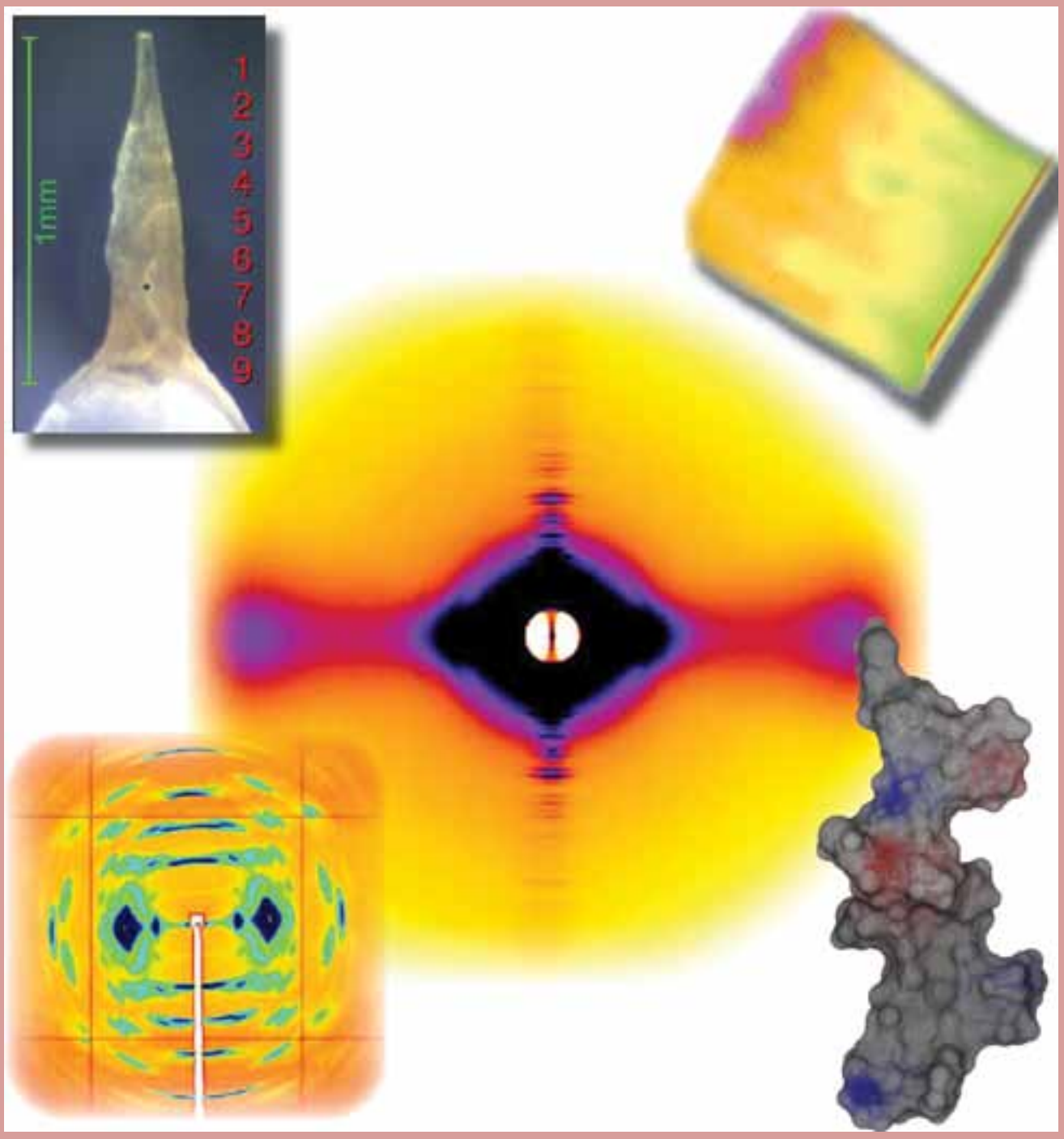
ACA RefleXions

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION

Number 2 Summer 2010



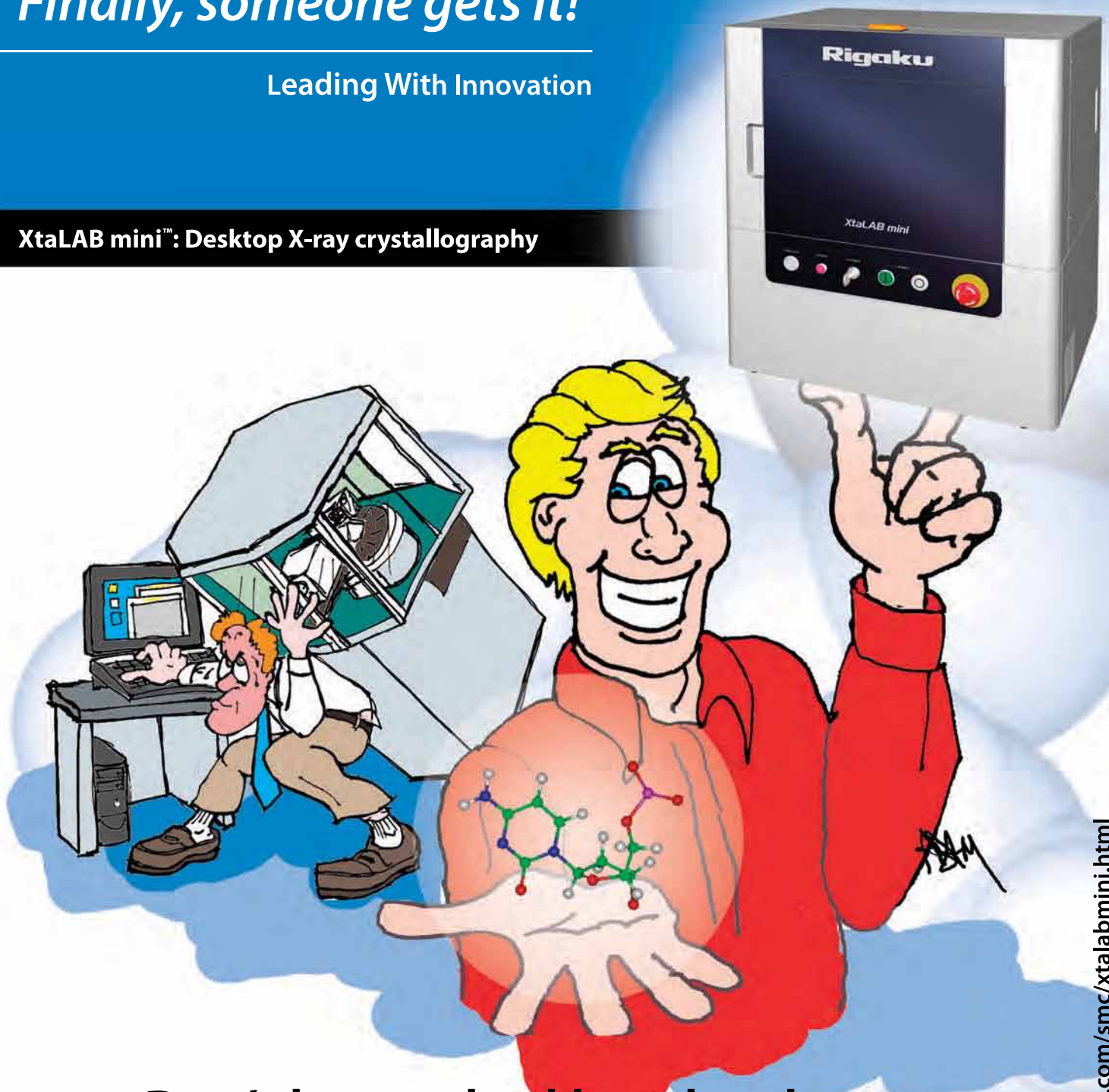
ACA 2010 Chicago, Illinois

Collect. Solve. Publish.

Finally, someone gets it!

Leading With Innovation

XtaLAB mini™: Desktop X-ray crystallography



Don't be crushed by a hard-to-use, hard-to-maintain diffractometer

www.rigaku.com/smc/xtalabmini.html

Rigaku

Rigaku Americas Corporation phone: 281-362-2300 e-mail: info@rigaku.com
Rigaku Europe phone: +[44] 1732 763367

ACA RefleXions

American Crystallographic Association

ACA HOME PAGE: www.amercrystalassn.org

What's on the Cover - Page 44

Table of Contents

ACA RefleXions staff:

Editor: Connie Rajnak.....conniechidester@earthlink.net
Editor: Judith L. Flippen-Anderson .....acareflexions@gmail.com
Awards: Bomina Yu.....bomina@gmail.com
Book Reviews: Joe Ferrara .....joseph.ferrara@rigaku.com
Historian: Virginia Pett .....PETT@wooster.edu
Photographer: Peter Mueller ..... pmueller@MIT.EDU

Please address matters pertaining to advertisements, membership inquiries, or use of the ACA mailing list to:

Marcia J. Colquhoun, Director of Administrative Services
American Crystallographic Association
P.O. Box 96, Ellicott Station
Buffalo, NY 14203-0906
phone: 716-898-8692; fax: 716-898-8695
email: marcia@hwi.buffalo.edu

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

ACA RefleXions (ISSN 1058-9945) Number 2, 2010. Published four times per year in the spring, summer, fall and winter for the membership of the American Crystallographic Association, Inc., P.O. Box 96, Ellicott Station, Buffalo, NY 14205-0096. Membership in the ACA includes a non-deductible charge of $1.75 from membership dues to be applied to a subscription to the ACA Newsletter. Periodicals postage paid at Buffalo, New York. POST-MASTER: Send address changes to ACA, P.O.Box 96, Ellicott Station, Buffalo, NY, 14205-0096.

Presidents Column:

In late March, I attended the American Institute of Physics (AIP) Assembly of Society Officers at the American Center for Physics (ACP) headquarters in College Park, Maryland. Representatives from all 10 AIP member societies and many of the 25 affiliated societies were present. The Assembly is one of the ways the AIP informs its member and affiliated societies about important issues such as science policy. A number of topics were presented, including a discussion about how members of professional societies can and should participate in advancing issues related to science. A key element focused on the need for scientists to reach out at the local, state, and national levels and to serve as resources for informed scientific opinions. Presentations included one by Lou Lanzerotti of Bell Labs (Chair of the AIP Governing Board), and a second one by Kenneth R. Miller of Brown University. Lanzerotti spoke of his involvement at the Town Council level in his community, which led to his election as Mayor of the small town in New Jersey where he lives. Miller is a cell biologist who wrote a widely adopted high school biology text that led to his being called as a lead witness in the 2005 Pennsylvania trial of Kitzmiller *vs*. Dover Area School District. The resulting decision discredited including intelligent design in the K-12 science curriculum. Miller had amusing anecdotes (appearing on the Colbert Report with no pre-interview prep before the show) and frightening ones (threats during the trial). He emphasized how critical it is, when speaking to a general audience, to choose real-life examples that illuminate issues, while avoiding abstruse detail.

