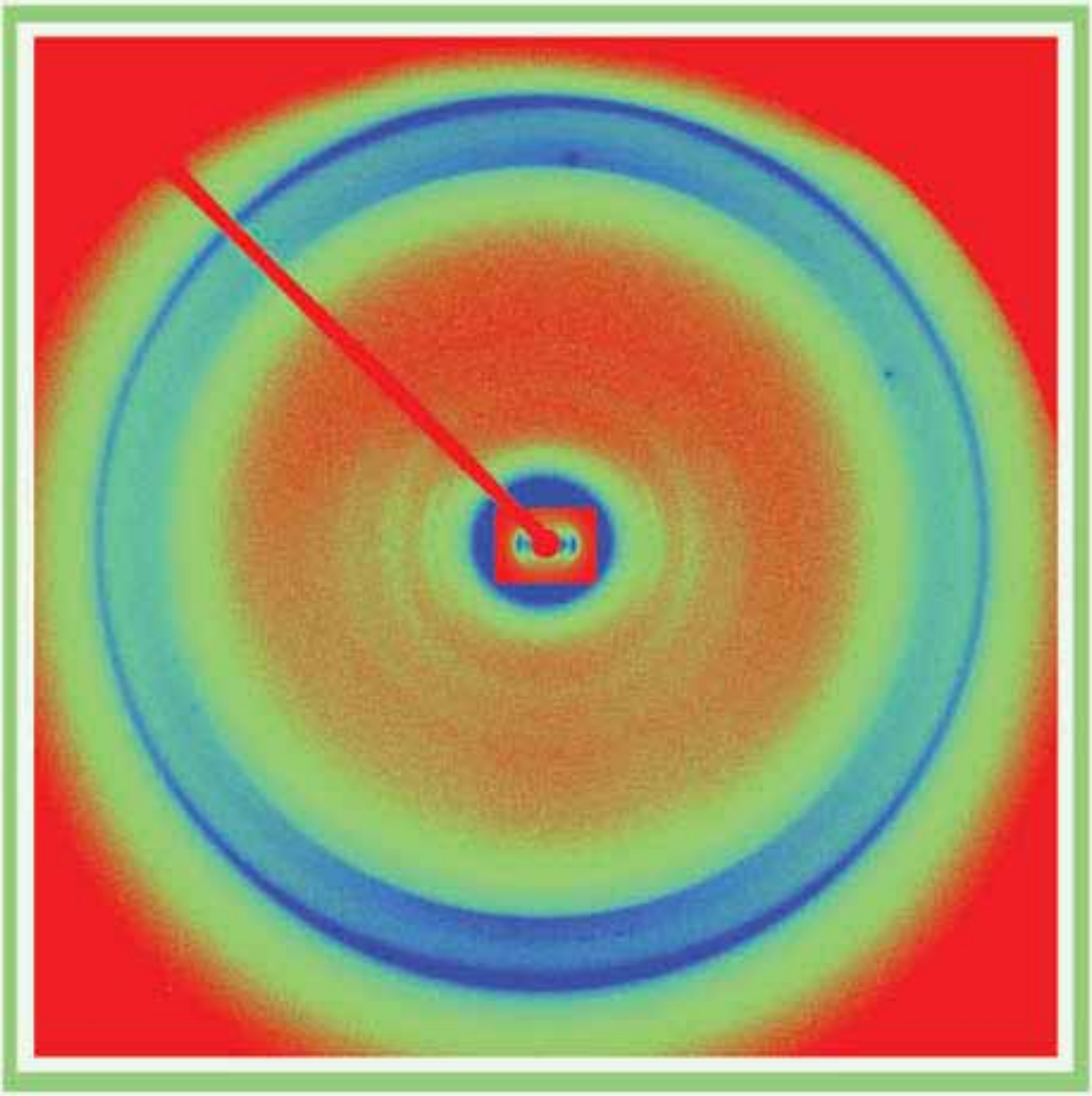
ACA RefleXions

American Crystallographic Association

Number 3
Fall, 2010



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The cover image was adapted from a slide shown by Gerald Stubbs in session 7.09 Fibril-forming Pathological Peptides: Prions, Amyloids & "Friends".

See page 8 for a more complete description.

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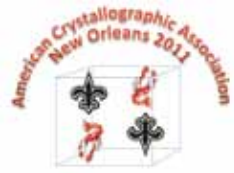

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Deadlines for contributions are: February 1 (Spring), May 1 (Summer), August 1 (Fall) and November 1 (Winter)

ACA RefleXions (ISSN 1058-9945) Number 3 2010. Published four times per year in the spring, summer, fall and winter for the membership of the American Crystallographic Association, P.O. Box 96, Ellicott Station, Buffalo, NY 14205-0096. Membership in the ACA includes a non-deductible charge of $1.75 from membership dues to be applied to a subscription to the ACA Newsletter. Periodicals postage paid at Buffalo, New York. POSTMASTER: Send address changes to ACA, P.O.Box 96, Ellicott Station, Buffalo, NY, 14205-0096.

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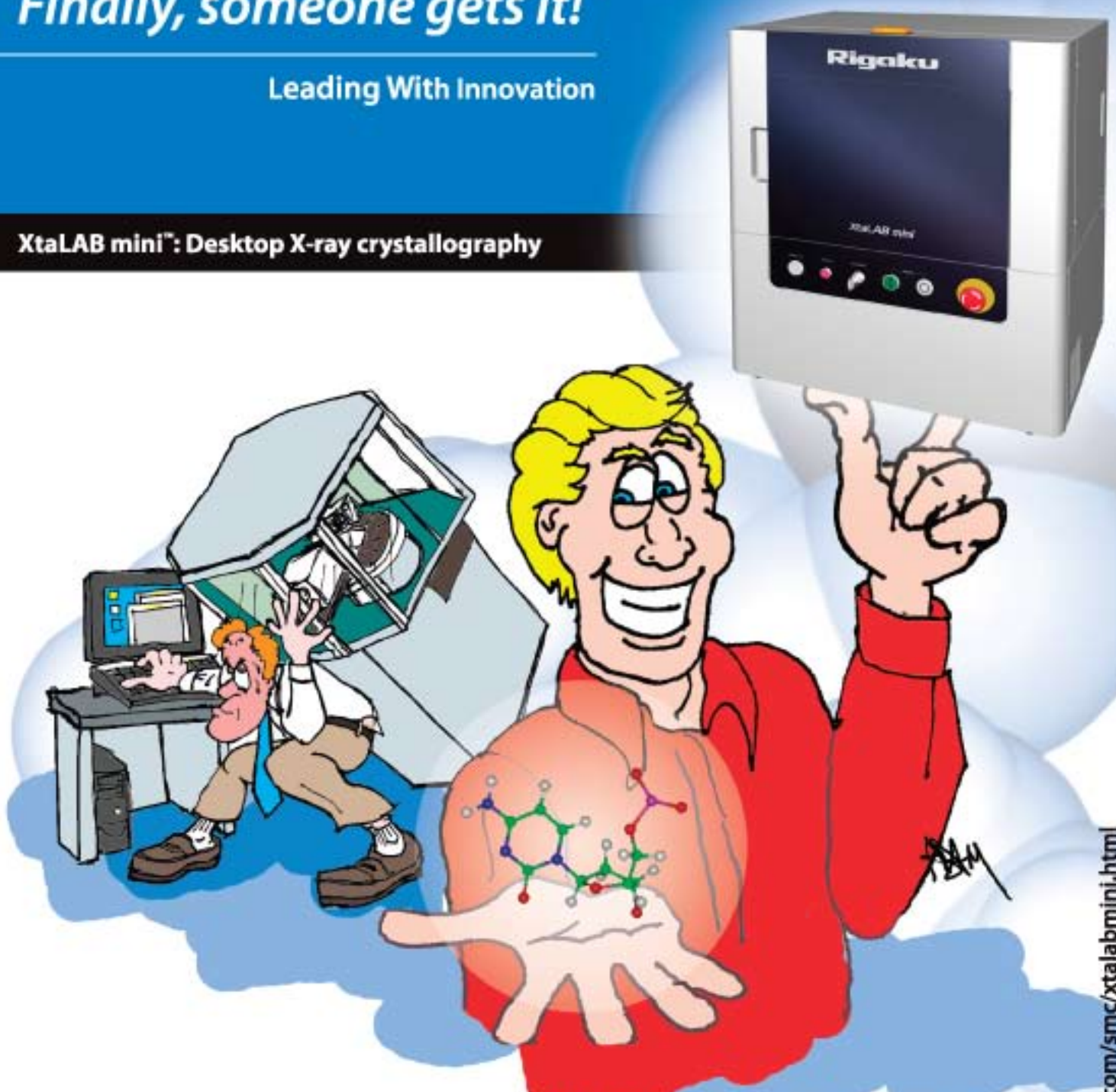

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When I ran for the Vice-Presidency of the ACA, no one told me how much fun this whirlwind was going to be. Here we are, just days back from our annual meeting in Chicago, and our *RefleXions* Editors are already getting reports in from Session Chairs. There is a lot about our 2010 meeting to celebrate. Those of you who were able to be in Chicago know how good the meeting was, and we owe a great deal to Ross Angel, the 2010 Program Chair, and Bernie Santarsiero, the 2010 Local Chair, and their teams. However, many of you might not know how successful it was in a number of respects. Torrential rains overnight on Friday closed O'Hare for a time and flooded roads to the extent that three giant carp made their way to Roosevelt Road via a storm drain, causing a unique traffic jam. In spite of this, only a few people were unable to make it to the Saturday workshops. Those that did slog their way to the on and off-site venues found the workshops stimulating and fruitful. This was especially true of the high school teacher workshop, which had been funded by the National Science Foundation through a grant to Cora Lind and by the USNCCr. The skillful presenters quickly overcame the intimidation factor that CRYSTALLOGRAPHY can engender when first encountered, and got the participants involved in the fun of symmetry, packing, and molecular structures. Summaries of the scientific sessions can be found in this issue; the workshop reports will be in the winter issue.

With 621 abstracts and 963 attendees, this meeting was among our very biggest. Two special guests attended, Carol Delbaere and Margaret Churchill, widows of Louis Delbaere and Bob Bau, respectively. They made our memorial sessions for Louis and Bob even more special by joining in our meeting. Margaret graciously endowed a new triennial award, the **Bau Neutron Diffraction Award** that will recognize exceptional research achievement in neutron diffraction. The award will be given for the first time in 2013 and will be coordinated by Tom Koetzle, Bob's long-time friend and colleague. We were also honored to have Mayor Daley's Commissioner of Public Health, Bechara Choucair, join us at the banquet, where he gave us official words of welcome and an invitation to come back to Chicago any time.

As they have for the last twenty years, AIP provided exhibits management services for our Chicago meeting. Over those two decades, the ACA Exhibit has grown in size and scope, and we are looking for more growth in 2011 in New Orleans. In an attempt to better serve our membership, we had survey forms in Chicago that asked for membership input on expanding the range of vendors at our annual meetings. We will have the space in New Orleans to add booths, so if you would like to see more microscopes, or powder mills, or peptide synthesis/sequencing equipment, or whatever, now is your chance to let us know what would be useful to you.

IUCr President Sine Larsen attended our meeting again this year. Sine reported that the IUCr is leading an effort to get 2013 officially designed by UNESCO and the United Nations as the International Year of Crystallography. This would coincide nicely with the centennial celebrations of the Laue (2012) and Bragg (2013) experiments. The ACA and the USNCCr have enthusiastically endorsed this effort. People interested in being involved or with ideas should contact an ACA council member. As an aside, the IUCr is urging all crystallographers to update their entries in the World Directory of Crystallographers.

Fred Dylla, Executive Director and CEO of the American Institute of Physics, also came to Chicago and met with the ACA Council so that we could discuss the benefits the ACA receives from AIP membership and the extensive support services that AIP can provide to the ACA. The ACA has been a member of AIP since 1966.

Proposals for 2011 summer schools are in hand, promising an exciting roster of options for next year, including small molecule and macromolecular oriented summer schools. A Call for 2012 Summer Schools is in this issue with a deadline for proposal submission of January 15, 2011. Members of the Continuing Education Committee and Marcia Colquhoun are happy to receive inquiries and provide guidance to people considering organizing a summer school. So, if you have an idea for a Summer School that you would like to try out, now is the time.

On a serious financial note, the ACA has experienced significant increases in meeting expenses over the years (about 50 percent from 2003 to the projected cost/attendee for 2011). These include increased A/V costs, telecommunications, credit card processing fees, coffee break expenses, etc. In addition, our meeting sponsorships decreased by 50 percent this year. As we presented at the Chicago Business Meeting, the Finance Committee recommended and the ACA Council approve a 10 percent increase in the membership dues (from $100 to $110 for regular membership) and meeting registration fees (from $450 to $500 for regular registration). These increases will take place in 2011. Late abstract fees will rise from $100 to $150. This decision was not made lightly, and we trust you will appreciate the need to keep the ACA solvent while bringing you the benefits and services that the membership deserves and expects.

Looking ahead to Boston in 2012, we will present the **Buerger, Warren, Supper** and **Etter** awards. The calls for nominations for these awards have a due date of April 2, 2011, (see the summer *RefleXions*, p 28). Please give thought to who might be outstanding candidates for these awards, and submit your nominations for these awards to Marcia Colquhoun (**marcia@hwi.buffalo.edu**).

The Nominations Committee for the 2012 ACA offices of Vice President, Secretary and Standing Committee Members has been formed and is made up of Marv Hackert, Bob von Dreele, and Gerald Stubbs. Please forward the names of any suggested candidates to them. Also, please remember to vote for the 2011 officers by November 15th.

Jen Shepard served recently as our ACA Web Manager and Membership Secretary, but she left the Buffalo office of the ACA

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as of August 1 to take up residence in North Carolina with her husband, Ben. Crystal Towns has been promoted to Membership Secretary, and we look forward to working with her in that new capacity. Council authorized a search for a third Headquarters staff member to take on Crystal's old responsibilities.

Lastly, a gentle reminder that 2011 is an IUCr meeting year, so our ACA meeting will take place in New Orleans from May 28 to June 2, 2011. The early registration deadline is March 31, 2011. Chris Cahill, our NO Program Chair, and Cheryl Klein Stevens and Ed Stevens, our Local Chairs, are already hard at work to be sure the high standards set by our 2010 meeting are met and perhaps exceeded. Hope to see you all in Louisiana in the Spring!

Judy Kelly

July 23, 2010 ACA Council meeting

President **Judy Kelly** announced that ***Keith Moffat*** will be the recipient of the ***2011 Patterson Award***. She went on to say that she has been made Co-Chair of the International Science Committee of the Council of Scientific Society Presidents.

Canadian Representative ***Jim Britten*** reported that:

1) The International Program Committee (IPC) for the 2011 Madrid IUCr Congress scientific program met in Madrid in May. The IPC has 3 Canadian members; Lynne Howell, Pam Whitfield and Jim Britten. The program is coming together on schedule and is waiting approval by the IUCr Executive Committee.

2) The second Chemical Crystallography Workshop (CCW) was held at McMaster University May 25-29 2010, as a satellite to the Chemical Society of Canada meeting in Toronto. The third CCW will be held at Université de Montréal.

3) The Mineralogical Society has named a new Argentinean mineral Cranswickite, in memory of Lachlan.

4) The reactor at the AECL Chalk River Neutron Diffraction Facility should be back online in a few weeks, but it is not clear how long it will be before diffraction experiments will be possible.

In his report as Financial Officer, ***S.N Rao*** said that a comprehensive employment tax bill had been recently passed in Congress that requires more stringent book keeping by not-for-profit scientific societies. Only reimbursements are now permitted. There can be no more waiving of registration fees for annual meetings - all awardees will have to pay up front and then reclaim. Award winners who are not US based will need a tax ID before award money can be turned over to them.

He reports that the Finance Committee recommended that 2011 dues should be raised by 10% across all membership categories, and that the ACA annual meeting registration feeshould increase by $50 for regular members (from $450 to $500), and proportionately for all other categories. The late abstract fee should be raised from $100 to $150. Council approved his recommendations.

Chief Executive Officer ***Bill Duax*** and Director of Administrative Services ***Marcia Colquhoun*** reported that the current membership of the ACA is about 1600. AIP member societies have one voting member on the AIP Governing Board for every 1000 members. Judy Flippen-Anderson is the current ACA rep to the Gov. Board and she has also been elected to the AIP Executive Committee. Charlie Carter will continue on the Governing Board as a non-voting rep from the ACA.

Marv Hackert, IUCr Representative, (Marv serves on the IUCr Executive Committee and the Statutes and By-Laws Committee), reported that following the recent discoveries of fraud, the IUCr is considering what actions should be taken to restore confidence within the scientific and crystallographic community. He also reported that the General Editor of the World Directory of Crystallographers, Iris Torriani, urges crystallographers to update/create entries.

Sine Larsen, President, IUCr, spoke about the upcoming 2011 IUCr Congress and General Assembly in Madrid. See Judy Kelly's comments in the President's column on the preceding page.

Since the current endowment is now self-sustaining, the ***Charles E. Supper Instrumentation Award*** will be placed on a triennial cycle with the other awards. The next ***Supper*** award will be in 2012 in Boston. The deadline for nominations for the ***2012 Buerger, Warren & Etter Early Career*** awards will be April 1st 2011, earlier than usual because 2011 is a spring meeting year.

In other meetings during the week it came up that the Continuing Education Standing Committee (CEC) has become unbalanced in its composition (3 small molecule members and 1 macromolecule member). Since a major task of the CEC is to rank travel grant applications, most of which are macromolecular in nature, this has become a real problem. Peter Müller, a CEC member, suggested that at each election candidates should alternate between macromolecule and small molecule practitioners, with the first being macromolecule. His suggestion was adopted.

The next ACA Council Meeting will be Saturday, October 9th 2010.

Carrie Wilmot

Reminder to Vote!

We are going GREEN for the elections this year. Each member will be mailed a postcard with instructions on how to cast an online ballot. We won't mail paper ballots or envelopes.

The deadline is November 15th.

The Bau Neutron Diffraction Award

Robert Bau (1944-2008) was an esteemed faculty member of the Chemistry Department at the University of Southern California from 1969 and President of the ACA in 2006. A much beloved teacher and mentor, Bob made major contributions to the development of the technique of single-crystal neutron diffraction and to its applications in chemical and biomacromolecular crystallography. **The Bau Neutron Diffraction Award** to recognize exceptional research achievement in neutron diffraction has been established by his wife, **Margaret Churchill**, with a request that **Tom Koetzle** design the award selection procedure. The **Bau Award**, to be presented triennially, consists of an honorarium of $1,500 in cash and reimbursement up to an additional $1,500 for travel expenses to accept the award and to deliver the award lecture at an ACA annual meeting. The first award is to be given in 2013.

Michael James Awarded Honorary Degree

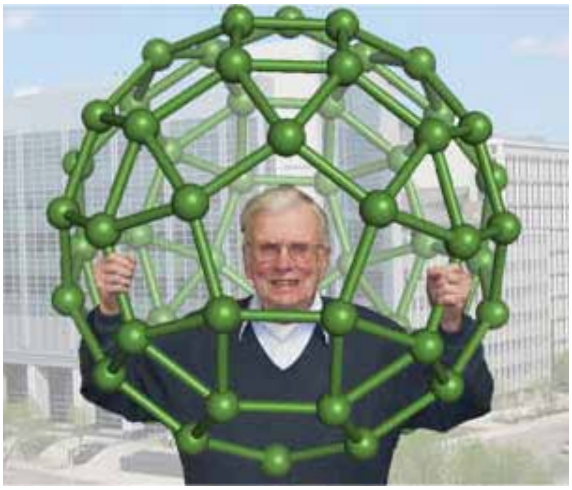
As a tribute to his leadership and contributions, the University of Manitoba awarded Canadian scientist Michael N. G. James of the University of Alberta with the D.Sc. honorary degree this June during their 132nd Spring Convocation.

Michael is known as the "father" of protein crystallography in Canada. He was the 2009 winner of the ACA M.J. Buerger Award. He studied x-ray crystallography with Bob Ferguson in the Department of Geology and Mineralogy, earning his M.Sc. in 1963. After obtaining his D. Phil. with Dorothy Hodgkin at Oxford University in 1966, he returned to Canada and in 1968 founded the first laboratory in the country devoted to the study of proteins by crystallography. Six years later, in 1974, James determined the first high-resolution crystal structure of a protein in Canada. In the years to follow James continued to establish protein crystallography in Canada, depositing over 200 protein structures in the PDB and training generations of graduate students and post-doctoral fellows, many of who are now leading researchers in the field.

Ludo Frevel Crystallography Scholarship

To encourage promising graduate students to pursue crystallography-related research, the International Centre for Diffraction Data (ICDD) has established the **Ludo Frevel Crystallography Scholarship Fund.** Multiple recipients are selected on a competitive basis, each receiving an award of $2,500. Since the scholarship's inception in 1991, $249,750 has been awarded to 109 aspiring crystallographers. **Applications for the year 2011 awards must be received by ICDD no later than 29 October 2010.** To qualify the applicant should be a graduate student enrolled in a graduate degree program during the 2011 calendar year, with major interest in crystallography, e.g. crystal structure analysis, crystal morphology, modulated structures, correlation of atomic structure with physical properties, systematic classification of crystal structures, phase identification or materials characterization. The term of the scholarship is one year, but a recipient may apply for an additional year by entering the subsequent year's competition. See the ICDD website: **www.icdd.com/resources/awards/frevel.htm** for more information.

Cotton Award to Larry Dahl



Lawrence Dahl, R.E. Rundle and Hilldale Professor of Chemistry at the University of Wisconsin-Madison, was named winner of the 2010 F. Albert Cotton Award. Funded by the F. Albert Cotton Endowment Fund and established by the American Chemical Society in 2002, the award recognizes distinguished work in synthetic inorganic chemistry, with special focus on creativity and imagination. Dahl, who is now a professor emeritus, was honored for the challenging synthesis and crystallographic characterization of large metal clusters, which has been his research focus for the past half-century. These molecules, which contain a record-setting 50-165 close-packed metal atoms such as nickel, platinum and gold, are possible precursors of new materials with useful catalytic, electronic, magnetic, and optical properties. His award lecture, *Nanosized CO/PR3-ligated clusters of zerovalent palladium..Structure/reactivity consequences due to ligand variations and heterometallic substitutions* was given as a plenary in the inorganic chemistry session during the 239th national ACS meeting in San Francisco, March, 2010..

Kavli Nanoscience Prize to Nadrian Seeman

The **Kavli Prize** is a joint venture between the Norwegian Academy of Science and Letters, the Norwegian Ministry of Education and Research, and the Kavli Foundation (US). The prizes in astrophysics, nanoscience and neuroscience are awarded biennially to recognize outstanding scientific research, honor highly creative scientists, promote public understanding of scientists and their work, and foster international cooperation among scientists. Among the eight 2010 Kavli Prize Laureates is ACA member **Nadrian Seeman**.

Seeman, the Margaret and Herman Sokol Professor of Chemistry at NYU and founding president of the International Society for Nanoscale Science, Computation, and Engineering, is recognized for his invention of structural DNA nanotechnology that could be harnessed to create raw materials for new nanoscale circuits, sensors and medical devices. Seeman's laboratory has constructed synthetic DNA sequences that are able to self-assemble into a series of three-dimensional structures. Programmed assembly of these synthetic sequences in a set order and orientation is a promising advance in the development of nanoelectronics. Seeman has also developed a type of DNA assembly line with colleagues at Nanjing University in China where one DNA walker molecule can move along another DNA track and pick up other DNA cassettes assembled on the track in a controlled manner. In this manner, novel nanoscale materials can be built efficiently.

Seeman shares this year's prize in nanoscience with Donald Eigler, of IBM's Almaden Research Centre in San Jose, "for their development of unprecedented methods to control matter on the nanoscale". The Laureates were honored at the Kavli Prize Award Ceremony and Banquet in Norway, September, 2010.

Argonne National Laboratory wins R&D 100 Awards

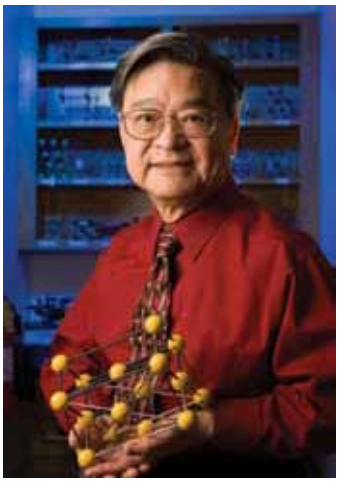
Widely recognized as the *Oscars of Innovation*, the **R&D 100 Awards** identifies and celebrates the most innovative and technologically significant products introduced into the marketplace and has long been a benchmark of excellence for industry sectors. On this year's list of the top 100 high technology products is the **Hard X-ray Mini-beam Quad Collimator System** developed by the Argonne National Laboratory in collaboration with the Life Sciences Institute of the University of Michigan. A breakthrough in protein crystallography, the collimator automates the process of switching between various micron-size x-ray beams. Previously, this switching of aperture sizes in collimating devices was done manually, slowing the research process and increasing risk of sample loss. The Hard X-ray Mini-beam Quad Collimator is compact, durable, economical, and its motions are reproducible and precise at the micron level. Furthermore, it can be placed on beamlines or other x-ray sources. The principle developers include ACA members **Robert Fischetti, Nagarajan Venugopalan, Ruslan Sanishvili, Michael Becker, Craig Ogata**, and **Janet L. Smith.** Argonne also won a second R&D 100 Award for the P Steradian Transmission X-ray Detector for Nanoparticle Analysis in Electron Optical Beam Lines. All award winners will be recognized at the R&D 100 Awards Banquet on November 11, 2010 in Orlando, Florida.

Catherine Drennan Reappointed by HHMI

In an attempt to improve the way undergraduates are taught science, the Howard Hughes Medical Institute (HHMI) created the **HHMI Professors Program** in 2002. Twenty accomplished research scientists who share a strong commitment to making science more engaging for undergraduates were appointed as **HHMI Professors**. These *Million-Dollar Professors* were each awarded $1 million over the next four years to bring the creativity they had shown in the lab to the undergraduate classroom. In 2006 the program was repeated. Twenty new professors were appointed and eight from the 2002 program received renewal awards. For the 2010 program, the existing HHMI Professors were invited to apply for four years of additional funding. Of the 30 who submitted applications, 13 were successful in obtaining a total of $9 million over the next four years. One of the continuing HHMI Professors from the 2006 program is ACA member **Catherine Drennan**.

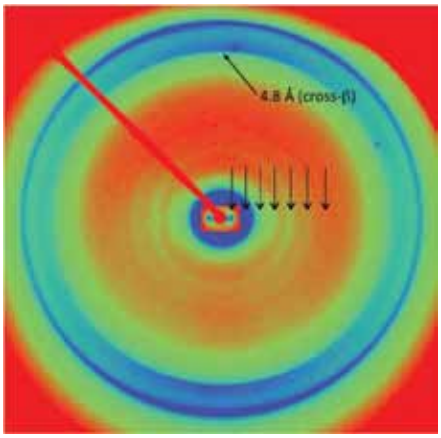
Drennan is a Professor of Chemistry and Biology and an HHMI Investigator at MIT. Recognizing the dissociation between chemistry and biology believed to exist among undergraduates and the negative long-term effect that this would have on the future of biological science, Drennan used part of her 2006 grant to develop resources that can be used to integrate biology and biochemistry into the general chemistry curriculum without removing any of the chemistry content. The remainder of the 2006 grant was used to develop a teaching assistant training "boot camp" for incoming chemistry graduate students. The 2010 funds will be used to improve and expand upon these areas both at MIT and at other institutions.

NIH Grant to UGA Researchers



B.C. Wang, the Ramsey-Georgia Research Alliance Eminent Scholar in Structural Biology at the University of Georgia, and four UGA colleagues have received a $1.47 million award from the National Institutes of Health. The award will be used to purchase a next generation, high-speed x-ray detector that will be housed at the UGA-operated **Southeast Regional Collaborative Access Team** research facility located at the **Advanced Photon Source, Argonne National Laboratory.** The new detector will optimize the facility, which provides data and structures to support more than 80 NIH-funded research projects aimed at understanding protein structure-function relationships and their mechanisms of action.

On the Cover



The cover image ***Diffraction pattern from an infectious mammalian prion sample*** was adapted from the slide at left which was shown by **Gerald Stubbs** in ***7.09 Fibril-forming Pathological Peptides: Prions, Amyloids & "Friends"***, one of the two sessions organized this year by the fiber diffraction SIG (see Joseph Orgel's report, page ???.)

Prions are associated with a variety of neuropathologies, including human Creutzfeldt-Jakob disease, bovine spongiform encephalopathy (mad cow disease), ovine scrapie, and others, as well as being related to the amyloids associated with many other diseases such as Alzheimer's and Parkinson's. In fiber diffraction from brain-isolated prions, meridional diffraction at 4.8 Å resolution shows the presence of the characteristic cross-β amyloid structure, long assumed but not previously confirmed; equatorial diffraction (arrows) implies a cylindrical shape consistent with a β-solenoid rather than a stacked β-sheet amyloid structure.

Diffraction data were collected at the Biological Small-Angle X-ray Scattering beamline 4–2 at Stanford Synchrotron Radiation Laboratory. Supported by NIH grants AG010770 and AG02132. The diffraction pattern was first published by Wille, Bian, McDonald, Kendall, Colby, Bloch, Ollesch, Borovinskiy, Cohen, Prusiner, and Stubbs, *Proc Natl. Acad. Sci. USA* **106**, 316990–16995, 2009.. © 2009, *PNAS*.

Dick van der Helm, University of Oklahoma George Lynn Cross Research Professor (retired after 40 years of service), passed away at his home in Cincinnati this June. Dick was born in Velsen in the Netherlands on March 16, 1933. He was awarded his University degrees from the University of Amsterdam, receiving his Candidaats (Chemistry/Physics) in 1952, and his Doctoraal (Chemistry) and Doctor (Crystallography) degrees in 1956 and 1960, respectively. He worked as a research associate at Indiana University from 1957-1959 and at the Institute for Cancer Research from 1959-1962. He then joined the OU Department of Chemistry in 1962 as an Assistant Professor where he developed his independent research program in single crystal x-ray diffraction of chelates and chelating agents and began his involvement in crystallographic computer programming. He was promoted to Associate Professor in 1966 and to Full Professor in 1969. He spent some time during 1969-1970 at the University of Groningen working in the field of protein crystallography. He was named a George Lynn Cross Research Professor in 1977 and retired from OU in 2002. Dick was still active as a research scientist even during retirement, and was appointed as an adjunct professor in 2002 in the Department of Biochemistry and Microbiology at the University of Victoria in Canada.

