensional solids. This was particularly appealing given the dominance of covalent, ionic and H-bonding interactions in this field. **Pingyun Feng** (UC-Riverside) presented an extensive class of chalcogenide materials based on variously sized tetrahedral and supertetrahedral Cd or In-S/Se clusters, and demonstrated how she used surface capping to functionalize these polynuclear clustersand ultimately assemble them into topologies of interest. **Jing Li** (Rutgers) brought us into the nano-regime with a lecture on tunable hybrid materials, specifically II-VI semiconductors. She was able to mimic quantum dots based on the inorganic layer thickness of ZnTe compounds assembled *via* diamine groups of variable length that serve as organic 'spacers.' She reported strong quantum size effects and little dependence on overall particle size.

Finally, **Sayon Kumalah** (Georgetown), who won an **Etter Student Lecturer Award**, discussed MOFs wherein metalated arylcarboxylates were used to produce Cobalt-grid compounds with functionalized channels.

Chris Cahill

13.13: Exploring structures from the near to the nanometer scale; PDF Analysis and SAS.

Shin-ichi Shamoto, Thomas Proffen, Katharine Page, Robert Papoular, Takeshi Egami, Reinhard Neder and Rex Hjelm.

Structure determination is usually based on the analysis of Bragg reflections yielding the average structure of the material. However, many materials are quite disordered or show limited long range order as in the case of nanomaterials. By analyzing the total scattering pattern one can obtain structural information as a function of length scale from the local structure to the medium and long range structure. The Pair Distribution Function (PDF) technique is a more and more popular way to obtain a picture of the "true" structure. PDFs can now be obtained covering atom-atom distances in excess of 15 nm, overlapping with the lower end of the length scale accessible by Small Angle Scattering (SAS).

Takeshi Egami (U. Tennessee & ORNL) gave an overview of the application of the PDF technique to disordered materials. He showed that the resolution of the diffraction experiment is related to the extent of the PDF that can be extracted. He showed an example of modeling domains in $LiNiO_7$ using PDF data to 20 nm. The data were obtained on the NPDF instrument at the Lujan Center at LANL. **Rex Hjelm** (LANL) gave a similar overview of SAS, showing that SAS measures the scattering length contrast of larger objects rather than the atomic level structure. **Reinhard Neder** (U. Würzburg) demonstrated how the PDF of nanoparticles can be refined using a full atom model and an evolutionary algorithm for minimization of the model parameters. Note that nanoparticles, depending on their size, contain only a few hundred thousand atoms, so that a complete particle can be modeled.

Lise Arleth (Royal Vet. & Agr. U.) discussed the experimental challenges as well as the advances in modeling of SAS data as applied to biological systems in solution. **Robert Papoular** (Leon Brillouin Lab) presented work on maximum entropy modeling for total scattering, and **Shin-ichi Shamoto** (Japan Atomic Energy Agency) gave another example of the application of the PDF technique to nanocrystalline samples.

Katherine Page (UC-Santa Barbara) presented "Structural Refinement of Nanoparticles Using Total Scattering," which won an **Etter Student Lecturer Award.**

Thomas Proffen

Thomas Proffen presenting Katherine Page with her award.

From the top left: Jim Pflugrath (Randy Alkire in background); Lee Daniels; Evi Struble and David Rose; Next: William Heller and Volker Urban; Xun-Li Wang and Claudia Rawn (above); Mark Arbing and Bill Furey (center); Bottom left: John DiMarco and Onome Ugono; Kurt Nienaber and Mike McDonough.

See page 7 for code identifying contributing photographers.

Crystallization of Biological Macromolecules: Poster Highlights

Both chemical and physical parameters are manipulated to crystallize biological macromolecules. One presentation that focused on chemical variables and another that focused on a physical variable both demonstrated success in the trenches.

Chemical variables, specifically the hypothesis that "various small molecules might establish stabilizing, intermolecular, non-covalent crosslinks in protein crystals and thereby promote lattice formation," were put to the test by **Bob Cudney** and **Alexander McPherson** (S-P201). Three separate studies were undertaken to test the effectiveness of 200 chemical additives on their ability to promote the crystallization of 81 different proteins and viruses. The experimental design was novel in its simplicity. To reduce variables and truly test the ability of the small molecules to promote lattice formation; the experiments were set up using only two crystallization conditions: 30% PEG 3350 and 50% TacsimateTM, both buffered at pH 7.0. The 200 chemicals were combined to form reagent mixes containing 3 to 20 different chemicals.