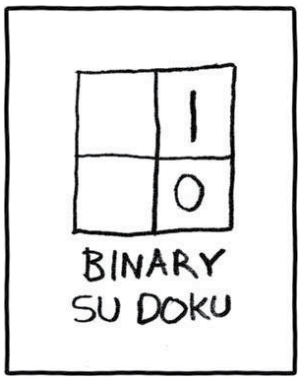
While many of us do not serve as expert witnesses or in official capacities in our communities, it is important to note how many local issues involve questions related to science matters, such as ground water contamination, electromagnetic fields from high voltage power lines, etc. So, we should look for opportunities to speak up for science and to contribute our expertise. Not least, we need to support solid K – 12 science education, particularly in these times of severe budget restraints.

Another presentation was made by some of the members of a Scholarly Publishing Roundtable that was convened to provide guidance to the Federal government on developing public access policies for scholarly publications resulting from publicly funded research. The Roundtable was convened by the Committee on Science and Technology of the US House of Representatives and the White House Office of Science and Technology Policy. Representatives from university administrations, libraries, for-profit and not-for-profit publishers participated. The full report and the committee's recommendations can be found on the Association of American Universities' web site: ***www.aau.edu/policy/scholarly_publishing_roundtable.aspx?id=6894*** under a 1/12/2010 entry. Eight specific recommendations are concluded by the following statement:

"The Roundtable's recommendations seek to balance the need for increased access to scholarly articles with the need to preserve the essential functions of the scholarly publishing enterprise. We urge publishers, librarians, universities, and scholars to consider these recommendations as creating an appropriate environment for moving past the decade of too often acrimonious debate by providing a basis for collaborating with federal research funding agencies to build an interdependent system of scholarly publishing that expands public access and enhances the broad, intelligent use of the results of federally funded research."

The ACP is a new facility that houses the headquarters of the AIP, the American Physical Society, the American Association of Physicists in Medicine, and the American Association of Physics Teachers. The building has handsome display cases with various physics-related exhibits, but no structural models. I have approached the ACP exhibition staff, and they are willing to consider displaying material from the ACA. We would be allotted space that is approximately 51 inches wide by 53 inches tall by 10.5 inches deep. If you have a visually exciting model that you would be willing to donate or lend for this purpose and that would fit in that sort of space, please send me a description and an electronic image so we can formally ask the ACP to consider including it in their exhibit space. Such an addition to their exhibits would help demonstrate the breadth of research interests that the ACA brings to the AIP. While I'm on this topic, I want to remind you that we are also seeking entries for the ACA Art In Crystallography contest (see announcement on page 21). Finally, the meeting brought home the similarities and differences between the ACA and our sister AIP societies. For one thing, the ACA is the second smallest of the ten AIP societies. In many cases an AIP society is the principal professional affiliation of its members. Many of the societies have a single major journal in their field (published by AIP) where all members strive to publish their research results. That is in marked contrast to the ACA, where our members have dozens of options for journals to publish in and multiple societies and interest groups that they participate in. There is an old joke about how crystallography is the "interstitial science" as it comes at the intersection of everything from mathematics to biology. That diversity is what makes the ACA so rich, and it is what we celebrate in our meetings. Our smaller size compared to many professional societies means our programs can be more representative of and responsive to the membership. The direction of the ACA is in the hands of the members through the Scientific Interest Groups (see page 4), which is why it is so important to participate in your SIG.

Judy Kelly



Brief notes from the 2010 ACA Spring Council Meeting - Chicago, IL - Saturday, April 10th, 2010

From left to right: Jim Britten, Marcia Colquhoun, Tom Koetzle, Judy Kelly, Bob Von Dreele, Carrie Wilmot, Bill Duax, Bernie Santarserio, S.N. Rao

Welcome: New ACA Vice-President Tom Koetzle and Past ACA President Marv Hackert who has been appointed to the IUCr Executive Committee by Sine Larsen (IUCr President), following the untimely death of Louis Delbaere.

President's Report: Judy Kelly attended the AIP Assembly of Society officers in Greenbelt, MD. Council explored several topics that came up during the meeting and plan to ask the Communications Committee to develop an internet social networking plan for the ACA (e.g. Facebook, Twitter, LinkedIn) and to explore new ways to publicize the activities of ACA and it members. Judy talks more about the Assembly in her President's column (see page 2).

Fred Dylla, the Executive Director and CEO of AIP, plans to meet with council before the start of the Chicago Meeting. In 2012 membership dues paid to AIP by member societies will increase to $9.00 per ACA member which includes a subscription to Physics Today.

The Materials Research Society had approached Judy about the possibility of holding a joint meeting with the ACA. It was decided that the Continuing Education Committee should explore options for joint interactions.

Canadian Representative Report: Council expressed sadness at the probable loss of Lachlan Cranswick who disappeared on January 18th, 2010 (see the spring 2010 issue of *RefleXions* – page 15), In addition the Canadian community keenly felt the loss of Louis Delbaere (see winter 2009 *RefleXions* – pages 9-12).

The Canadian Light Source's Brockhouse Diffraction and Scattering Sector final design (3 independent beamlines) is progressing slowly but surely. AECL Chalk River Neutron Diffraction Facility was still not online following the discovery of an internal leak

Financial issues: The ACA balance sheet for the year ending 12/31/09 is on page 30. Apple has agreed to loan the ACA 40 laptops for the SAD workshop in Chicago and Bristol-Myers Squibb has also donated laptops to the ACA for the workshops.

The Continuing Education Committee oversees student travel awards. They rank the applications and fund about one third based on this ranking. For the Chicago meeting there were ~100 applications, with $35,000 available to be disbursed (10K from the IUCr and the remaining 25K from the ACA, much of which comes from the donations to the student travel fund).

The annual meeting in Toronto had larger than expected attendance, which resulted in a small profit for the ACA. Judging by the number of abstracts submitted for Chicago it should also be a large and scientifically diverse meeting. Despite reduced advertising revenue, *RefleXions* also ended 2009 in the black. Suggestions for companies that might be interested in advertising in *RefleXions*, or in becoming Corporate Members would be most welcome (send information to ***marcia@hwi.buffalo.edu***).

Although ACA membership was up in 2009 (1,888 *c.f.* 1,767 for 2008), the number of 2008 members who did not renew in 2009 almost doubled (959 *c.f.* 550 in 2008) which is a concern. Council would be most interested in ideas for promoting the benefits of belonging to the ACA. An increasing number of ACA members are taking advantage of being able to renew online.

2010 Chicago Meeting Update: Marcia negotiated an 'early bird' $40 a night reduction at the conference hotel and approximately 69% of the reserved block was booked at the reduced rate. Ross Angel (Program Chair) reported that several sessions had been changed; "Structures with high solvent content" was broadened to "Methods to deal with difficult structural problems"; two incommensurate sessions were merged under the title "Incommensurate modulated materials"; "What can our beamlines do for you" was moved into the daytime schedule. Larry Favello and Tom Koetzle have been helping Christina Hoffman in the organization of the *Transactions Symposium* honoring the memory of Bob Bau (former ACA President). As of 5/26/10, there were 614 submitted abstracts, and 40 exhibitors.

In Chicago there will be 4 workshops 3 of which will be off-site with attendees being bussed to and from the hotel (2 at UIC and 1

at Northwestern). In addition, an unusual out-reach / professional development workshop has been organized by Cora Lind entitled "Crystallography: World of Wonders" for high-school teachers in the Chicago area. Cora has been able to get NSF support so there will be no registration fee, and high-school teachers who attend the workshop will receive professional credit. The workshop can accommodate a maximum of 100 attendees, and also includes admission to the plenary lecture on Saturday evening to be given by Venkatraman Ramakrishnan, one of the 2009 Nobel Laureates in Chemistry.

An Art Festival organized by Andrezj Joachimiak will be part of the Chicago meeting.

Future Meetings: Council is exploring the introduction of several changes for the 2011 New Orleans meeting. (1) Late abstracts up to a month before the meeting would be allowed for a small fee, so that last minute "hot" data could be presented in poster form. These abstracts would not be in the hard copy program schedule, but would be on the CD. (2) *Transactions* and award lectures will be recorded for later on-line access, in which the slides would be displayed and advanced in conjunction with the presenter's voice. (3) Young scientists (students and postdocs) who are selected for an oral presentation will be able to display their poster at the back of the session room. This will allow them to discuss their research in more detail with attendees following the session.

2011 ACA Awards: The Patterson, Wood and Etter Early Career awards will be presented at New Orleans 2011 (see pages 24-26). In addition a Supper Award for instrumentation development will be awarded in 2011.

Council is putting together a proposal for instituting annual memorial awards for student posters in the research area of a member who died in the previous year, as a way to honor and remember their contributions to crystallography.

ACA Fellows: Council is currently working on the details of how ACA Fellows will be selected. It is projected that at steady-state, ACA Fellows will represent ~5% of the membership.

ACA Summer Schools: The Continuing Education Committee has written a call for proposals that was published in the fall 2009 issue of *RefleXions* (page 49). At this time no new proposals for 2011 Summer Schools have been received and so Council has decided to ask simply for a Letter of Intent rather than a full proposal. This would enable the ACA office and the Continuing Education Committee to help a potential organizer put together a full proposal. The only 2010 Summer School to be held is the Small Molecule Crystallography Summer School run by Charles Lake.

SIGs and Committees: The name Special Interest Group has been changed to Scientific Interest Group. Guidelines and specific responsibilities expected of the SIG Chairs have also been streamlined.

Council is looking to identify underrepresented and new scientific growth areas that the ACA should be supporting through the formation new SIGs.

Carrie Wilmot

AIP report – May 2010

With the recent decision of the American Institute of Physics to increase it's membership dues, it seems an appropriate time to reflect on the relationship between the ACA and the AIP. Recent conversations with officers and Council members suggest that the ACA membership is largely unaware of the benefits of being a member society under the AIP umbrella. The gist of what might be a consensus among a large fraction of members is that the only benefit is a subscription to *Physics Today*, and that few ACA members actually read *Physics Today*. I want to outline an alternative perception of what it means to be represented by an umbrella society like the AIP. I'll begin with the benefits of *Physics Today*, why I feel it has always been a real bargain, and why the dues increase makes sense. Then, I'll review some real additional benefits that ACA currently does derive from its membership. Finally, I'll describe ways in which the partnership between ACA and AIP can and should be strengthened.