Dick in 1985 receiving the Oklahoma Scientist of the Year Award.

Dick was a recipient of an NIH Career Development Award from 1969-1974; he also received the Oklahoma Scientist Award in 1980 and the Oklahoma Chemist Award in 1985. He served on the USNCCr; on the AIP Committee on Public Policy, as Chair of the Small Molecule SIG of the ACA; and on several NIH grant review panels. Dick also organized a highly successful national meeting of the ACA that was held in Norman in 1978.

His major research areas encompassed studies of (i) siderophores, (ii) natural products from marine organisms, (iii) single crystal diffraction of N, S and P-heterocycles, and (iv) structural studies on cycloisomerism, cyclodiastereoisomerism and retroenantriomerism using cyclic peptides.

Dick was an absolutely fantastic mentor to many students, staff, and faculty. He will be sorely missed. Three years ago, the ***Dick van der Helm Undergraduate Summer Research Internship*** was set up by John Burks, one of his former undergraduate researchers.

Dick shared, a couple of years ago, a few stories of his time at OU in the form of a ***Life at OU*** article that we placed on his departmental webpage. It makes for very interesting reading indeed - see the following!

Life at OU by Dick van der Helm

When I arrived in the Department in 1962, there were only a few young and middle-aged faculty members. George Murphy, the Chair, was middle-aged and so was Harold Affsprung (who tragically died in a mountain climbing accident in 1967). The younger faculty members were Al Weinheimer, Sherrill Christian, Norman Fogel and Jordan Bloomfield (who left after a few years to join Monsanto). In the following years many new faculty members were hired (all as assistant professor). There was good cooperation between the older and younger faculty members, however the latter group was rather wild. Every interview for new faculty members was used as an excuse for a party, quite often at the house of Sherrill and Dee. There were also customs that no longer exist. Every year there would be a river bottom party organized by Phi Lambda Upsilon (PLU) society, at which there was no difference between faculty and graduate students. The only light came from a small fire and the moon and sometimes you had to wade through the water to reach the beer and the party. Strange things happened. Another yearly occurrence was the Professor Snarf contest, also organized by PLU. Erlenmeyer's with the name of each faculty member were set up at the entrance of the old building. Anyone could put money in the flasks. It took about a week and the last two days quite a bit of bills instead of quarters were spent The fun was that there was no telling if this was a popularity contest or just the opposite. The winner was sometimes quite confused about that ambiguity. I never got farther than second place, and the trophy for that was a huge railroad spike (it had also an obvious other name). I have forgotten what the trophy for first place was. Well it seems that both these happenings have been discontinued and were not considered professional (!). It was great fun, however.

A number of the older people were quite active in research and certainly all the others were. They were ambitious with their feet on the ground. The normal limitations, space, money and time were present. Two classes per semester was a minimum. Although I was educated in x-ray crystallography and physical chemistry I was hired in the Analytical Division (x-ray analysis, you see). It was safe for me to teach Instrumental Analysis and slowly I moved over into teaching only physical chemistry. When I moved to O U I was 29, and had two publications. I don't remember that this bothered me at all. In the 5 years that I had been in the U S I had spent a lot of time on programming. Two of these programs were the basic ones for crystallography, made for a new small computer. These are now part of the history of crystallographic computing. These programs were sent at no cost to many labs all over the world and had given me good name recognition. My laboratory had to be made from scratch, a stockroom, while also an elevator was being built (Annex). It took almost 2 years before I had a real lab and a manual diffractometer (with the help of GE and NIH) to take data. It was not until 6 years after I started at OU that the first

publications from the lab appeared (6), and I ended up with more than 325 publications, which have gathered more than 5000 citations in the literature. I had several good mentors, Caroline MacGillavry (she discovered M.C.Escher and his etchings) in Holland who made me enthusiastic for molecular structure determination, L.L.Merritt, Jr. (Instrumental Analysis book), at Indiana University who gave me all the responsibility in the lab for graduate students in crystallography and equipment, and A.L (Lindo) Patterson (every crystallographer knows his name) who taught me a lot of math (he always used a yellow block of lined paper and pencil and started with first principles without ever consulting a book). I still have these notes. He was a terrific teacher and great fun. I have had the pleasure and good fortune to work with many good and excellent students and postdocs, and it is not possible to mention them all here, but I remember them all clearly. I have listed all who worked in the lab if their work resulted in publications. I will mention a few. There was among the postdocs M.B.Hossain (Bilayet), known to everyone in the department; he worked from the middle sixties (with 2-3 years absence) all the while till 1997 when he retired from OU. He has more than 110 publications from the lab and taught many of the students crystallography. His first love, however, was politics and he was always ready for that. Another was M.A.F. Jalal (always known by his last name). He was in the lab 5 years and taught students and me biochemistry and molecular biology; his publications, mostly all written by himself, still shine in quality and clarity. But there were other postdocs. Larry Eng-Wilmot with his interest in siderophores; two excellent crystallographers Chuck Barnes (Missouri) and Doug Powell (now at OU), and finally Ranjan Chakraborty who taught us a lot of molecular biology for the membrane proteins and was an excellent microbiologist. Among the graduate students I can only mention a few. Steve Ealick was the best and the fastest. Both of us were hard-headed, but quarrels were over in one day because there was work to do. He had more than 20 publications from the lab. Two students were very courageous. Bill Franks, one of the first graduate students, had three children and organized his time for 7 days of the week and kept the schedule. The structure which he solved was the largest in crystallography that year. It learned us a lot about pleated sheets and we encountered the confusing fact that Pauling had used D-amino acids in all his models rather than L-amino acids. After his PhD he worked as a postdoc at Harvard. He could have had any faculty position but, instead, chose to commit himself to Langston University. Another was Xinhua Ji who lost 12- 15 years during the Cultural Revolution, but he spent all his energy to catch up and is now very successful at NCI. Then there were 7 students from TUB who did work in the lab that was published. All good students and three of them earned an MSc degree. For a while a trick was used so that research by undergraduate students could replace the second semester P Chem lab. Although other divisions could use it as well (spectroscopy was physical chemistry), after 10 years or so this opportunity was voted out (I now see that the organic division is doing a similar thing). It brought in a good number of excellent students, who with summer support from my grants, had a grand old time, and contributed in a significant manner to our lab. Doing real research where failure was a possibility, they experienced the pleasure of discovery. There were some 10 students among many more who did research which was published. I can only mention a few, for instance John Burks who did a number of structures among which was an important natural product for which the structure had eluded many people before, or Don Washecheck who later as graduate student at Wisconsin got his picture on the cover of C&E News. I hope that the tiles in our labs have been renewed because many champagne corks pockmarked them. Each structure that was solved required a celebration. Over the years my research changed although from the beginning to the end I was always involved in the structures of marine natural products in collaboration with Fritz Schmitz and Al Weinheimer. There also was always a collaboration with Darrell Berlin at OSU on biologically active synthetic products. However from peptide chelates I changed over to siderophores, iron transport compounds for ferric iron in microbes, partially due to the fact that I had an NIH Career Development Award from 1969-1974. The grant on siderophores I had continuously for 29 years. We started with the structures of siderophores then also their transport and finally during a sabbatical in 1984 I thought it possible to do the structure of the membrane proteins, which transport the ferric siderophores across the outer membrane in gram-negative bacteria. It took 15 years to publish the first structure and another 3 years for the second. The last years in collaboration with Hans Deisenhofer in Dallas. It was difficult, much more so than I anticipated, but very rewarding, and in the process I became more an "iron " man and less of a crystallographer. In my mind Sherrill Christian will always be remembered as the best faculty member we ever had. He was very bright, full of ideas, quick, enormously energetic, critical but positive and always ready for a conversation. I am thankful to all collaborators but most of all to all the students and postdocs. To work with them was by far the most fun. I also thank them for their patience with my impatience.

Dick and Allen Rees with the new CAD-4 low temperature diffractometer.

Remembering Dick van der Helm

It is sad for me to realize that Dick is no longer with us, but I am so glad I knew him. He was a good colleague in the early days of my career. Born in the Netherlands, he was educated at the University of Amsterdam where he worked with Professor Caroline MacGillavry. He then went to Indiana University, working as a postdoc for Lynne Merritt and then came to The Institute for Cancer Research in Philadelphia,

Remembering Dick van der Helm, cont'd

(Lindo Patterson's laboratory) in 1959 where he taught me the correct (Dutch) way to pronounce some of the local place names, such as the Schuylkill River. He was a valuable colleague, interested in deriving new ways of solving crystal structures and in writing computer programs for the determination and refinement of crystal structures. At that time crystal structure analysis was not very simple, but we were working in the laboratory of Lindo who had invented the Patterson function, and Dick showed how well such a map could be used to solve crystal structures. Lindo regarded Dick like a son and felt that he had contributed greatly to our appreciation of the power of the Patterson map (which Lindo called the "F-squared map"). Dick became very adept at solving crystal structures by Patterson methods, even if no heavy atoms were present.

Dick also encouraged us in our early attempts to use direct methods for structure determination. There was one structure that we worked on together but, because the chemical formula that had been provided with the crystals was not correct, gave us great difficulties. So we decided to try Harker-Kasper inequalities. This method involved U values and the scientific literature said it would only work if some of the U values were greater than 0.5. None were. So, Dick said to multiply all U values by 2 and then several of them met this criterion and we were able to solve the structure. Then, however, I had to present this structure determination at an ACA meeting. I was very nervous about it, but finally just told the audience what we had done, to Dick's great amusement. To my surprise nobody questioned us about this.

In 1960 Lindo Patterson acquired an IBM 1620 computer. This was a wonderful binary-coded decimal machine (produced by IBM between 1960 and 1970), so much easier to program than our Hollerith machine in which the pathway of each digit had to be wired into a plugboard (oh my aching fingers). The IBM 1620 was known as CADET (affectionately interpreted as *Can't Add Doesn't Even Try* because of the way addition, etc. was done). Dick and Lindo immediately started programming this new computer for structure factor calculations, electron-density maps and least-squares structure refinement (to mention just a few of the tasks they tackled). The then available Fortran processor took up half of the IBM 1620 memory (20, 000 digits) and so, to avoid this loss of space, they wrote the programs in machine language, filling most programming spaces. The programs were written so that they could work (in line with Lindo's stipulation) for all of the 230 crystallographic space groups, and were distributed (on paper tape) to crystallographic laboratories throughout the world. The Structure Factor Program and Least-Squares Sum Maker and the Three and Two Dimensional Fourier Summation Programs are still available on the Worldwide Web (as IBM 1620 source Code by Dick van der Helm). Dick's structure factor and least-squares program typed *And they all went to the* when the calculations began and then, when the calculation was complete, typed *the Seashore* (from Melina Mercouri's phrase in the movie *Never on Sunday*). The night watchman at the laboratory told us he was proud to have learned to turn the computer off when he saw the word "Seashore."

Dick was also interested in the uses that anomalous dispersion effects could provide in structure and absolute configuration determination. We were studying citrates at that time together with Carroll Johnson who had also joined the laboratory. Some of the naturally occurring derivatives of citric acid were ideal targets for absolute configuration determinations. We obtained the isomer of isocitrate that is active in the Krebs cycle and measured diffraction data for Friedel pairs for the potassium salt with chromium radiation. A sine Patterson map (suggested by Okaya and Pepinsky) was calculated for the chromium data and this gave signs for the Patterson peaks from which the absolute configuration could be found.

Dick then left for the University of Oklahoma where his work covered ferric ion-binding natural products and marine organisms, particularly those with potential anti-cancer activity. His work, in many cases, established a previously unknown chemical formula. Siderophores are produced by organisms in order to chelate any available ferric iron (which is essential for their survival). Dick told me that they can pull ferric iron out of stainless steel. This form of iron is less soluble than the lower valence ferrous state but is the one we have to use in our oxygen-rich blood stream. He extended his studies to those proteins that are siderophore transporters and receptors in bacteria and successfully studied several examples and provided some information on their mode of action.

Dick provided a fine example of a scientist to his students and he cared that they should be properly taught and well supported when they moved on to independent positions. He was intensely interested in new crystallographic methods and the analysis of the structural results he obtained. He was a hard worker and checked everything he did very carefully. His scientific and administrative advice proved invaluable to me, and, when Lindo Patterson died, he came back to Philadelphia to help me face the unexpected task of running the laboratory. And throughout his life he displayed a wonderful kindly sense of humor. Dick was involved with many of the early stages of computer and diffractometer use in crystallographic research and later became a worldwide acknowledged expert on the manner in which living organisms access and control iron utilization. He received many awards that indicate how much the scientific community has appreciated him.

Jenny Glusker

It is very sad to hear that Dick has passed away. We were friends since our student days at the University of Amsterdam in the early 50's. It was a time in which everything started to revive after the war years, and we were enthusiastically engaged in science, the profession very much in demand at the time. We were both inspired by Caroline McGillavry, an outstanding professor of crystallography. He decided to continue his career in the US, I came later but we met again on the east coast where he was working with Patterson in Philadelphia before coming to Oklahoma. We met for the last time in Norman in 2001, shortly before Dick's retirement. Dick was a person of great integrity which is more than evident in his scientific work. He will be missed by all of us.

Philip Coppens

David H. Templeton (1920-2010)

David died at the age of 90 at his house in El Cerrito near Berkeley, California. Just the evening before, he had a nice dinner with his son Alan who visited him and certainly did not expect his father to leave us so soon (although he tired easily). He survived his wife Lieselotte (Lilo), who died at the age of 91, by seven months.

I met David for the first time in 1972, in his office at the Lawrence Berkeley Laboratory, on the hill dominating the UC Berkeley campus. I arrived from Switzerland, shortly after obtaining my PhD from the ETH in Zurich, for a postdoctoral stay in David's laboratory. I immediately felt at ease around him with his soft way of speaking, his gentleman's manners, and his ability to make you laugh with some funny stories. I was also happy to meet the senior members of his laboratory, Allan Zalkin, Helena Ruben and Lilo, who was also part of the research team. I greatly benefited from their help and advice.

David received his Bachelor of Science *summa cum laude* in 1941 from the Louisiana Polytechnic Institute. While working on his Master's degree in chemistry at the University of Texas, David was drafted in 1943 and served in the Army Corps of Engineers. He was however soon reassigned to the Manhattan Project in Chicago where he met Glenn Seaborg, William Zachariasen and other leading scientists. It is certainly there that David got his first insight into crystallography and x-ray diffraction. I remember when David was discussing his Chicago period how impressed he was by the ability of Zachariasen, the author of the famous book, *The Theory of X-ray Diffraction in Crystals*, to identify compounds from a simple inspection of their powder diffraction patterns. Apparently the pre-computer scientists of that time did possess abilities that are missing today!

While in Chicago, Glenn Seaborg convinced David to come to Berkeley for his PhD once he had finished his Master's studies at Texas. David was apparently very successful in his research and completed his PhD in Chemistry in 1947 after just three semesters at Berkeley. He then immediately joined the college faculty.

Shortly after the war, the accelerators for charged particles, cyclotrons, synchrotrons, and other exclusive machines were the source of most of the newly discovered radionucleotides, and Berkeley was one of the most prominent centers in this field. David's first research studies examined radiochemistry. His publications with Isadore Perlmann and Glenn Seaborg were dedicated to the fission of various heavy metals by high-energy particles and to artificial radioactive isotopes. Together, they discovered a dozen new ones. In 1949, David published as sole author, *The story of radioactive isotopes*, a review describing the production and properties of neutron-deficient isotopes produced by high-energy bombardment in the 184-inch cyclotron. In 1951 a review article followed with Glenn Seaborg as a second author (Seaborg won the Nobel Prize for Chemistry that same year) concerning "radioactivity and nuclear theory," an obvious sign that Glenn recognized David's expertise.

David and Lilo in their office at the Lawrence Berkeley Laboratory.
Courtesy of the College of Chemistry, UC Berkeley.

The research on new materials produced at the Lawrence Berkeley Laboratory and the study of their properties could not be conceived without x-ray diffraction to characterize their crystal structures. David was soon given the assignment to start a crystallography laboratory. In this new unit, David and his graduate student, Allan Zalkin, published the first structural studies on a series of Rare Earth (RE) Tetraborides. In 1953, both authors published one of their most cited publications - 258 citations with an average of approximately 5 per year - on the structures of Yttrium trifluoride and related RE trifluorides. This remarkable piece of work illustrates the quality of their studies from Weissenberg and powder diffraction patterns recorded on films with visual estimation of the intensities.

Based on his experience working with heavy elements, David very soon realized the importance of obtaining precise atomic x-ray scattering factors close to certain absorption edges. In 1955, David published his first paper concerning the x-ray dispersion effects in crystal structure determination, which was immediately followed by his most cited paper (565 times) with Carol Dauben on the dispersion corrections for x-ray scattering of atoms from elements 20 to 96. These two papers dedicated to the topic of resonant (or anomalous) scattering marked a new orientation in David's career, which he pursued till the end of his scientific research activities.

In the early 1970s the SPEAR ring at the Stanford Synchrotron Radiation Lightsource (SSRL) was constructed, yielding intense synchrotron radiation. SPEAR was the new source of x-rays that David had been waiting for. The energy tunability of the source allowed crystallographers to extend their field of research by exploiting physical properties that were not possible from conventional x-ray tubes. In collaboration with James Phillips and Keith Hodgson from the department of chemistry at Stanford, David and Lilo published in *Science* their famous paper on the LIII absorption edge of cesium in which they showed that the change in scattering power was "approximately equivalent to removing a rubidium atom from the structure" by appropriate tuning of the wavelength. The importance of dispersion, i.e. the dependence of the atomic scattering on x-ray energy, was immediately recognized as a powerful tool in phasing macromolecular structures. David's scientific curiosity and his deep knowledge of diffraction theory was at the origin of his observation of x-ray dichroism (a change in absorption that

David in Paris in 1983, and David circa 1950. Courtesy of Michael Barnes at UC Berkeley, from the collection of Diana Killen and Alan Templeton.

depends on the polarization state of the incident beam) near the LI and LIII edges of uranyl, platinate and aurate, and the K edge of vanadium, bromate, bromide and iodate, properties which are closely related to the polarization anisotropy of resonant scattering and are expressed in terms of second rank tensors. David's continuing interest led him to discover some higher order effects in the anisotropy of diffraction in, for example, potassium chromate and germanate, where non-negligible third rank tensor effects could be measured. The last of David's studies dedicated to the anisotropy of resonant scattering was published in 1998. It is probably the increased traffic congestion on the Bay Bridge between the Berkeley hills and the Stanford storage ring that brought to an end his fruitful contribution to this field.

David's interests in research were by no means limited to the field of resonant diffraction. To mention just a few other topics, he published several studies showing how to improve the calculation of Madelung's constant for the electrostatic energy of ionic crystals. He was also interested in the problem of least-squares and the fixing of the origin in polar space groups and, in his last publication in 1999, how to improve the calculation of a full matrix in least-squares refinements. His life long collaboration with Allan Zalkin was a success story. The number of interesting crystal structures published by the team included a few noble gas compounds like XeF_4, XeF_5^+ and XeO_3 following Neil Bartlett's first syntheses. The structure and chemistry of the porphyrins were published with Melvin Calvin.

While I was preparing this article, I discovered David's very interesting contribution to the field of mathematical puzzles. Indeed, in Martin Gardner's book, *My Best Mathematical and Logic Puzzles*, the well known journalist for *Scientific American* mentions that David found a way to force a draw in the Hip game on an order-6 board based on symmetry arguments, a typical sign of David's ability to put theoretical considerations into practice!

The quality of David's work can be estimated from some bibliometric indices. His articles were cited close to 11,000 times, a record. He was cited about 200 times each year for the last 20 years!

David's scientific reputation attracted a large number of young crystallographers, doctoral students, trainees and postdoctoral fellows. He was very generous in giving advice and was the motivating source for many innovative studies by several visitors to his laboratory. It is not an exaggeration to characterize David's influence as the "David Templeton School". To cite just a few examples, Ivar Olovsson's collaboration with David and their studies on solid ammonia and various sodium chromate and sulfate polyhydrate were certainly the basis for Ivar's life-long interest in hydrogen bonds. Recently, the publication by Marc Schiltz and Gérard Bricogne: *Exploiting the anisotropy of anomalous scattering boosts the phasing power of SAD and MAD experiments* was dedicated to David and Lilo's pioneering studies.

In 1982, I had the pleasure of inviting David to give a series of lectures at the doctoral school of the physics department at Lausanne on the topic of anomalous x-ray scattering during the winter semester. One of the participants was Howard Flack, who was carefully listening to David's lecture on absolute configuration mentioning Roger's scale factor. The lecture was apparently well understood by Howard, who shortly afterward published what is now called the *Flack parameter* for the estimation of the enantiomorph-polarity character of some structures. David's series of lectures describing his experiences with, and the possibilities offered by, synchrotron radiation was also the inspiration for our laboratory's involvement in the creation of the Swiss Norwegian beam lines at the European Synchrotron Research Facility (ESRF) in Grenoble.

In 1977 the University of Uppsala recognized David's remarkable contributions to scientific research and education by presenting him with their Doctor Honoris Causa degree. In 1987 he received, together with Lilo, the ACA A L Patterson Award for their contribution to "Theory, Measurement and Use of Anomalous Scattering". In 1988, he was also selected to give the G.N. Lewis lecture of the College of Chemistry at the University of California, Berkeley.

David's management skills, diplomacy and sense of fairness helped him greatly in serving as Dean of the College of Chemistry between 1970 and 1975, a particularly tumultuous period on the Berkeley campus. He was also president of the ACA in 1984.

One day before his death, David's son Alan was able to confirm for his father that the University of California had received the final installment of his contributions to establish an endowed chair for the College of Chemistry at Berkeley that will be known as the Lieselotte and David Templeton Chair in Chemistry. The Hewlett Foundation equally matched his contribution, making it a substantial and fully funded chair. Its purpose is to support a faculty member in chemistry, with preference for a woman who has growing children and who is trying to balance the demands of an academic career with raising a family - a challenge that was very familiar to David and Lilo.

I would like to thank Alan Templeton, Allan Zalkin, Ivar Olovsson, Ken Raymond, Michael Barnes and Mindy Rex for their kind help in preparing this article.

Gervais Chapuis

Editor's note: Contributions may be made in David's memory to the Lieselotte and David Templeton Endowed Chair, College of Chemistry, 420 Latimer Hall no. 1460, Berkeley, CA 94720-1460

Remembering David Templeton

I first met David Templeton in June, 1955, when I arrived in Berkeley to start graduate school in chemistry, and he was my course advisor. From the first it was clear that he was a perceptive, easy-going, and tolerant person, and he was willing to grant me leeway in course selection, though I'm sure that he watched carefully to keep me out of trouble. (I took courses in physics and math in both six-week summer sessions; opted to skip chemistry 114H (thermodynamics) and took a quantum mechanics course in physics instead; didn't teach freshman chem lab at all as a graduate student; and took my PhD oral exams in my first year, all rather atypical for a first-year student.)

When I was recruited for a postdoc on "the Hill" in March, 1958, David was one of the Nuclear Chemistry faculty who offered me the job. David, along with John Rasmussen, directed graduate students who worked with me doing nuclear orientation. I remember that David taught me to use a crystal goniometer, and he made a critical and ingenius design recommendation for my first Mössbauer spectrometer. He was delighted when his student Jim Haag got beautiful data aligning a cerium isotope (*Phys Rev 121, 591 (1961*). He was always generous with his ideas and asked nothing in return.

In the spring of 1971 David had become Dean of the College of Chemistry, and he had to find a new chemistry chair to replace Bruce Mahan, who was stepping down, so he asked the faculty individually for recommendations. I took a walk on campus before my meeting with him to decide whom I would recommend. To my surprise I realized, as I mentally eliminated my colleagues one by one, that I would be the one to draw the short straw (I suppose one has to be this dumb to be suitable for such a job). He confirmed this in our meeting an hour later. And here comes the part that displays his integrity and his loyalty to the university. He made it very clear to me that in taking the job I was making a commitment to improve the department, including enforcing Berkeley's very high standards for promotion to tenure. He was forthright, in other words, about disclosing the least pleasant aspect of the job. I always admired him for this, because I knew I would always have his support, and in the end the department benefited tremendously.

His creativity came to the fore that fall in a big way. By 1971 student protests were declining, and students were returning to the hard sciences to prepare themselves for careers. In Chemistry 1A, enrollment jumped from ≈1200 to ≈1800 (approximate numbers but not too far off) -and it was totally impossible to accomodate all students in our usual schedule because Chem 1A is a lab course and we just didn't have the facilities. David came up with the idea of adding lab sections in the evenings! Given that these were three-hour labs, this was very far out of the mainstream of traditional academic scheduling practice and there were plenty of barriers against this,-but it worked! Because Chem 1A was prerequisite for many other courses, a lot of kids were able to move their education along and graduate on schedule because of his idea. I helped make it work, as a foot-soldier, but he was the general and I'm sure that he had to move a few mountains to get it approved on campus (that was all above my pay grade).

Dave Shirley

Although I departed from Berkeley more than 55 years ago, I have a number of fond memories of David. Once when a chemistry professor of mine from Texas Tech visited me in Berkeley, David took off an afternoon to give him a tour of "the Hill". Knowing this professor, I am sure that was a treasured moment for him, and I am sure he talked about that at numerous classes back at Texas Tech. David always blended giving a small bit of crucial advice at a critical time with the freedom for me to learn on my own and even to pursue an idea or two that I had. I was always impressed with his brilliance, especially after one weekend when he went skiing. Upon his return, I excitedly told him that I had obtained data for a low-temperature crystal structure of sodium superoxide that he had predicted would exist. He, too, was excited and quickly grabbed a copy of one of his papers and read out his calculations of the data for the new crystal structure, which agreed perfectly with what I had found during his absence.

I find it remarkable that he would take the time, as busy as he was, to correspond with me at Christmas over a period of 56 years, and I was not even his first PhD research student!

Giles Carter

Other letters to Alan Templeton:

We were greatly saddened to learn from your kind letter that your father passed away last month and send you and your family our deepest sympathy. It must be particularly hard to have lost both parents within such a short time but, at least, it is comforting to know your father did not have to endure a lingering or debilitating illness.

We first met your mother and father at one of the early ACA meetings, most likely in the '50's, and immediately found we had much in common. My recollection of him outside the conference room at those meetings is that, rather than occupying the center of one of the informal and often brisk discussions that tended to form, he would characteristically stand a little aside with your mother although, as we all knew, he was well informed and entirely willing to respond most knowledgeably and graciously on any crystallographic matter *inside* the conference room. All who knew him at these meetings held him in the highest regard, with great respect for his views which were invariably carefully considered and exhibited deep physical insight. However, although remarkably well informed, he never pressed his views but, instead, was invariably the perfect gentleman.

Sidney C. Abrahams

I just returned from travels last night and got your message. I was saddened to hear of your father's passing. You have my sincerest condolences. As you can imagine he played a big part in my life and I consider him my academic father. I will certainly try to come up to Berkeley on September 25th for the memorial service, barring any unforeseen circumstances. One way or the other I will send or bring with me some of the memories of the great time I had in the Templeton lab.

I have also learned of your mother's passing last fall. Lilo was an important part of the lab, and I was very sorry to hear that sad

Remembering David Templeton, cont'd

news. I can imagine that it has been a difficult year for you, having lost two such wonderful people within the span of a year. The history that you assembled of your mother's life trajectory is fascinating - I previously had no idea of the details. When we used to have our afternoon tea in the lab, the discussions rarely went to family history, but rather were centered around current events and science.

I hope I get to talk with you at the memorial service for your dad, to find out how your life has progressed, and to reminisce about your parents.

Art Olson

I was a graduate student of Dave Templeton's from the fall of 1964 to the summer of 1968, and while he was an effective instructor and a wise and sympathetic councilor, what sticks in my mind is his subtle sense of humor.

For example, as program chair for the Feb. '68 ACA meeting in Tucson, AZ, he sent out "instructions to authors" on the format for their abstracts that included as an example the equation: $R = \sum |Fo|-|Fc| / \sum |Fo| = 1 + e^{i\pi}$, with an *Acta Cryst*. reference. When I suckered in and looked it up, I found an otherwise blank numbered page. Only then did I realize that thiswas his way of objecting to the all-too-common careless omission of the second set of absolute value signs in the numerator.

Then there was the seminar in which he likened x-ray crystallography to alpine skiing. The title escapes me, but the sub-title was "How to Break Your Leg on the Bunny Slope". He told the tales of the fluoride ion that completely vanished from the structure of LaF_3 (until a secondary extinction correction was included), the nice low R-factor obtained for some xenon oxide compound with one oxygen on the wrong side of a false mirror plane, and likened digital computers to the ski lift by saying that "While it gets you more runs during a day, it doesn't necessarily improve your technique."

He appeared to be quite delighted at the mystification and frustration his WWII draft board must have felt when repeatedly told that they couldn't draft him (?), but with no explanation or reason given. (He had been pulled out of graduate school and was part of the Manhattan Project in Chicago, analyzing metal samples for neutron-absorbing oxygen.)

But how many of his subtle jokes did I miss, and is he still grinning over those?

Barry DeBoer

Photo © The Ottawa Citizen

Editor's note: See Council Highlights, p. 4 - Jim Britten has learned that the Mineralogical Society named a new Argentinean mineral, CRANSWICKITE, in memory of Lachlan. An article about Lachlan by Armel LeBail and Ian Swainson appeared in the Spring 2010 RefleXions, page 13.

The following is from an article by Matthew Pearson and Zev Singer in The Ottawa Citizen, June 21, 2010:

OTTAWA - Lachlan Cranswick was a kind, shy and generous man, his older brother, Rupert, said Tuesday. Speaking by phone from Australia, where Cranswick is originally from, Rupert said he went through his brother's personal records earlier this year and discovered that Lachlan had been donating a lot of money to charities monthly. A few years ago, Lachlan also sent large sums to his brothers to help them support their families. "It was just unbelievable," Rupert said. "He was that sort of brother." He also said Lachlan was supposed to travel to Australia last month to visit his family. "I would have preferred another sort of closure, but at least we know where he is and we can bring him back to rest, bring him back to his family," Rupert said.

Lachlan, a National Research Council scientist at the Chalk River Laboratories, went missing in January, and his case baffled police. The 41-year-old physicist was unmarried and was last seen on Jan. 18. He appeared to have put out his garbage the next morning. Four days later, after he failed to turn up for a curling event, a search began. However, the trail was cold, with nothing to suggest either foul play or suicide. His wallet and laptop were in his unlocked home, and his car was parked there, too. Extensive ground searches using dogs and helicopters found nothing.