From Bob Cudney: Crystal of bovine ribonuclease A grown in PEG 3350, poly-L-lysine, poly-L-ornithine, poly-DL-alanine.

None of the details of this study were hidden. All 200 chemical additives and the results of the 18,240 manually delivered vapor-diffusion experiments (that's right – no robots) were presented in several tables (note – nearsighted people had a distinct advantage reviewing the results presented in these tables). Tabulated results were very clearly stated. Overall, 65 of the 81 samples were crystallized. It is important to note that 35 of these 65 samples required one or more of the chemical additives to crystallize, which demonstrated the importance of these chemicals to promote crystallization. The results indicated that polyvalent, charged groups (di- and tri-carboxylic acids, diamino compounds, molecules with sulfonyl or phosphate groups) and common bio-chemicals (coenzymes, biological effectors and ligands) were the two most promising types of reagent mixes. Less promising results were observed with osmolites, polyamines, detergents and sugars.

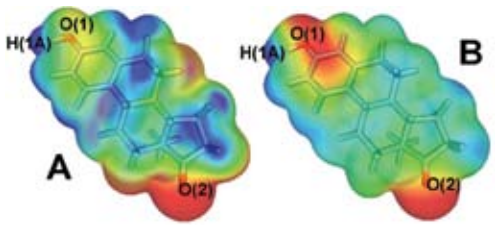
These experiments demonstrate a fundamentally different chemical approach to screening and identification of crystallization conditions. Two simple cocktails were used to promote supersaturation of the protein molecules while simultaneously using low concentrations of "silver bullets" to promote lattice formation/crystallization. The method has the potential to be adapted and tested *en masse* by the crystallization community. If this approach proves as effective in the hands of the many as it has in the hands of these two researchers we will experience the excitement of that first glimpse of a crystallized sample more frequently and with less effort.

Physical variables also play an important role in crystallization. The effect of one such physical variable (stirring) on the crystallization of Hen Egg White Lysozyme was investigated and the results presented (**S-P177**, **Ryota Murai** *et al.*). This is not the first time stirring has been presented as a physical variable; likewise it certainly is not the first crystallization experiment to use HEWL. However, the importance of producing large crystals of biological macromolecules for neutron diffraction is a topic of increasing interest and relevance. This method may be used to produce such crystals and therefore is worthy of mention. In this study, the protein concentration was varied along with temperature to control the level of supersaturation in the crystallization solutions. The plates were stirred (at either 50 or 100 rpm) on a rotary platform. The effect of stirring on the crystallization trials was dependent on the level of supersaturation. At high levels of supersaturation there was a significant reduction in the number of crystals produced and a subsequent increase in the size of the crystals in stirred versus static plates. No effect was observed when the crystallization experiments were stirred at lower levels of supersaturation.

Joe Luft

Poster Highlights of Small, Service & Cool Posters

T-P171: Elizabeth Zhurova (U.Toledo) presented a charge density study of the important steroid estrone, from both experimental and theoretical approaches. The orthorhombic phase II was studied by x-ray diffraction at 20°K and compared to models from DFT calculations in both the solid and gas phases, allowing electrostatic potential distributions to be determined. This allowed a precise determination of the intramolecular O ··· O distance, which is important for estrogenic activity, as well as an assessment of the aromaticity of the A ring, which exhibits some bond localization. A surprising finding in the ESP distribution was a locally stabilizing H ··· H intramolecular bond path linking the A and C rings.



The ESP mapped onto the molecular surface, (r = 0.001 a.u.). A –experimental, B – solid state theoretical data; red: (-0.1 eÅ-1); green: (zero); blue: (0.1 eÅ-1). (-32.2 - 32.2 kcal/(e·mol).

M-P176: Marvadeen Singh-Wilmot (U. West Indies, Jamaica), presented a poster which demonstrated how crystallography is being used to enhance research and education at her university. Although the x-ray lab is a relatively new facility, it produces results which stimulate growth of active research projects, facilitate the birth of new research areas, and enhance the learning experiences of both undergraduates and graduate students by involving them in crystallography. Examples of recently determined structures were presented, including metal clusters and Ln(III) complexes as luminescent probes. Also presented were structures of plant natural products, a very important research area in the West Indies.