***Physics Today - a bargain at twice the price*.** I began to read *Physics Today* as soon as I joined the ACA in the early 1970s. Today I have five folders bursting with torn out articles I return to oftener than you might suspect. One of my favorites is Freeman Dyson's remembrance of Richard Feynman, published in 1988 after his death, that recalled a most astonishing toss-away proof that Feynman produced and never published. He took Newton's third law of motion, added the Heisenberg Uncertainty Principle, and deduced Maxwell's laws of electrodynamics (Dyson (1990) "Feynman's Proof of the Maxwell Equations", *Am J. Phys*. **58:**209-211). Maxwell's laws are the earliest physical laws that are "invariant" under the Lorentz transformation, and hence consistent with Einstein's special and general theories of relativity. Newton's third law is not relativistically consistent. The uncertainty principle lies at the heart of quantum mechanics. The most important conundrum in physics today is the inability to reconcile quantum mechanics with general relativity!

Another of my folders is full of short commentaries by Frank Wilczek, often published under the *Reference Frame* rubric. I first encountered Wilczek when he published "Whence the Force of F=ma I: Culture Shock" (***tinyurl.com/2wzrrq4***), which opened a wide new window on the puzzles that drive physicists. Wilczek is a wizard with words, and brings sublime subjects down to my level.

I suspect that many other crystallographers would also find such contributions fascinating and provocative. Its appeal transcends many fields relevant to crystallography. Within the last year, the Biophysical Society has become an adjunct member society of the AIP. Their Council found two things to be most attractive. One was *Physics Today*. When I told my colleague who was then Past President of the Biophysical Society that my subscription at that time cost only $5, he wouldn't believe it was such a bargain!

Check it out: ***www.physicstoday.org/*** - it's a hellova website. While you're at it, check out the new AIP scientific networking site, UNIPHY ***(www.aipuniphy.org/Portal/Portal.aspx)***. Peter Strickland of the IUCr journals has promised to provide the metadata necessary for UNIPHY to pre-populate new members' pages with crystallographic publications. John Haynes, VP for AIP Publishing and the guru behind UNIPHY has promised that this will be implemented soon.

The History Center - preserving our crystallographic heritage. AIP has received two important bequests from the Avenir Foundation to enhance the Center for the History of Physics: *www.aip.org/history/*, which also includes the Niels Bohr Library and Archives. Thanks to efforts of Judy Flippen-Anderson, among others, the ACA will benefit directly from these gifts because the AIP History Center will assume the preservation and curation of important documents from crystallographers that the ACA has accumulated over the years, thanks to efforts by Jenny Glusker and more recently Virginia Pett (see the ***ACA History Archive*** note following this article).

Meetings support - the sine qua non benefit of ACA umbrella membership. The primary activity of the ACA is to bring off a successful scientific meeting once a year. When I joined the Council in 2001 as Vice-President, one of the first things I learned was how important a man named Bob Finnegan was to the ACA. Bob at that time organized the vendors exhibits for the ACA annual meeting. The Vendors as a group are perhaps the most important reason that our meetings are so much fun. The ACA pays the AIP for these services, to be sure, but again it is cheap at the price. Ask Marcia Colquhoun! I'm quite certain that when push comes to shove, and the Council has to decide whether or not to continue as a member society, meetings support will be one of the most difficult services to replace.

Media relations and public policy - what ACA membership might think about: Truth in advertising. I currently chair the Media Relations Advisory Committee to the Physics Resources Center. The real motive behind this bit of cheerleading has to do with the other things that AIP does that could benefit the ACA membership on a far broader scale, provided that the ACA can find among its members a few who are willing to contribute to the activities of the Physics Resources Center. The other big reason why the Biophysical Society negotiated an adjunct membership was that they liked what AIP does to bring science to the public. Media relations is something that has become more important than ever before. Many AIP member societies actually have staff to deal with getting word out to the public about the scientific activities of their members. ACA is not in a position to do this; their priorities are to use their limited discretionary funds to help young scientists attend the annual meeting. However, that doesn't mean that media relations is not an increasingly relevant priority. By far, the most important way that news gets out about an exciting new result is that it makes it to the mass media. Some of us may have university or corporate media relations offices to help get such stories out there, but most of us probably do not. It's actually worse than that: most newspapers and network media have jettisoned their scientific reporting staffs, making it even less likely that JQ Public is going to be able to appreciate the next breakthrough by an ACA member.

For the past decade, AIP has pioneered two media efforts, under the rubric *INSIDE SCIENCE*. One of these, *Discoveries and Breakthroughs Inside Science* (DBIS; ***www.aip.org/dbis/***), consists of 30-second spots that highlight a new discovery and how it affects human welfare. These stories are distributed to mainstream television networks, both here in the US and throughout the world. DBIS is paid for in part by the Physics Resources Center and in part by a collection of ~20 "partners" including the American Biophysical Society, whose benefits include spots dedicated to results from partners and special links to their own websites.

The second media effort at AIP is called *Inside Science News Service* (ISNS; *www.insidescience.org/)* ISNS consists of news stories based on important new results in all branches of science, written by scientific journalists to be ready to go, so that they can be picked up by newspapers and cable media outlets. In the last year, ISNS has achieved an important breakthrough: their most important client turns out to be FOX news! This means that these stories are actually getting through to a large audience.

ISNS is poised to compete with a handful of similar media vehicles to become the *go-to source* for science news stories. A media consultant has helped ISNS to map out a plan to increase its production of stories to help ensure that ISNS wins the battle to become the "trusted" source. The task is within reach. ACA can help make that a reality, while at the same time helping itself to first-rate science news coverage of important crystallographic results. The Communications and Continuing Education Committees afford a natural mechanism to identify and help write stories that AIP can include in ISNS.

I hope that these points may catalyze a renewed interest in the relationship between the ACA and the AIP. Judy Flippen Anderson and I plan to meet with the Council in Chicago to press for favorable decisions on the ideas described here. The time is ripe, and few things could mean more to ACA in the years to come than to strengthen its position with respect to the media.

Charlie Carter

ACA History Archive

The ACA is working with the AIP to archive material on the history of crystallography. As part of this effort, we invite crystallographers to recount their own personal history. Shortened versions of these personal histories will be featured in *RefleXions*, and the full-length accounts will be deposited in the archive. The AIP History Center already has information on a number of crystallographers (***www.aip.org/history/*** – keyword crystallography). The first in the series of articles being developed by Virginia Pett follows this note. If you would like to deposit your own history, please contact Virginia at (***pett@wooster.edu)***, for some very flexible guidelines. If you are interested in helping with the history of crystallography project, please also contact Virginia.

In addition, one of the services the AIP provides to its member societies is the storage of other historical documents. There are significant gaps in the files that are currently archived. If you have, and are willing to donate, copies of early ACA *Newsletters* edited by Jenny Glusker, meeting abstracts (and/or calls for papers), and printed *Transactions* please contact Judy Flippen Anderson (***acareflexions@gmail.com***). She will let you know if what you have is still needed and how and where to send it. Suggestions of other historical artifacts that could/should be archived are also welcome.

James M. Stewart received the 2001 Fankuchen Award for his suite of crystallographic computer programs, XRAY63, later known as XTAL. As part of the ACA History Project, he recounts here the influences that shaped his scientific career. Jim's full narrative will be deposited at the AIP Center for the History of Physics. This is the first of a series of narratives by individual crystallographers. If you would like to contribute your story, contact Virginia Pett (pett@wooster.edu).

I had the mixed good fortune to be born in Port Angeles, Washington in February, 1931 at the time when the Great Depression was firmly established in the land. My father Charles R. Stewart was born in Selkirk Scotland; my mother Mary E. Stewart nee McDonald was born on the upper peninsula of Michigan. I like to say it was a marriage concocted in hell. A committed Women's Christian Temperance Union devotee and a dram-fancying Scot!

Jimmy Stewart and Uncle Charlie, 1934.

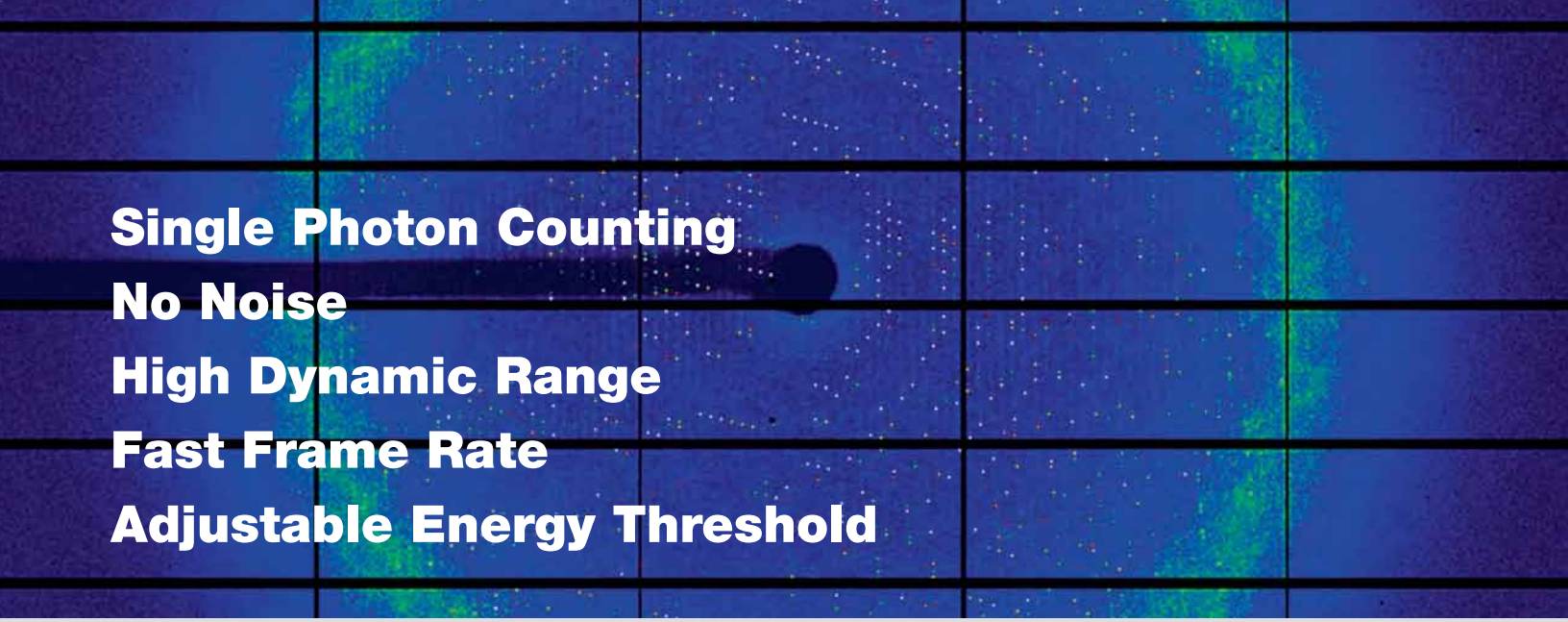
My family constituted my introduction to science. My father was a literate and charming Scot who could quote Burns and some of the romantic poets. He could also sing in addition to his skill as a plumber and being dedicated to stamp collection and the geographic knowledge that instilled. He was, in the tradition of his father, a fisherman. Early on I had opportunities to see lead melted and used, pipes threaded with the difference between tapering pipe threads and cylindrical machine threads explained. When my parents got to Port Angeles they set up a plumbing business which proved unsuccessful. My mother, as she put it "kept the wolf from the door" by working in a local grocery store. Although she had only six years of schooling, she was a quick study and took in the details of the trade. My Uncle Charles W. Alward was an engineer on the Port Angeles and Western logging railroad. That meant at a very early age I got to see and be held in the cab of the Shay locomotive that he drove. As the years went by I got information from him on all sorts of aspects of the logging operations and the operations connected to the Alward farm. Some of the lessons were frivolous, such as the day I found out about an electric effect. Walking with Uncle Charlie from the house to the barn he held out his hand and said: "Take my hand Jimmy." Which I did, only to find out that he, in his rubber boots, had his hand on the electric fence. Hello! Pay attention!