On Tuesday, though, Rupert said police had notified the family over the weekend that a man's body was discovered Friday in shallow water by two people canoeing on the Ottawa River near Welsh Bay, downriver from Deep River. Lachlan Cranswick's jacket and identification, including his Atomic Energy of Canada Limited photo ID badge, were discovered with the body, but police were still planning to do a DNA analysis to confirm the identification, his brother said. "It has hit the family very hard," Rupert said. "I suppose you always live in hope, but now it's a certainty that something happened. "He didn't deserve it. He was a very loving sort of brother."

Lachlan had two older brothers - Rupert and Noel - but their parents are deceased. The family is planning to have Lachlan cremated in Canada and to have his ashes sent to Australia for burial near his parents. Rupert said Deep River police and the OPP put a lot of resources into the investigation, stayed in regular contact with him and Noel and were helpful when each of them traveled to Deep River earlier this year. "I can't praise them enough, I think they've done a wonderful job," he said. Rupert described Lachlan as shy and private, but said he loved living in Deep River, where he moved in 2003. He loved his work at AECL and his involvement in a curling club in the area.

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Lodovico Riva Di Sanseverino (1939–2010)

Editor's note: the following is from J. Appl. Cryst. (2010). 43, 946

Lodovico Riva Di Sanseverino passed away on 18 June 2010 at the age of 70. Lodovico was Professor of Chemistry and Mineralogy at the University of Bologna and since 1974 had been the organizer of the International School of Crystallography in Erice. He was born in Palermo in 1939 and, after starting his chemistry career at the University of Palermo, he graduated from the University of Florence in 1962. After some periods spent in The Netherlands and in England, he pursued his scientific career as full Professor at the University of Bologna, starting in 1975. He died unexpectedly in hospital in Sicily a few days after closing the latest course of the Crystallographic Schools in Erice, which, also thanks to the invaluable collaboration with Paola Spadon, was the usual outstanding success. To underline the height reached by this 42nd course entitled '***Structure and Function from Macromolecular Crystallography: Organization in Space and Time'*** (directed by T. L. Blundell and M. A. Carrondo), three Nobel Laureates had gladly accepted to be teachers. Lodovico had decided not to return immediately to Bologna after the school, but to stay in Erice, because his support could be helpful to the next course, once again related to crystallography, namely ***'Structural and Molecular Archaeology'***, directed by G. Tsoucaris. We wish to remember Lodovico with the contented expression of the present photo, which was taken during the banquet of the XX IUCr Congress in Florence in 2005, when the Union presented him with an Award for Exceptional Service to Crystallography for his organization of the Erice Schools. Lodovico leaves behind his wife Fiorbellina, his son Clemente, his daughter Claudia and two grandchildren.

Carlo Mealli

I met Lodovico for the first time in 1973 at a crystallographic conference in Rome, and we soon became very good friends. My adventures with him in Erice and with the International School of Crystallography started in 1976 when I was a young student and I did help him then as the first "orange scarf". I remember very well how young I was and, I must confess, how inexperienced. He trusted me anyway and in 1994, I became officially the Executive Secretary of the School. In so many years of collaboration we really did enjoy working together; I can recollect many beautiful memories of him, -particularly his humor. I remember how important for him it was not only to try to guarantee Courses with a high standard of scientific content but also to create a friendly atmosphere among participants. He put great care into planning what he called "social events" aiming always to help the younger students to interact easily with the senior scientists. His main pride was to be able to cite a long list of scientists who started their career as "students" in Erice and later became "big bosses" of well renowned crystallographic labs, thanks to the links established in Erice. And he was also particularly proud of the fact that 15 Nobel Laureates were invited to contribute to the Courses *before* receiving their prestigious awards.

Lodovico at the Palermo airport with students (l to r) Fabio Nicoli, Elena Papinutto, and Federica Morandi. Photo courtesy of Frederic Vellieux.

I miss him very much, and I know that the Courses in Erice will never be the same without him. The cumbersome task of continuing his work remains with us, the Erice staff. We know very well that it is as impossible to replace his charismatic personality as it will be impossible to replace his talent for making everybody sing strange songs from everywhere in the world!

Nevertheless we will try our best to continue in his spirit, with the same care and the same love for Crystallography. Unforgettable Lodovico!

Paola Spadon

Lodovico singing in Erice. from Paola, and at right in the Marsala room with students Francesca Fabbiani and Burger Dittrich. Marsala room photo courtesy of Madga Korczynska, UCSF.

Gordon S. Smith (1928-2010)

Gordon died July 19, 2010 in Livermore California. Born June 10, 1928, he was the son of Blanche and Paul Smith of Kirkwood, Mo. He served two years in the Army stationed in Japan beginning in 1946. While serving, he played trumpet in a military band and a dance combo at the officers' headquarters. Gordon graduated from Washington University, St. Louis in 1952 and received his Ph.D. in physical chemistry from Cornell University in 1957, studying with J.L. Hoard in the field of crystallography. After several years at the Mellon Institute in Pittsburgh, Pa. where he collaborated with Leroy Alexander on accurate x-ray intensity measurements and an important redetermination of alpha-quartz parameters, Gordon came to LLNL in 1963 where he spent the remainder of his career until his retirement in 1994.

Gordon Smith campaigning for Livermore School Board. ***photo provided by Darren Smith.***

At LLNL, Gordon published structure studies of many intermetallic compounds as well as several actinide chlorides including $PaOCl_2$, $PaCl_5$, $ThCl_4$, and UCl_5. With Jagan Akella, Gordon performed diamond-anvil studies of elements at very high pressure including Th, U, and Am. An early synchrotron powder pattern study solved a long standing problem with the structure of BeH_2. In the late 1960's he collaborated with Q. Johnson and E. Kahara in an article published in *Science* describing *Automatic Determination of Crystal Structures*. Another forward-looking publication with Q. Johnson and G. McMillan presented the very first *Computer Drawn Stereo Movie of Crystal Structures*. One of his most cited works concerns a criterion for rating powder diffraction pattern quality and indexing, co-authored with Robert Snyder of Georgia Tech. *The Smith-Snyder Figure of Merit* is routinely cited to confirm correctness of unit cell indexing. A number of Gordon's publications dealt with powder pattern analysis, especially including indexing. He was Chairman of the Apparatus and Standards Committee of the ACA in 1969 and Program Chairman of the ACA for the 1974 meeting in Berkeley, CA.

Gordon was one of the scientists who initiated the renaissance of powder diffraction in the 1970s. This began with the development of laboratory computers allowing the automation of the powder diffractometer and the simultaneous evolution of large computers allowing in depth evaluation of powder diffraction standards. In 1978 he was a co-author of *An Analysis of the Powder Diffraction File*, an extensive study that led ultimately to the adoption, by the ACA and the IUCr, of *The Standard Form for Powder Diffraction Data*. This laid the groundwork for the expansion of the Powder Diffraction File from about 40,000 to more than 600,000 entries today.

During his near-half century in Livermore, he was active in local politics and civic affairs where he had a special interest in childhood education. He was an avid fan of jazz music and had an extensive collection of old records. He was also an accomplished writer of short stories. Gordon was preceded in death by his wife of more than 50 years, Renee Corey Smith. He is survived by his sons, Kevin Smith of Westport, CT, and Darren Smith of Newport Beach, CA; his grandchildren, Charlotte Smith, Oliver Smith and Aidan Smith and his brother, Howard Smith of Fremont, CA. We would like to thank Gordon's sons, Darren and Kevin, his brother, Howard, and Donald Sands for their help in preparing this material.

Quintin Johnson & Robert Snyder

Contributors to this issue

Sidney Abrahams, Randy Alkire, John Allingham, Sara Andres, Ross Angel, Megan Barker, Lesa Beamer, Christine Beavers, Donnie Berkholz, Emil Bozin, Jim Britten, Carol Brock, Sue Byram, Chris Cahill, Branton Campbell, Patrick Carroll, Giles Carter, Charles Carter, Jennifer Cash, Peder Cedervall, Gervais Chapuis, Yuan Cheng, Shan-Ho Chou, Rashed Chowdhury, Ed Collins, Marcia Colquhoun, Philip Coppens, Gérard Coquerel, Louise Dawe, Barry DeBoer, Carol Delbaere, Tom Emge, Larry Falvello, Philip Fanwick, Jim Fettinger, Barry Finzel, Frank Fronczek, Juanma Garcia-Ruiz, Anna Gardberg, Jenny Glusker, Brandon Goblirsch, Danielle Gray, William Heller, James Holton, Peter Horanyi, Ashfia Huq, James Hurley, Chris Incarvito, Thomas Irving, Michael James, Quintin Johnson, Andrew Jones, Renuka Kadirvelraj, Jim Kaduk, Katherine Kantardjieff, Wei Ke, Judy Kelly, Saeed Khan, Serah Kimani, Cheryl Klein-Stevens, Tom Koetzle, Eaton Lattman, Sukyeong Lee, Adam Lietzan, Cora Lind, Tony Linden, Alexander Mankin, Krystle McLaughlin, Carlo Mealli, Keith Moffat, Peter Müller, William Ojala, Art Olson, Joseph Orgel, Eric Ortlund, Allen Orville, Brian Patrick, Lois Pollack, Thomas Proffen, Donald Raymond, Joe Reibenspies, Ross Reynolds, George Richter-Addo, David Rose, Gerd Rosenbaum, Bernie Santarsiero, Amy Sarjeant, Art Schultz, David Shirley, Carla Slebodnick, Janet Smith, Stacey Smith, Eddie Snell, Robert Snyder, Holly Soutter, Paola Spadon, John Spence, Ed Stevens, Gerald Stubbs, Narayanasami Sukumar, Alan Templeton, Ray Trievel, Francis Tsai, Hiro Tsuruta, Jennifer Urban, Vera Vasylyeva, Bi-Cheng Wang, Xiaoping Wang, Manfred Weiss, Angus Wilkinson, Carrie Wilmot, Lin Yang, Victor Young, Bomina Yu.


Glen Nemerow

In Science August 27, 2010: **Glen Nemerow** and **Vijay Reddy**, Scripps, reported the x-ray structure at 3.5 Å of the 150 - megadalton hunam adenovirus capsid containing ~1 million amino acids. The crystal structures of the major HAdV capsid proteins, the fiber, the penton base and the hexon had been solved by others, and were used to derive pseudo-atomic models at 7-10 Å by CryoEM.The structure they solved is a recombinant HAdV-5 vector, (Ad35F) which has shorter fibers than the wild type HAdV. Details of their 12 year epic struggles with crystallization, diffraction, (which required hundreds of trips to the 23 ID-D beamline at the APS at Argonne), and structure determination of Ad35F are available in *Science* Online.They found that although the interhexon contacts were extensive and were augmented by the cement proteins, the interactions between the penton base and peripentonal hexons were rather tenuous. This favors efficient capsid disassembly and release of the penton complex during cell entry. Their Ad35F structure also gives insight about the folds and interactions of cement proteins with the hexon subunits. The improved knowledge of HAdV assembly from its individual capsid proteins is extermely important to the development of novel antiviral strategies to block infection at multiple cell entry steps.


From Stephan Harrison's Perspective in the same issue of Science.

Call for Summer School Proposals for 2012

The deadline for proposal submission is January 15, 2011. The members of the Continuing Education Committee (CEC), **William Furey, fureyw@pitt.edu; Peter Müller, pmueller@mit.edu, Allen Hunter, adhunter@ysu.edu;** and **Frank Fronczek, ffroncz@lsu.edu,** and **Marcia Colquhoun, marcia@hwi.buffalo.edu** are happy to receive inquiries and provide guidance to people considering organizing a summer school. Please also see **Hosting ACA Summer Courses**, written by William Furey for the CEC (fall 2009 issue of *RefleXions*, page 47) as the requirements & guidelines are outlined in that article.

Call for Nominations for ACA Offices for 2012

The Nominations Committee, **Marv Hackert**, **m.hackert@mail.utexas.edu**, **Bob von Dreele**, **vondreele@anl.gov**, and **Gerald Stubbs**, **gerald.stubbs@Vanderbilt.Edu** would be happy to receive suggestions for the 2012 ACA offices of **Vice President, Secretary**, and **Standing Committee Members**. The Continuing Education Committee, The Data, Standards & Computing Committee and the Communications Committee each add a new member every year. **Suggestions are due by February 1, 2011**.

Calls for nominations for ACA Awards

The **Martin J. Buerger Award,** the **Bertram E. Warren Award**, the **Charles E. Supper Instrumentation Award** and the **Margaret C. Etter Early Career Award** will all be presented at the Boston ACA meeting in 2012. **Please submit nominations for these awards by April 2, 2011**. Nominations forms and more details about the awards are on the website, **www.AmerCrystalAssn.org** and should be faxed to 716-898-8695, emailed to Marcia Colquhoun, **marcia@hwi.buffalo.edu** or mailed to: ACA Award Nominations, P.O. Box 96 Ellicott Station, Buffalo, NY 14205.

The *RefleXions* editors, Judy and Connie, are hoping someone will volunteer for the position of

Opinions Column Editor

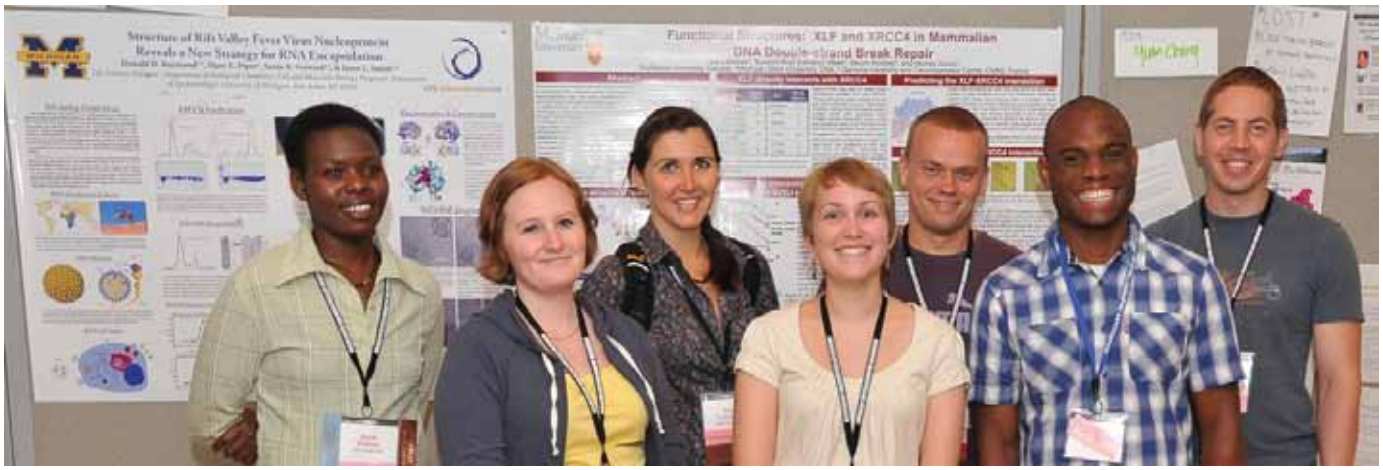
In the past our *Opinions* columns have featured two subjects: **Intelligent Design / the Evolution debates** and **Global Warming**. We can supply sources for both of these, and the column could consist of updates from these sources - or - the *Opinions* editor could choose another subject and put together something different. Please contact either editor (**conniechidester@earthlink.net** or **acareflexions@gmail.com**).

2010 Art in Crystallography Contest

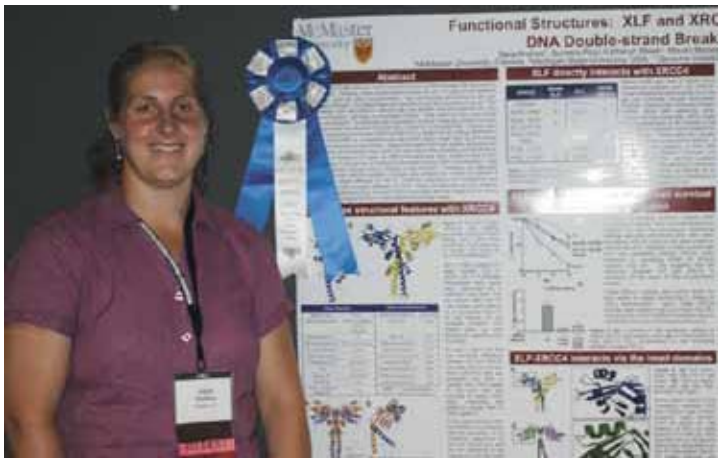
We are accepting entries to the 2011Art in Crystallography Contest in the form of images emailed to either editor (conniechidester@earthlink.net or acareflexions@gmail.com). Entries should be accompanied by a paragraph explaining the science and the method of producing the image. A photo of the artist would be appreciated but is not required. Prizes consist of small monetary awards and banquet tickets at the annual meeting. Winning entries will be posted on the web and will be displayed at the ACA Meeting. (Winners are not required to attend the meeting). We will also feature images in *ACA RefleXions* from time to time; the 2009 entries were featured on the cover of the *IUCr News* in issue 17, #2. Please let us know if you are interested in being a judge. The deadline for 2011 Contest is May 1st, 2011.

The next 39 pages are about the 2010 ACA meeting in Chicago, starting with the poster awards and continuing with photos of attendees, reports from session chairs, and images the speakers used in their talks. Except where noted, the ACA staff photographer, Peter Müller, took all the photos.

Bernie Santarsiero with the local committee: front row: Marta Witek, Mike Tuntland, and Anu Mittal; back row: Kent Truong, Jaime Torres, Shahila Mehboob. Not in photo: Hyun Lee and Rima Chaudhuri. The local committee took the group photos of speakers in the sessions on pages 26, 40, and 51.



Poster Prize Winners, l to r: Serah Kimani (RCSB -PDB), Jennifer Cash (RCSB -PDB hon.mention), Vera Vasylyeva (Oxford Cryosystems), Jennifer Urban (AIP), Andrew Jones (JCC), Donald Raymond (Pauling), and Peder Cedervall (Pauling). Sara Andres (Canadian Pauling), Yuan Cheng (RCSB -PDB hon. mention) and Brandon Goblirsch (IUCr) are not pictured..

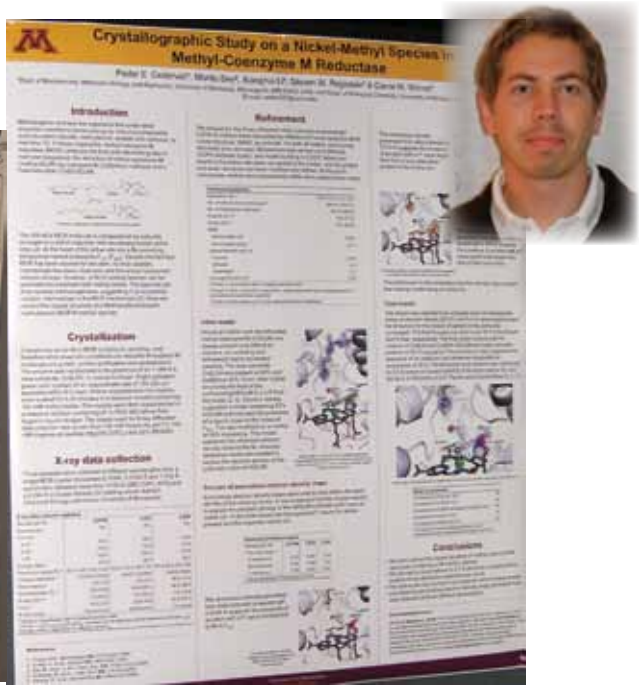


Above: Canadian Pauling winner* Sara Andres *with* S-232*: *Functional Structures: XLF and XRCC4 in Mammalian DNA Double-strand Break Repair.*

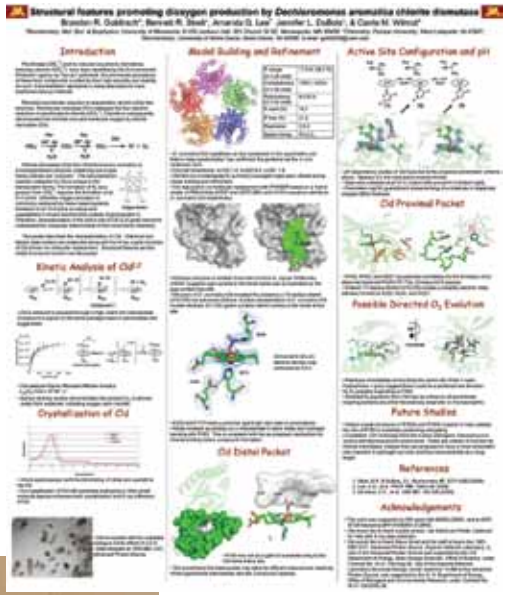
At the 2009 Toronto meeting, the ACA Council created a new volunteer position: **Poster Chair. Victor Young,** at right, organized the Poster Award Selection Committees this year.

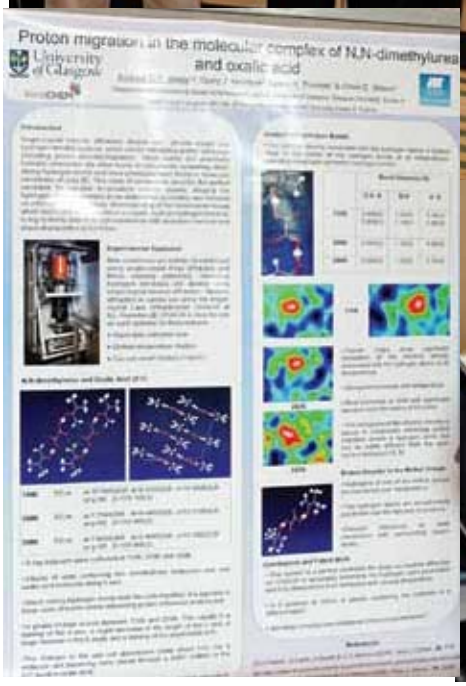
The Pauling Prize Winners were selected by **David Rose, Brian Patrick, Bernie Santarsiero,** and **Branton Campbell**. The ACA Pauling awards went to **Peder Cedervall (see below)** for **S-104**: *Crystallographic studies on two nickel-alkyl species in methyl-coenzyme M reductase* (below) and **Donald Raymond** (see corner left).

Below*: Donald Raymond *is describing* S-310*: *Structural Biology of Rift Valley Fever Virus Nucleoprotein* ***to Donnie Berkholz.***



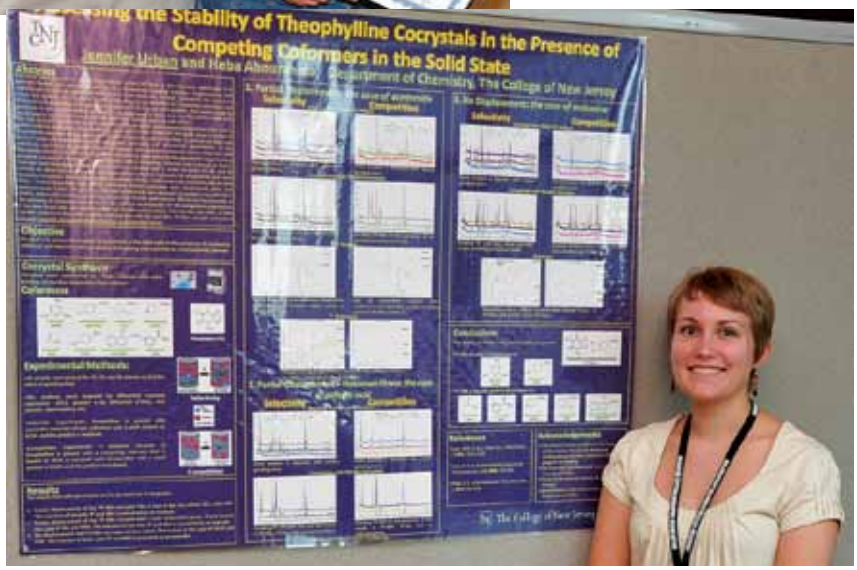
David Rose, Brian Patrick, Bernie Santarsiero, and **Branton Campbell** also selected the IUCr Poster winner. **Sine Larson**, IUCr President, with **Branton** and **Victor Young,** is seen at right looking up to **Brandon Goblirsch,** who won for **S-041**: *Structural features promoting dioxygen production by Dechloromonas aromatica chlorite dismutase*, shown below.

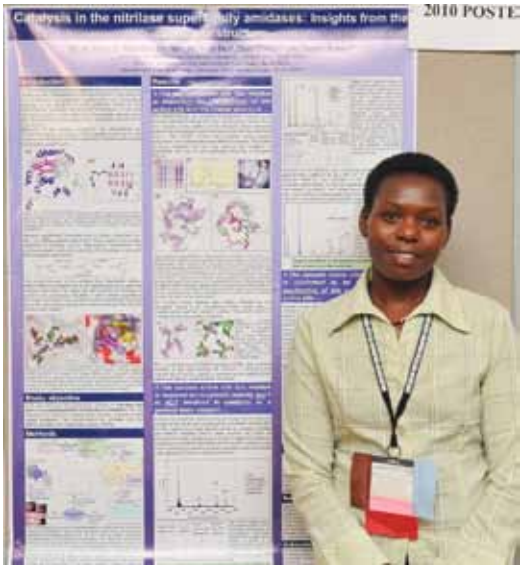




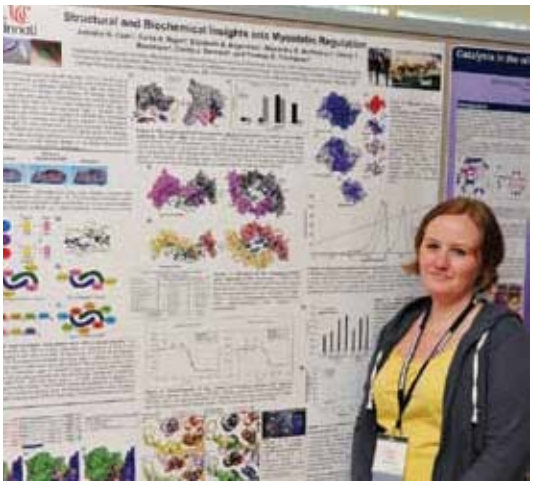
The ***Journal of Chemical Crystallography*** Poster Prize went to **Andrew Jones**, shown receiving his award from **Patrick Carroll** at the banquet. (**Louise Dawe** and **Phillip Fanwick** were also on the JCC Selection Committee.) Andrew's poster, **S-241**: *Proton transfer in molecular complexes of urea and its derivatives* is shown at left.

The **American Institute of Physics** Poster Prize Selection Committee, **Katherine Kantardjieff, William Ojala** and **Tom Emge**, chose **S-196** by **Jennifer Urban**: *Assessing the stability of theophylline cocrystals in the presence of competing coformers in the solid state*. Jennifer is shown at right with her poster.

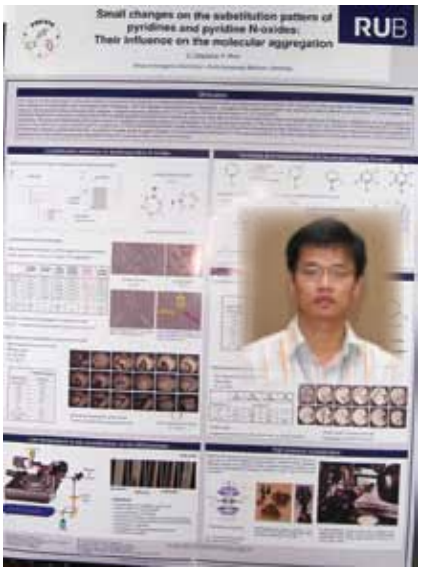




The RCSB Protein Data Bank Prize Selection Committee: **Michael James, Cheryl Stevens, Bi-Cheng Wang, Eric Ortlund**, and **Charles Carter** chose poster **S-068** by **Serah Kimani**: *Catalysis in the nitrilase superfamily amidases; implications from active site structure* as the winner. Serah is at left with her poster.

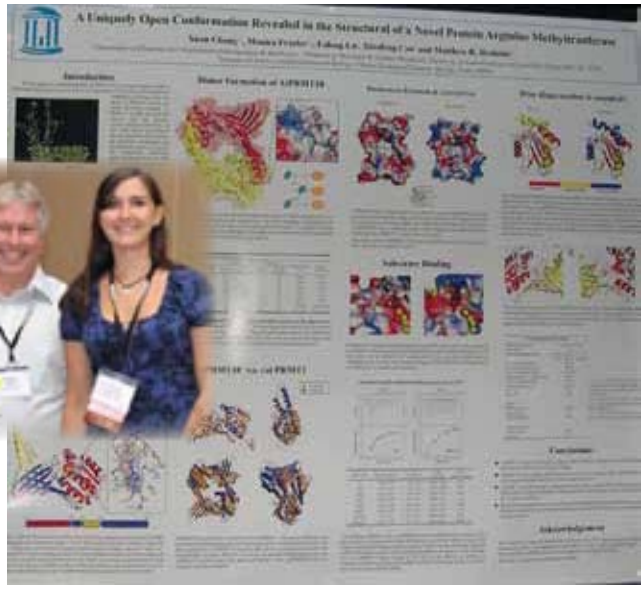


Honorable mentions went to **Jennifer Cash** for **S-322**: *The Structure of the Muscle Growth Inhibitor Myostatin bound to Follistatin 288: Insights into Receptor Utilization and Heparin Binding*, at right, and **Yuan Cheng** for **S-033**: *A Uniquely Open Conformation Revealed in the Structure of a Novel Protein Arginine Methyltransferase*.

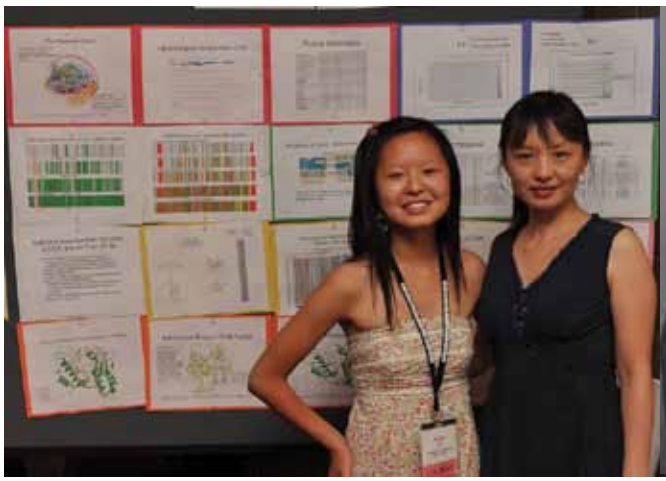


Above, Yuan Cheng with S-033.