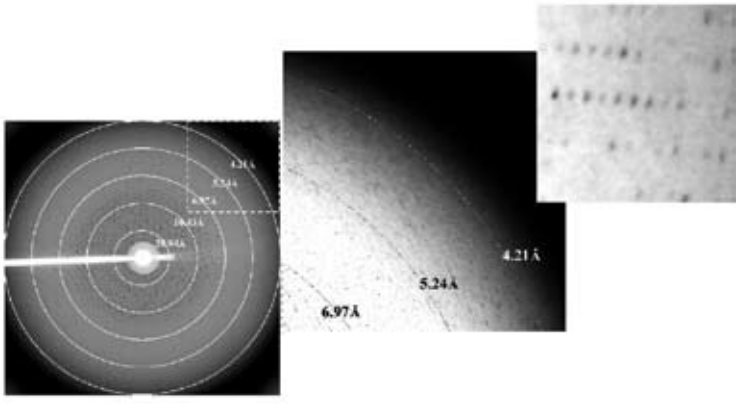
Frank Fronczek

Synchrotron Posters

Synchrotron crystallography facilities were well represented from the U.S. and beyond; some examples follow. News out of Brookhaven National Laboratory included the recent upgrade of National Synchrotron Light Source beamline X-25, described in poster **T-P025** by **Lonnie Berman** (and 23 co-authors!). As the first step in a multi-stage upgrade, the wiggler insertion device was replaced this past winter with a mini-gap undulator, which provides x-rays at double the flux and is continuously tunable over a 2-20 keV energy range. Additional improvements in the experimental station include the installation of motorized slits and an air-bearing omega axis with a miniature kappa sample mount. During the next phase, scheduled for January 2007, a new monochromator and mirror will be installed to take full advantage of the new source. Longer term goals for the beamline include the addition of microfocusing capabilities.

Two posters described some very interesting work at CHESS. In **T-P029**, **Marian Szebenyi** presented the initial steps in development of an Energy Recovery Linac as a new type of x-ray source. Advantages would include small source size, high coherence, high brilliance and very short pulses, thus allowing some experiments not possible at existing synchrotron sources. Still in the early phases of design studies and prototype fabrication, we look forward to hearing more about this project in the future. **T-P014**, presented by **Richard Gillilan**, reviewed use of capillary optics for microfocusing, now routinely providing 18 μm beams for very small samples. For accurate visualization and centering of such samples, the group is experimenting with the use of fluorescent dyes soaked into the crystals.

From the Advanced Photon Source, **Ward Smith** *et. al*, **T-P039**, reported on the progress of construction and commissioning at GM/CA-CAT, one of the newest PX facilities at the APS. See image at right from his poster.Their sector includes two independent beamlines from canted undulator sources, capable of delivering a focused beam 25 μm by 65 μm in size, and covering an energy range of 3.5-35 keV. So when can you use them? The 23-ID-D beamline was declared operational earlier this year, with 50% of beam time now available to general users. Beamline 23-ID-B is in the final commissioning phase and has begun taking some initial outside users; the line should be fully operational by the end of the year. At an additional bending magnet beamline, first monochromatic light was delivered this spring, with plans for full user operations by the end of 2007. All three beamlines will be equipped with ALS-style sample automounters currently under development.



Diffraction pattern of HK97 virus capsid crystal (a=b=1006 Å, c= 775 Å, λ=0.694 Å). Recorded at APS Sector 23, GM/CA-CAT undulator line focused at detector; 25 seconds 0.25 °exposure on MarMosaic 225mm CCD at 689mm distance. Courtesy of Lu Gan and Jack Johnson, Scripps Res. Inst.

In **T-P031**, **Randy Alkire** *et al* (Structural Biology Center), keeping a watchful eye on the quality of data at APS Sector 19, described their work on a real-time shutter timing monitor. All experimental shutters have inherent delays in operation, which can change over time depending on the condition and age of components. Having shown by simulation studies the observable effects of inaccurate shutter timing on data R-factors, this group has developed a system to continuously monitor shutter timing based on their existing beam position monitor design. They intend to track shutter function for all data sets collected and automatically alert users to detected shutter problems. Since the effect of timing problems becomes more significant with shorter exposure times, these are important considerations as synchrotron beamlines get brighter.

Numerous beamline upgrades at SSRL were presented by **Aina Cohen**, **M-P160**. Beamline BL7-1 has been upgraded to take advantage of the SPEAR3 source, including a new wiggler and optics now being commissioned. BL12-2, a new undulator beamline optimized for the most challenging experiments, is scheduled for completion next year. Recent enhancements to automation and remote access at the SSRL beamlines include automated sample washing and annealing, and improved sample illumination. Scientific capabilities will also be expanded by the availability of *in situ* UV/VIS spectrophometry on crystals during data collection. In a collaborative effort with groups at other synchrotron facilities, they also announced that the 'unipuck' sample holder, compatible with most auto-mounters, is in a version 1 testing phase, with production release planned for the fall.