I was carrying kindling from the woodshed very soon after I could walk and delivering groceries for Stewart's grocery store from the time I was in grade school. My family all treated me as being able to understand and do. They must have thought that I had talent, but like Uncle Charlie and the electric fence lesson, they were careful to be sure I didn't get any ideas of myself that are like the ones being touted in the 21st century about building self image. One particularly valuable role was being the one to run and clean the cream separator on the Alward farm. Aunt Margaret milked two Guernsey cows. In those days the valuable product was the butter fat. The separator is a type of centrifuge that can divide the skim milk from the cream. The cream could be sold to the local dairy and the skim milk could be added to otherwise waste foodstuffs to make slops for the farm's pigs. The device consists of a crank for motive power, an upper chamber for the raw milk, a stack of pleated disks on a central shaft and two chambers with spigots, one for the less dense cream, the other for the more dense skim milk. Assembling it, using it, being its power source, and finally cleaning it was training not commonly available to the majority of my classmates.

At Bellingham High School we got to do many interesting experiments that have now become inaccessible to beginning chemistry students. For example — we synthesized rayon and nylon, we built a mercury barometer, and we generated oxygen from mercury oxide by heating it in a test tube with a Bunsen burner. After Western Washington College of Education, the next significant step in life was getting married to Bernice Dorren and starting graduate school at The University of Washington.

At UW Ed Lingafelter, an x-ray crystallographer, was an outstanding mentor and a teacher with great knowledge and talent. There were also great moments in the ethics of science. I was in the process of checking out a bond lengths and angles program for the IBM-650 when there appeared a paper by Lippert & Truter on the crystal structure of monoaquobisacetyl-acetonatozinc where the authors published their bond lengths and angles. Since Henry Montgomery in our group was scooped by this publication I tried to compare their results against mine. There was something clearly wrong so I consulted Lingafelter. In an in-

Jim and Roberta Lingafelter - ACA meeting -1980s.



Single Photon Counting
No Noise
High Dynamic Range
Fast Frame Rate
Adjustable Energy Threshold

DECTRIS X-ray detector systems

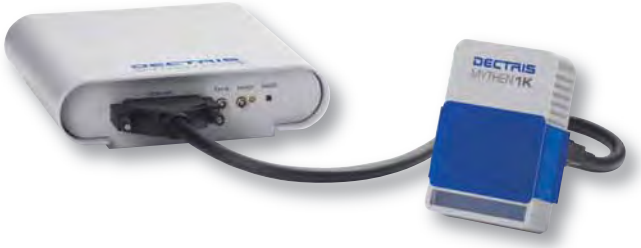
DECTRIS offers a wide variety of detector systems for a broad range of applications

PILATUS 2-D detector systems

PILATUS detector systems are based on CMOS hybrid-pixel technology and deliver outstanding results in various applications. A wide range of models ensures that a suitable PILATUS detector can be chosen for every measurement.

MYTHEN 1-D detector systems

MYTHEN is a one dimensional silicon strip detector system, which can be combined to form multi-detector arrays covering large angles (MYTHEN 6K).



XBPM Beam Position Monitors

XBPM4 is a 4-quadrant x-ray beam position monitor based on CVD diamond technology, suitable for hard x-ray synchrotron beam lines.

DECTRIS
Next Generation X-Ray Detectors

DECTRIS Ltd. | Neuenhoferstrasse 107 | 5400 Baden | Switzerland | info@dectris.com | www.dectris.com

stant he saw what I didn't: that the authors had used the monoclinic cell angle β* for β. Setting that right made the two results agree within the precision of the two data sets. At that point Lingafelter wrote to the authors and pointed out what he had discovered and suggested that they might cooperate in posting a correction in mutual interest. Montgomery & Lingafelter published their structure, giving credit to Lippert & Truter. In a subsequent paper Truter & Lippert expressed their gratitude for the error notification.

The first computers that I got to work with were located in the administration building. The research people got to use them on second and third shift. They were early IBM accounting machines. Professor Lyle Jensen had mastered their use for doing Fourier analysis of crystallographic data and I got a chance to be a "helper." It wasn't very long until the research people got their own computer, an IBM 650.

It was on the IBM 650 that I got my first taste of computer programming. It was the most amazing intellectual pleasure I'd ever had in my life. It involved bringing to bear all the step-by-step details required to process raw data into useful results. However, the 650 brought its own complications to problems. The storage was minimal, just two thousand 10-decimal "words" or 20 kBytes. That space had to hold the program and any data needed in the calculation. The memory medium was a rotating drum. In order to fetch words from the drum quickly, the programmer had to take into account that if instructions were not issued in a timely way, the registers in which the calculations were carried out would be delayed until the next required word rotated to the "read or write head." So you had to be sure to store your variables at locations separated by the optimum number of words if you wanted maximum speed. Now all of this is useless information. I just give it here to give a flavor of where many hours of my life went. You may think they were wasted, but I'd argue that it was fun, it made my reputation, and it put shoes on the baby, as one of my mother's aphorisms would put it. The next step up was to the IBM 709, the first really big machine the university got in. This was the machine on which the XRAY system was developed.

After accepting a two-year appointment with P. M. Harris at Ohio State University I was put to the task of getting the IBM 650 programs that I had brought from UW up and running. I also got to work on refining the structure of the explosive RDX (1,3,5-trinitroperhydro-1,3,5-triazine). The structure had been solved by direct methods, but not yet refined. Doing crystal structures in 1958 was a several-year and sometimes several-student process. It was on the IBM 704 at OSU that STARTX, the first program of XRAY was coded.

Returning to Seattle, I was given teaching duties because of an illness that kept Ed Lingafelter out of school for a year. The only course I remember doing during that time was an elementary one in physical chemistry for medical technicians. But the best part was getting back into the very active cooperative programming scene. Darrell High, a graduate student from the protein crystallography group, and I hit it off very well and continued generating a "system" of programs for the solution, refinement, and reporting of crystal structures called XRAY63, a plan that would turn into my major contribution in the field.

It was not till years later that Syd Hall and I decided to create the XTAL version to enhance transportability among computers. At one of the IUCr summer schools I met Syd Hall. Each of us had been working on writing code to produce all the triplets for doing direct methods. My post-doctoral student, Roger Chastain, had generated an excellent code that was very fast, Syd had generated a code that was equally fast but used an entirely different algorithm. On comparing how it was done in each case we realized that the methods were quite different, but could be used in combination. Thus began a long collaboration that lasted till I faded away at the University of Maryland College Park, and Syd took up the care and feeding of XTAL from his base at The University of Western Australia in Perth.

Because of people's interest in XRAY and XTAL I was privileged to travel the world and learn more about what was needed to do crystallographic computations. However, without a doubt, I treasure most the interactions with the people who built and used the system. It was through their effortsg that XRAY came together.

Jim in Scottish dress in front of his "memorabilia wall" that includes the plaque for the 2001 Fankuchen Award.

We still have judgement here, that we teach but bloody instructions, which, being taught, return to plague the inventor.

–MacBeth Act I, Scene VII

Those of us who used XRAY/XTAL remember the error messages, generated randomly from a file of quotations ranging from "Ozymandias" by Shelley to Charlie Brown.

Bruker AXS

APEX DUO - Dual Wavelength Perfected

The Most Versatile System for Small Molecule Crystallography

The APEX DUO combines the highest intensity Microfocus sealed tube sources for Mo and Cu radiation with the most sensitive CCD detector for crystallography.

The APEX DUO allows collection of charge density quality data with Mo radiation and exploits all the advantages of Cu wavelength for absolute structure determination and diffraction experiments on ever smaller organic crystals. Data from both wavelengths can be collected successively in one experiment and switching between wavelengths is fully automated, fast and without user intervention.

think forward

Crystallography

www.bruker-axs.com

Michael James - ACA Buerger Award - 2009

It is not often that one has the opportunity to fill the pages of *RefleXions* with one's own research results. I have already had an article in the winter 2008 issue and I thought that it was all over. All I had to do then was to attend the Toronto ACA meeting, give the Buerger lectures and that was that! But no! Judy Flippen-Anderson, Editor, has insisted that, as the 2008 article was pre-award I should contribute post-award as well. This additional tale from the James lab in Edmonton is the result of her editorial fiat.

I ended the previous article by discussing the early history of the structures of the proteolytic enzymes from *Streptomyces griseus*, SGPA, SGPB and SGT. SGPB has a 32 year history in my lab. I had the good fortune to meet Michael Laskowski, Jr. (Chemistry Department, Purdue University) at the inaugural "Proteolytic Enzymes and their Inhibitors" Gordon Conference in 1980. He introduced me to the research that he was doing on avian ovomucoids. Michael's interest in ovomucoids stemmed from his passion for physical chemistry. He had recognized that these small protein inhibitors of the serine proteinases could lead him to develop a sequence to reactivity algorithm that would then allow him to predict the K_{assoc} for that ovomucoid with any one of a panel of six proteinases (SGPA, SGPB, α-chymotrypsin, subtilisin, porcine elastase and human leucocyte elastase). He needed structural conformation that the ovomucoids and proteinases bound to one another in an identical fashion regardless of the variation of the sequences. Our lab was going to provide those data.

Michael's laboratory provided the thermodynamic association constants for each of the P_1 variants of the third domain of the turkey ovomucoid (OMTKY3) bound to SGPB. The P_1 residue of the OMTKY3 wild type is Len^{18} and Laskowski had produced all of the measured K_{assoc} for the wild type and for the 19 naturally encoded variants. The range for these values was huge, from 10^4 for Pro^{18} to 5.6×10^{10} for Leu^{18}.