The **Oxford Cryosystems Poster Prize** went to **Vera Vasylyeva** for **S-235**: *Small changes on the substitution pattern of pyridines and pyridine-N-oxides: Their influence on the molecule aggregation*. **Randy Alkire** is at right presenting the award to Vera at the Awards Banquet. **Thomas Proffen, Frank Fronczek**, and **Amy Sarjeant** were also on the Selection Committee.



A special feature of this meeting was the category created for poster presentations by high school students. Although there were no prizes awarded, photos were taken. At left below: Isabel Xu and her mother Shirley standing by **Dana Hogan**'s poster, **HS-005**. At right, **Kevin Gibas**, St. Joseph's Collegiate Inst., showing off **HS-006** with Bill Duax.



Top right: Peter Müller's view of the President's Reception, an annual invitation only event that honors corporate donors and ACA meeting supporters. The background photos are Peter's "Art" shots taken on and around the Chicago site. At left above: Marcia Colquhoun, Director of Administrative Services; at right: S.N.Rao and Ton Spek; Below, from left: Marv Hackert and George Phillips; and (Three Presidents), Judy Kelly, ACA, Sine Larson, IUCr, and Elspeth Garman, BCA.

Program Chair Ross Angel is next to Peter Müller's photo of "The Bean" above. Immediate above: Local Chair Bernie Santarsiero pondering some request from Judy Kelly, ACA President. The logo for the meeting, designed by Bernie, features the same "Bean." Peter's skyscraper photos are additional decorations.

2010 ACA Meeting in Chicago, July 24-29th

For the second time, the annual meeting featured unopposed plenary lectures or award lectures every day. **Thomas Steitz, Venki Ramakrishnan,** and **Ada Yonath** the three Nobel Laureates who shared the 2009 Nobel Prize in chemistry presented lectures; **Jim Ibers**, a long time professor at Northwestern, gave a plenary lecture appropriate to the topics in the ***Transactions* Symposium *The First Element***, organized in memory of **Bob Bau**; and Symposia were organized in honor of **Ton Spek (Trueblood Award)** and **Ray Trievel (Etter Early Career Award).** Both Ton and Ray gave award lectures at the start of these symposia. **David Watkin's Fankuken Award** lecture was postponed and will be presented in New Orleans. In addition to these meeting highlights, a special symposium ***New Tools - New Lights*** was organized in memory of **Louis Delbaere**. Both Bob's widow, **Margaret Churchill**, and Louis' widow, **Carole Delbaere** attended the meeting and the symposia.

Reports on these lectures and symposia, other session reports, and reports on selected posters are on the following pages. Reports on the workshops held on Saturday afternoon and letters from the Travel Award recipients will be in the winter issue. Group photographs of session speakers were taken by the students in the local committee except where otherwise noted

Below, from left: Tom Koetzle, ACA Vice-President, and Carol Huber, Jenny Glusker and Cheryl Klein-Stevens at the opening reception.

At left: Sue Byram walking into the President's Reception; above: Chief Executive Officer Bill Duax in a typical pose.

ACA Past-President Bob von Dreele, ACA President, Judy Kelly, and Tom Koetzle, ACA Vice-President.

Jim Kaduk, wearing a typical sweater.

Chris Cahill with the indomitable Buffalo office crew: Crystal Towns, Marcia Colquhoun and Jen Shepard.

Judy Flippen-Anderson, Bruce Foxman, Charles Campana, and Jon Clardy.

SP.01: What We Have Learned from Structures of the Ribosome

by Venki Ramakrishnan

The 2010 ACA Annual Meeting in Chicago started with an unprecedented Saturday evening Plenary Lecture by Venki Ramakrishnan, who shared the 2009 Nobel Prize in Chemistry with two of our other featured speakers, Ada Yonath and Tom Steitz. It was a spectacular beginning to our meeting. After a small delay while fifty additional chairs were brought into the lecture hall, we were presented with Venki's engaging talk on the evolution of his ribosomal odyssey. Venki and his group focused on the central process of translation that utilizes the adaptor molecule called transfer RNA, or "tRNA." The term "ribosome" was initially coined in 1958 at the first symposium of the Biophysical Society by R. B. Roberts, because, he said, *it has a pleasant sound*. As the individual components of the ribosome—rRNA, mRNA, tRNA, complementary proteins, GTPases—were identified, they were structurally characterized and assembled into ternary ribosome complexes to understand their function.

Throughout the talk there were words encouraging to all of us, particularly the younger scientists, about how Venki chipped away at seemingly insurmountable road blocks until he and his colleagues made breakthroughs that allowed the project to keep moving forward for decades. Some of these breakthroughs included removing variable components, like protein S1, to aid crystallization of 30S; fast detectors, intense synchrotron sources, and the use of new molecules, like osmium hexamines, for phasing; and herculean efforts (thousands of crystals frozen, hundreds of crystals screened, dozens of data sets collected from multiple crystals) to determine the various structures, from the 5.5Å structure of the 30S subunit to the 2.8Å structure of the 70S ribosome with mRNA and tRNA.

It was a talk of great achievements and perseverance that appealed to all in the audience—expert or nonexpert, junior or senior scientist. Of note was his comment about having no results after five years of effort and how that would be an impossible situation in the funding arenas most of us operate in these days. We owe Venki our heartfelt thanks for arranging to come to the ACA meeting in Chicago, despite the great time pressures he was under at the end of July. This was a talk that we will remember for a long time.

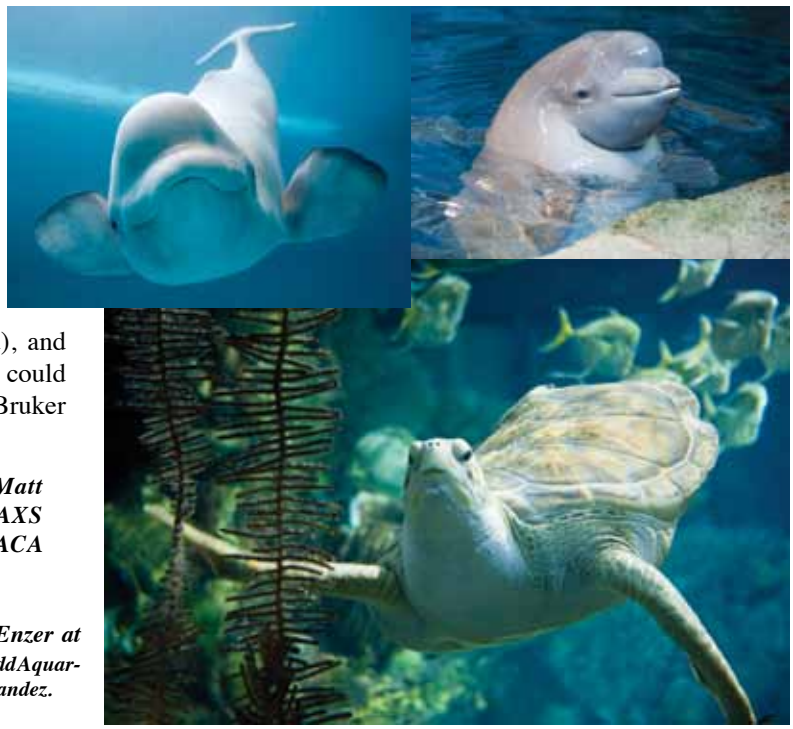
Bernie Santarsiero

Bruker Dinner at the Shedd

On July 25th, friends of Bruker AXS were treated to a most enjoyable tour and dinner with entertainment provided during dinner by a Shedd diver feeding the creatures - separated from the diners only by the floor-to-ceiling glass wall.

ACA members had only to fill an online registration form prior to the meeting (one guest was allowed), and then event tickets could be picked up at the Bruker Exibits Booth.

Cary Bauer and Matt Benning, Bruker AXS waiting to direct ACA people to the shuttle.



From Amanda Enzer at the Shedd. ©SheddAquarium/Brenna Hernandez.

AW.02: Ray Trievel Receives Etter Early Career Award

Raymond Trievel, U of Michigan, was the 2010 **Margaret Etter Early Career** awardee. His lecture gave an excellent overview of protein methylation and demethylation in biology. Site-specific methylation of lysine residues occurs in histones, transcription factors, ribosomal subunits, chromatin modifying enzymes, and other protein substrates. Methylation of these targets has been implicated in diverse functions, including gene regulation, DNA damage response, protein turnover, and genome stability. The methylation status of lysine residues is dynamically regulated through the concerted activities of lysine methyltransferases (KMTs) and lysine demethylases (KDMs) and is biologically important because both the site and degree of methylation are critical for intermolecular recognition in cellular signalling pathways.

Ray went on to describe the structural mechanisms of the catalytic events as worked out in his laboratory. In the course of studying the mechanisms of KMTs and KDMs, Ray and his colleagues identified short-range interactions between the methyllysine methyl groups and active site oxygen atoms that are indicative of carbon-oxygen hydrogen bonds. This unusual type of hydrogen bonding can occur when a carbon atom and its hydrogens are polarized by an adjacent covalently bonded heteroatom that enables hydrogen bonding with a nearby oxygen atom. In KMTs, carbon-oxygen hydrogen bonds facilitate the alignment of the methyllysine substrate for multiple methyl transfer reactions, contributing to the product specificities of these enzymes. Similarly, hydrogen bonding to methyllysine substrates within the active sites of KDMs promotes demethylation and defines the methylation state specificities of these enzymes. These findings prompted Ray to examine whether carbon-oxygen hydrogen bonding represents a general mechanism by which polar methyl groups are recognized in biology. He concluded his talk with a survey of the PDB that led to numerous examples of these interactions in the structures of different classes of methyltransferases and demethylases, highlighting the widespread nature of carbon-oxygen hydrogen bonds in methyl group coordination and catalysis.

James Hurley

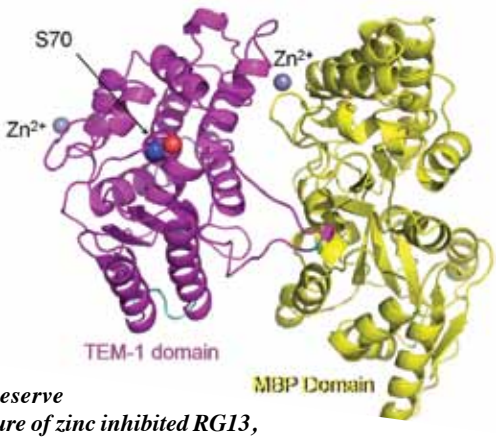
Top row, l to r: Ryan Jackson, James Swindell, Dayne West, and Wei Ke bottom row: Bret Wallace, Tara Michels-Clark, Weina Wang, Jennifer Colucci, and Pranoti Navare.

2.02: Etter Award Symposium

This symposium, organized every year to honor the memory of **Margaret C. Etter**, spotlighted the work of eight young scientists. Peggy Etter was an ardent advocate of student research. Perhaps by design, this year the YSSIG **Etter Student Lecturer Award** reflected her lifelong work in hydrogen bonds. **Dayne West**, in his ESL Award presentation described the likely transfer of protons within the carbonic anhydrase II enzyme. West's work focused on distinguishing which residues are involved in zinc metal coordination and in the transfer of protons through the active site of the enzyme.

Tara Michels-Clark described a new approach for the analysis of diffuse neutron and single crystal x-ray scattering; the way in which the disruption of a bacterial enzyme in the human gut effectively alleviated a form of cancer drug toxicity was the topic of **Brent Wallace**' talk; **Pranoti Navare** discussed the crystallization of entantiomers in racemic mixtures -how it is greatly enhanced on chiral surfaces

James Swindell presented comparisons of two data sets that were processed with HKL2000, d*TREK, XDS, MOSFLM and PROTEUM2 software packages. His results showed that the software packages handled the data differently and that each had particular strengths and weaknesses when dealing with one set or the other. He urged that during structure solution the software programs used to process data should be put to an experimental test just as other parameters are (*e.g.* growth conditions) during a crystallographic experiment. This talk spurred an interest within the YS and Biomac SIGs to have a specific session next year that will concentrate on highlighting several software packages for processing and refinement of data.



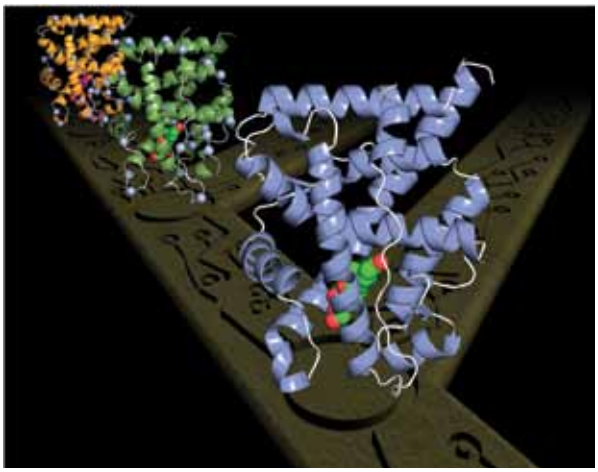
From Wei Ke, Case Western Reserve U: Crystal structure of zinc inhibited RG13, a TEM-1/MBP fusion protein.

Wei Ke, who won the **Etter Student Lecturer Award** designated by the Insdustrial SIG, presented a detailed crystallographic analysis of how the engineered molecular switch of maltose binding protein fused to TEM-1 beta-lactamase is regulated by maltose and zinc ion. The crystal structure of the molecular switch showed that when bound to maltose the linker region is likely more accessible to correctly fold into the active site of

the enzyme; where zinc binding enhances the inhibition of the enzyme by stabilizing hydrogen bonds that block the active site.

In other talks, **Weina Wang** described the mechanism by which nucleoside sugars are discerned in DNA polymerase, and **Jennifer Colucci** talked about the resurrection of an ancestral protein in order to effectively study steroid hormone receptors. She showed the image at right, and commented that ***the Ortlund lab (Emory U) uses structural biology to focus on nuclear receptor mediated transcriptional activation. They utilize structure and ancestral gene resurrection to understand the evolution of novel function within proteins***.

Ryan Jackson



SP.02: Plenary Lecture by Jim Ibers

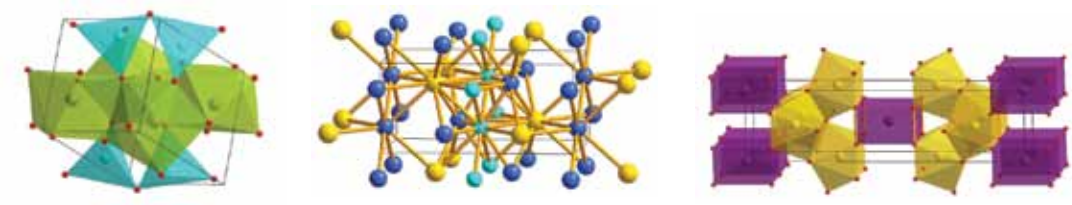
To celebrate his long, productive, and continuing scientific career as well as his 80th birthday, **Jim Ibers** gave a plenary lecture on Monday morning 26th July. The fact that he walked from home to the hotel made the venue especially appropriate. In his introduction, former student **Jim Kaduk** was both humorous and serious; the name Ibers is famous (the Ibers were pre-Roman people in Catalonia - the Iberian penninsula is named for them); Kaduk went on to emphasize how much he had learned from his teacher, comparing him to Yoda, the ultimate Jedi master.

Jim Kaduk and Jim Ibers walking in to the lecture hall.

Ibers' lecture *Uranium and Neptunium Solid-State Compounds: Adventures in Synthesis, Crystallography, and Characterization* discussed the challenges and rewards of studying such compounds. Uranium-238 compounds can be synthesized with luck, intuition, and experience in the normal way at Northwestern, but compounds of the highly-radioactive Np-237 have to be made at Argonne (Lynn Soderholm at Argonne collaborates with Jim). Compounds discussed included $NpSe_2$, $NpCuSe_2$ (Np_2CuSe_2 was the intended target), $(UO)_2YbS_3$, $(UO)_2YS_3$, $Ba_8Hg_3U_3S_{18}$, $Cs_3U_{18}Se_{38}$, and AAn_2Q_6 where A = K or Cs, An = U or Np, Q = Se or Te. The crystallographic problems posed by such compounds are many, and include absorption (face-indexed corrections or empirical corrections with lots of redundancy are critical), unknown stoichiometry, non-stoichiometry (ICP/MS is essential; chemistry by computer is not sufficient), disorder, sub/superstructures, and modulated structures.

The structural results are only as good as the model: one must bear in mind that assumptions such as kinematic diffraction, known scattering factors, isotropic extinction, and harmonic vibration models may be approximations, and experimental errors are *always* present. Charge balance, oxidation states, residuals, and structural common sense (as well as checkCIF) all factor into determining the quality of the result. Systematic errors, the number of electrons, and the complexity of the structures makes refining site occupancies risky. Iber's structures provide good examples of the importance of reading the list file.

Jim Kaduk



$Np\ Cu\ Se_2$

$U\ Cu\ 0.60\ Sb_2$

$K\ U_2\ Se_6$

U is yellow; Cu is turquoise; Se is red; K is purple; Sb is blue; Np is olive.

Hans Beat Buergi, Garry McIntyre, Tom Koetzle, Alberto Albinati, Joel Miller, Larry Falvello, Chick Wilson, Nobuo Niimura, Paula Piccoli, Carl Schwalbe, Art Schultz, Xiaoping Wang, Margaret Churchill, Muhammed Yousufuddin. Dean Myles & Michael O'Keeffe not shown. Photos by Peter Müller.

In memory of Bob Bau,

TR.01: The First Element

This full-day *Transactions* Symposium was organized as a tribute to the late ACA President, **Bob Bau** (1944 – 2008), Professor of Chemistry at the University of Southern California (USC), whose untimely death interrupted his varied and productive activities in several areas of chemistry, diffraction, and service to the scientific community. Bob's many interests were well reflected in the program, which covered not only diffraction but especially research related to neutron scattering, from instrumentation development through hydrogen characterization to neutron diffraction with proteins. A recurring theme was *important science involving diffraction*, which could serve as an aphorism for a large fraction of Bob's research activities throughout his career. The two half-day sessions were chaired by **Art Schultz** and **Tom Koetzle**.

At the time of his death, Bob was Chairman of the Instrument Development Team for the Topaz single-crystal diffractometer at the Spallation Neutron Source at ORNL, an instrument that has generated high expectations for both qualitative and quantitative advances in the science available through neutron diffraction. **Christina Hoffmann**, lead instrument scientist for Topaz, was the principal organizer of the *Transactions* Symposium. **Xiaoping Wang**, also an instrument scientist associated with Topaz, presented a talk on the commissioning of the instrument.

One of the most common traditional uses of neutron diffraction in chemical research has been the location of hydrogen atoms as a means of solving chemical mysteries; and in Bob Bau's research this resulted in the characterization of unexpected compounds whose nature would have been difficult if not impossible to discern by other means. **Tom Koetzle**, BNL, who co-authored forty research publications with Bob in what is one of the best known long-term programs in the application of neutron science to chemistry, treated us to a tour of the USC – Brookhaven National Laboratory collaboration: *Twenty-Five Years of Metal Hydride Structures*. Some of the compounds that emerged from that collaboration were featured on the cover of the winter '09 *RefleXions* including a compound with four hydride bridges on a metal-metal bond. More recent efforts from Bob Bau's group, involving an unusual elongated dihydrogen ligand in an osmium complex and a four-coordinate hydrogen in a yttrium cluster, were discussed in a talk by **Muhammed Yousufuddin**, one of Bob's later students who is now at UT-Arlington.

Among the positive expectations for a new generation of neutron sources is the further development of high-throughput neutron diffraction for hydrogen location, a topic covered energetically by **Chick Wilson**, U Glasgow. Neutron scattering has a value-added component in the magnetic moment of the neutron, which permits magnetic as well as structural analysis of the sample. **Garry McIntyre**, Inst. Laue-Langevin, presented results from polarized-neutron scattering measurements on a sample with spin-polarized hydrogen. Garry's data serve as a proof of principle for the utility of this technique as an alternative to deuteration to reduce the incoherent background scattering from hydrogen.

Chemical imaging of different sorts was a theme in other talks. **Dwayne Miller**, U Toronto, gave an animated presentation *Making the Molecular Movie: The First Frames*, describing the origins and present status of his work on femtosecond electron diffraction imaging. **Hans-Beat Buergi**, U Berne, discussed diffuse scattering, which has in the past largely been discarded in Bragg scattering experiments, but which in reality convey information of great importance in understanding many solids. Hans-Beat indicated that the interpretation of diffuse scattering data can be tricky, but new x-ray and neutron scattering instrumentation has already improved and will continue to improve the quality of the data. A talk on dynamics, presented by **Alberto Albinati**, U Milan, described the application of a normal-mode model to variable-temperature single crystal neutron diffraction data from a ruthenium complex with dihydrogen ligands. The study yielded rotational frequencies for the dihydrogen groups.

Five talks dealt with important science involving small-molecule structure determination in conjunction with complex or unusual chemistry. **Paula Piccoli**, ANL, gave a characteristically animated presentation describing the diffraction analysis of a fifteen-coordinate thorium complex prepared in the group of Gregory Girolami at U Illinois. **Larry Falvello**, U Zaragoza, presented results involving solid-state chemical reactivity that

raised mechanistic questions. **Joel Miller** talked about molecular magnets; many of his compounds were characterized structurally using powder x-ray diffraction, in collaboration with Peter Stephens, Stony Brook U & the NSLS. Synchrotron radiation also figured in the talk by **Carl Schwalbe**, who described structural changes, including one case of polymorphism, that occur in salts of the anti-inflammatory agent flurbiprofen when the cation is systematically modified to include more hydrogen-bonding sites.

Michael O'Keeffe gave a talk on the growing field of microporous materials, including metal-organic frameworks (MOF's), covalent organic frameworks (COF's) and zeolitic imidazolate frameworks (ZIF's), all of which may have potential for portable energy storage, carbon dioxide capture, and applications in separations and catalysis.

Bob Bau's most recent neutron research was in protein diffraction. **Nobuo Niimura** gave a talk covering technical developments that enhance neutron protein crystallography and should permit more facile exploration of the role played by hydrogen and by water of hydration in biological processes. **Dean Myles** also addressed macromolecular crystallography and the role of hydration in protein properties in a talk on the structure of a rubredoxin mutant that is stable in boiling water.

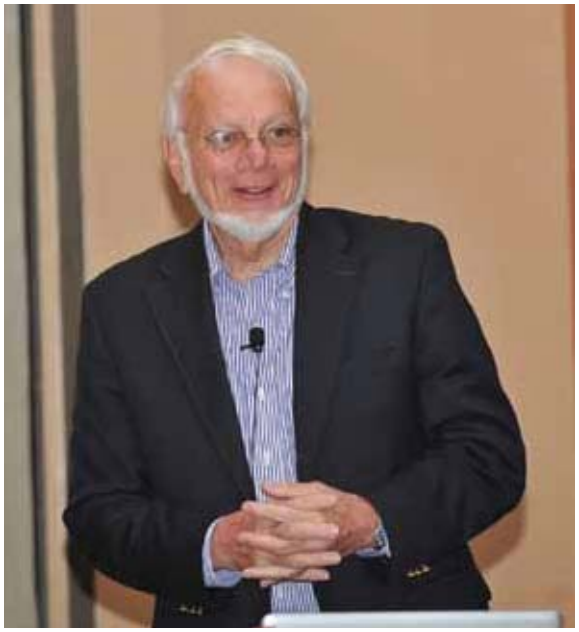
Bob Bau and Tom Koetzle. Photo courtesy of Thomas Mak.

In closing comments, **Tom Koetzle** described Bob Bau as an "unusual, unique individual". Bob is survived by his wife, **Margaret Churchill**, who attended the symposium. Tom announced that a generous gift from Margaret to the ACA has endowed a new triennial award, the **Bau Award for Neutron Diffraction**. This honor comes in addition to the **Robert Bau Endowed Graduate Fellowship**, which is being created at USC.

The 2010 *Transactions* Symposium was a fitting tribute to Bob, and while his absence was mourned in the heartfelt comments of many of the speakers, the science described throughout the day underscored the continuity and the continuing importance of the many areas in which Bob was a pioneer.

Tom Koetzle, Art Schultz & Larry Falvello

SP.03: Plenary Lecture by Tom Steitz



Like Cinderella, who needed a magic touch to unveil her true beauty, the ribosome had been waiting a long time for its structure to be solved. It was a formidable task to crystallize, solve and interpret the structure of this 2.5 million Dalton ribonucleoprotein machine, which is responsible for synthesis of each and every protein in the cell. In 2000 after the first high resolution structures of the ribosomal subunits and later of the complete ribosome had been unveiled, this princess of the cellular enzymes shined forth in the true magnificence of its hundreds of thousands of atoms. One of the people who helped this magic to occur is **Thomas Steitz,** Sterling Professor of Molecular Biophysics and Biochemistry and Professor of Chemistry at Yale and an HHMI Investigator. In his plenary lecture, Tom focused on the structure of the large ribosomal subunit. The intricate mesh of short and long-range contacts help to shape the thousands of nucleotides that comprise the rRNA of the large subunit into a scaffold that forms the subunit core. The organization of rRNA is assisted by ribosomal proteins that bind at the subunit surface and whose long positively-charged tails penetrate deep into subunit structure gluing rRNA segments together. One of the main revelations was the discovery that catalysis of peptide bond formation, the key reaction of protein synthesis, takes place in the catalytic center which is built exclusively of rRNA, revealing the ribosome as a true ribozyme. Structures of the ribosomal functional complexes illuminated the likely mechanisms of catalysis of peptide bond formation. A nascent peptide exit tunnel, that starts at the catalytic center and penetrates through the entire body of the large subunit, provides the exit route for the newly synthesized polypeptides. The ribosome is the target of action of many important antibiotics. Like Cinderella's glass slippers, these antibiotics fit perfectly into their binding sites (composed primarily of rRNA). Structural analysis of the ribosome-antibiotic complexes paved the way for rational drug discovery work being carried out in the pharmaceutical company Rib-X founded by Tom Steitz and his colleagues. Time will show if the new drug leads discovered through ribosome crystallography are indeed going to live happily ever after.

Alexander Mankin

SP.04 Plenary Lecture by Ada Yonath

Ada Yonath gave the last of the three Nobel plenaries at the meeting, describing her years of pioneering work on ribosome crystallography as well as her latest studies. She spoke about how she became engaged in the crystallography of the ribosome and about her long journey before the first crystals materialized. Among other stories, she told about feeling encouraged that it might be possible to obtain crystals by the fact that polar bears pack ribosomes in an orderly fashion in their body cells ahead of winter hibernation. She mentioned her long time collaboration with Abteilung Wittmann in Berlin, and doing the *T. maritima* ribosome crystal structure with the first crystals she obtained.

Ada also described her effort in cryopreservation of diffraction quality crystals, which she pioneered in collaboration with Håkon Hope, leading the way eventually to the cryo-crystallography techniques currently in routine use by many macromolecular crystallographers. In a Herculean effort, her group manually screened 25,000 crystals in a 6-month period on their way to the first crystal structure. She also emphasized the importance of new methodologies that were necessary to advance ribosome crystallography. At that time these new methods, including MAD experiments using large heavy metal clusters, were used by her group; more recently they have been adopted by others. Her description of the ribosome structure was centered on the peptide bond formation (PTC) site, located within a universal internal symmetrical region connecting all of the remote ribosomal features involved in its functions. She proposed that the high conservation of the symmetrical region implies its existence as the ancient ribosome, irrespective of environmental conditions. She then discussed the functional role of an elongated tunnel, above which the PTC is located. Nascent chains emerge out of the ribosome through the tunnel, which may act as the first cellular chaperone and incidentally hosts a major family of antibiotics. This tunnel is a target of extensive pharmaceutical interests, as discussed earlier in the plenary lecture by Tom Steitz.

Session 7.18, Macromolecular Complexes and Assemblies, served as an overture to Ada's plenary lecture, presenting modern day challenges of solving large macromolecular assembly structures. The lecture hall was filled for her lecture, despite the fact that it was scheduled at 11:30am - 12:20pm, demonstrating the respect that crystallographers have for her. Her Nobel Prize is gratifying to all of us at ACA, particularly those who engage in structural studies of protein-nucleic acid interactions. For many years, Yonath traveled the world to seek best possible experimental facilities, motivating many of those who develop and support synchrotron instrumentation. In concluding her lecture, Ada emphasized her great love and strong commitment to her family over those years, and offered strong encouragement, especially to those researchers with children who continue to pursue their scientific interests while managing family priorities.

Hiro Tsuruta

7.18: Macromolecules, Complexes & Assemblies

An exceptionally high number of abstracts were received, demonstrating the intense interest that many crystallographers have in this research topic. In taking on highly complex macromolecular assemblies at multiple resolutions, many of the studies employed a hybrid approach to complement crystallography. **Luis Castillo**, University Hospital, Heidelberg, Germany, discussed HIV-1 capsid maturation based on his crystallographic studies of HIV capsid proteins with point mutations on the inhibitor binding sites. Of particular interest was the presence of different mutants locked into two distinctive immature or mature capsid protein conformations. Luis and his colleagues recently identified two additional mutants that adopt an intermediate phenotype between the unliganded and liganded conformations. Explaining how these mutant crystal structures fit into either the immature or the mature capsid lattice seen by cryoEM, their study presented snapshots of the conformational change pathway that the HIV-1 capsid undergoes during maturation.

The other structural study on viral assemblies was given by **Fang Li**, U Minnesota. Fang reported crystal structures of coronavirus receptor binding domains (RBDs) complexed with angiotension-converting enzyme 2 (ACE2) from human. NL63 coronavirus is a prevalent human respiratory virus, that targets ACE2, which is also targeted by a Group-II SARS corona virus. This talk described the molecular basis whereby two different coronaviruses that lack structural homology can recognize the same receptor protein .Fang and coworkers studied RBDs from various SARS coronavirus strains complexed with ACE2 from human and palm civets.Their research revealed a series of stepwise mutations in the RBDs, allowing SARS coronavirus to transmit from palm civets to humans and causing the worldwide SARS epidemic in 2002-03. The array of these studies not only provided structural insights on viral evolution, virus-receptor interactions, viral host ranges and cross-species infections, but also implications on novel antiviral strategies against coronavirus infections.