With news from across the pond, **Jose Brandao-Neto** *et al*, **M-P158**, summarized progress and plans for the first macromolecular crystallography beamlines being built at Diamond, UK. Three Phase I undulator beamlines are under construction, equivalent in design and functionality, and tunable over the 0.5-2.5 Å range. On the experimental end, all three will have single axis air bearing goniostats, with on-axis sample viewing and ADSC Q315 detectors, and will be equipped with Rigaku ACTOR robotics. Beamline 103 will also accommodate category 3 pathogenic samples. Future MX beamlines now in the design phase include a fixed wavelength side station optimized for protein-ligand complex studies, as well as a dedicated micro-focus beamline.

Anne Mulichak

Material Science Posters in Honolulu

Two themes were apparent in the material science posters: utilization of high intensity, wavelength tunable x-ray and neutron sources and the extraction of much structural information from diffuse scattering.

Branton Campbell, **M-P106**, employed diffuse scattering measurements to explore local distortion modes in single crystals. Important to this procedure was his technique for accurately interpolating reciprocal space coordinates for every pixel of area detector data onto any desired reciprocal space coordinate system. Each point in the new coordinate system is a linear combination of points from the area detector data.

Claudia Rawn, **M-P088**, studied magnetic nanoparticles that have biomedical and engineering applications using time of flight neutron diffraction.

Miguel Castro-Colin, **M-P098**, employed pair distribution function (PDF) analyses of diffuse scattering from HgSe clusters in zeolites. Applications are related to the interaction of the clusters with visible light.

Jeff Deschamps, **M-P108**, demonstrated that diffuse diffraction data from liquid crystal elastomers could be analyzed in terms of periodic pair distribution functions (PPDFs). This new technique revealed structural information within the liquid crystal layers.

John Konnert

From Branton Campbell: Diffuse scattering distribution concentrated in the L = 5 plane of a natural single-crystal sample of zeolite mordenite. This Weissenberg-like image was extracted from a series of CCD images collected at beamline 33ID-D (20 keV) of the Advanced Photon Source. Three distinct features are evident: broad hazy patches, open diamonds, and star-shaped distributions around each Bragg peak. Each reveals an important component of what turns out to be a complex fault-defect architecture with implications for mordenite's adsorptive and catalytic properties. B. J. Campbell et. al., J. Appl. Cryst. (2004). 37, 187-192.

Poster Highlights

In **T-P003, Thomas Weiss** presented kinetics of formation of unilamellar vesicles, probed by time-resolved small-angle x-ray scattering. He mixed 50 mM+50 mM pairs of TTAB, TDMAO, LiPFO and LiPFOS. Then 100ms post-mix, he recorded images, at a 200Hz frame rate. He observed growth mechanisms and evolution of polydispersity. A growing disk bends over to decrease the volume of lipids in the energetic rim of the disk. Wrapping into a vesicle makes the rim vanish. **Divya Singh** showed analyses of lipid bicelles made from short and long chains (14C DMPC and 6C DHPC) in **T-P005**. At 10°C, the bicelles were discoidal, and the lipids segregated edge/center. At higher temperature, the lipids started mixing. Thermodynamics equations that would almost exactly model bicelle size (at 10°C) were proposed. **Dominika Borek**, **T-P221**, showed the structure of ytrL, a protein involved in sporulation in some bacteria. The molecule packs into the crystal in a fiber-like arrangement resembling a physiological fiber. The poster detailed difficulties in symmetry averaging, solvent flattening, and model building. **Urszula Derewenda**, **T-P215**, determined the structure of the longest coiled-coil thus far: 225Å for the dimer, 350Å for the tetramer. Every step of the structure determination repeatedly failed, (the long thin structure was hard to crystallize, and only the nth data set from selenomethionine crystals was usable to determine the Se sub-structure), but perseverance paid off.

Dan Anderson

Web Watch

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

Crystallographic Teaching:

Several crystallographers have recommended **http://www.ruppweb.org.**

Crystallography:

New Z' Website: Structures with Z' > 1 (i.e. more than one molecule in the asymmetric unit) are of intense current interest. As part of an Engineering and Physical Sciences Research Council of the UK funded project, a web site has been developed concerning these fascinating systems including an annotated database of structures with high Z' as well as an index of useful literature. Please visit **http://www.durham.ac.uk/zprime** for more details. ***(Editor's note: see news article, p. 13.)***

Louis Delbaere

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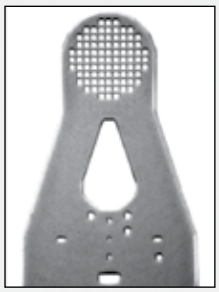