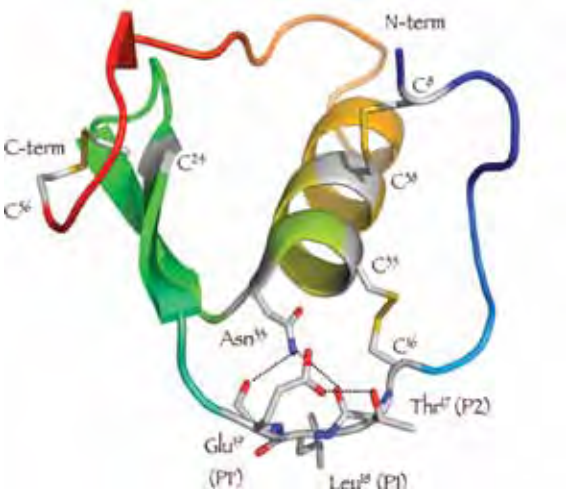


Figure 1: a view of the secondary structural elements of the 56 amino acid OMTKY3 wild type.

Our structural work showed firstly that the K_{assoc} values for the OMTKY3 variants arose from only 10 amino acid residues of the ovomucoids making contact with residues of the proteinases and secondly that all 18 of the variants that we were successful in crystallizing bound almost exactly in the same way. The only two variants that we were unable to crystallize were Cys^{18} and Met^{18}. Fig. 1 shows a view of the secondary structural elements of the 56 amino acid OMTKY3 wild type: there are 3 invariant disulfide bridges and the reactive site loop extends from P_6 (Lys) to P_3' (Arg). Fig. 2, below, shows this reactive site loop bound in the active site of SGPB. The P_1 residue is a Leu^{18} in the wild type and it was this residue that was substituted by all other 19 encoded variants. Our structural work also provided explanations for the huge variations in the thermodynamically measured K_{assoc}.

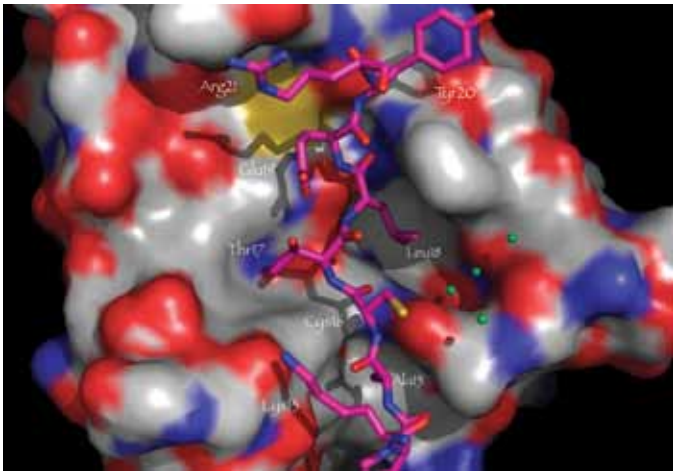


Figure 2: The reactive site loop bound in the active site of SGPB.

Figure 3: The wild type OMTKY3 is represented in cyan and the Ala^{32} variant is in magenta. SGPB is shown in green and magenta. $Pro192^B$ does not move. The methyl group of Ala^{32} forces the OMTKY3 domain to move away from the enzyme, yet the residues of the reactive site remain solidly in place

Michael Laskowski, Jr.'s algorithm was based on additivity among single amino acid substitutions between variants at all 10 of the contacting residues with the panel of six proteinases (~1140 measurements of ΔG°). Some of the substitutions were not additive; for example the Gly^{32} Ala variant exhibited a ΔΔG° value of 1.3 kcal/M. My student T. Wai Lee set out to determine the reason for this unexpectedly large difference resulting from a single methyl group addition in the sequence (glycine to alanine). In the wild-type OMTKY3 Gly^{32} structure, the C^{α} of the Gly^{32} makes contact with $Pro192^B$ of SGPB. The addition of the methyl group in the Ala^{32} variant forces the whole ovomucoid domain to shift as the $Pro192^B$ remains fixed in place and the methyl group

of Ala[32] occupies the same position as the C^{α} of the Gly[32]. It acts as a hinge and the distal parts of the OMTKY3 domain differ in position by ~6Å (Fig. 3). The non-additivity results from the loss of contacts that P_6 Lys[13] has with residues of SGPB. This result would not have been realized without the structural result of Wai. Other students and post-docs who made tremendous contributions to this project were Masao Fujinaga, Randy Read, Anita Sielecki, Kui Huang and Kathy Bateman. I am deeply indebted to them all.

One last story! I hope that the readers can put up with it. For the past six or seven years my laboratory has been a member of the Tuberculosis Structural Genomics Consortium (TBSGC) led by Tom Terwilliger, initially, and now by Jim Sacchettini. Thus far we have determined 29 structures (28 deposited) and this last structural story is about one of the enzymes from the arginine biosynthetic pathway. Most people in the Western world are surprised to learn that TB is still a problem in the world's health. In fact, according to recent publications from WHO, almost 1/3 of the world's population is infected by TB (2 x 10^9 people!). The vast majority of these cases are latent and there usually are few symptoms. However, active TB cases account for approximately 2 million deaths per year and there are an estimated 9 million new cases per year. There is a drastic increase in TB that goes hand in hand with HIV AIDS. People with HIV AIDS are far more susceptible to contracting TB. As well, there is an increase in multidrug resistant forms of TB and an alarming increase in extreme drug resistant forms of TB (XDR) for which all known antibiotics against TB are useless.

Ramasamy Sankaranarayanan (Sankar) is the PDF in my lab who determined the structure of ornithine transcarbamoylase (OTC) from *Mycobacterium tuberculosis*. Elham Mordian and Craig Garen cloned, expressed and purified the enzyme from a library that we received from Stuart Cole's laboratory in Paris. Maia Cherney grew two crystal forms of OTC from Mtb. The hexagonal form was co-crystallized with one of the substrates, carbamoyl phosphate and an inhibitor, norvaline. The hexagonal form of the enzyme was a challenge in that the unit cell had a *c* axis length of 463.0Å. There was a trimer of OTC in the asymmetric unit. The very large value of the solvent content (63%) made us worry about the resolution that this crystal form would yield. However, the data extended to 2.2Å resolution and we collected the data by remote access on beam line BL 9-1 at SSRL. Sankar solved the structure by molecular replacement and refined the atomic parameters of OTC to an R of 17.6% and R_{free} of 23.9%.

The norvaline and the carbamoyl phosphate were each bound to their respective domains in OTC (Fig. 4) and clearly showed how the enzyme catalyzed the reaction (Figs. 5 and 6). Figure 4 shows molecule A of the trimer in the asymmetric unit. Carbamoyl phosphate binds to the CP domain and the phosphoryl group is bound at the N-terminus of a helix.

Figure 5 shows the hydrogen bonding environments of norvaline (NVA) and carbamoylphosphate (CP). There are 4 arginines in the immediate vicinity of the active site suggesting that the ornithine substrate would bind as a neutral δ–amino group ready for nucleophlic attack directly on the carbonyl carbon of the carbamate of CP (Fig. 6 below). The final product is citrulline as the phosphate group is released (Fig. 6). This research represents the joy one has in doing structural biology. The interpretation of enzyme mechanisms provides not only the structural details of the groups in the active site but also is the start of structure-based inhibitor design that, with luck, turns sometimes into effective pharmaceuticals.

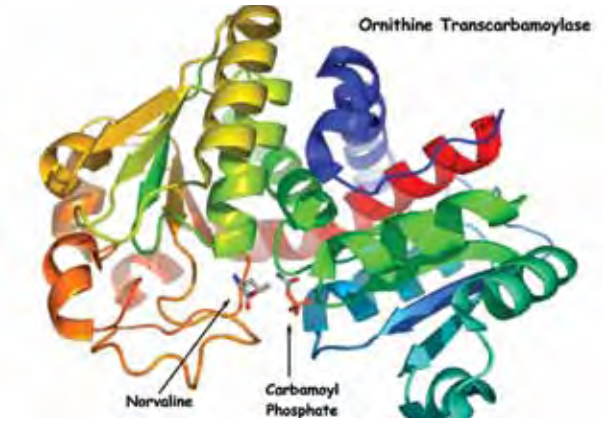


Figure 4. Ornithine transcarbamoylase (OTC) from the arginine biosynthetic pathway in Mycobacterium tuberculosis (Mtb). This crystal form had carbamoyl phosphate bound to the CP domain and the inhibitor norvaline bound in the ornithine binding domain.

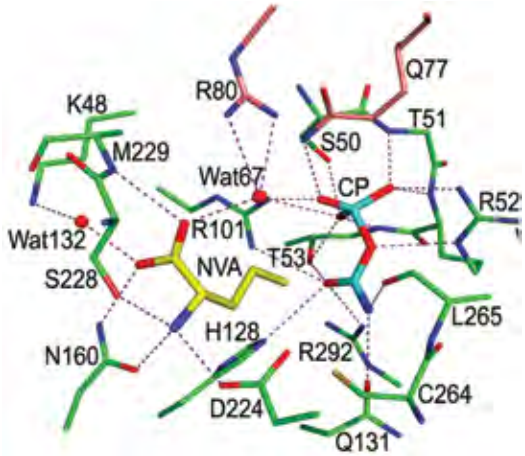


Figure 5. Active site of Ornithine transcarbamoylase.

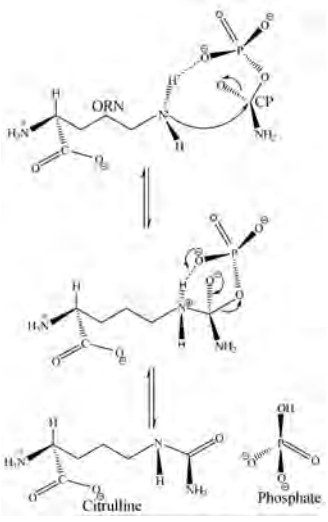


Figure 6. Proposed mechanism of OTC.

It is hard to believe that 42 years have passed since I first joined the Department of Biochemistry at the University of Alberta. I was deeply honored by being selected as the 2009 M.J. Buerger awardee. It is really the graduate students, undergrads, post-docs, research associates and technicians who have worked so hard and diligently in my lab that deserve this award. I was there for guidance; mainly it was them guiding me!!!

Michael James

7th Annual SER-CAT Symposium, March 19, 2010

The symposium, hosted by the Oak Ridge National Laboratory (ORNL) in Oak Ridge, TN was held at the ORNL Spallation Neutron Source (SNS). ***Leighton Coates*** (Lead Instrument Scientist: MaNDi, SNS, ORNL) was the primary organizer and coordinator. SER-CAT is very grateful for his time and effort. Similar to previous meetings, the overall theme was "Interesting structures, methods and advances in SER-CAT facilities" and it attracted over 50 participants mostly from the southeastern US. The symposium showcased the diverse and often outstanding science emanating from the use of the SER-CAT facility.