Macromolecules, Complexes, Assemblies, cont'd.

Ron Stenkamp, U Washington, presented the 2.7Å structure of *E. coli* fimbrial tip assembly, composed of FimH, FimG, FimF and FimC subunites. The subunits are held together by donor strand complementation, for instance a β-strand from one subunit completes the β-sandwich in another subunit. The lectin and pilin domains of FimH change their relative orientation and position in forming the tip complex, providing a model for FimH's force-mediated mannose binding properties. Some residues differ by as much as 14 Å between their positions in the tip complex and their positions in their FimC complexes This research provides insight into the allosteric effects of mechanical force on receptor-ligand interactions and into how multiple subunits can bind the same chaperone (FimC) and still bind specifically to particular subunits in the larger fimbrial structures.

Liang Tong, Columbia, and his colleagues used crystallography and cryo-EM for structural studies on propionyl-CoA carboxylase (PCC), a 750kDa dodecameric enzyme complex that performs sequential enzyme catalysis reactions, including biotin carboxylase activity. The 3.2Å crystal structure of a bacterial enzyme and the 15Å cryoEM structure of the human enzyme confirm that they have a common quaternary structure, (6 monomeric α subunits decorating the hexamric β subunit PCC core). This structure establishs a molecular basis for understanding the large collection of disease-causing mutations in PCC.

Making a nice transition to Ada Yonath's plenary lecture on the ribosome, **Yuichiro Takagi**, Indiana U, described the crystal structure of the Head module of Mediator, a gene expression module in the RNA polymerase II transcriptional machinery; his study also combined crystallography with cryo-EM and solution x-ray scattering. The 4.5Å structure of the 7 protein complex Head, solved by tantalum cluster SIRAS and Se-Met SAD, reveals three distinctive domains recently seen in a cryo-EM study: fixed jaw, movable jaw, and handle domain. A single particle cryo-EM study on the Head bound to the minimum pre-initiation complex supports the model where Mediator modulates access of promoter DNA to the pol II cleft through the Head-Rpb4/7 interaction.

Hiro Tsuruta

AW.03: Trueblood Award Plenary Lecture by Ton Spek

The recipient of the 2010 **Kenneth Trueblood Award**, **Anthony (Ton) L. Spek**, took us on an entertaining journey through his long career in crystallography. His lecture: *From Paper Tape Input to Forensic Crystallography: Forty Years of Crystallographic Computing* described how his interest in crystallography began as a student at Utrecht University in The Netherlands in 1966, where his accommodation was for a time in the house of J.M. Bijvoet. Under the guidance of A.F. Peerdeman, Ton's first task was to determine the structure of crystals of an unknown organic reaction product. It took six months. The direct methods programs then available could not generate a solution, so Ton set about writing his own direct methods program in ALGOL. Access to the university's computer was limited to one 13 hour shift per week and the program and all input was punched on paper tape. At that time, one had to be a scientist, programmer and computer operator. In 1971, Ton was asked to set up and run the National Single Crystal Service Facility in Utrecht, a position which he held until his retirement 38 years later. Ton attended many of the significant meetings on direct methods theory and software development during the 1970's, including the five week CECAM workshop, attended by people such as Hauptman, Germain, Main, Destro and Viterbo, at which the final form of the program MULTAN was established. Ton then described the evolution of his very popular structure analysis program, PLATON. The program had humble beginnings in 1980 as an in-house tool for efficiently producing a comprehensive listing of derived geometry for a structure. Over time, numerous tools have been, and are still being added to the program to extend its capabilities. New ideas, such as the SQUEEZE routine to handle disordered solvent, charge flipping for structure solution, a new method for absolute structure confirmation, and twin detection are promptly encoded, tested and incorporated into the program and thus become readily available to users. Ton explained the SQUEEZE algorithm in some detail, demonstrated charge flipping in action, and then went on to describe the impetus and rationale behind the development of structure validation. Automated structure validation was pioneered by Syd Hall, the then Editor of *Acta Cryst. C*, who invited Ton to use some of the tools already in PLATON to check for things such as missed symmetry and voids. The extensive validation routines in PLATON have grown from this beginning and were recently extended to include the validation of structure factor files. This validation scheme has been very successful in setting standards for quality and reliability. Ton finished by showing how validation can be used to detect mistakes in structures. PLATON was a key tool in the investigation of the recent sad cases of fraudulent structure reports. Although Ton has recently retired, he remains active and we look forward to seeing his cheerful face at future meetings and to the ongoing developments in PLATON for years to come.

Tony Linden

1.01 Lighting the Way: *In Memory of Louis Delbaere*

Louis Delbaere (1943-2009) was a Professor and Tier 1 Canada Research Chair in the Biochemistry Department at the University of Saskatchewan. He was a key figure in establishing the Canadian Macromolecular Crystallography Facility (CMCF) at Canada's national synchrotron research facility, the Canadian Light Source, and he led the Molecular Design Research Group devoted to the discovery and structural elucidation of molecules involved in bacterial infections, cancer, Parkinson's and Alzheimer's Disease, diabetes and immune disorders.

Louis passed away suddenly on October 5, 2009, in Mississauga, Ontario while returning from a meeting with the ACA Board in Buffalo. Shortly thereafter, this special session, involving several of Louis' closest friends and colleagues, was organized to highlight the seminal contributions Louis made to the advancement of Canadian crystallography and the international crystallographic community. The speakers and the audience were especially grateful that Louis' wife, Carol Delbaere, attended the session, providing pictures taken of the two of them and many of their friends and colleagues during previous ACA and IUCr meetings and special occasions, which were presented as a slide show prior to commencement of the talks.

The first speaker, **Michael James**, U. Alberta, gave an historically rich account of Louis' early contributions to our understanding of monosaccharide structures and human Lewis blood-group determinants during his days as a postdoctoral fellow in Ray Lemieux's laboratory. He also paid tribute to Louis' role in elucidation of the first protein structures determined in Canada (*Streptomyces griseus* proteases), and described his pivotal work with Gary Brayer, I-Nan Hsu, and Theo Hofmann on the structures of alphalytic protease and penicillopepsin as a reminder of his contributions to the birth of protein crystallography in Canada. The scientific aspects of Michael's story were nicely balanced by enjoyable and more personal anecdotes of his long-standing friendship with Louis, including their weekly squash matches, aptly followed by beers at the University of Alberta Faculty Club, and his many fond memories of get-togethers with Louis, his wife Carol, and their two children.

J. Wilson Quail, U. Saskatchewan, took the audience back to Louis' early days as a postdoctoral fellow at Oxford, where Louis and Carol formed friendships that flourished from that time forward and established his reputation as an ambassador of Canadian crystallography. Wilson also discussed Louis' first years at the University of Saskatchewan, when the first crystallography lab there was established. He went on to describe their first synchrotron data set collection at DESY in Hamburg. A particular highlight of Wilson's talk was his portrayal of the manner in which Saskatoon was chosen for the site of the Canadian Light Source, and the pivotal role Louis played in rallying support among the scientific community. His account of Louis' perseverance, selflessness, and unwavering devotion to his family during this monumental endeavor was heartfelt.

Sine Larsen, U. Copenhagen and IUCr President, who held perhaps the longest-standing friendship with Louis, described his participation as Chair of the Canadian delegation at the 2008 IUCr in Osaka, where the bid for the venue of the IUCr Congress in 2014 was presented, and also his election to the IUCr Executive committee. That Montreal was selected for the 2014 site was both an affirmation of the respect crystallographers around the world held for Louis, and a reminder of the void that has been left by his passing.

Zongchao Jia, Queen's U., recounted some of his experiences as a graduate student with Louis and presented recent work from his own lab on an unusual bifunctional isocitrate dehydrogenase (AceK) from *E. coli* that possesses kinase and phosphatase activity. The structure of AceK alone reveals a eukaryotic protein kinase-like domain containing ATP and a regulatory domain with a novel fold. The structure of its complex with isocitrate dehydrogenase (ICDH) showed that the binding of AceK to ICDH further activates AceK and influences higher-order substrate recognition. Apparently AceK's kinase/phosphase activity switch is regulated through a conformational change mediated by a distant AMP binding event.

Gerald Audette, another alum of the Delbaere lab, discussed strides made by his lab at York U. on engineering bionanowires from type IV pilin proteins of *Pseudomonas aeruginosa*. The self-oligomerization of these filament structures from alkylthiol functionalized gold surfaces and their potential for metal ion derivatization holds great promise for future development of bionanoelectronics. The next steps in this research will investigate methods for patterned nanofibre oligomerization via differential alkylthiol functionalization of gold surfaces.

Lynne Howell, U. Toronto and Hospital for Sick Children, spoke about proteins involved in the biosynthesis and export of the exopolysaccharide alginate in *Pseudomonas aeruginosa*, which facilitates development of chronic lung infections in cystic fibrosis patients. She described her laboratory's structure-function studies of AlgK and AlgE, two of the outer membrane-associated components of this cell-envelope-spanning multi-protein complex. Using complementation and subcellular fractionation studies, AlgE was shown to function in alginate secretion; furthermore, AlgK helps localize AlgE to the outer membrane. These details from the structures done by Lynne's group help to explain how proteins assemble.

Louis Delbaere receiving his trophy for being the "Ambassador" to the General Assembly of the IUCr from Michel Leblanc, President and CEO of the Board of Trade of Metropolitan Montreal.

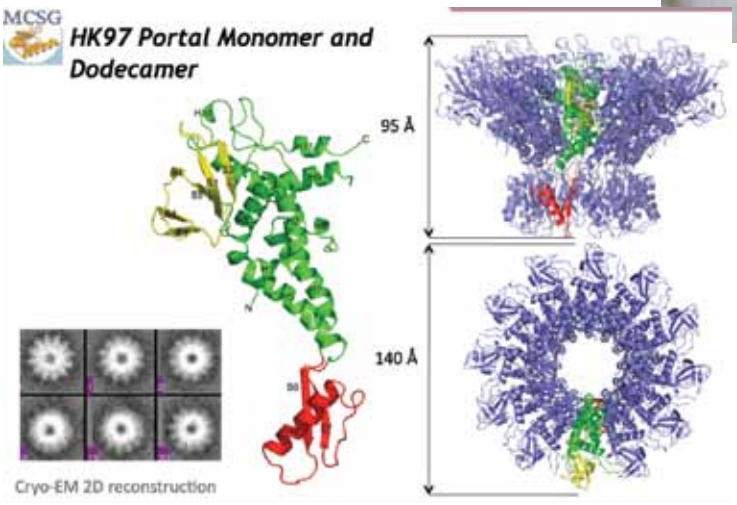
and function within the alginate biosynthetic complex, and show how this system stands apart from other bacterial exopolysaccharide secretion systems.

Michael Murphy, U. British Columbia,described his structures of a class of lipoprotein receptors (HtsA and SirA) from *Staphylococcus aureus*, both alone and in complex with two iron-chelating siderophore substrates (staphyloferrin A and B). *S. aureus* employs these proteins to scavenge iron from our bodies as a nutrient source, whereafter cell surface-bound lipoprotein-siderophore-iron complexes are shuttled to a membrane permease for nutrient intake. Murphy proposed that large localized conformational differences accompanying binding of the two different staphyloferrin-iron complexes to their receptor proteins may underlie the mechanism by which only substrate bound receptors are internalized by the membrane permeases for iron uptake.

John Allingham

At right: Louis during a May 2009 visit to Grenoble to meet with Sine Larsen and to tour the ESRL.

1.02: Molecular Motors and Machines



From Andrzej Joachimiak: their new bacteriophage HK97 Portal Protein.

Molecular machines are vital to all living organisms. While common mechanisms exist, distinct structural features which confer function are apparent. **Francis Tsai**, Baylor College of Medicine, began by highlighting recent advances in the structure determination of molecular motors and ATP-dependent molecular machines. Francis' talk was followed by the keynote lecture given by **Andrzej Joachimiak**, Argonne National Laboratory, who presented an excellent overview of Protein Structure Initiative (PSI) efforts by the Midwest Center for Structural Genomics to elucidate the structure and function of macromolecular assemblies and predicted molecular motors. Notable examples included bacterial chaperonins and the bacteriophage HK97 portal protein.

Rui Zhao, University of Colorado Denver, presented her recent structural work on the Brr2 helicase, an essential component of the spliceosome. The crystal structure of the Brr2 Sec63 domain revealed an unexpected resemblance to DNA helicase Hel308 domains, suggesting that Brr2 is composed of two consecutive Hel308-like modules. Next, **Sukyeong Lee**, Baylor College of Medicine, presented the structures of two AAA+ (ATPase Associated with diverse functional Activities) machines determined by electron cryomicroscopy (cryoEM) and atomic structure fitting. The structure of the intact m-AAA protease, (a membrane-bound AAA machine), revealed a novel mechanism that hetero-oligomeric AAA proteases use to dislocate and degrade membrane integral protein substrates. Sukyeong went on to describe the fitted cryoEM structure of an Hsp104 hexamer and also that of a novel Hsp104-T4 lysozyme chimera. The latter has an unexpected gain-of-function and can rescue heat-aggregated proteins on its own.

Ines Munoz, Spanish National Cancer Research Center, reported the 5.5 Å resolution crystal structure of bovine CCT (chaperonin containing TCP-1), an approximately 1 MDa ring-shaped group II chaperonin. Remarkably, the structure revealed the presence of one tubulin molecule in each CCT octamer, thus providing the structural basis for substrate recognition. Finally, **Siyang Sun**, Purdue, reporting for Michael Rossmann's lab, discussed their recent structural studies of gene product 17 (gp17), the bacteriophage T4 DNA packaging motor protein. Her work suggested a mechanism in which electrostatic forces drive DNA packaging by alternating between the tensed and relaxed states of gp17. A similar mechanism may also underlie other molecular motors.

Sukyeong Lee and Francis T.F. Tsai

George Sheldrick, John Rose, Cheng Yang, Joseph Ng, B.C. Wang, Manfred Weiss, Soichi Wakatsuki, Elspeth Garman, Daniele de Sanctis.

Photo taken with B.-C Wang's camera.

1.03: Longer Wavelength Phasing

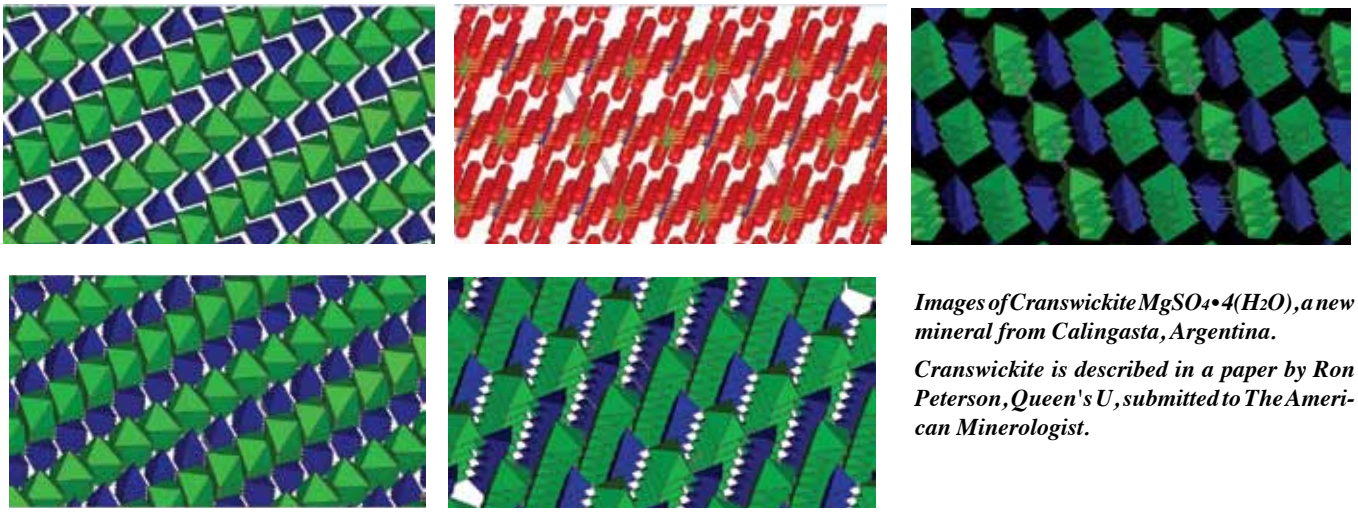
The first half of the session was chaired by **John Rose**, U Georgia. **Manfred Weiss**, Hemholz-Zentrum, began by giving an overview of the possibilities and the challenges associated with collecting diffraction data at wavelengths longer than 1.5 Å. He also presented some analysis of successful S-SAD cases, which have been published or deposited in the PDB. **Soichi Wakatsuki**, Photon Factory, Tsukuba, then presented the Japanese plans for building dedicated long-wavelength synchrotron beam lines at the Photon Factory. **Cheng Yang**, Rigaku USA, reported a number of successful cases based on data collected on a chromium anode home source. The challenging structure determination efforts of **Joseph Ng**, U Alabama-Huntsville, was detailed in the next talk. His structure of the protein FeoA by S-SAD was particularly difficult because FeoA crystallized in a monoclinic space group with four molecules in the asymmetric unit.

Manfred Weiss then introduced **George Sheldrick**, U Göttingen. George is best known for his popular SHELX-programs, but he talked about a seemingly easy S-SAD case which in the end was not solved. Despite the facts that the crystals diffracted well and that the data collected at the Hamburg beam line X12 were very good, the structure could not be solved by S-SAD. In a post mortem analysis George attributed this to the very high concentration of chloride present in the crystal, which apparently degraded the low resolution anomalous differences. **Elspeth Garman**, U Oxford, discussed her experiences with successful and unsuccessful S-SAD cases based on data she had collected on her home source. **Daniele de Sanctis**, ESRF, described the ESRF synchrotron upgrade project and the experimental possibilities for doing long-wavelength work in Grenoble.

B.-C. Wang, U Georgia, then introduced his concept of MDS data collection for S-SAD experiments. He convincingly showed that collecting a few short-exposure data sets gives better data than collecting one long-exposure data set, despite the fact that the overall dose on the crystal is the same. In all probability redundancy is more important than intensity.

To conclude: experimental phasing by sulfur-SAD has been shown to be a feasible alternative to other phasing methods, at least in favourable cases.

Manfred Weiss and Bi-Cheng Wang



Images of Cranswickite $MgSO_4 \cdot 4(H_2O)$, a new mineral from Calingasta, Argentina.

Cranswickite is described in a paper by Ron Peterson, Queen's U, submitted to The American Minerologist.

1.04: Structural Enzymology: Mechanistic

Paul Carey, Case Western Reserve, began with *Using Raman Microscopy to Map Reaction Pathways in Crystals in Real Time*. Paul described the way he used Raman microscopy and Raman difference spectroscopy to follow enzyme reactions, *e.g.* with beta-lactamase drug reactions. Typically the reactions were started by using soak-in conditions at room temperature. Then, Raman data as a function of time provided both structural and kinetic information, which was leveraged by his collaborators so that intermediates could be flash frozen and trapped in single crystals. Paul noted that a particular Raman-active vibration band derived from a catalytically essential Asp side chain was dramatically altered by metal coordination during the reaction cycle of the RNA polymerase.

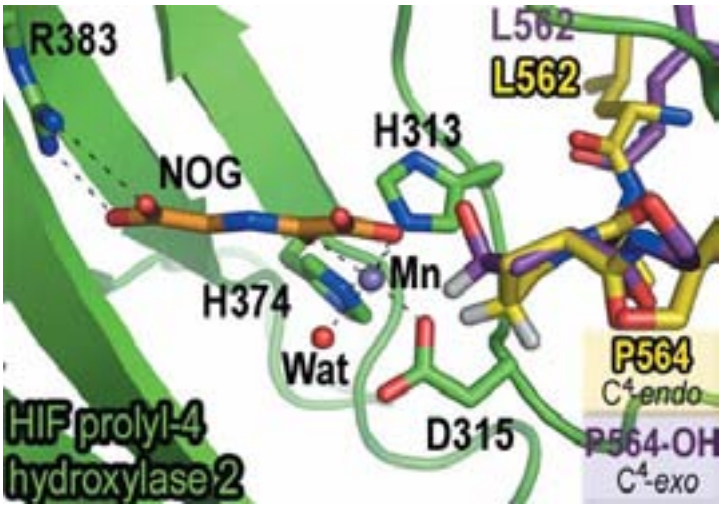
Brian Fox, U Wisconsin, in *Structural Evidence for the Staging of Active Site Configurations that Control Diiron Monooxygenase Reactivity* spoke about the way in which multicomponent enzymes catalyze the oxidation of a wide range of hydrocarbons. Some microbes express these enzymes and use the resulting hydrocarbons as their sole source of carbon and energy. For example, Toluene-4 monooxygenase, a large hydroxylase protein containing the diiron center active site T4moH, (composed of an electron transfer chain between an NADH oxidoreductase and a Rieske type [2Fe-2S] protein). T4moH complexes with a small protein called the effector protein, T4moD. Brian's recent high-resolution crystal structures of stoichiometric T4moH-T4moD complexes, some with aromatic substrate analogs; a peroxide intermediate of the diiron center and a series of crystal structures of mutant T4moH-T4moD complexes suggest how residues outside of the first coordination sphere rearrange to create an active site pocket poised for turnover.

Rasheduzzaman Chowdhury, Oxford U, emphasized that hypoxia inducible transcription factors play an essential role in the cellular response to reduced dissolved oxygen concentration. This is accomplished in part by the post-translational prolyl-4R-hydroxylation of the α-subunits of α/β-heterodimeric hypoxia inducible factors (HIF). Three O_2-dependent HIF prolyl hydroxylases (PHD 1-3), which are Fe(II) and 2-oxoglutarate dependent oxygenases, catalyze the hydroxylation of specific proline residues within the oxygen-dependent degradation domains. Chowdhury reported the crystallographic and biophysical characterization of PHD2 in complex with a portion of the C-terminal oxygen-dependent degradation domain of HIF-1α subunit. His data suggest that catalysis involves conformational changes of PHD2 that serve to isolate and prepare the hydroxylation site, as well as to stabilize the PHD2-HIF-1α complex

George Richter-Addo, U Oklahoma, presented new results obtained at beamline X26-C at the National Synchrotron Light Source. This beamline supports nearly simultaneous and fully correlated x-ray diffraction and UV-vis spectroscopy experiments from the same single-crystal sample and under nearly identical conditions. His data indicate that the exposure of a single crystal of a nitrite adduct of ferric myoglobin at 100 K to high-intensity synchrotron x-ray radiation results in changes to the UV-vis spectrum of the crystal; he attributed this to reduction of the ferric compound to the ferrous derivative. Electron density maps reveal that the nitrite adduct maintains the unusual O-binding mode of the nitrite to the heme-ferrous center. Richter-Addo made the important observation that nitrite reduction by Mb (and Hb) occurs via the ferrous derivative and not the ferric derivative.

According to **Tzanko Doukov**, SSRL, the ferryl (Fe(IV)=O) intermediate is important in many heme enzymes and therefore the precise nature of the Fe(IV)-O bond is critical to understanding these biologically critical reaction mechanisms. He described solving 1.40 Å crystal structures of cytochrome c peroxidase Compound I as a function of x-ray dose while monitoring the visible light absorption spectrum at BL9-2 at SSRL. Doukov and coworkers used 19 crystals to determine 14 structures differing in total x-ray exposure; their strategy involved sample automounters, x-ray photoreduction, and single-crystal spectroscopy. Composite data sets were assembled by merging, taking care that reflections in each of the 19 data collections were measured in a way that allowed monitoring as a function of time/dose. Their results showed that the Fe(IV)=O bond increased linearly from 1.73 Å in the low x-ray dose structure to 1.90 Å in the high dose structure. The low dose structure correlated well with a Fe(IV)=O bond; the authors postulated that the high dose structure is the cryo-trapped Fe(III)-OH species previously thought to be Fe(IV)-OH.

Allen Orville



From Rashed Chowdhury: Structure of prolyl hydroxylase 2 (PHD2, green) in complex with HIF-1α substrate (residues 556-574, yellow) (PDB ID: 3HQR). The figure illustrates a comparison of Pro564/HIF-1α conformations when bound to PHD2 (C4-endo, yellow) and von Hippel-Lindau protein (C4-exo, purple). The C4 Pro564 hydrogen(s) are gray. (Structure, 2009, 17(7), 981-989).

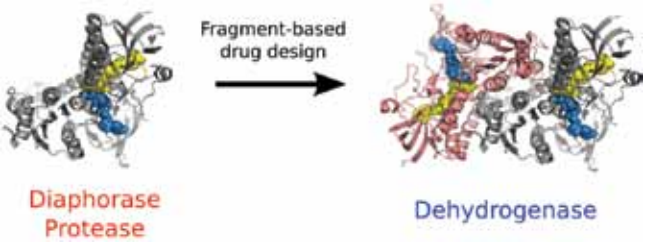
1.05: Biological Impacts of Structural Enzymology

Speakers in this session touched on the involvement of conformational motion in catalysis, how the unique metal site of hydrogenase is constructed, mechanistic aspects of how several enzymes exacerbate oxidative damage, and opportunities for structure-based drug design. The first two talks, by **Lesa Beamer**, U Missouri, and **Violetta Weinreb**, UNC-Chapel Hill, focused on conformational change and catalysis. Both talks identified interdomain interfaces that impact mechanism. Beamer spoke about phosphoglucomutase from a human pathogen. She described Arrhenius plots of mutants indicating that increased flexibility in the hinge increased the entropy of activation for catalysis. Beamer also described the ambitious and successful assignment of NMR triple resonances for the enzyme, which enabled her to quantify dynamic motions using relaxation-dispersion methods. Weinreb described combinatorial mutagenesis of a dynamic region between two domains of a bacterial tryptophanyl-tRNA synthetase that implicate the catalytic Mg^{2+} ion as the active-site receiver of intramolecular communication about the conformational state. A major fraction of the metal's catalytic effect depends on coupling between the metal and the protein. then combinatorial mutagenesis with Mn^{2+} substituted for Mg^{2+} showed that net interactions with active-site lysine residues actually oppose catalysis. Studies with mutants demonstrated long-range synergistic coupling between the remote *Master Switch* and the Mg^{2+}ion. The possibility that this coupling is a general mechanism for coupling conformational changes to NTP utilization and would apply to many other transducing proteins is very inteesting.

The [FeFe] hydrogenase, HydA, is an attractive crystallographic problem because it diffracts to high resolution, is robust to radiation damage, and preserves high isomorphism in its different oxidation states. **David Mulder**, Montana State U, described a partially assembled form of HydA, created in the absence of three proteins that synthesize a unique two-iron prosthetic group containing a variety of non-protein ligands. Partially assembled HydA contains an Fe_4S_4 cubane cluster at the bottom of a cleft whose surface is positively charged. Insertion of the Fe_2 prosthetic group is apparently followed by a condensation of loops around the cleft to produce the native enzyme. Mulder described extensive structural parallels between this process and the insertion of the similar MoFe prosthetic group of nitrogenase. Loop region conservation in organisms containing the 2Fe subcluster biosynthetic genes coupled with evolutionary analysis of HydA together indicate a bacterial origin for HydA that postdates the emergence of eukaryotes..

Mark Safro, Weizmann Inst., presented several very interesting observations about the specificities of the human cytoplasmic and mitochondrial phenylalanyl-tRNA synthetases. Both bacterial and eukaryotic cytosolic PheRSs demonstrate a high level of proofreading activity against the similar, naturally occurring amino acid tyrosine. However, despite the high level of oxidized phenylalanyl derivatives in the mitochondrion, the mitochondrial enzyme lacks the editing domain which protects the bacterial species from incorporating m-, o-, and p-tyrosine into proteins. Safro suggested that the human cytosolic and mitochondrial phenylalanyl tRNAs act in tandem to incorporate these and other pharmaceutically active derivatives into cellular proteins.

Donnie Berkholz, Mayo Clinic, discussed additional pathways leading to reactive oxygen species. Dihydrolipoamide dehydrogenase (DHD) is a dimeric enzyme with a relatively weak dimer association constant. Berkholz explained how adventitious protease and diaphorase activities associated with the monomeric, but not the dimeric species can lead to significant iron imbalance and oxidative stress. He uses fragment-based drug design (smaller molecular fragments compared to high-throughput screening) to cover chemical space with a much less extensive library of compounds.



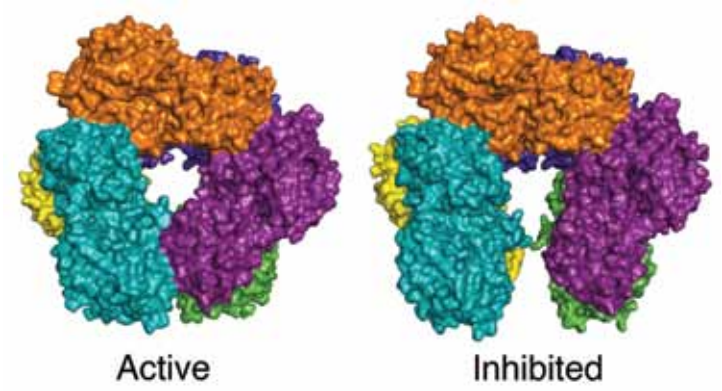
From Donnie Berkholz: DLD is an abundant mitochondrial enzyme involved in critical metabolic activities. In addition to its primary activity (bottom right), it has two moonlighting activities (bottom left) that implicate it as an underappreciated contributor to mitochondrial oxidative stress. These activities occur primarily when DLD is in a pathophysiological monomeric state (left, in gray), suggesting a strategy of stabilizing the dimer (right, in pink and gray) to reduce oxidative stress.

A related strategy for specificially inhibiting the farnesyl transferase in pathogenic fungi was described by **Michael Hast**, Duke U Med Ctr. These fungi all share a conserved enlargement of a channel adjacent to the farnesyl lipid binding site that offers a substantially different and more accommodating volume against which to target modifications of existing anti-fungals.

Kevin Kirouac, U Western Ontario, concluded the session with an intriguing discussion of the stereochemistry of base selection during repair of 8-oxo guanine damage. The likely polymerase, Pol I, is a Y-family polymerase whose complexes with DNA reveal restricted C1'-C1' distances that promote accuracy by enabling a clash between a conserved glutamine, Q59, and the 8-oxo group. The clash tilts the 8-oxo group, making it less likely to form catalytically productive complexes except to dCTP. The Q59A mutation strongly favors dATP, which exploits the Hoogstein edge of the damaged guanine.