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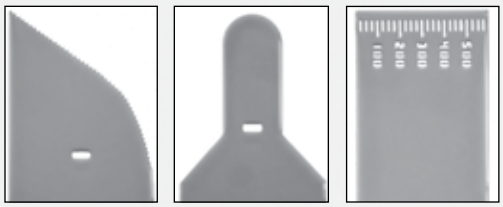

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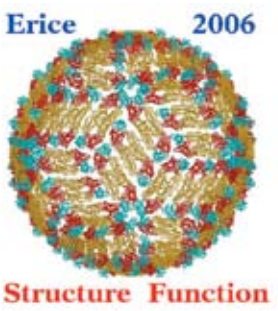
Structure & Function of Large Molecular Assemblies

The 38th International School of Crystallography course was held 9-18 June,2006 in Erice, that beautiful old city at the top of a mountain in Sicily. The organizer, Michael G. Rossmann, (at left) had also organized the first Erice meeting on Macromolecular Crystallography in 1976. At that time, Dorothy Hodgkin was the Director of the School, a role filled by Tom L. Blundell since 1982. Similar meetings occurred at six-year intervals. Paola Spadon and Lodovico Riva di Sanseverino (at right) have been the gracious local hosts for all of the meetings.



There were 152 participants from 28 countries, 60 oral presentations in 20 sessions, and 54 posters. A wide range of topics were covered, from structural investigations of small molecule interactions with proteins to multiprotein cellular assemblies, viruses and their interactions with host-cell receptors and antibodies, and even to entire cells. A fantastic array of new protein structures were presented; they had been solved using various experimental techniques including crystallography, electron microscopy, and nuclear magnetic resonance and single-molecule spectroscopic techniques. State-of-the-art advances in technology were highlighted, and limitations and challenges of the individual approaches were discussed.

Despite the enormous variety of biological systems described and investigated, a number of common themes emerged. Major advances have often been the result of close interactions among structural biologists using diverse techniques and biologists, chemists, and physicists - multidisciplinary collaborations can lead to great synergy. The "molecular machines" analogy linking the functioning of large multi-component assemblies with macroscopic machines was frequently invoked and the importance of understanding integration of the components was constantly emphasized. Beautiful computer graphics representations - both still and animated - of molecular and cellular processes were prevalent and left meeting participants with many vivid images of our expanding molecular atlas of living organisms.

Very exciting progress has occurred since that first macromolecular meeting in Erice in 1976. The macromolecular crystallography community was small then, and efforts were focused on studies of proteins with great natural abundance, a few tRNAs, and several plant viruses. Three-dimensional electron micrographic reconstruction techniques were in their infancy. In the intervening 30 years, numerous advances have revolutionized the field of structural biology at all levels. Recombinant DNA technology has made it possible to clone and overexpress even naturally scarce gene products in sufficient amounts for structural investigation, and improvements in microbiological and biochemical technology have permitted scale-up for production of high-quality samples for many purposes. The frontier in size for all structure determination techniques has expanded by orders of magnitude, resulting from technological advances such as synchrotron radiation, computer technology, superconducting magnets, algorithmic development in crystallography, NMR, and EM. What does all of this means for structural biology? ***More and better structures!***

A common theme emerged from the presentations and discussions: how our understanding of biology and biochemistry is constantly being reduced to molecular level explanations. Nowhere was this more apparent than with macromolecular structure and the role of conformational changes in regulating and promoting biological processes. Molecules are able to recognize each other through basic chemical interactions, but dramatic changes in molecular shapes can occur as a result of environmental factors such as pH, ionic strength, and the presence of other molecules including co-factors such as ATP, a common unit of energy currency in biology. A number of systems were described in which binding of ATP and other factors led to large conformational changes; subsequent chemical processing such as hydrolysis of ATP leads to regeneration of the original resting conformation. An interesting insight from these collective presentations is that whereas the largest conformational changes are often seen to occur upon binding of a co-factor such as ATP; the energy of hydrolysis is harnessed to bias directionality, and ensure time's arrow, rather than to cause large movements.

Speculations about prospects for the next 30 years of structural biology resulted in some questions: Will the popular subjects of detailed investigations be whole cells and collections of cells? What will be the focus of attention? Will crystallography still play a major role? Will experimental methods be sufficiently powerful to determine structures at an atomic level of detail from single copies of complex molecules? Will the structures and interactions of biological systems be computable from first principles and available knowledge of components?