After his welcoming remarks Leighton served as chair of ***Session 1- SER-CAT Science*** that began with a keynote by ***Brian Davison*** (ORNL) who spoke about "Biomass to Biofuels: Overcoming Biomass Recalcitrance". He explained that the three components of biomass – cellulose microfibrils, hemicellulose and lignin – present a challenge in understanding how to convert these components to a monomeric form. There is a need for detailed structural analysis of the biomass structures themselves, the plant formation mechanisms, enzymes for deconstruction and the impact of pretreatment. "Allosteric Modulation of Ras Positions Glutamine 61 for a Direct Role in Catalysis" was presented by ***Carla Mattos*** (NC State). The mechanism through which Q61 contributes to catalysis has been somewhat elusive. It is now essential to know the position of hydrogen atoms in the catalytic residues and water molecules in the active site. Work is underway to produce crystals of Ras-GppNHp for determination of the neutron crystal structure to fine tune H positions in the hydrolysis site. ***Ronny Hughes*** (Alabama - Huntsville) described "The Mechanism of IPPase Catalyzed Phosphoryl Transfer". He stated that many aspects of the IPPase catalytic process remain unclear or have been difficult to validate due to the lack of information about hydrogen positions in the active site. Large volume crystals (>6 mm^3) of the enzyme suitable for neutron structural studies have been obtained in an effort to determine the precise location of hydrogen atoms within the active site.

Session 2 - SER-CAT Awards and APS Status chaired by ***John Rose*** (UGA). It began with a presentation by ***B.C. Wang*** to this year's SER-CAT winner of the Outstanding Science Award, ***Xinhua Ji*** (National Cancer Institute). In his talk, "Structure of ERA in Complex with the 3` End of 16S rRNA: Implications for Ribosomal Biogenesis", he explained how he and his co-workers have been able to explain an important step in the biogenesis of ribosomes and to establish a role for protein ERA in the process. The overall results, together with the structure of ERA in complex with GNP, have established a functional cycle of the protein, suggesting that ERA serves as a chaperone for the maturation of 16S rRNA and a checkpoint for the assembly of the 30S ribosome subunit. In the future his work could result in the development of novel antibiotics that could be used in tumor suppression. This was followed by ***John Quintana*** (Advanced Photon Source) who gave a summary of future developments expected at APS.

A tour of the SNS was conducted by ***Leighton Coates*** and colleagues, including an up-close look at the TOPAZ single crystal neutron diffraction system and goniometer sphere, a view of the Macromolecular Neutron Diffraction (MaNDi) site and the Small Angle Neutron Diffraction (SANS) instrumentation facility.

Session 3 - Interesting Methods, chaired by ***Joe Ng*** (UAH), began with "An Introduction to Small-Angle Neutron Scattering for Structural Biology" by ***William Heller*** (ORNL). Small-angle neutron scattering (SANS) shares fundamental concepts with small-angle x-ray scattering (SAXS) but the properties of neutrons opens up an additional avenue for understanding the structure of biological macromolecular systems. Heller's presentation was an introduction to SANS that included basic theory, practical experimental considerations, data analysis and modeling and an overview of the facilities available in the Center for Structural Molecular Biology (CSMB) at ORNL. Next, ***B.C. Wang*** (UGA) discussed a novel approach to data collection titled "The MDS Strategy: Collecting Multiple Data Sets with Short Exposures

Can Produce Better Data than Traditional Long Exposures Within a Fixed X-ray Dose". Wang explained both the theoretical and practical aspects of a novel data collection strategy; the Multi Data Set or MDS approach. The MDS approach differs from traditional data collection in that for the same fixed x-ray dose, *N* data sets are collected using a fraction (1/*N*) of the exposure time used in traditional data collection. It can be shown mathematically that a significant improvement in the overall σ_I for the data set can be achieved using MDS. This effect has also been shown with actual data measurements. ***Christina Hoffmann*** (ORNL) spoke on "Single Crystal Neutron Diffraction at ORNL". She described various neutron diffraction facilities at ORNL. At the SNS, a high-pressure diffractometer "SNAP" and a general purpose single crystal diffractometer "TOPAZ" are in the user program. A macromolecular diffractometer "MaNDi" is scheduled for commissioning in 2012 and an elastic diffuse scattering spectrometer "Corelli" is scheduled for commissioning in 2013. At the High Flux Isotope Reactor (HFIR), a four-axis monochromatic single crystal diffractometer is currently in the user program and a Quasi-Laue SCD "Imagine" is scheduled for commissioning in 2011. ***Christopher Stanley*** (ORNL) ended the session with "Utilizing Small-Angle Neutron Scattering to Investigate the Polyglutamine Aggregation in Huntington's Disease". Stanley's research uses time-resolved SANS to probe the aggregates of huntingtn exon 1 protein fragments with varying polyGln lengths. The time-resolved snapshots yield quantitative information on the size and shape of precursors and the internal structure of the resulting fibrils. This research is providing new insights into the pathway of polyGln aggregation and should later assist in determining the role that precursors play in neuronal toxicity.

Session 4 -SER-CAT: The Way Forward, chaired by ***B. C. Wang***, featured talks by experienced SER-CAT beamline personnel: ***John Chrzas*** and ***Zheng-Qing (Albert) Fu***. In "Update on SER-CAT Upgrades and Others" Chrzas reported that there had been a large increase in the SER-CAT "Virtual Home Synchrotron" program during 2009. SER-CAT has worked with users to help improve their beam time efficiency, especially in view of the new 12 hour shift allocations. Recent software upgrades and future hardware/software upgrades in support of mini-beam operations on 22-ID were described. Next, Fu spoke about "Single-Line-Command Driven UI's for Data Processing at SER-CAT". He explained the new single-line-command driven user interfaces for data processing at SER-CAT. As part of SER-CAT efforts to monitor the data quality on-the-fly at SERCAT, command-line interfaces have been developed for DENZO/SCALEPACK, D*TREK, XDS and X-GEN. These non-graphic user interfaces provide a quick way to automatically process, diagnose and characterize a data set.

A poster session was held in the lobby outside the meeting room. Later, just before dinner, ***Dean Myles*** (ORNL) presented an interesting, exciting and informative overview of future plans and developments at ORNL.

SER-CAT thanks the ORNL for their sponsorship and support and Leighton Coates and his organizing committee for another outstanding meeting! SER-CAT also thanks all the speakers and attendees for their strong participation and support.

Gary Newton

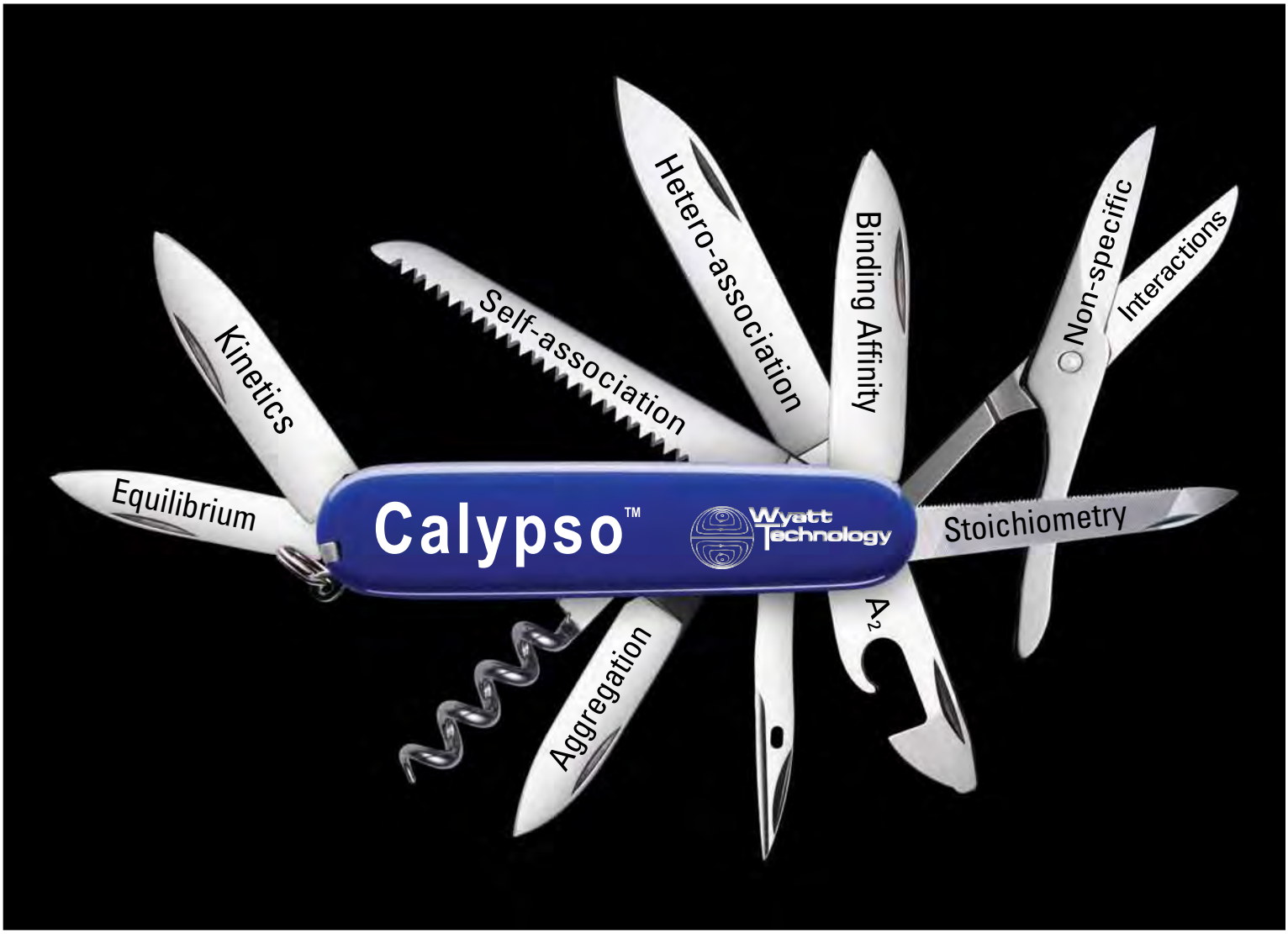
Highlights of the 67th Pittsburgh Diffraction Conference October 29-31, 2010

The three-day conference held at the Georgia Center for Continuing Education located on the University of Georgia Campus provided an outstanding forum for experts in the fields of RNA crystallography, biological SAXS, diffraction studies of materials, crystallization of protein-protein complexes, and neutron small molecule crystallography.