A series of three related posters from Zac Wood's group at the University of Georgia highlighted work on the structural and functional evolution of the short chain dehydrogenase family enzymes involved in UDP-sugar metabolism. In T-064, (Samuel Polizzi), UDP-4-keto-xylose; you have to CE it to believe it, the authors are interested in the evolutionary origin of UDP-xylose synthase. The title refers to the fact that the authors have used capillary electrophoresis, which has one thousand times greater resolving power than conventional HPLC, to separate the 4-keto and 4-hydroxy forms of xylose. A key difference between the synthase and the closely related UDP-glucuronic acid decarboxylase is an

extended loop that covers the NAD cofactor binding pocket. The decarboxylase, ArnA, actually produces a small amount of xylose. The authors show that retention of the reduced NADH following the oxidative decarboxylation of UDP glucuronic acid leads to increased synthesis of xylose and propose that the leakage by ancestral ArnA may have afforded a selection for the extended loop that allows the recycling of reduced NADH necessary to reduce 4-ketoxylose. The preceding enzyme in the pathway is another dehydrogenase,



T-070, **Renuka Kadirvelraj**, *Human UDP-Glucose Dehydrogenase Reveals a Bifunctional Active Site: The Pin in Fischer's Lock* shows that this enzyme uses an intriguing form of intramolecular communication to regulate activity in response to the downstream product, UDP-xylose, which acts as a feedback inhibitor. The four different structures of the UDP-xylose•hUGDH complex show that the inhibitor binds to the active site, allowing a buried loop that is normally packed against the bulky C5-hydroxymethyl in the substrate to repack and accommodate the smaller C5-hydrogen of the xylose. To repack, the loop slides through a tunnel and shifts an α-helix (ie., the Pin) buried between subunits in the interface. This sliding motion induces a screw-type disruption of the symmetric trimer of dimers, forming an inactive, lower symmetry complex resembling a horseshoe (see above).

T-079: *Twisting of the DNA Binding Surface By A Beta-Strand-Bearing Proline Modulates DNA gyrase Activity*, **Nei-Li Chan**, National Taiwan U, provided a rationale for the fact that DNA gyrase is the only topoisomerase capable of introducing negative supercoils. For this activity to happen, it is necessary to have a gyrasespecific *GyrA-box* motif present in the C-terminal domain of the gyrase A subunit (GyrA-CTD). The crystal structure of *Xanthomonas campestris* GyrA-CTD has a canonical GyrA-box motif resembling the GyrA-box-disordered *E.coli* GyrA-CTD in that both have a non-planar pinwheel fold composed of 6 seemingly spirally arranged β-sheet blades. This non-planar architecture is due to the tilted packing seen between blades 1 and 2, with the packing geometry likely being defined by a conserved and unusual β-strand-bearing proline. Mutagenesis studies support the idea that the abrupt bend at the proline contributes directly to gyrase's (-) supercoiling activity. Chan and his co-authors suggest that a similar β-strand-bearing proline in phenylalanine hydroxylase may explain the deleterious structural effect of the P to L mutation responsible for phenylketonuria.

Charlie Carter

From left: Carol Brock, Bruce Foxman, Jenny Glusker, Peter Müller, Larry Falvello, Larry Dahl, and Chuck Campana. Photograph by Peter Müller.

2.03 Blast from the Past

In the opening talk, *Undistorted Reciprocal Lattice Views, from the Precession Camera to Pixel Picking*, **Larry Falvello**, U Zaragoza, described in detail the theory behind precession photographs and showed how a precession camera works.

Carol Brock, U Kentucky, also focused on precession photographs, albeit in a more practical context. Her talk *When the Structure is Difficult Look at the Whole Diffraction Pattern* described examples of structures that could only be understood when the space between the Bragg reflections was considered as well. Carol noted that his can be done by means of precession and pseudo-precession photographs.

Jenny Glusker, Fox Chase Center, in her talk *Electron-density maps. What insight can we gain from them?* explained in detail how electron density maps are calculated and what can be learned from the different types of electron density maps. Jenny reminded the audience that several steps are needed to go from the diffraction pattern to the three-dimensional electron density map and that the electron density is not what is measured in the diffraction experiment but rather *is* already an interpretation of the actual data.

In *Topotaxy HOWTO: Following Two-Phase Solid-State Reactions in the 1970s and Today with a Modern Diffractometer* **Bruce Foxman**, Brandeis U, demonstrated his new approach to an old method aimed at understanding phase transitions by comparing the respective orientation matrices. His method results in simple yet impressive two-picture movies, showing the before and after states of topotactic reactions.

To conclude the session, **Chuck Campana**, Bruker-AXS, and **Larry Dahl**, U Wisconsin, told a story in tandem: *The Structure of $Fe_3(CO)_{12}$ Revisited*, an interesting and entertaining historical overview of more than sixty years of crystallography and chemistry on the title compound, triiron dodecacarbonyl. First attempts to determine the structure of $Fe_3(CO)_{12}$ were made in 1950 by the then young Larry Dahl. Many experiments, diffraction and other, followed over the decades and in 2010 the (thus far) final dataset was collected – at low temperature and to 0.4 Å resolution – finally giving the complete picture.

David Watkin, Oxford U, who was originally scheduled to speak about *Structure Analysis. -Why do we always ...?* could not attend the session because of a health problem. **Peter Müller**, MIT, who organized the session, together with all speakers wish him well and look forward to hearing his presentation next year in New Orleans.

Peter Müller

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2.04: General Interest II

Carroll Johnson, ORNL, described how to analyze crystal structures as dynamic systems. Using the thermal parameters as indicators of dynamic flows, the intimate, concerted motions of the molecule can be quantified.

Ronald See, Indiana U of Pa., attempted to use the Bond Valence model(BVM) to predict hydrogen bonding trends. Neutron data on imidazole systems correlated well with Cambridge Structural Database (CSD) entries and computed data.

Carol Brock, U. Kentucky, hunted down kryptoracemates, (racemic compounds in which the enantiomers are not related by symmetry) in the CSD. Using InChI strings, she searched the Sohnke (enantiomorphous) space groups, and found that kryptoracemates are unusual, but hardly rare. From her search she estimated that the probability of spontaneous resolution is about 6%.

Sean Johnson, Utah State U, determined the structure of the helicase Mtr4, which proved to have a novel arch domain. Removing this arch did not affect the helicase activity, but did affect other processes necessary for RNA degredation.

Cory Gerdts, Emerald BioStructures, described how microfluidic mixing methods could allow a researcher to have hundreds of crystallization experiments on a card the size of a microscope slide. He showed that this technique leads to higher quality crystals, using much less sample.

James Fettinger, UC Davis, explained that although using low temperature devices has improved data quality, they have also introduced some negative aspects, *e.g.*, twinning and phase changes. A phase change at 161˚K was followed by collecting data sets above and below the transition temperature.

Christine Beavers

General Interest Posters

M-063: with *X-ray Diffraction Measurements of Substrate-Supported Crystals using a Hexapod*, **Lin Yang** explained how to determine the orientation of the in-plane axes of a thin crystallite grown on a solid support. A hexapod (or, six-jack) sample manipulator mounted on a rotatable stage is used to center the crystallite in a grazing-incidence x-ray beam and to produce an in-plane-averaged "powder" pattern. Then the crystallite is rotated about a vector that is perpendicular to the surface normal. Because the geometry of the system can be manipulated, additional data can be collected via an area detector. This method was applied to crystallites of 6,13-TIPS-pentacene (TIPS = triisopropylsilylethynyl) grown on SiO_2 supports. Lin Yang published this work in the *Journal of Synchrotron Radiation*, 2009, pp788-795.

Carol Brock and Jim Fettinger

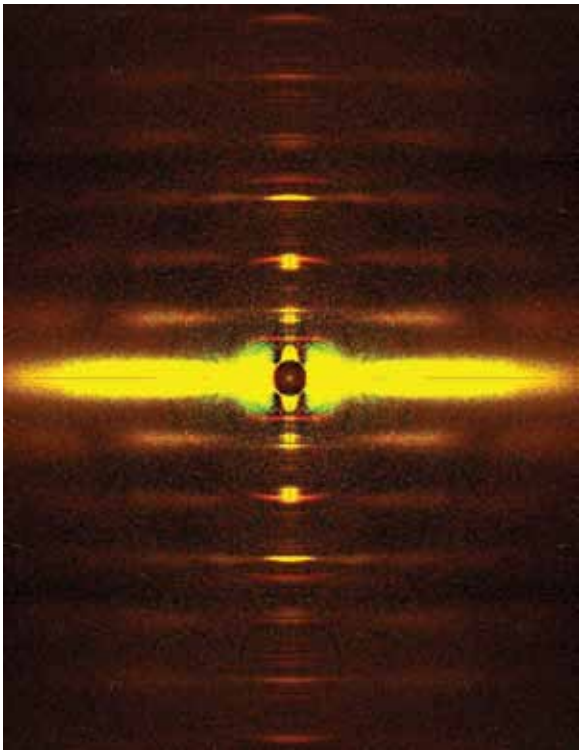
From left: Manfred Burghammer, Thomas Irving, Paul Langan, Joseph Orgel, Srinivas Janaswamy, Carlo Knupp (leaning to his right), and Leif Hanson. Photo taken by the Local Committee.

Fiber Diffraction Flexes Its Muscles

The fiber diffraction SIG organized two sessions at this year's meeting that saw both stimulating scientific presentation and robust discussions.

7.09: Fibril-forming Pathological Peptides: Prions, Amyloids & "Friends" served as our general, 'hard-core' fiber diffraction techniques and developments series of presentations. Each presenter outlined their group's research into the mechanisms of fibril-associated (mainly neurological) disease, the cause and effect of fibril formation from normal to 'evil', soluble protein transitions that allow fibril polymerization, and the range of techniques employed by each group to characterize the structures. The latter was as impressive as it was informative: to see that as with other difficult structural problems, TEM and x-ray diffraction based methods (single crystal crystallography and fiber diffraction) are well supplemented with NMR, CD, and FRET amongst other biophysical techniques as a matter of necessity. **Gerald Stubbs**, Vanderbilt U, talked about *Structural studies of prions and other amyloids by X-ray diffraction* which was the highlight of the session. Also see *On the Cover*, page **??** In Gerald's words *Amyloids are misfolded proteins associated with a variety of diseases including Alzheimer's, Parkinson's, and variant CJD ("mad cow") diseases. Studies of amyloid molecular structure are essential if we are to understand the process of amyloid formation and design rational therapeutic interventions. However, conventional methods of structural analysis cannot be used on amyloids, because of their size and degree of disorder. Our fiber diffraction methods have shown that there is a much greater diversity of amyloid structures than had been believed, but there are nevertheless common structural motifs. We have examined amyloids associated with Alzheimer's disease, type II diabetes, and CJD, obtaining the first x-ray diffraction data from CJD-associated amyloids ("prions").*

Session 3.01: **New Developments in Fiber Diffraction: Cryo-, Micro-diffraction and Complementary Techniques.** A common theme in these talks was to describe the ways in which multi-modal techniques (TEM particle reconstruction, high resolution crystallography structure in the context of low resolution fiber diffraction structure etc.) have allowed the solution of fiber diffraction based problems, and how developments in beamline technologies and techniques are advancing both new and old problems. A developing theme to watch seems to be fiber diffraction's capabilities in assisting the development of new biofuel technologies. Exciting advances have been made in connective tissue and muscle structures. Thomas Irving, BCPS, highlighted these themes well in his presentation: *Time-resolved Fiber Diffraction Reveals the Molecular Basis for Stretch Activation in Insect Flight Muscle*. Thomas said that *the majority of flying insects, representing about half of all known animal species, turn their muscles on and off with each wingbeat, not by adding and removing calcium with each contraction as in vertebrate muscle but by a phenomenon called "delayed stretch activation" whereby mechanically stretching the muscle at constant [Ca^{2+}] leads to active contraction. The structural mechanism underlying stretch activation has been elusive despite decades of study. Using time resolved x-ray fiber diffraction with the BioCAT beamline 18ID at the Advanced*



From Thomas Irving: Two-dimensional x-ray diffraction pattern from twitching rat cardiac muscle in the diastolic state. Courtesy P. de Tombe, Loyola U Med. School. l

3.01, 7.09 Sessions: Fiber, cont'd

Photon Source, investigators from Duke University and the Illinois Institute of Technology discovered clear evidence for previously unsuspected mechanical connections between the thick and thin filaments in resting muscle that transmit strain in the thick filaments directly to the troponin/tropomyosin complex turning the muscle "on" when the muscle is stretched and "off" when the muscle is released. Even more surprisingly, they found clear evidence for twisting and untwisting of the myosin-containing thick filaments as the muscle is stretched and released in cyclical contractions. During stretch, this would result in placing myosin heads closer to their "target zones", stereospecific binding sites on the actin-containing thin filament. This, combined with stretch-induced recruitment of myosin heads, may finally provide an explanation for stretch activation in these muscles. Since stretch activation is also a feature of human cardiac muscle, this may have relevance to understanding this feature of cardiac function.

Joseph Orgel

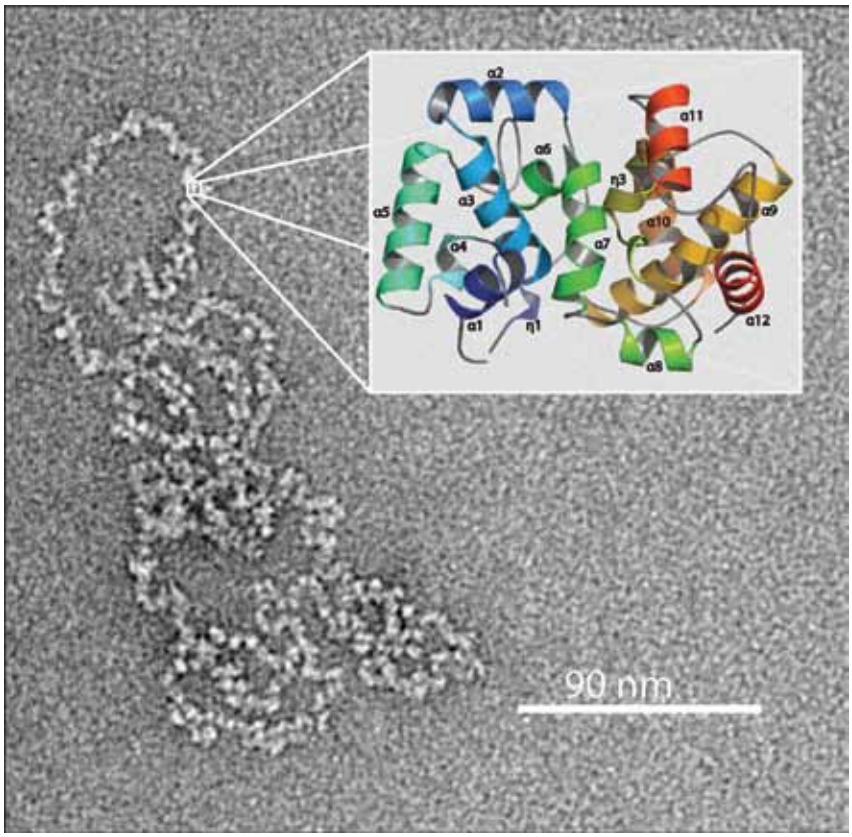
4.01: Biomacromolecules

The keynote speakers for this session were **John Tainer** and **Zimei Bu**. **John Tainer**, Scripps and LBNL, started the session with a rousing presentation describing work on DNA repair and replication complexes using a combined approach of small-angle x-ray scattering (SAXS) and crystallography. In addition to providing an overview of the SIBYLS beam line at the ALS, he presented the structures of several complexes, including DNA-Mre11, a protein from the double-strand break repair machinery. **Zimei Bu**, formerly at Fox Chase Cancer Center and now at City College of New York, presented a small-angle neutron scattering (SANS) study of the NHERF1-ezrin complex that made it possible to probe the structure of the two subunits within the intact complex. NHERF1 is a scaffold protein that participates in the localization and trafficking of membrane proteins.

Dilano Saldin, U Wisconsin-Milwaukee, presented work of interest for those using x-ray free electron lasers for small-angle x-ray scattering and diffraction. Through the use of an angular correlation function from what appears to be azimuthally uniform data, it is possible to reconstruct the 2-dimensional structure from the pattern. **Nicholas Reiter**, Northwestern U, presented a crystallographic study of the tRNA-RNase P holoenzyme complex. The structure shows the active site and suggests that tertiary interactions drive function.

Richard Baxter, UT Southwestern Med. Ctr., presented a combined crystallography/SAXS study of TEP1, a thioester protein involved in the humoral innate response in mosquitos to the malaria parasite, and its complexes with two proteins LRIM1 and APL1. While TEP1 is homologous to the C3 human complement factor, the mechanism of activation differs considerably. **Sai Venkatesh Pingali**, ORNL, presented a SANS study of dilute acid pretreatment of lignocellulose. Sai's work demonstrated that in addition to increasing the cross sectional radius of the elementary cellulose fibril, dilute acid pretreatment also opens the fibril network and causes lignin to aggregate into ~30nm particles. **M. Gordon Joyce**, NIAID/NIH, presented a crystallographic study of the NKp30 cell activating receptor from natural killer cells. This protein helps the cells identify targets through binding to several receptors. The antiparallel dimer found in the crystallographic structure is thought to be involved in the function of the protein.

William Heller

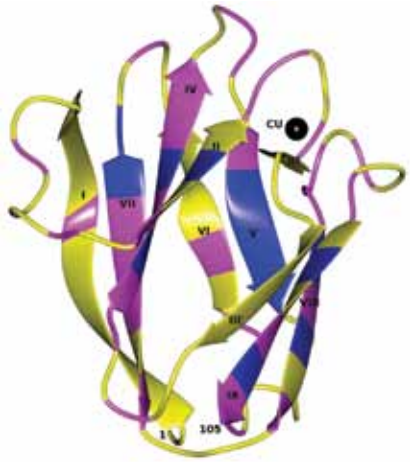


From a Biomac poster by Donald Raymond, U Michigan: Electron micrograph of an authentic ribonucleoprotein (RNP) purified from Rift Valley fever virus (RVFV) infected cells. Apparent is a lack of helical symmetry, which is different from the helical RNPs seen in other negative-sense RNA viruses to date. The inset shows the crystal structure of the RVFV nucleocapsid protein monomer. Raymond DD, Piper ME, Gerrard SR, Smith JL. Structure of the Rift Valley fever virus nucleocapsid protein reveals another architecture for RNA encapsidation. Proc Natl Acad Sci (2010).

Editor's note: Donald won a Pauling Award for his poster S-310; see page 19.

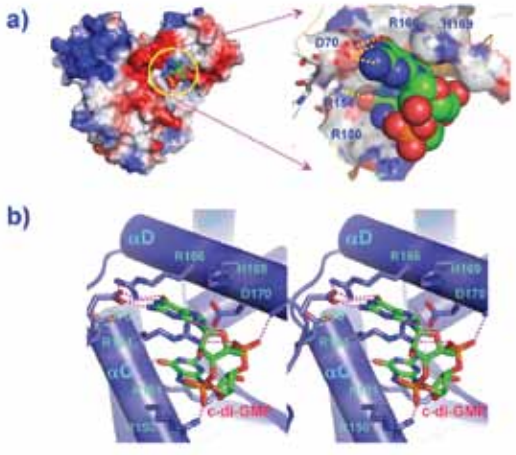
Biomac Posters

As I cruised the poster area at the Sheraton I enjoyed seeing "old themes" like copper binding proteins, intriguing ties to my own research, excited young researchers, and colleagues from around the world. The incredible diversity of research is what makes ACA meetings so much fun. I visited for a while with **Narayanasami Sukumar** from Cornell about his poster: **T-012**: *A Joint X-ray and Neutron Diffraction Study on a Copper Protein to Reveal the Role of Protein Dynamics in Electron Transfer*. which showed a combined x-ray and neutron diffraction model of the copper protein Amicyanin. The size requirements for neutron diffraction on protein crystals has gone from the cm size I remember talking about in grad school to only millimeters, but these sizes are still a challenge for most proteins. Here the neutron diffraction data allowed Sukumar to follow the protonation state of key His and Tyr residues in order to derive a model for the electron transfer process. As a physicist, my heart was warmed by his prominent display of an equation for the reorganization energy based on temperature, change in free energy (DG) and electronic coupling. Biochemical work added to the story of the MADH-amicyanin-cytochrome c551i complex provides insight into the dynamic nature of the process.



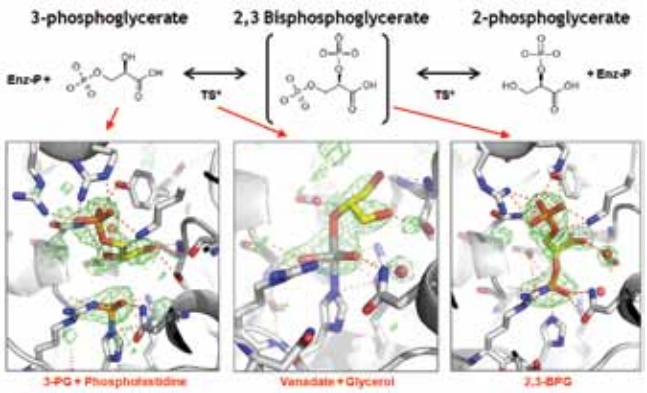
Ribbon diagram of amicyanin with residues color coded based on deuterium occupancy values of backbone amide hydrogens: blue for non-exchanged, pink for partially exchanged and gold for completely exchanged. The numbering scheme for the β-strand is in Roman numerals. The copper is shown as a black sphere. N.Sukumar, F.S.Mathews, P.Langan and V.L.Davidson (2010) Proc. Natl. Acad. Sci. USA, 107, 6817-6822.

After some years working in the Xu lab on nuclear receptors, I couldn't help being drawn in to **Shan-Ho Chou**'s poster T-137: *The c-AMP Receptor-Like Protein CLP is a Novel c-di-GMP Receptor Linking Cell-Cell Signaling to Virulence Gene Expression in Xanthomonas campestris on the Receptor-Like Protein XcCLP*, an analog of catabolic activation protein (CAP), which is involved in regulating gene expression in eubacteria. Shan-Ho came all the way from National Chung-Hsing University in Taiwan to present at this ACA meeting which makes my drive from Grand Rapids nothing to complain about. He showed that XcCLP is intrinsically active in binding DNA and that the presence of c-di-GMP acts to change the XcCLP conformation to release DNA binding. Again biochemical assays and modeling helped fill out the story of c-di-GMP as a negative regulator in downstream pathogenic gene expression.



From Shan-Ho Chou: the docked model of c-di-GMP/XcCLP complex: a) XcCLP dimer (positive, blue; negative, red); c-di-GMP as van der Waals with N= blue, O=red, C=green. Yellow designates docked region. Yellow dotted lines indicate specific H-bonds. b) Specific interactions between c-di-GMP and XcCLP. The stick residues have H-bonds or salt-bridges as dotted red lines c) Superpositon of DNA-binding domains of apo-XcCLP (red) and XcCLP/c-di-GMP complex (blue). Carbons are pink in apo-XcCLP and gray in c-di-GMP/XcCLP. Ko-Hsin Chin, Yen-Chung Lee, Zhi-Le Tu, Chih-Hua Chen, Yi-Hsiung Tseng, Jinn-Moon Yang, Robert P. Ryan, Yvonne McCarthy, J. Maxwell Dow, Andrew H.-J. Wang, & Shan-Ho Chou, J. Mol. Biol., 2010, 396, 646-662.

Finally, I visited with **Anna Gardberg** at her poster, **T-134:** *Case studies from the structural genomics of infectious disease*.



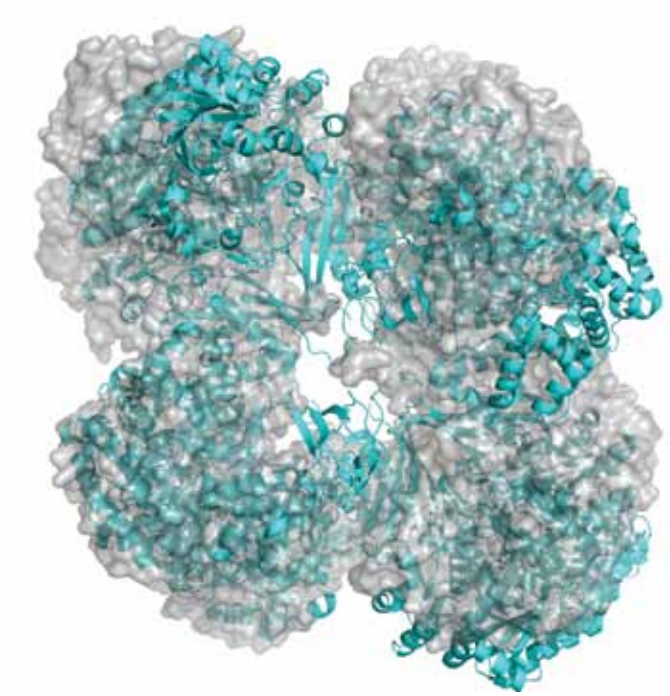
From Anna Gardberg: BupsA.00114.a B1 is a phospho-glycerate mutase from Burkholderia pseudomallei that was selected for ligand crystallization (Tier 11), resulting in several ligand-bound structures (PDB IDs: 3EZN, 3FDZ, 3GP5, 3GP3, 3GW8). Close-ups of the active site reveal the 3PG substrate and a transition-state intermediate as a covalently-bound phosphate (left panel), which can be mimicked by vanadate + glycerol (center panel). The final product, 2,3-BPG is shown in the right panel. David Davies, was the lead crystallographer on this enzyme.

Anna works at Emerald Biostructures solving structures right and left. Somewhat reminiscent of my days working with industry, Anna said she usually gets at least purified protein to start with and often is presented with a dataset to start her work. Her enthusiasm about solving and refining structures, then looking at the structural similarities and mechanisms all at a high energy pace was infectious (pun intended) and I couldn't wait to get back to my own project. That's another thing about ACA meetings, they energize you. I always come away with new ideas and more things to try than I ever have time to actually complete but especially with memories of old and new friends to help make it through the next year, until New Orleans!

Ross Reynolds

Biomac Posters, cont'd

Adam Lietzan from the Kumar laboratory of Marquette University presented **T-049:** *Structural insights into allosteric activation of pyruvate tetramer organization of Rhizobium etli PC is independent of acetyl coenzyme A*. This work follows up on initial studies of pyruvate carboxylase that revealed significant changes in the organization and symmetry of this tetrameric enzyme in structures from different organisms. A possible explanation for these differences is that different ligands are present in the various structures. Adam and his co-authors show that the asymmetry of pyruvate carboxylase from the bacterium *R. etli* is not related to which ligand is bound, but is inherent to its structure. This raises interesting questions about the regulation and stoichiometry of this key enzyme in different organisms.



From Adam Lietzan: the tetrameric arrangement of PC from S. aureus possesses nearly 222 symmetry in the presence and absence of acetyl coenzyme A, while PC from R. etli maintains an asymmetrical tetrameric arrangement in the presence of acetyl coenzyme A. Alignment of S. aureus PC in the absence of acetyl coenzyme A (cyan; PDB: 3BG5 Xiang & Tong. (2008) Nat. Struct. Mol. Biol. 15, 295) within a surface model display of R. etli PC in the absence of acetyl-CoA (grey) shows R. etli PC is clearly asymmetrical.

Zhiwei Chen from the Di Cera laboratory at Washington University presented **T-034:** *Crystal Structure of Human Prethrombin I at 1.66 Å*. Thrombin is coverted into an active enzyme in a multi-step activation pathway. Prethrombin 1 is an early species in that pathway, and had previously not been structurally characterized. The authors presented the first structure of prethrombin 1, which among other novel features shows a collapsed conformation for the region between residues 186 and 193. This sheds new light on the allosteric equilibria between different forms of the mature enzyme.

Lesa Beamer

7.01 Membrane & Associated Proteins

Mark Hunter, Arizona State U, who was designated an **Etter Student Lecturer** by the Synchrotron Radiation SIG, described on-going femtosecond serial crystallography studies of the structure of Photosystem I using the free electron laser source at the Linear Coherent Light Source (LCLS). In these experiments, a stream of nanocrystals of Photosystem I were injected into the femtosecond FEL beam. The energy absorbed by the drop that contains the crystal destroys the crystal, but not before a diffraction pattern is recorded. Over six million single-shot diffraction patterns from randomly oriented nanocrystals are grouped together by crystal orientation to give a complete set of diffraction data, from which the crystal structure is solved. This method is very promising because protein crystals in general are not large and are highly susceptible to radiation damage.

Ernst ter Haar, Vertex Pharmaceuticals, presented crystal structures of calcitonin gene-related peptide (CGRP) in complex with its receptor (CGRP-R) in the presence of synthetic drugs. CGRP is a potent vasodilator directly implicated in the pathogenesis of migraine. These structures reveal how small molecules bind to CLR, a class B GPCR that makes up half of the CGRP-R, and how they block access to the CGRP binding cleft at the interface of CLR and RAMP1, a receptor activity-modifying protein which is the other half of the CGRP-R.

Huey Huang, Rice, summarized the pioneering research done by his group using neutron scattering and x-ray diffraction to study the structure of membrane pores formed by antimicrobial peptides. These relatively small peptides collectively form non-selective pores in the cell membrane, thereby killing the targeted cell. The Huang group previously used neutron scattering to estimate the size of these pores. More recently, they have utilized anomalous scattering from Br labels within the lipid molecule to help resolve the electron density distribution of these peptide-induced membrane pores so that the architecture of the pores can be determined.

Jarek Majewski, LANL, described x-ray reflectivity and grazing incident scattering experiments that followed the process of cholera toxin attack on model lipid monolayers and bilayers. In-plane and out-of-plane changes in two-dimensional packing of cholera toxin molecules and the lipid membrane were investigated.