Eddy Arnold

Photos courtesy of Eddy Arnold.

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23rd ECM, Leuven, Belgium

The European Crystallographic Meeting, August 6-11, 2006, had a very rich and diverse program covering all areas of crystallographic theory, instrumentation, technology and applications. There were six simultaneous sessions each morning and afternoon of the four-day meeting, of which two were devoted to macromolecular crystallography. Here are some of the highlights of the sessions I was able to attend.

Christopher Schofield (UK) reviewed the medical relevance of a newly discovered family of enzymes that hydroxylate proteins post translationally. **Bauke Dijkstra** (Netherlands) discussed the structure and catalytic mechanisms of three families of dehalogenases and their mechanistic and evolutionary relationships between one another and with three different subfamilies of short chain oxidoreductase enzymes. **Matthew Bochtler** (Poland) described DNA cleavage enzymes that are selective for palindromes and psuedo palindromes (odd numbered with the noncomplimentary base in the center). **Andrea Schmidt** (EMBL, Germany) discussed a ligand binding site buried below a protein surface. She was modeling the dynamic opening of the site based on the analysis of differential thermal motions of the residues in different domains of the structure.

Annette Hendricks (Denmark) described the structure of enzymes involved in lipid metabolism. She illustrated the similarity of proteins involved in the tetrameric structure of the first and third step in lipid biosynthesis (enoyl- ACP reductase and bk-ACP reductase.) In eukaryotes there are two ßk[acylACP] synthetases that elongate hydrocarbons of different lengths. **Casper Elo Christenson** (Denmark) is using structure determination to explain the differences in substrates specific to the two classes.

Federico Ruiz, (Spain) gave an interesting talk on neutron diffraction analysis of a fully deuterated aldose reductase. Ruiz described the advantages of using duterated proteins in neutron data analysis. The analysis brought to light greater detail in the active sites, enabling refinement of models for mechanism of action and for a disordered cystine accepting C-H··S bonds from the two carbons on the catalytic nicotinamide ring.

Maria Armenia Carrondo (Portugal) described the recent determination in her laboratory of ligand free and single stranded RNA bound forms of a ribonuclease. The elaborate, multicomponent complexes had many unusual and interesting features. The bound RNA was found in the inactive mutant form. It has three cold shock proteins (not two) and a bound single strand of RNA threaded through the multimer. Charge balance in the complex and whether there are really two Mg^{+} ions in the active site are controversial questions. So far only one Mg has been unequivocally determined by x-ray analysis.

Guido Capitans, (Zurich) gave a talk on chaperone-assisted assembly of type 1 pilus. This is a multi-domain membrane transport protein incorporating a stack of interlinking pieces, the assembly of which depends upon a chaperonin. **Patrik Cramer** (Germany) gave an amazing description of the complex assembly of proteins inside a water-filled single crystal of an RNA polymerase; he obtained excellent diffraction data on the complex.

Eight students were awarded poster prizes from the IUCr, the Cambridge Crystallographic Data Center, the RCSB-PDB and Oxyford Cryosystems.

Bill Duax

Top photo: CCDC Poster Prizes. In back, from left: Sam Hawksville (U. Shefield, UK) and John Liebeschuetz, CCDC; Sara Wishkerman (U. of the Negev, Beer Sheva, Israel), Emiliana D'Oria (Universität de Barcelona & CERQT Barcelona, Spain), and Teresa Duarte, Portugal, the judging panel chair, are in the front row. Sam, Sara and Emiliana were the prize winners.

Middle photo: Davide Viterbo, at right, who presented the IUCr poster prizes. Winners were: Maarten Dewilde, Katholieke Universiteit Leuven (Belgium); Sonia Hammer, U. of Frankfurt (Germany); and Andreas Lemmerer, U. of Witwaterstrand (South Africa).

Below left: The Oxford Poster Prize was presented by Bernard Tinart, Université Catholique de Louvain, to winner, Roeland De Borger, on left.

Below right: The RCSB-PDB prize winner was Gregor Hagelüken (on left), and it was presented by Bohdon Schneider.

Advances in Protein Crystallography

24-25 January 2007
South San Francisco, CA, USA

Welcome to the 4th annual Advances in Protein Crystallography conference and exhibition. As in previous years, we are organising influential speakers and high profile companies to join us at this event, which will be held once again at the South San Francisco Conference Center.

There will also be a pre-conference training course on Modern Protein Drug Target Crystallography held on 23 January.