Joseph Wedekind (PDS Secretary) organized an exciting session on ***RNA biology and methodological developments***. ***Martin Egli*** (Vanderbilt) lectured on RNA phasing, providing examples from his own lab on the use of novel nucleotides with site-specific selenium modifications that have proven useful in phasing and are available to the community. ***Ailong Ke*** (Cornell) described the structure of a portion of pRNA from f29, an essential component of the phage's genome packaging motor. He described a model that showed how pRNA fits within a pentameric toroidal EM envelope to produce a molecular scaffold. ***Christine Dunham*** (Emory) discussed her work on the 70S ribosome including the 4 Å proximity of the L27 protein to the peptidyl-transfer center, binding of the ribosome to mRNA, tRNA, and EF-G, as well as how mutant tRNAs cause frame shifting. ***Charles Dann III*** (Indiana) discussed the crystal structure of a novel Mg^{2+}-sensing riboswitch called the M-box. His accompanying functional evidence demonstrated that the M-box regulates transcription by altering the equilibrium of terminator and anti-terminator stem loop structures within the mRNA in response to cellular Mg^{2+} levels. ***Graeme Conn*** (Emory) spoke on crystal structures of RNA methylases. Various models were presented to show how these SAM-dependent enzymes bind ribosomal targets modifying the respective 2´-OH, N1, and N7 positions of rRNA and block antibiotic binding in order to confer drug resistance. ***Joseph Wedekind*** (Rochester) anchored the session with a lecture on the use of Raman crystallography to measure the pK_a of a key adenosine in the hairpin ribozyme active site. His work indicated that specific changes in the RNA conformation are the source of changes in the base pK_a, which has implications for how the RNA fold can fine-tune its limited chemical repertoire to attain function that is on par with a protein catalyst.

The session on ***SAXS*** as applied to biomolecules organized by ***Jeff Urbauer*** (Georgia) featured an inclusive mixture of new methods development and application to proteins, nucleic acids and macromolecular assemblies. ***Dmitri Svergun*** (EMBL), one of the leaders in development of SAXS methods, gave a tour-de-force presentation of contemporary SAXS methods as applied to macromolecules and macromolecular assemblies. Modern, automated data collection and analysis methods and data interpretation were detailed, as was the information content of SAXS data and its utility for understanding macromolecular structure and function and macromolecular assembly. More recent advances were also addressed, including characterization of flexible systems and intrinsically disordered proteins. ***Greg Hura*** (LBNL) described efforts towards high throughput SAXS analysis of proteins and protein complexes. The goal is a pipeline for rapid acquisition and analysis of SAXS data, with application to structural genomics, metabolic pathway analysis and rapid screening of solution conditions for monitoring assembly and reactivity. Examples of successes presented establish a clear and forefront role for such high throughput approaches. ***Alexander Grishaev*** (NIH) has played a significant role in pioneering the use of SAXS data for refinement of structures determined by NMR spectroscopy. His recent efforts include using neutron scattering for refinement of, and resolution of, ambiguity in structural models. He described studies using selective isotopic labeling (deuteration) to achieve contrast variation, thus increasing information content and permitting improved discrimination of components of complexes. ***Thomas Grant*** (HWI) reported on SAXS studies of the tRNA synthetase Gln4 and using the results to complement single crystal diffraction studies. A large disordered region of the protein, not observed in the crystal structure, was demonstrated using SAXS to sample a conformational ensemble, representing the functional excursions of this segment. ***Sam Butcher*** (Wisconsin) described hybrid NMR-SAXS approaches for defining RNA structures. These studies are particularly challenging for NMR due to their large size and the inherent limitations of the NOE for defining long range structure. The complementary shape information SAXS offers is very valuable in this regard. Successful application of this approach was demonstrated for RNA molecules and complexes. To conclude the session, ***Jeff Habel*** (LBNL) described efforts towards utilizing the considerable information available from SAXS data to guide construct design for protein crystallization. Properties such as aggregation behavior, folding state, and flexibility are readily available from SAXS data. When combined with the advantages of small sample requirement, fast data acquisition, and efficient sample screening, the data present exciting possibilities for routine use of SAXS methods in crystallization efforts.

Angus Wilkinson (GIT) organized the session on ***Diffraction Studies of Materials***. ***Chris Tulk*** (SNS, ORNL) discussed recent experiments examining both the stability and crystal structure of various noble gas hydrates. ***Scott Childs*** (Renovo Research) elaborated on how the Materials Module in *Mercury* (CSD) could be used to gain insight into the structural systematics underlying molecular cocrystals. ***Katharine Page*** (LANL) showed how pair distribution functions (PDFs) derived from neutron total scattering data could provide considerable new insight into the structure property relationships underlying functional materials, such as the ferroelectric $BaTiO_3$. ***Matthew Suchomel*** (APS) further pur-

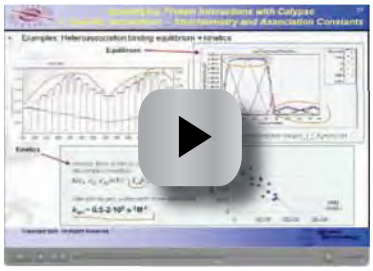


For characterizing protein-protein interactions, only the Calypso™ does it all.

Calypso. Label-free, immobilization-free macromolecular interactions.

No other biophysical method for quantifying macromolecular interactions provides as broad a range of analyses as Wyatt's Calypso. Using Composition-Gradient Multi-Angle Light Scattering (CG-MALS), Calypso gives you label-free, in-solution characterization of equilibrium and kinetic properties, hetero- and homo-association, binding affinity from picomolars to millimolars, stoichiometries of associating complexes, aggregation and self-assembly, and also measures non-specific interactions. So whether you're conducting formulation studies, developing drugs, or performing fundamental biomolecular research, the tools you need can be found in one handy place: Wyatt.com/Calypso.

WATCH THE CALYPSO WEBINAR NOW



Learn about CG-MALS theory and applications at: Wyatt.com/Calypso

Wyatt Technology CORPORATION

sued the general theme of potentially functional inorganic solids studied by diffraction in the context of his work on complex perovskites made under pressure. He pointed out the important role that data with both very high resolution (Dd/d) and high peak to background ratio, such as that available to both on-site and mail-in users of the 11-BM powder diffractometer at the APS can play in understanding the sometimes subtle peak splittings and orderings that occur in materials of this type. Finally, ***Angus Wilkinson*** discussed the thermal and high-pressure behavior of some ReO_3-type oxyfluorides and fluorides.

The ***Crystallization of Protein-Protein Complexes*** session, organized by ***Joseph Ng*** (Alabama - Huntsville) highlighted recent innovations in the field. ***Peter Sun*** (NIDDK) provided details of his study of 650 published protein-protein complexes deposited in the PDB, which led to the development of the Protein Complex Crystallization Database. Peter also described sparse-matrix and systematic buffer/pH screens that were formulated based on the statistical analysis of the database. ***Larry DeLucas*** (Alabama - Birmingham) described the problems associated with the crystallization of membrane protein complexes from protein production to crystallization. He also described the use of a novel diagnostic technology: high-throughput self-interaction chromatography, that can be used to optimize the protein production and crystallization of membrane protein complexes. ***Marc Pusey*** (iXpress Genes Inc.) described two novel fluorescence-based approaches to protein crystallization screening, the use of trace amounts of fluorescently labeled protein to facilitate finding protein crystals in the drop and the use of fluorescence anisotropy to screen for likely crystallization conditions using fluorescently labeled protein. Fluorescence anisotropy measures the rotational rate (and thus size) of the labeled analyte and has been shown to be capable of producing crystals from a number of conditions previously scored as clear solutions or precipitate in traditional crystallization trials. ***Leighton Coates*** (ORNL) described neutron scattering/diffraction instruments available at ORNL for data collection on macromolecules, including an update on the Spallation Neutron Source and the MANDi detector. He also provided exciting results from some recent case studies. ***Jeanette Hobbs*** (Molecular Dimensions, UK) described the use of nucleation grains to aid in the optimization of 'tricky' proteins and how the use of dynamic light scattering together with combined white/UV illumination can improve your chances of obtaining diffraction quality protein crystals. ***Miranda Byrne-Steele*** (Alabama - Huntsville) described some interesting work on the homotrimeric proliferating cell nuclear antigen (PCNA) from *Thermococcus thioreducens* (a hyperthemophile) and *Methanococcoides burtonii* DSM 6242 (psychrophilic). Her work showed that euryarchaeal PCNAs can be divided into two groups on the basis of interfacial interactions: (1) charge-shape and (2) charge-charge complementarity.

The session on ***Small Molecule Neutron Crystallography*** organized by ***Christine Hoffmann*** (ORNL) covered recent developments in the field with talks by a number of beamline scientists. ***Garry McIntyre*** (ILL -Grenoble) described his work on the VIVALDI Laue diffractometer at ILL which has enabled new science and provides neutron Laue data collection rates up to 100 fold over conventional diffractometers. He also provided examples of the application of the Laue technique to rapid chemical crystallography, reciprocal-space surveys, and studies of structural and magnetic transitions. ***Thomas Proffen*** (LANL) described his work using *diffuse scattering* to explore crystal defects or local structural deviations including recent developments in instrumentation and modeling software that makes the analysis of diffuse scattering more accessible to the non-specialist. Several examples were presented on the analysis of single crystal diffuse scattering data and the atomic pair distribution function obtained from powders. ***Alison Edwards*** (Australian Nuclear Science and Technology Organization) described her work on the design and commissioning of the KOALA Laue diffractometer, which is based on the VIVALDI instrument at ILL. She also pointed out the need for the careful consideration of the parameterization of the model during refinement since the choice of parameterization will have a direct impact on the utility of the final refined structure. Several examples were presented from recent studies together with the modeling approach employed. ***Anna Gardberg*** (ORNL) described a joint single crystal neutron and x-ray diffraction analysis of the small, iron-containing protein rubredoxin (MW = 6 kDa). The neutron resolution was achieved by complete deuteration of the protein and subsequent crystallization in D_2O-based phosphate buffer. The room temperature 1.65Å neutron data proved superior (7X) to the 1.1Å x-ray data in locating the deuterium atom positions. ***Christina Hoffmann*** closed the session with an overview of neutron scattering/diffraction instrumentation at ORNL including the newly funded IMAGINE quasi-Laue diffractometer for the HFIR research reactor and the multi-purpose single crystal diffractometer (TOPAZ) undergoing commissioning at the SNS. The TOPAZ diffractometer is designed for data collection on sub-millimeter sized crystals, similar in size to those used in conventional x-ray analysis.