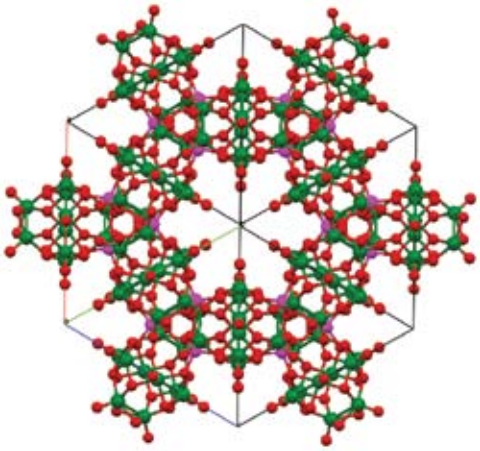
Masa Fukuto, BNL, utilized lipid Langmuir monolayers to create two-dimensional crystals of streptavidin (SA) and cowpea mosaic virus (CPMV). X-ray reflectivity, grazing incidence diffraction and Brewster microscopy data were presented. For SAs that are attached to a biotin-bearing lipid monolayer, a biotin density-driven phase transition from a disordered SA structure to a 2D SA crystal was observed. Data suggest that all SAs are bound to the lipid monolayer by two biotins. In the case of CPMV, the viruses were adsorbed to the oppositely charged lipid monolayer by electrostatic interaction. 2D crystals were obtained by manipulating the pH value and ionic strength in the bulk solution to optimize the electrostatic interaction between CPMVs.

Lin Yang

5.01 Cool Structures

The Cool Structures session opened with **William Ojala**, U St. Thomas, MN, presenting the effects of "bridge-flipped" isomerization, a reversal of a group of bridging atoms connecting two major parts of the molecule, on the molecular conformation and packing in crystal structures of benzylideneanilines (Ar-CH=N-Ar' vs. Ar-N=CH-Ar' bridging), and the phenylhydrazones (Ar-CH=N-NH-Ar' vs. Ar-NH-N=CH-Ar' bridging). **Jim Simpson**, U Otago, New Zealand, described the reversible bridging and terminal bonding of carbonyl groups found in a tricobalt cluster $RCCo_3(CO)_6$(triphos). Carbonyl bridging of the Co-Co bonds is favored in the presence of a highly electron donating apical substituent group R or substituting ligands.

Carla Slebodnick, Virginia Tech, presented a solution for the problematic crystal structure of a new anionic framework $[(As_6V^{IV}_{12}V^{V}_{3}O_{51})^{9-}]_\infty$, which consists of disordered 'half-balls' that appeared as a network of $V_{10}O_{26}$ "balls" in the highly symmetric space group *Im3m*.



From Carla Slebodnick: Crystal structure of the anionic framework as viewed down the [111] axis. V. Soghomonian, C. Slebodnick and E. C. Spencer: Re-determination of the structure of an anionic oxo-vanadium arsenate framework, Dalton Trans., 2010, 39, 8652-8654.

Gary Nichol, U AZ, showed examples of facile chemical transformations in $[Re_6(\mu\text{-}Se_8)]^{2+}$ cluster complexes that produced disorder or twinning in crystal structures. **Patrick Carroll**, U Penn., described some crystallographically challenging structures solved recently in his laboratory. These included disordered structures, twinned crystals, large and "unexpected" molecules, and two structures that remain "uncompleted". **Christopher Incarvito**, Yale, presented an x-ray structural and theoretical analysis of the asymmetric H-bond in hexafluoroacetylacetone (HFAA). The compound is a liquid (m.p. 177°K) at ambient temperature, and the crystal was grown *in situ* using the zone-melting technique at 93°K. The weakening of hydrogen bond strength compared to that of the acetylacetone molecule is contributed to the electron withdrawing CF_3 groups in HFAA. **Marilyn Olmstead**, UC-Davis, showed the audience an amazing picture of an ancient "buckyball" from her recent visit to Turkey. She described the structures of two concomitant isomers of C_{86}, namely Cs(16)-C_{86} and C_2(17)-C86 found to be disordered in the crystal structure of C_{86}·Ni(OEP)·2toluene. The Cs and C2 isomers of C_{86} are related by a 90° rotation of a set of two pentagons and two hexagons, consistent with the proposed Stone-Wales transformation.

Xiaoping Wang

6.01: New Tools - New Lights

Crystallography has always been a technique-driven discipline. Once in a very great while, a new technique comes along that promises to transform the discipline through offering a truly disruptive technology. Framed by a historical perspective offered by one of the pioneers of hard x-ray diffraction at synchrotron sources, **Gerd Rosenbaum**, Argonne, the next three speakers, **John Spence**, AZ State U, **Linda Young**, APS/ANL, and **Francesco Gramiccia**, ESRF, offered spectacular results from their initial experiments using the world's first hard x-ray free electron laser, the Linac Coherent Light Source (LCLS) at Stanford.

In brief, the suggestion ten years ago by Neutze, Hajdu and colleagues that the ultrashort (tens to hundreds of fs) x-ray pulses produced by x-ray lasers would enable scattering to outrun damage has been confirmed. Nanocrystals were efficiently introduced into the LCLS beam by an ingenious one-crystal-at-a-time microdroplet spray developed by the Arizona State group. Diffraction patterns could be obtained from micro- to nanocrystals, the latter containing (for example) only ~100 unit cells of the very large integral membrane protein complex, Photosystem I. The source possesses full spatial coherence and the diffraction pattern neatly reveals the fringes arising from the shape transform of the exterior of the nanocrystals. Further, pseudo-powder patterns could be achieved by summing suitably-weighted patterns from the individual, randomly-oriented nanocrystals. These in turn revealed that radiation damage was not evident (at least, to 8.9Å resolution) if pulses of 10 fs or 70 fs duration were used, but only began to be apparent with 200fs pulses, much longer than originally anticipated. Young offered an explanation: the leading edge of the x-ray pulse ejects the innermost electrons thus starting an Auger decay clock (in her case, in neon atoms) and producing "hollow atoms". In the meantime, the inelastic scattering cross section (generating damage) is greatly reduced relative to elastic scattering (generating signal) for subsequent x-rays, though ultimately the neon atoms undergo full ionization to yield naked nuclei. The effect is very unlikely to be element-specific and presumably occurs in the C, N, O, S atoms of proteins such as Photosystem I.

The DOE's LSCS, the world's first hard-x-ray laser, opened as a user facility last year. The machine, in a long underground tunnel near Stanford, produces femtosecond snapshot x-ray pulses at 60 Hz, each containing about 10^{13} photons, up to 8 kV, in a 3-micron diameter beam. In the photos from John Spence above: the control room on Dec 13, 2009, the time that the first protein nanoxtal patterns were seen from an x-ray laser. Researchers in the diffractive imaging team prepare to collect a few million diffraction patterns from a continuous stream of Photosystem I nanocrystals fired in a liquid jet across the LCLS. Below, John Spence, Henry Chapman, and Inger and Janos Hajdu. (Team leaders I. Schlichting, P. Fromme, and J. Ulrich were absent).

You can only be a "new tool" once: this was THE opportunity at the ACA for the LCLS and its first users.

But crystallography also depends on seemingly more prosaic advances. Macromolecular structures are now invariably determined at ~100K - but does the cryo structure resemble the room temperature structure? and if not, why? Unfortunately, crystal cooling rates are limited by heat transfer properties and are neither infinitely fast (the room temperature structural distribution is frozen in) nor infinitely slow (the distribution remains in equilibrium throughout and the structure is that of the final state). **Rob Thorne**, Cornell, described the cooling processes and offered keys to better low temperature structures. Finally, **Christoph Ollinger**, Bruker AXS, urged us not to neglect the latest forms of lab x-ray sources and described a liquid metal jet microfocus source; again, a source determined by heat transfer properties.

Keith Moffat and Gerd Rosenbaum

7.02: Non-ambient Environments for Specialized Experiments.

John Evans, U. Durham, described a series of *in-situ*, time-resolved powder diffraction experiments designed to shed light on the synthesis of a high-temperature, metastable cubic phase of zirconium molybdate. Full powder patterns, which were collected every quarter of a second, allowed the evolution from the starting materials to the desired phase to be witnessed.

Tiziana Boffa Ballaran, Bayerisches Geoinsitut, posed the question "Is the non-homogeniety of the earth's mantle due to chemical or thermal processes?" To answer this question, she subjected perovskite crystals to 75GPa, simulating the conditions in the lower mantle.

Dominic Fortes, Univ College London, introduced the audience to the importance of sulfuric acid and magnesium sulfate hydrates in the planetary sciences. These compounds have been observed on the surface of icy moons, and have been predicted to be present in the depths of the subsurface oceans. High-pressure neutron powder diffraction experiments revealed new polymorphs and new hydrate forms.

Russell Morris, U. St. Andrews, presented a series of experiments examining the absorption of NO into metal organic frameworks. This work was motivated by a need for materials that can controllably release this gas for medical applications. The experiments made use of a special gas cell for performing single crystal diffraction at different NO loadings and pair distribution functions, derived from total scattering data, to understand framework behavior. He showed that the pore system in some MOFs can structurally respond to changes in adsorbate loading, and that the structural response can modulate the material's properties. Interestingly, in systems that combine hydrophobic and hydrophilic channels, one of the two types of channel systems can be selectively occupied by some gases.

Craig Robertson, U. Durham, presented the development of a laboratory diffractometer suitable for single crystal data collections down to ~2°K. In order to achieve such low temperatures, the instrument made use of the 3 stage Displex and a special crystal mounting technique in which the crystal is glued to a graphite fiber. As the sample is not optically accessible in the cryostat, a sample centering procedure based on the single crystal diffraction images was developed.

Lauren Borkowski, Stony Brook SUNY, presented a series of variable temperature and pressure diffraction studies of metal formate frameworks, which had perovksite related structures. In some cases, a phase transition involving an increase in volume per formula unit was observed on compression, suggesting that the pressure transmitting fluid was being forced into the framework.

Stephen Moggach, U. Edinburgh, presented a single crystal diffraction study of ZIF-8 under pressure. The unit cell volume showed a very complex dependence on pressure that was associated with the pressure transmitting fluid being forced into the pore system and the occurrence of a structural phase transition.

Christine Beavers and Angus Wilkinson

7.03 Software Integration and Databases

Wladek Minor, U VA, gave a humorous peek at the six clicks required to determine your structure using HKL3000. His main point was that it is very easy to hit the button six times, but that the experimentalist must engage his/her brain to be sure that mistakes are not made. He used an analysis of publicly available data and showed that statistical outliers can frequently be not outliers at all but operator error. **Albert Fu**, UGA, showed how you could do everything automatically with either HKL programs or XDS programs just by using the command line. His emphasized the oversight built in by the architects of the programs, but also that the operator must be involved.

Barry Finzel, UMN, showed us his new communication tool that can be used to help non-structural biologists design new drugs. When biologists attempt to overlay experimentally derived protein:ligand complex structures, as is usually done, they tend to use methods thaat rely on sequence and secondary structure matching. Barry believes that the optimal superposition of such complexes results rather from an overlay of select protein substructures surrounding the binding site. The chosen substructure should include key structural elements contributing to complex stabilization, but not include elements subject to conformational change when different ligands bind. Barry and his research group have been working to develop a database of "overlay methods" that captures optimized procedures for aligning important drug targets. A web-based interface provides access to computational tools to apply these methods to either user-contributed complex structures or structures from the PDB, and allows users to share aligned structures with collaborators.

Santosh Panjikar, EMBL, gave us a guided tour through **autoRickshaw**. This program aims to show the user in as close to real time as possible, how their data collection is going. The user can then either stop, collect more data, or load on a new crystal. The goal is to mimic what an experienced crystallographer would do. Santosh demonstrated how a difficult phasing problem was handled by phase combination with partially built models, finding additional sites in successive rounds of phasing. **Ronen Keegan** gave us an update on the latest and greatest from CCP4 and gave us a heads up for a new version of REFMAC that will come out soon. **James Holton**, UCSF/LBNL, described his new *MLFSOM* which he developed in order to determine where the errors in final refined structures come from. To this end, a quantitative simulator of the entire diffraction experiment called "MLFSOM" (MOSFLM in reverse) was created that puts damage, noise and signal on a common, absolute scale.See **http://bl831.als.lbl.gov/~jamesh/powerpoint/ACA_mlfsom_2010.ppt**.

7.03: Related Posters

M228: ***autoBUSTER re-refinement reliably reveals interesting features in newly-released PDB structures*** by **Thomas Womack**, Global Phasing, demonstrated the power of using the "interesting features" (*e.g.* errors) in structures that were recently deposited in the PDB. This program routinely yields better refinement statistics and improved validation scores due to its crystallographic data refinement using TLS and fully automatuted NCS setup.

M234: In ***MAIN 2010: finalizing the structure by validation driven structure improvement***, by **Dusan Turk**, Jozef Stefan Inst.,the model is fitted to the density and energy minimized using real space refinement. Residues ILE, VAL, THR and LEU are fitted using fragment side chain fitting. The program also evaluates hydrogen bonding networks using explicit hydrogens to optimize the working model. Asymmetric residues like HIS, ASN, and GLN along with the solvent molecules are flipped to yield an optimized final model.

M222: In ***Refined Crystallization Screens*** by **Hao An**, ANL, two sets of refined crystallization kits from the Midwest Center for Structural Genomics structure determination pipeline were evaluated. These refined kits are the fruit of the evaluation of other popular commercially available crystallization kits used by MCSG in order to reduce the number of setups and to improve coverage of crystallization space. One of the sets is based on the 384 most successful crystallization conditions gathered by the MCSG LIMS system. This LIMS system allows for the potential further improvement of the crystallization conditions used at MCSG.

S-298: ***SrRietveld: A Next Generation Rietveld Refinement Program*** by **Jiwu Liu**, Columbia, described SrRietveld, an opensource program aiming to ease the use of current Rietveld refinement engines and to extend their functions while allowing for incorporation of future components.

T-219: ***The PSI Structural Biology Knowledgebase – Search Online for Protein Seqeunces,Structures, Models, Methods, and More*** by **John Westbrook**, Rutgers, demonstrated the efforts of the PSI Structural Biology Knowledgebase, **www.sbkb.org**, to be available to the biology community as a portal to all of the information that PSI sponsored structural genomics centers have amassed.

M231: ***SrReal - an open-source software library for local structure analysis*** by **Pavol Juhas**, Columbia, is a part of DANSE. SrReal is capable of highly customizable calculations of atomic pair distribution functions, Ewald sums, empirical ionic radii or bond valence sums. It utilizes both C++ and Python and is fast and easy to use.

M-216: ***Chem-BLAST – a rule-based method to develop advanced structural ontologies for chemical bioinformatics, the PubCheM and the PDB*** by **Talapady N. Bhat**, NIST, demonstrated the power of **C**hemical **B**lock **L**ayered **A**lignment of **S**ubstructure **T**echnique. The website **www.rcsb.org/pdb/explore/externalReferences.do?structureId=3GGT** allows both rule based and vocabulary based searching of ligands in public databases. Interpreting the structural data of chemical compounds by dissecting them into scaffolds allows for easy classification and annotation. This speeds up the search for ligands in the structural databases and opens a ligand gateway to the PDB and PubChem.

Ed Collins and Peter Horanyi

7.04: Radiation Damage

This year saw a return of the highly popular session on radiation damage - the practical problem of intense x-rays "killing" a crystal during data collection, and it did not disappoint! We were fortunate to have a leader in the field, **Elspeth Garman**, Oxford, as our first speaker to bring the audience up to speed on the long history and still very physics-oriented nature of the subject. Most of the vast body of literature on radiation effects to biological systems pertains to room temperature and 10^6 lower dose levels than that which protein crystals typically endure, making it difficult to find studies relevant to cryo-macromolecular radiation damage. Fortunately, a series of "RD" workshops and the CCP4 Study Weekend have produced review articles summarizing the status and history of the field (most recently Garman & Nave (2009) *J. Synchrotron Rad*. **16**, 129-132; Garman (2010) *Acta Cryst*. **D66**, 339-351). A list of relevant papers is available at **http://lmb.bioch.ox.ac.uk/www/garman/gindex.html**. The focus this time was on "global" damage (loss of resolution), which for cryo-cooled protein crystals is proportional to dose (the amount of energy absorbed per unit mass of sample, measured in Gy or J/kg) and, remarkably, independent of "dose rate" (Gy/s). This allowed **James Holton**, UCSF/LBNL, to create a web page **http://bl831.als.lbl.gov/xtalsize.html** for computing the size of a protein crystal (or crystals) needed to solve a structure by MAD/SAD or to obtain complete native data, given the observed resolution limit, spot size, background level and molecular weight.

Some progress toward understanding the temperature dependence of global damage was presented by **Matt Warkentin**, Cornell, who found three distinct temperature ranges with different temperature dependence behavior: diffusion dominated at temperatures above 200˚K; an undefined effect operated between 200˚K and 80˚K; and there was no temperature dependence below 80˚K.

Tobias Krojer, Structural Genomics Consortium, Oxford, gave a perspective "from the trenches" on the difficulty of translating knowledge of damage mechanisms into practical tools that can be easily used at the beamline. The biggest challenge will be a general program for combining beam shape, crystal shape and dose calculations into a data collection strategy.

Finally, two talks explored the possibility of reducing radiation damage with micro-beams. Specifically, as beams and crystals become smaller than the track-length of the primary photoelectrons, much of the energy “deposited” will actually fall outside the crystal, breaking the fixed diffraction-per-unit-dose rule. However, the exact length-scale where this effect occurs is crucial to it's practical exploitation. **Ed Stern**, U Washington, presented calculations and experiments with the unexpected result that photoelectrons of energy 17 keV had an apparent penetration depth of less than 2 microns. **Bob Fischetti**, ANL, presented experimental measurements of the spatial extent of damage from a 1-micron 18-keV incident beam in which photoelectron damage was observed outside the beam footprint up to 4 microns from the beam center, but not further. These dimensions are very small, but not so small as to prevent an advantage when collecting multi-crystal data sets.

Janet Smith and James Holton

7.05: Local Structure (Neutron, Powder, Mats)

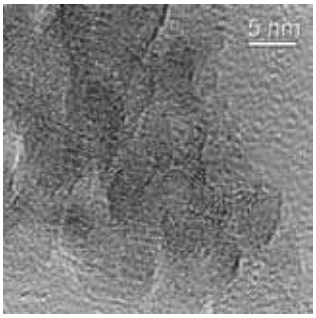
Atomic order of interest in emerging complex functional materials is often limited to the nanometer length scale, where crystallography, the basis of Rietveld refinement, fails. In these cases, the total scattering approach can be used. This approach treats Bragg and diffuse scattering on an equal basis. In recent years, the analysis of total scattering data, *e.g.* via the atomic pair distribution function (PDF) method, has become an invaluable tool to study nanocrystalline, nanoporous, and disordered crystalline materials. **Karena Chapman**, ANL, talked about probing chemical reactions in real time using PDF analysis. Current state-of-the-art PDF set ups (with optimized beam intensity, sample environments and detectors), such as that existing at 11-ID-B of the APS, now allow total scattering data suitable for PDF analysis to be collected at rates up to 30 Hz. This allows for the structural changes during reactions to be probed *in-situ* to reveal changes in bonding during catalytic reactions and particle nucleation and growth-from the earliest x-ray amorphous multi-atom clusters to nanoparticles and beyond. The insights gained into the reaction kinetics and mechanism can ultimately lead to greater control of structure and functional behavior.

Hyunjeong Kim, LANL, showed results of a structural study of crystallographically challenged hydrogen storage materials. One of the ways to prepare new hydrogen storage materials is mechanical alloying or ball milling, which often yields nano- or amorphous- phases or mixtures of both. Some of these exhibit interesting hydrogen storing properties. Alternatively, packing hydrogen storage materials into porous materials leads to great improvement in their properties; such nano-confinement allows materials to release high purity hydrogen at lower temperatures without a significantly long induction period. Despite favorable changes in properties, little is known about the structure of either type, partly because their amorphous or nano-sized nature limits the use of conventional crystallographic analysis and, therefore, structural determination becomes very challenging. This atomic PDF study focused on two promising hydrogen storage systems: Mg_xCo_{100-x} alloys prepared by ball milling, and nano-phase ammonia borane (NH_3BH_3) confined in pores of mesoporous silica MCM-41.

Efrain Rodriguez, NIST, presented local structure effects in magnetoresistive manganites and selenides. The two classes of materials were studied using the total scattering approach and the PDF method. Discussion was focused on how neutron and x-ray powder diffraction were employed to obtain the local and long-range structure of both materials to have a better understanding of the microscopic interactions leading to the magnetoresistance effect. $La_{0.5}Ca_{0.5}MnO_3$ was studied below the charge-ordering temperature. By combining Rietveld and PDF analysis with the total neutron scattering data, two competing models describing the low temperature phase displaying charge and orbital order were examined: 1) the Mn^{3+}/Mn^{4+} checkerboard model and 2) the Mn-Mn dimer model (so-called Zener polaron model). In the case of $Zn_{1-x}Cu_xCr_2Se_4$ selenides, PDF analysis of x-ray data was used to find how the local environment of the Cu and Cr cations lead to the observed magnetic and transport properties.

John Provis, U Melbourne, reported on efforts to couple total scattering and density functional theory computations to solve the structure of complex disordered aluminosilicates. Understanding the atomic structure of complex metastable materials is of great importance to both academia and industry. However, structures of such materials cannot be solved by most standard techniques. John presented a novel synergy between total scattering and density functional modelingwhich he and his co-workers had used to solve the structure of the metastable aluminosilicate material metakaolin. This combined aproach resulted in new insight into the local environment of the aluminum atoms in metakaolin, including evidence of the existence of tri-coordinated aluminum. When a detailed atomic description of the structure is available, it is possible to tailor the chemical and mechanical processes involving metakaolin and other complex metastable materials at the atomic level so as to obtain optimal performance at the macro-scale.

Stacey Smith, Brigham Young U, Neutron Scattering SIG-designated recipient of an **Etter Student Lecturer Award**, gave a presentation that was a highlight of the session.



From Stacey Smith, an Etter Young Student Lecturer: TEM image of alumina nanoparticles whose structural evolution as a function of calcination temperature was investigated using a combination of PDF and Rietveld analyses.

Their group has developed a simple and uniquely cost-effective synthetic method for producing γ-Al_2O_3 nanoparticles of exceptional size (3-5 nm) and purity. In order to establish the temperature range through which they could produce the catalytically-active gamma phase, they had to determine phase progression as a function of synthetic temperature. This is difficult because the alumina phase diagram includes many closely-related phases that are not readily distinguished from powder-diffraction data due to the extremely particle-size broadened Q-space peaks. In these cases, PDF analysis was able to resolve the distinct local structures of the candidate phases. A combination of PDF and Rietveld refinements proved successful in determining the alumina nanoparticle phase progression pathway.

Ilkyoung Jeong, Pusan National U, demonstrated the power of total scattering methods when used in combination with reverse Monte Carlo modeling to study ferroelectric-relaxor crossover in $Ba(Ti_{1-x}Zr_x)O_3$ (BZT). Comprehensive structural studies on normal ferroelectric to relaxor crossover in BZT have been performed using neutron total scattering measurements. The study estimated the degree of the displacement correlation between Ti ions and revealed that it is stronger and extends much longer for the ferroelectric state than for the relaxor state. The overall centering behavior of the Ti ion is found to change from directional to random displacements between the ferroelectric and the relaxor phases, providing an atomistic picture for ferroelectric-relaxor crossover with increasing Zr concentration.

Eric Chan, Australian National U, elaborated on applications of single crystal diffuse x-ray scattering for studies of polymorphism in pharmaceuticals. Due to the recent advancements in modern computing power, the analysis and interpretation of single crystal x-ray diffuse scattering for molecular crystals now involves the construction of a computer model of a dynamic crystal. Their method allows inclusion of structural features on a local level that can be tested against effects on the observed diffuse scattering. Observations of the dynamic behavior of organic molecules in the solid state suggest the models can also be used to explain the structural nature of packing defects or lattice strain. Three polymorphic systems were discussed: benzocaine, paracetamol and aspirin.

***In a related poster,* M-240: *Structure of nanoparticles: frontiers in PDF modeling,* Christopher Farrow**, Columbia U, discussed frontiers in PDF modeling to obtain structure of nanoparticles. Nanoparticles are poised to become vital in the future of energy, medicine, computing and countless other fields. Despite their current and potential usefulness, there are no robust methods for determining the structure of nanoparticles with atomic resolution. Furthermore, the process of nanoparticle growth is still not well understood. These obstacles stand in the way of high precision design and fabrication of nanoparticles for industrial applications. Christopher's presentation described established and new methods for modeling nanoparticles with the PDF. Recent work in which these methods have been applied to model noncrystallized nanoparticle precursor molecules was also reported, and his poster also outlined a plan to combine structural information from various sources with the PDF in order to model complex strained, segregated and disordered nanoparticles.

Thomas Proffen & Emil Bozin

Annual Statement of Ownership, Management, and Circulation

1. Publication Title: ACA RefleXions
2. Publication Number: 1938-9965
3. Filing Date: September 09, 2010
4. Issue Frequency: Quarterly
5. Number of Issues Published Annually: 4
6. Annual Subscription Price: $1.75
7. Location of known office of Publication is: 700 Ellicott Street, Buffalo, NY, 14203
8. Location of Headquarters or General Business Office of Publisher: PO Box 96, Ellicott Sta., Buffalo, NY, 14205
9. Full Names and Complete Mailing Addresses of Publisher, Editor and and Managing Editor: Publisher: ACA C/O 700 Ellicott Street, Buffalo, NY, 14203; Editor: Judith Flippen-Anderson, 3521 Lauralee Way, Annandale, VA 22003; Managing Editor: Connie Childress, 4210 Old Field Trail Dr., Kalamazoo, MI 49008
10. Owner: American Crystallographic Association, Inc.
11. Known Bondholders, Mortgagees, and Other Security Holders Owning or Holding 1 Percent or More of Total Other Securities: None
12. Tax Status: Not Changed During Preceding 12 Months

15. Extent and Nature of Circulation			Average No. Copies Each Issue During Preceding 12 Months	No. Copies of Single Issue Published Nearest to Filing Date
a. Total Number of Copies (Net press run)			2300	2300
b. Paid and/or Requested Circulation	(1)	Paid/Requested Outside-County Mail Subscriptions Stated on Form 3541	1557.25	1619
	(2)	Paid In-County Subscriptions Stated on Form 3541	0	0
	(3)	Sales Through Dealers and Carriers, Street Vendors, Counter Sales, and Other Non-USPS Paid Distribution	0	0
	(4)	Paid Distribution by Other Classes Mailed Through the USPS	583.5	532
c. Total Paid and/or Requested Circulation [Sum of 15b.(1),(2),(3),and(4)]			2140.75	2151
d. Free Distribution by Mail	(1)	Outside-County as Stated on Form 3541	61	51
	(2)	In-County as Stated on Form 3541	0	0
	(3)	Other Classes Mailed Through the USPS	0	0
e. Free Distribution Outside the Mail			0	0
f. Total Free Distribution (Sum of 15d. and 15e.)			61	51
g. Total Distribution (Sum of 15c. and 15f.)			2201.75	2202
h. Copies not Distributed			74.75	77
i. Total (Sum of 15g. and h.)			2276.50	2279
j. Percent Paid and/or Requested Circulation			97.23%	97.68%

16. Publication of Statement of Ownership will be printed in the Fall 2010 issue.
17. I certify that all information furnished on this form is true and complete.
(signed) Marcia Colquhoun for American Crystallographic Association, Inc.

7.06 Absolute Structure Determination;

Where are we now? **Simon Parsons**, U Edinburgh, began by discussing *Precise Absolute Structure Refinement Using Quotient Restraints*. Simon and his colleagues have developed a method for absolute structure determination. In their method one absolute structure is refined competitively against the inverted alternative, where the results are expressed by the *Flack Parameter*. Simon showed us that one can write a set of restraints based on observed and calculated values of a quotient he termed *D(h)* which can be calculated from a single diffraction data set. Using D(h) quotients systematic errors in the intensities tend to cancel out, resulting in significantly more precise values of the Flack parameter.

Martin Lutz, Utrect U, spoke about how experimental conditions affect absolute structure determination by Bayesian statistics (Hooft method). Martin described the experimental conditions necessary for absolute structure determination, particularly how errors in the data can influence the outcome. Use of the *Student t-distributions* was shown to increase the robustness of the Hooft method.

Michael Ruf, Bruker AXS, discussed how their new Microfocus sources can significantly improve the experimental conditions for determining light-atom absolute structure. Comparisons to sealed tube sources demonstrated a significant improvement in the data, which in turn results in more precise Flack parameters.

Amber Thompson, Oxford, spoke about interpretation of the Flack and Hooft Parameters in the analysis of 150 light-atom (CHNO) crystal structures. Amber demonstrated that the Flack and Hooft parameters follow a tight Gaussian distribution and that earlier interpretation of the parameters maybe unduly pessimistic.

Frank Fronczek, Louisiana State U, reported light-atom absolute structure determination with short wavelengths. His remarks about the correctness of structures that have high standard uncertainties and Flack parameters near zero resonated with the audience. Frank found that oxygen-rich chiral crystals of high quality frequently yield Flack values near zero with standard uncertainties ~ 0.3 - 0.5 and Hooft P2(true) ~ 1.0. He said that datasets maximize their probability of success if they are collected at low temperature, high resolution, high redundancy and high completeness of Bijvoet pairs. and observed that larger molecules were generally easier than smaller ones, presumably because more Bijvoet pairs are available.

Raymond Scaringe, BMS, presented a series of experimental tests for absolute structure without heavy atoms. Raymond compared Flack parameters with Hooft parameters for several compounds and thinks that using both parameters results in a higher level of confidence in the structure.

Finally **Jeff Deschamps**, NRL, discussed the absolute configuration of epoxyresibufogenin where he had used the Hooft method. Jeff decided to add a level of confidence to this light-atom structure determination, and verified its configuration by determining the absolute structure of it's bromo derivative.

Joe Reibenspies

7.10: Data Collection Strategies

Håkon Hope, UC Davis, began by providing an introspective examination of how slight deviations in area-detector orientation can manifest themselves in data collection and refinement. He also proposed a detector calibration strategy to offset variations that may often be ignored. Håkon delicately mixed classic and modern technology by using his new iPad to deliver his presentation of area detector fundamentals.

Janik Zikovsky, ORNL, switched gears and discussed a new software application, ***Crystalplan***, which aids researchers at TOPAZ. This software enables one to intricately plan data collection at the neutron source with respect to coverage, redundancy, and most importantly, time. This impressive software aptly complements the powerful hardware at TOPAZ.

Mathias Meyer, Agilent Technologies (formerly Oxford Diffraction), demonstrated the usefulness of ***CrysAlisPro*** and its data collection strategy algorithms. He contends that in the end efficiency should not be based solely on time, but rather on the balance between time and data quality.

Kanagalaghatta Rajashankar, NE-CAT & Cornell, explained the benefits of simultaneous two-wavelength (MAD) data collections at APS. While he admits that SAD is still a productive technique, his test case convinced the attendees that MAD should still be the experiment of choice at the beamline.