Topics include:

- Protein Engineering for Crystallography
- Eukaryotic Expression, Membrane Proteins, and Post-translational Modifications
- Protein-ligand Complex Crystallization
- New Exploratory Concepts in Crystallization and Cryo-protection
- New Robotic Techniques in HTP Drug Target Crystallography
- Conquering Remaining Bottlenecks Towards Full Automation
- Efficient High Throughput Technology in Laboratories
- Next Generation for Crystallographic Software and Model Building Tools
- Novel Disease Targets
- Use of Target Structures in HTP Virtual Ligand Screening

Keynote Speakers

Dennis Danley, PhD
Principal Research Investigator,
Protein Chemistry and Structure
Pfizer Groton Research & Development

Katherine Kantardjieff, PhD
California State University - Fullerton
Professor of Chemistry & Biochemistry
Director, W.M. Keck Foundation for Molecular Structure

Zygmunt Derewenda, PhD
Professor of Molecular Biology & Biological Physics
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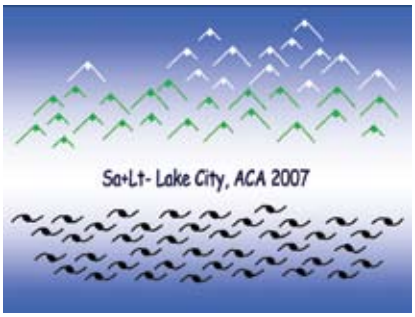

Abstract Deadline: March 1, 2007
Advance Registration Deadline: June 1, 2007
Advance Hotel Registration Deadline: June 13, 2007

The Call for Papers, on-line abstract submission instructions, on-line registration, and a preliminary meeting program are posted on the ACA website at: www.AmerCrystalAssn.org/. The 2007 ACA meeting will begin with workshops on Saturday, July 21. Symposia and sessions will begin on Sunday morning, July 22. Consult the Call for Papers for detailed information on workshops and sessions.

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Symposia:

The *Transactions* Symposium will be on Diffuse Scattering. It is being sponsored by the Small Molecule, Service Crystallography, Fiber Diffraction, Powder Diffraction, Materials Science, & Neutron Scattering SIGs.

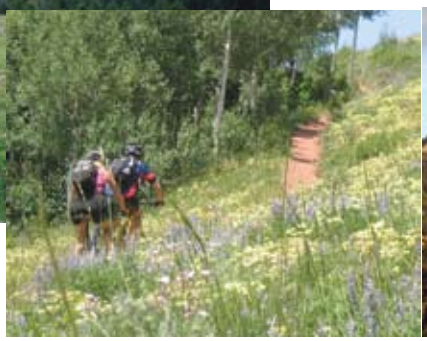
Fankuchen Award Symposium to honor Frank Herbstein, 2007 Awardee.

Trueblood Award Symposium to honor Angelo Gavezzotti, 2007 Awardee.

Jack Duntiz will help to organize the Fankuchen and Trueblood Symposia.

At right, Subway Canyon in Zion National Park; From left below: backpacking on Wasatch Crest Trail; bikers; Mount Olympus.

Photos courtesy of Heidi Schubert; her friend Mike Dropkin took the photo of bikers.



NOVEMBER 2006

17 **Protein Crystallization - Present and Future.** A one-day workshop in Hamburg, Germany. **www.proteincrystallography.com/event/default.aspx.**

JANUARY 2007

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

23-24 **Advances in Protein Crystallography**, South San Francisco, CA, **www.proteincrystallography.com/event/default.aspx.**

FEBRUARY 2007

19-22 **6th Pharmaceutical Powder X-ray Diffraction Symposium,** Barcelona, Spain.

MARCH 2007

25-29 **233rd ACS National Meeting and Symposium,** Chicago, IL. **www.chemistry.org/portal/a/c/s/1/acsdisplay.html.**

JUNE 2007

7-17 **Engineering of Crystalline Materials Properties: State-of-the-Art in Modeling, Design, and Applications**, the 39th crystallographic course at the Ettore Majorana Centre, Erice, Italy. **www.crystalerice.org/Erice2007/2007.htm.**

JULY 2007

21-26 **ACA Annual Meeting - Salt Lake City, Utah.** ***Local Chairs: Chris Hill (U of Utah, chris@biochem.utah.edu) & Heidi Schubert (U of Utah,* heidi@biochem.utah.edu*), Program Chair: Jill Trewhella (Univ. of Sydney, b2jtrewhella@usyd.edu.au).***

AUGUST 2007

13-17 **BSR2007: 9th International Conference on Biology and Synchrotron Radiation,** Manchester, UK. **www.srs.ac.uk/bsr2007/.**

MAY 2008

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

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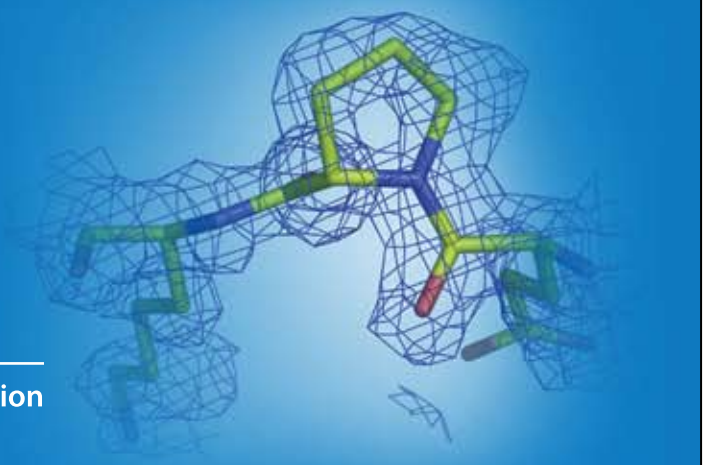

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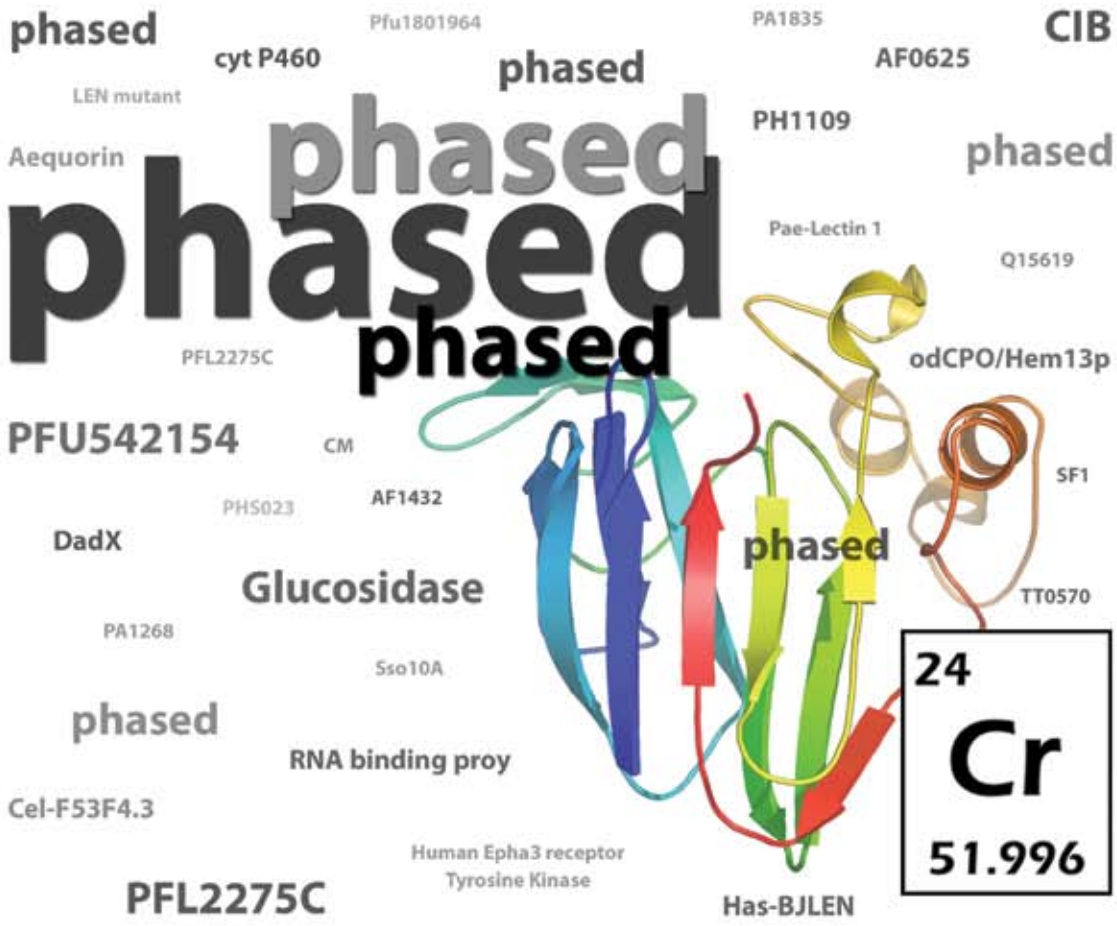

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