Lee Daniels, Rigaku Americas, provided an overview of new algorithms used in Rigaku's strategy programs. He emphasized the use of 3D bitmaps that allow the software to plan data collections based on actual laboratory environments rather than conditions optimized by the vendor. The software corrects for any device or configuration added to standard systems without sacrificing efficiency and data quality.

Simon Teat, LBNL, provided detail on the small-molecule detector system at ALS. While the high flux of ALS extends the dynamic range of most CCDs, a two (or more) detector position strategy can be used with exceptional results.

Joerg Kaercher, Bruker-AXS, concluded with a look at Bruker's data collection strategy algorithm and its impact on routine and challenging samples. Joerg's presentation allowed attendees to see Bruker's strategy regarding the automation of data collection, integration, and structure solution. He emphasized, however, that trained crystallgraphers are still needed!

Chris Incarvito

From left: Charles Campana, Luc Bourhis, Konstantin Udachin, Brandon Mercado, Saeed Khan, and (in back) Richard Gildea, Tom Emge, Peter Muller not shown. -Must have been taking photos elsewhere. *Photo taken by the Local Committee.*

7.26: Handling Disorder in Crystal Structures

The session began with a presentation from **Charles Campana**, Bruker AXS, which detailed methods of modeling disordered solvent molecules using tools available from SHELXTL and Platon. Chuck also showed an elegant way to calculate hydrogen atoms on water molecules using XP commands: do CENT to generate a dummy atom between neighboring oxygen and then fix the O-H distance with the command HIMP.

Tom Emge, Rutgers, gave a brief survey reporting on the deleterious effects of highly disordered solvent in a variety of crystal structures. His presentation included structures containing large pores, such as MOFs and cavitands, and those containing disordered solvents or counter ions of high molecular weights. **Brandon Mercado**, UC Davis, the **Etter Student Lecturer** designated by the small molecule SIG, see at right, showed newly solved endohedral metallofullerenes structures of $Sc_4(\mu_3\text{-}O)_n@C_{80}$ (n=2,3) and $Sc_2(\mu_2\text{-}O)@C_{82}$. These crystallized as co-crystal systems and due to inherent disorder were challenging to solve.

Luc Bourhis, Durham, gave a wonderful overview of the cctbx and smtbx free and comprehensive toolbox programs of Olex2 that are used for strategy and organization of small molecule structure solution and refinement procedures using Olex2 or other established crystallographic software. **Richard Gildea**, Durham, followed, with an excellent description of cctbx/smtbx routines to the van der Suis and Spek procedure (SQUEEZE) for handling disordered solvent in structure refinements.

Peter Müller, MIT, detailed several particularly challenging cases of solvent disorder, where the use of hand-picked complex restraints in SHELXL was required. Finally, **Konstantin Udachin**, NRC, gave a comprehensive talk on H-bonding and disorder in low-temperature clathrate hydrates that meticulously described the host/guest interactions that often lead to distortions of the overall clathrate shape.

Saeed Khan and Tom Emge

7.24: Mechanisms of Phase Transitions

This session aimed to investigate the atomistic mechanisms of crystal phase transitions between phases that have group-subgroup symmetry relationships. Several of the speakers used symmetry-mode analyses as a means to characterize the order parameters of transitions.

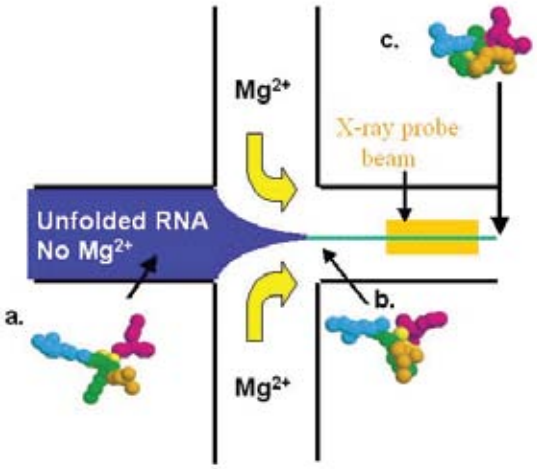
Chris Howard, U Newcastle, used this method to classify distortions that arise in perovskite-like compounds like $SrZrO_3$ and $(Ca,Sr)TiO_3$, where displacive and strain modes cooperate to induce a complex series of low-temperature phase transitions. These order parameters are nicely interpretable in the context of Landau theory. **Ian Swainson**, CNRC, showed that symmetry-motivated basis functions defined at the surface of the Brillouin-zone boundary provide a clean approximation to the rigid-unit tilt-mode and buckling-mode phonons known to soften at phase transitions in perovskite-related compounds. Active modes were identified by comparing simulated and experimental phonon structure factors. **John Evans**, Durham U, showed that symmetry-mode analysis can be combined with other computational and experimental techniques (*e.g.* DFT and solid-state NMR) to characterize highly-complex distortions with large supercells. Recent results included an unusually-large supercell that arises in $(MoO_2)_2P_2O_7$ and a novel family of magnetic oxychalcogenides. **Tiziana Boffa-Ballaran**, U Bayreuth, spoke on behalf of **Ross Angel**, Virginia Tech, on a DFT analysis of the high-pressure evolution of $YAlO_3$. They found an unexpected combination of coupled order-parameters with the net effect of reducing octahedral tilts rather than increasing them at high pressures. **Matteo Alvaro**, Virginia Tech, described a chain-silicate clinopyroxine whose composition was specifically tuned so as to exhibit distinct high-temperature and high-pressure phase transformations with dramatically different structural and physical characters. **Javier Ellena**, U Sao Paolo, presented a remarkable sequence of structural transitions in an important antifilarial drug, diethylcarbamazine citrateg. Each transition in the sequence involves the cleavage or formation of intermolecular hydrogen bonds; and all but one are observed to be fully reversible.

Branton Campbell

From left: Eaton Lattman, Lois Pollack (front), Lee Malkowski (rear), Robert Rambo, Edward Snell, Tobin Sosnick, Hiro Tsuruta. Photo courtesy of Eddie Snell.

7.11: Pushing the Envelope on SAXS

Lois Pollack, Cornell, talked about reconstructing time-resolved SAXS data using state-of-the-art mixing instrumentation experiments in which access times varied from sub-milliseconds to one week. The Cornell mixer comprises two symmetrically placed outer jets and a central one, which combine to produce a very thin, rapidly moving stream across which diffusive mixing is extremely fast. Each location along the channel corresponds to a fixed time after reaction is initiated. As an example Pollack presented SAXS results on Tetrahymena ribozyme folding, in the form of a time series of I(Q) curves of surprisingly good quality. These enabled the measurement of both the size and shape of the molecule as it folded, revealing transient states. She also discussed initial efforts at reconstructing the envelopes of these species from the I(Q) curves using the program DAMMIM. She emphasized that the ill-conditioned nature of these reconstructions requires the use of additional constraints or confirmatory information. The figure below illustrates the operation of the mixer.



Robert Rambo, ALS & LBNL, defined a new structural invariant available from SAXS data, the volume-of-correlation, Vc. In SAXS analyses, the Kratky plot, which graphs q2*I(q) versus q (=4πsinq/l) is a powerful tool for distinguishing compact from unfolded or expanded particles. For compact particles the trace asymptotically approaches the q-axis for large q, while for expanded particles the curve continues upward. The integral under this curve is termed the *Porod Invariant Q*. Q is related to the mean square electron density of the particle, but is defined only for SAS data associated with compact particles. Vc is based on a related plot of qI(q) versus q, for which the integral $R = \int qI(q)dq$ appears to converge for all experimental cases so far examined. From this one can derive Vc which appears to be independent of concentration and contrast. It is already clear that Vc is sensitive to molecular conformation, in the same way as radius of gyration. Moreover, it seems to provide a more robust method of extracting molecular weight from SAXS data. Rambo showed that both for simulated and actual SAXS data a plot of ln(QR) versus logarithm of molecular mass was highly linear, providing errors in mass of less that 10% over a very large range of masses.

Edward Snell, HWI, reported work in which he, together with colleagues, combined crystallography, SAXS and computations to investigate a domain that is appended to the N or C-terminus of a tRNA synthetase in eukaryotes but not prokaryotes. The elusive N-terminal domain was not visible in their crystal structure of yeast Gln4, but was known to be present in the crystal. SAXS data were used to reconstruct *ab initio* the envelope for this molecule. The structure, missing the N-terminal domain, was fitted into the SAXS envelope. A portion of the SAXS model is unaccounted for by this superposition, and was hypothesized to represent the missing domain. In agreement with the sequence, it was found adjacent to the N-terminus, and was perfectly positioned to fill a huge channel along the z-axis in crystal structure. Snell also showed a number of control experiments, in which similar SAXS reconstructions were able to accurately recreate missing domains in other proteins.

Lee Makowski, ANL, discussed MADMAX (**M**ultiwavelength **A**nomalous **D**iffraction using **M**edium Angle **X**-rays) as an approach that can overcome the experimental difficulties of measuring anomalous scattering in solution. Makowski *et al*. used a principal components analysis of patterns taken at x-ray energies near the absorption edge to isolate the anomalous signal from other effects and measure it to ~ 5 Å spacing. Lee reported that their measured differences compare well to theoretical expectations calculated from the atomic coordinates of proteins of known structure. They were able to demonstrate applications to Fe-containing proteins; seleno-met-labelled proteins and membrane proteins.

cont'd next page

7.11 SAXS cont'd

Tobin Sosnick, U Chicago, described the process of modeling folding intermediates of the RNA from RNase P using experimental constraints, including SAXS and nuclease and chemical mapping. The crystal structure defines a 154 nucleotide-specificity domain comprising several secondary and tertiary structural modules. The modeled structure of the intermediate contains modules composed of secondary structures and short-range tertiary interactions, which implys a sequential order of tertiary structure formation during folding. The intermediate lacks the native core and several long-range interactions among peripheral regions, such as a GAAA tetraloop and its receptor. Folding to the native structure requires the local rearrangement of a T-loop in the core in concert with the formation of the GAAA tetraloop-receptor interaction. Sosnick also described a series of experiments designed to show why flexibility doesn't blur the cryoEM reconstructions of large RNAs. Evidence from mutagenesis and salt dependency indicate that electrostatic repulsion, often suggested as the basis of this effect, is insufficient to account for the intermediate's extended structure, which is evidently due instead to specific native and non-native interactions in the core.

Hiro Tsuruta, Stanford, in *Kinetics of hepatitis B virus core assembly by time-resolved small angle x-ray scattering* reported their recent TR-SAXS experiments conducted on the assembly of the HBV core capsid. Their solution x-ray scattering studies in equilibrium indicated that a low concentration of urea kept the capsid protein in an assembly-ready dimeric form at least for several hours. They conducted time-resolved studies of the assembly induced by a rapid salt concentration jump at a mildly alkaline pH value and found that the assembly reaction was surprisingly fast, the half-life was of the order of a few seconds or shorter, depending on the salt concentration. Their results suggested the presence of a transient assembly intermediate larger than the T=3 or T=4 capsid which undergoes partial disassembly prior to incorporating the dimeric capsid protein to form the T=4 capsid. The assembly process also involves a slow annealing process after capsid formation.

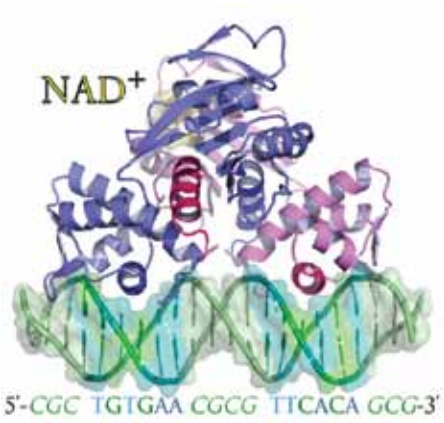
Eaton Lattman

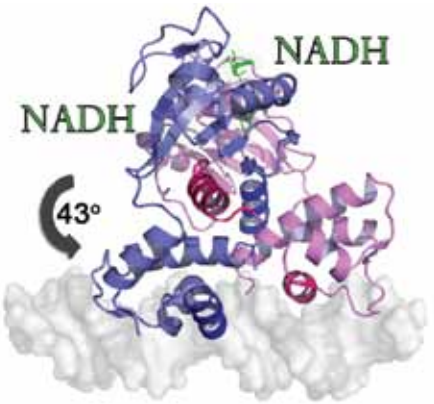
7.12: Exciting Structures

This year's session, selected exclusively from submitted abstracts, highlighted some recent high impact structures. There were 10 presenters: **Eric Montemayor, Sulochanadevi Baskaran, Sherwin Montano, Kehui Xiang, Millie Georgiadis, Krystle McLaughlin, Jinghua Lu, Robyn Stanfield, Maksymilian Chruszez and Carrie Wilmot.** All did a good job of describing their research; it was difficult to select just a few to highlight in this report.

Krystle McLaughlin, U Rochester Med. Ctr. the Biomac SIG choice to be a **Etter Student Lecturer**, discussed her work on the redox sensing repressor, REX, and explained how the cell senses the NADH/NAD^+ ratio as it dynamically controls gene regulation in response to the redox state. See Krystle's image below.

Krystle McLaughlin,
2011 Etter Student Lecturer.





Millie Georgiadis, Indiana School of Medicine, discussed her recent work on the *Hsmar1* transposase, of which there is a single active copy in the entire human genome. This active version of the transposase landed in copy of a SET gene creating a chimeric protein termed SETMAR. Millie described work investigating the structural basis for activity and speculated on how this fusion protein lost its specific transposase activity and evolved into a DNA repair protein.

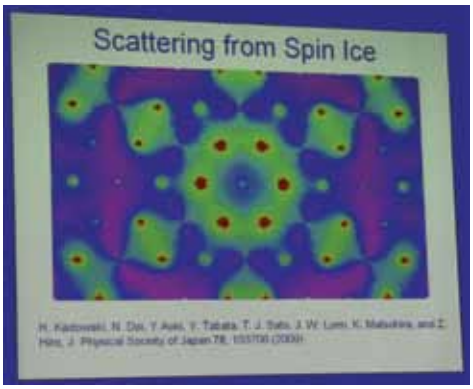
Kehui Xiang, Columbia, in addition to imaging, PIN1, which plays a role in regulating Simplekin *via* phopsphorlyation, shared with us that PEG3350 contains high levels of free phosphate – who knew!

Finally, **Carrie Wilmot**, UMN, described the structure of MauG, a di-heme enzyme that catylazes the formation of the tryptophan tryptophylquinone (TTQ) cofactor of methylamine dehydrogenase (MADH). Remarkably, this enzyme is fully active within the crystal allowing the Wilmot lab to compare the structure before and after activation with exogenous H_2O_2. By visualizing reactive intermediates, a mechanism was proposed requiring both the proper orientation of both tryptophans within the active site along with modulation of the chemical environment to facilitate TTQ production.

Eric Ortlund

7.13: Weird Materials:

This session was organized to give people working on unusual materials that do not fit in a trendy or general session a chance to present their work. **Jeff Lynn**, NIST, began by stating that it is always good to start a session with frustration, thus introducing his topic of spin ice and magnetic monopoles. He presented intriguing scattering data that suggest the presence of dynamic monopoles in spin ice.



Marcus Bond, Southeast Missouri State U, discussed unusual copper(II) complexes $ACuCl_3 \cdot H_2O$, in which the A cation determines the stacking order. Square planar, flattened tetrahedral and tetrahedral building blocks can further aggregate via hydrogen bonding. **Louise Daw**, Memorial U of Newfoundland, continued the topic of copper(II) complexes that are good for a surprise in her talk on *self assembly gone wrong*. She convinced the audience that copper can adopt a variety of different geometries in the same structure, and that, depending on the ligands, different exchange pathways can dominate. Magnetic models can be proposed through knowledge of exchange pathways.

Jim Kaduk, IIT, entertained the audience with a thorough analysis of *what to do when your data are too good*, illustrating the power of high resolution synchrotron data collected at APS beamline 11 when it comes to detecting minor impurities or subtle structural distortions in lanthanides. BaR_2ZnO_5 crystallizes in the tetragonal space group *I4/mcm* for R = La and Nd, and in orthorhombic *Pbnm* for smaller lanthanides. Four weak peaks in the $BaSrLa_4Zn_2O_{10}$ pattern could not be attributed to any impurity phase but corresponded to reflections in the tetragonal unit cell; the body centering condition was thus violated, so clearly the true space group is *P4/ncc*.

Christine Beavers, ANL, reminded everybody that simple projects on isostructural compounds are rarely as simply as anticipated, and showed how quickly structures can get complicated in a series of non-isostructural lanthanide complexes exhibiting unit cell sizes of up to 20,000 $Å^3$. Data analysis can further be complicated by sluggish phase changes between different, related structures. Finally, **Abe Clearfield**, Texas A&M, discussed the ion exchange material $Na_2Ti_3O_3(SiO_4) \cdot 2H_2O$, which selectively removes cesium ions from alkaline solutions. He demonstrated that the binding sites for cesium and sodium are different, leading to the observed distinct uptake behavior. Exposure to protons distorts the tunnels, resulting in cesium retention in the material.

Cora Lind

7.15: Would You Publish This II?

A very fun evening was had as presenters used specific examples to address issues associated with handling problem crystal structures of limited chemical importance.

Gary Nichols, U AZ, and **Ilia Guzei**, U Wisconsin, provided specific examples of "problem structures" due to poor crystal/data quality. Gary presented crystal structures of poorly diffracting chiral organic molecules that provided vital relative configuration information to the chemist. Unfortunately the crystals were extremely small and so the data resolution was disappointing. Ilia presented his progress toward refining the structure of a non-merohedrally twinned crystal of a hexanuclear gold cluster with heavily restrained organic ligands and unidentified diffusely scattering counter-ions and solvent. These presentations stimulated broader discussions about when results are too bad to publish and when alternative data collection methods (*e.g.* Cu instead of Mo datasets; synchrotron *vs* in-house datasets) should be considered. Ilia also introduced his newly created *Idealized Molecular Geometry Library* for modeling commonly disordered solvents and anions, available at ***http://xray.chem.wisc.edu/SHARE1/www/Projects/Idealized_Geometries.html***.

Allen Oliver, Notre Dame, reported a new polymorph of chloro(octaethylporphyrinato) iron(III) and outlined the benefits of including the data in the literature or depositing it in the CSD even though many other related octaethylporphyrin structures have already been published. After general discussion, the advice was that a new polymorph or a significantly improved structure of an already reported structure should at least be submitted to the CSD.

Chris Cahill, George Washington U, provided an entertaining example of a structure that was *NOT* the first cis-$[UO_2]^{2+}$ complex ever reported, despite excellent refinement statistics. Instead, a more careful data collection identified systematically weak reflections yielding different unit cell parameters and space group, and more importantly, an even better refinement for a trans-$[UO_2]^{2+}$ complex.

Jim Simpson, U. Otago, concluded the session by drawing from his experience as a co-editor of *Acta Cryst. Section E*. He presented a variety of entertaining structure submisssion stories, including examples of publishable structures that don't look great in checkCIF and structures with mistakes that are not so obvious in checkCIF, as well as entertaining anecdotes about what not to publish *under any circumstances*. The presentations by Chris and Jim emphasized that refinement statistics and checkCIF are extremely valuable tools for predicting many crystallographic errors, but they cannot replace crystallographic expertise; there are still plenty of mistakes the non-crystallographer cannot detect and the validation software cannot be programmed to identify.

Carla Slebodnick & Danielle Gray

7.22: Structural Insights into the Cause and Treatment of Cardiovascular Disease

This session integrated a variety of structural studies related to thrombosis, diabetes, hypertension and cardiovascular disease.

Several speakers described studies aimed at exploring the molecular underpinning of various aspects of heart disease. **Kenton Longenecker**, Abbott, spoke about their characterization of a crystallized complex of a monoclonal antibody, and its antigen - a segment of the B-type natriuretic peptide (BNP). BNP is a biomarker for cardiovascular stress, and the antibody is under investigation as a diagnostic for heart disease. **Nualpun Sirinupong**, Wayne State U, presented progress regarding structural studies of SmyD1, a histone H3H4 methyltransferase known to play a role in heart development. **Angeline Lyon**, U Michigan, presented a summary of structural and biochemical data on the Gaq signaling pathway linked to heart development and the maintenance of normal heart rhythm and arrhythmia. **Emannualle Laffly**, UMBC, described structural studies on guanylate cyclase aimed at explaining the mechanism of NO-induced vasodilation and **Zsolt Bocskei**, Aventis-Sanofi, described the critical role played by crystallography in the development of potent non-peptidic inhibitors of renin, which catalyzes the first step in angiotensin production. Bocskei also briefly discussed the structural basis for the design of dual inhibitors of thrombin and Factor Xa, important enzymes in the blood coagulation cascade.

Other presenters had investigated proteins involved in glucose metabolism in efforts to identify possible medicinal agents that can provide glycemic control in diabetes. **Shenping Liu**, Pfizer, used the SAXS method to determine the conformations of wild type GK, (glucokinase) and activating mutants, (GKA) in solution, in the presence of glucose and GKA. Shenping and his co-workers found that that the glucose dose dependently shifted the population of GK from inactive to an active conformation, clearly supporting the mneumonic model of GK's cooperativity.This research shows the significance of conformational states of the enzyme frozen in different glucose-bound and unbound crystal forms of the enzyme.

David Rose, U Waterloo, presented *Intestinal Glucosidases: Structure/Mechanistic studies towards clinical applications for diabetes and obesity;* and **Kyra Jones**, in David's lab, with *Inhibition of recombinant maltase-glucoamylase by acarbose, salacinol, kotalanol, and de-O-sulfonated kotalanol,* described their progress towards characterizing those specific glucosidases responsible for the metabolism of complex glucose saccharides - important enzymes in the production of glucose from dietary starches.

Holly Soutter and Barry Finzel

7.16: What Can Your Beamline Do For you?

This was a session organized to inform the user community of various user facilities and what they offer. **Marc Allaire**, NSLS, began with a brief overview of the facility and went on to inform the audience about the protein crystallography opportunities at NSLS. Marc also gave an update on the new construction project, NSLS II. **Thomas Proffen**, Lujan center, LANL, talked about the opportunities for diffuse scattering and Pair Distribution Analysis at his beamline NPDF. **Dean Myles**, the division head of the Neutron Scattering Science Division gave an overview of neutron scattering opportunities at two of Oak Ridge's Neutron facilities: the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HIFR). **Brian Toby** described the various x-ray scattering programs at the APS; and **Ken Littrel, Gary McIntyre** and **Richard Gillilan** followed, discussing, respectively, more specific beamlines such as the small angle scattering at HFIR, single crystal diffraction at ILL and macromolecular diffraction at CHESS. All speakers emphasized the availability of time, the access process and the unique programs at their facilities.

Ashfia Huq

7.21: Professional Odysseys 2010

This was the YSSIG's panel discussion about careers in crystallography (and beyond). Our panel represented academic, industrial, government, institute, and synchrotron/service crystallography experience, - and all with only three members. (This just goes to show how diverse a single person's scientific path can be!) With help from the enthusiastic audience, we had a lively discussion ranging from how to show what you can bring to a job to the value of postdoc positions. Thanks very much to our knowledgeable and generous panelists, Joe Ferrara, James Holton, and David Rose.

Megan Barker & Anna Gardberg

At top, an overview of the poster area. Then, at left: George Oh discussing his poster S-312 with Branton Campbell; at right: Clemens Vonrhein telling his M-148 poster story. Below them, at left: Thomas Schneider, Tom Peat and Christine Muchmore; at right: Weinu Wang and Marv Hackert. .

At top, from left: Crystal Towns, Marcia Colquhoun, Jen Shepard, as they accept their appreciation gifts from Judy Kelly. Below left: Bob von Dreele; below right: Judy Kelly. Below them, Joyce and Jim Ibers; Jeff Deschamps. In the view of the banquet crowd across the bottom of the page, at the table in front: Sine Larson, David Kelly, Ton Spek and Marv Hackert.

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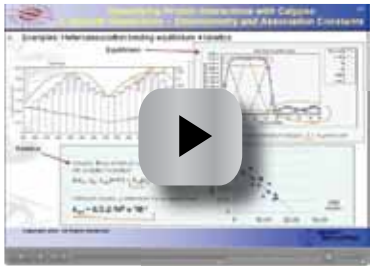

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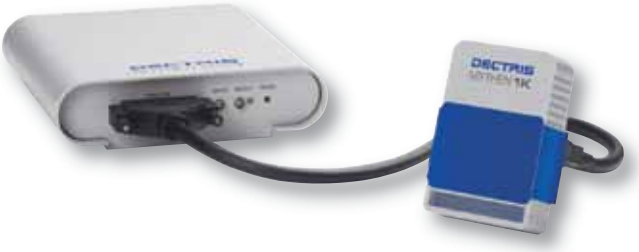

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ISC 2010 in Granada

L to r: Stefan Schorsch, Natalie Ferté, Juan Manuel García-Ruiz, Jaime Gómez-Morales, Eleni Arvaniti, Luigi Nassimberi.

The second **International School of Crystallization** was held May 24th-28th under the auspices of the IUCr and the Spanish Ministry of Science and Innovation. The conference, directed by Juan Manuel García-Ruiz and Jaime Gómez-Morales took place in Hotel San Anton in the heart of Granada as had the 2009 school. Most of the 115 attendees (from 15 countries) were students or postdoctoral researchers; there were 17 lecturers as well.

Day 1 was devoted to fundamentals. Basic concepts such as: phase diagrams, supersaturation, nucleation, crystal growth kinetics, and crystal morphology were rigorously defined and exemplified. ***Day 2*** focused on crystallization methodologies. This meant that a wide range of crystallization techniques were taught including crystallization in gels, from melts, under high pressure, with hydrothermal routes, and from solutions. ***Day 3*** was the 'polymorphism day'. Everything about polymorphism was explained from fundamental and practical aspects to industrial applications - properties of solvates and co-crystals included.

Day 4 was dedicated to the ***Demonstration Fair***, when 17 simultaneous practical demonstrations were performed in front of small groups. The interactions between teachers and students were at their best on this day. ***Day 5*** featured 'special and hot topics' when international experts gave talks on how minerals form, bio-inspired crystallization and biomineralization, among other subjects.

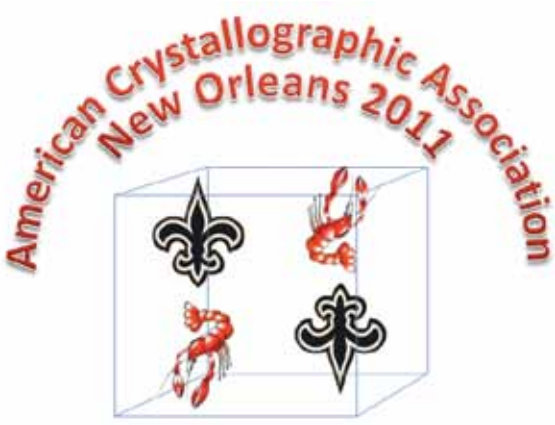
Poster sessions at the end of the first 3 days gave students additional opportunities to discuss aspects of their research with experts. The selection committee, chaired by Luigi Nassimberi, had difficulty selecting only three from the 49 posters on display all week. Social events included a welcome party the first evening, a night visit of the Alhambra after day 3, and a dinner after a vivid flamenco demonstration the 4th evening.

Visual check of crystallization progress during the demonstration fair

Any participant can download the lectures, the demonstrations and the posters from the ISC2010 website. The organizing committee and the staff of the Factoria are to be congratulated for this very successful school. It is very likely that a similar event will take place in 2012 - see **www.iscgranada.org/**

Gérard Coquerel

Below, overview of the lecture room



ACA 2011 May 28 - June 2

Sheraton, French Quarter, New Orleans

Abstract Deadline: January 31, 2011
Student and Young Scientist Travel Grant Applications: January 31, 2011
Advance Registration Deadline: March 31, 2011
Advance Hotel Registration Deadline: April 15, 2011

Register online and see Call for Papers at
www.AmerCrystAssn.org

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Transactions Plenary: Philip Coppens

A day long symposium on Time Resolved Photochemistry (Session I) and Electron Density (Session II) is being organized to honor Philip for his contributions to the field of crystallography and to celebrate his 80th birthday.

Transactions Session I Chairs: Peter Lee & Yu-Shang Chen

Transactions Session II Chair: Jason Benedict

Patterson Award to Keith Moffat

followed by a special session on Fast Science chaired by Tim Graber and sponsored by the Synchrotron Radiation SIG

Etter Early Career Award to Yurij Mozharizskyj
Etter Symposium Chaired by Jamaine Davis and sponsored by General Interest & YS-SIGs

Wood Award to Daniel Nocera

Evolution of Powder Diffraction Software to honor the memory of Lachlan Cranswick sponsored by Materials, Neutron Scattering, & Powder Diffraction SIGs, and the Canadian Division.

Award Symposia or Plenary Lectures every day. The workshops are not yet set as we go to press in mid-September. See the meeting website for an update.

OCTOBER 2010

1-3 **AsCA2010**, Asian Crystallographic Association Meeting, Busan, Korea. **www.asca2010.org.**

NOVEMBER 2010

9-10 **APC2010, Advances in Protein Crystallography,** Florence, Italy. Keynote speakers: Bernhard Rupp, and Emmanuel Saridakis **www.selectbiosciences.com/conferences/APC2010/ Deadline for abstracts: 14 May 2010.** Register early and save.

23-26 **NACCI 2010:** First North African Crystallographic Conference, Casablanca Morocco.

MARCH 2011

5-9 Biophysical Society 55th Annual Meeting, Baltimore, MD **www.biophysics.org.**

APRIL 2011

25-29 **MaThCryst School on Fundamental Crystallography**, Mahdia, Tunisia.

MAY 2011

28-2 **ACA 2011, Sheraton Hotel New Orleans, New Orleans, LA. Program Chair: Chris Cahill; Local Chairs: Cheryl Klein-Stevens & Ed Stevens.**

23-27 **MaThCryst**-sponsored Workshop on Fundamental Crystallography, Tokyo, Japan.

AUGUST 2011

22-29 **XXII Congress and General Assembly of the IUCr,** Madrid, Spain. **www.iucr2011madrid.es.**

JULY 2012

28-2 **ACA2012, Westin Boston Waterfront Hotel, Boston, MA**

SEPTEMBER 2012

9-13 **EMC 2012**, European Mineralogical Conference, at Johann Wolfgang Goethe-University, Frankfurt, Germany.

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Review of applications will begin on October 1, 2010 and will continue until the position is filled.

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