A new feature of the PDC this year was the ***Pittsburgh Diffraction Society Future Leaders Symposium*** organized by ***B. C. Wang*** (Georgia), which highlighted outstanding research being carried out by a graduate or undergraduate. ***S. Jason Polizzi*** (Georgia) presented a preliminary 2.7 Å crystal structure and enzymatic characterization of a novel mutation of UDP-xylose synthase (UXS) found in zebrafish that prevents skeletal development. His studies have suggested that UXS and other nucleotide-sugar decarboxylases deviate from the classical model of catalysis proposed for other members of the short chain dehydrogenase/reductase family. ***Guoxing Fu*** (Georgia State) described his work on the structural and kinetic studies of the executioner caspases 3, 6, 7 and 8, which play a role in inducing apoptosis. His studies show that caspases-3 and -6 bind P5 using critical loop-3 anchoring Ser/Thr and loop-4 side-chain interactions, while caspases-7 and -8 lack the P5-binding residues. These differences will be valuable for the future design of novel inhibitors that are more specific for target caspase members. ***Yuan Hu*** (Indiana U of PA) presented his work on $Na_2(Zn_{1-x},Co_x)SiO_4$ (x = 0.50), a possible dilute magnetic semiconductor. The studies verified that the Co^{2+} and Zn^{2+} ions were randomly distributed in divalent sites forming a single Zn-Co phase. The resulting Rietveld model was refined to convergence with χ^2 of 1.894 and R = 2.49 %. All atoms were observed to possess tetrahedral environments, but those associated with the sodium ions were distorted. ***Susan D. Orwig*** (GIT) presented her work on acid-β-glucosidase

(GCase) an enzyme involved lysosomal storage disorders such as Gaucher's disease. Her work is focused on solving co-crystal structures of GCase with ER permeable small molecules, called pharmacological chaperones to understand how binding of these molecules can restore cellular trafficking of the complex to the lysosome in endogenous mutant GCase's. ***J. Tucker Swindell II*** (Georgia) described an interesting study on how the choice of data reduction approach (software used) can affect the success rate of sulfur SAD phasing. He presented a comparative analysis of data reduction programs (HKL2000, d*TREK, XDS, Proteum2) on the success rate of sulfur-SAD phasing for data collected on a moderately diffracting crystal using 1.9Å SER-CAT (22ID) x-rays. ***Norie Sugitani***, (Alabama- Huntsville) presented her work on the structural studies of Mbur_1912 from the cold-adapted acrhaeon, *Methanococcoides burtonii* DMS6242. The presentation included the general challenges of studying and analyzing psychrophilic proteins at the level of expression, purification and crystallization.

The Chung Soo Yoo award for best student poster went to ***Jason D. Salter*** (Rochester) for "*Crystallizing HIV-1 viral infectivity factor (vif) in complex with Elongin B and Elongin C*" which described his attempts to prepare and crystallize a tripartite complex of HIV *vif* with Elongin B and C using several truncated forms of the *vif* protein. Small crystals have been produced that diffract x-rays.

The PDS would like to thank all the vendors whose donations help support the conference. The full program and abstracts are available from the PDS web site ***www.pittdifsoc.org***

John Rose

Call for Nominations PDS Sidhu Award

The Pittsburgh Diffraction Society gives the Sidhu award, named in the memory of Professor Surhain Sidhu, to an outstanding scientist who is within six (6) years of having earned a PhD or its equivalent. The award honors significant contributions to the science of crystallography and/or diffraction and carries a cash prize of $2000. The prize is bestowed biannually when the Society holds its conference in Pittsburgh. The successful candidate must attend the ***68th Pittsburgh Diffraction Conference that will be held on October 27 – 29, 2010 at the Holiday Inn University Center, Pittsburg PA (www.pittdifsoc.org)*** to present the Sidhu Award Lecture and receive the prize.

Nomination Process: Nominees, or interested third parties, should submit a letter that describes the candidate's educational background, in particular the institution(s) granting the PhD, name(s) of thesis advisor(s), thesis title, and the date the degree was bestowed. Briefly summarize the scientific contribution that qualifies the candidate for consideration. Include reprints of pertinent publications and two (2) letters of recommendation from scientists who are familiar with the research of the candidate. Please also include the candidate's CV. The entire application package should be electronically submitted as a pdf file to Bi-Cheng Wang (***wang@bcl1.bmb.uga.edu***) by the application deadline of ***1 September 2010***.

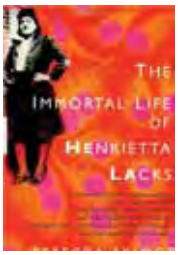
Professor Sidhu was a founding member of the PDC. In 1942 he was Professor of Physics and Director of the X-ray Laboratory at the University of Pittsburgh. Later, he moved to Argonne National Laboratory, where he pioneered the use of the null matrix in neutron diffraction. This procedure involves choosing isotopes of an element in the proportion that gives a zero net coherent scattering factor. It has been widely used for studying biological materials in which the isotopic ratio of H to D is appropriately adjusted.

Past Winners: A. I. Bienenstock, R. M. Nicklow, T. O. Baldwin, S.-H. Kim, L. K. Walford, D. E. Sayers, B. C. Larson & N. S. Seeman, P. Argos, K. Hodgson & G. DeTitta, G. Petsko, D. C. Rees, D. Agard & J. M. Newsam, Q. Shen, M. Luo, L. Brammer, R. C. Stevens, M. Pressprich & T. Yeates, A. Vrielink & J. Wang, M. Georgiadis, M. J. Regan, C. Ban & M. Wahl, W. R. Wikoff, L. Shapiro, Y. Lee, E. O. Saphire, Y. Xiong, C.-Y. Ruan, P. Chupas ,

Membrane Structural Biology by Mary Luckey (2008) Cambridge Press, 344 pp, ISBN-13: 9780521856553

Believe it or not, the recommendation for *Membrane Structural Biology with Biochemical and Biophysical Foundations* came from Amazon as the result of purchasing Rupp's *Biomolecular Crystallography*. Being adventurous, I ordered a copy and found it well written and enlightening. In particular, the extensive use of "highlight boxes" provides useful background information in more detail without cluttering the main text. Not being a membrane structural biologist by formal training, I found this textbook to be both quite informative and accessible. ***Chapter 1: Introduction*** - provides an excellent review of our current understanding of membranes as well as a historical context for the remaining chapters. ***Chapter 2: Diversity of Membrane Lipids*** - a description of the most common lipids and their properties as a prelude to understanding the thermodynamics of lipid bilayers. ***Chapter 3: The Tools for Studying Membrane Components: Detergents and Model Systems*** - describes the detergents used for extracting and crystallizing membrane proteins as well some of the analytical tools used for determining the states of the proteins. ***Chapter 4: Proteins in or at the Bilayer*** - describes proteins that sit on the surface of the membrane, with examples of toxins, colicins and peptides. The latter part of the chapter gives the basics of transmembrane proteins, essentially an introduction to the next chapter. ***Chapter 5: Bundles and Barrels*** - I think this is the meat of the book. A detailed view of both bundles of alpha-helices and barrels of beta-sheets is given here, with numerous examples from the recent literature. An excellent description of photosynthesis is provided as a description of various transporters. ***Chapter 6: Functions and Families*** - introduces the concept of families and superfamilies as applied to membrane proteins. It also provides a view into the bioinformatics of membrane proteins and readers are introduced to current tools for analysis of sequence, structure and function. ***Chapter 7: Protein Folding and Biogenesis*** - covers translation, translocation, folding, insertion and diseases of misfolding. ***Chapter 8: Diffraction and Simulation*** - provides a brief description of liquid crystallography of the bilayer. A detailed explanation of modeling of the bilayer is given next along with several examples of x-ray structures with lipids associated to the protein. ***Chapter 9: Membrane Enzymes and Transducers and Chapter 10: Transporters and Channels*** - provide a detailed survey of the current known space of the title classes. ***Chapter 11: Membrane Protein Assemblies*** - the penultimate chapter provides detailed information about the structure and mechanism of the F_1F_o-ATPase, the complexes of the respiratory chain, the translocon, and complexes responsible for vitamin B12 and drug transport. ***Chapter 12: Themes and Future Directions*** - is a final review of the book and a look forward. I am surprised that SAXS as a method for looking at proteins, specifically complexes, was not mentioned in the book, as I think this is an up and coming technique for the field.

The Immortal Life of Henrietta Lacks by Rebecca Skloot (2010) Crown Publishers, 369 pp, ISBN: 9781400052172



I had seen reviews for *The Immortal Life of Henrietta Lacks* just about everywhere I looked, from The *New Yorker* to *Nature*, and even *The Houston Chronicle*. I decided I would not read the reviews but I did listen to an interview with the author on NPR. I decided this book was a big deal and decided to review it here since its central topic, the immortal cell line, HeLa, has so influenced modern medical science.

The author weaves four stories in an out-of-time sequence that makes the book very interesting. The writing is not technical, but enlightening and current. We first learn about the HeLa cells themselves. We also find the author as a precocious sixteen year old in a college biology class, where she first learns about the HeLa cell line, and her subsequent journey into becoming an investigative reporter.

The next story is that of Henrietta Lacks, the woman from whom the HeLa cell is derived and her family, particularly her daughter Deborah. The author and Deborah become friends but only after an arduous journey and the diagnosis of hypertension and hyperglycemia in the latter. There are parts of this story that will make you mad: for example the family of Henrietta couldn't get decent health care even though her cells have done so much for medical science.

The story of HeLa cell line itself is also unveiled for us in the context of the importance of this immortal cell line to medical science and medical ethics. HeLa cells were used to develop the polio vaccine in the 50s. They were sent into space before humans and they were subjected to nuclear explosions. They have been used for cancer research in the hopes of curing cancer, creating mouse/human hydrids and infertility studies. The author suggests all the HeLa cells produced thus far would, if laid end to end, circle the earth three times.

Finally, we are given a history of informed consent and an analysis of the current arguments for and against the use of human tissue in research without the patient's knowledge of the disposition of the tissue or the profits that might happen. These issues are raised throughout the book and discussed in detail in the afterword.

The Structure of Scientific Revolutions by Thomas S. Kuhn (1996) University of Chicago Press, 212 pp, ISBN:0226458083

I came across references to this book in reading three other books at the end of last year. I thought to myself that I should read it, and I have, twice. The first scientific book I started reading this year mentioned TSoSR. Until the first version of this review appeared, I thought that I must have been the only person who hadn't read it.

The main concepts described include the terms "paradigm", "normal science" and "revolutionary science." Kuhn describes a paradigm as being the prevailing model or theory describing a phenomenon. Normal science is the process by which incremental improvements add to the existing paradigm. Kuhn suggests that most science is normal - which is a point of

contention for many. Revolutionary science is the result of a crisis or crises in which the extant paradigm no longer describes the observations. Kuhn does stress that the observer's frame of mind is important, as two observers may see the same picture yet interpret it completely differently. When revolutionary science works, a paradigm shift occurs. Kuhn also suggests that those creating the paradigm shift may not be aware of the shift, and that the actual revolution may only be observable from a historical perspective.

Kuhn also spends time discussing the concept of incommensurability (not related to lattices at all). This idea is used to describe a new paradigm that is essentially orthogonal to the old paradigm ... where the descriptors of the old fail to work with the new, and communication between scientists fails. Obviously, this creates a problem in the transition from old to new. Kuhn first this published this philosophy book in 1961. A third, final edition was published in 1996, the year Kuhn died. This book has been referred to as one of the hundred most influential books since World War II by the *The Literary Times* and the best exposition of the scientific method by the *New York Times*. Is it? You'll have to decide for yourself.

Small-Angle Scattering of X-rays by André Guinier and Gérard Fournet; translated by Christopher B. Walker (out of print)

Published in 1955, this book is long out of print and quite difficult to find. Fortunately, Angela Criswell located a copy for this retrospective review. Given that SAXS is such a "hot topic" these days, it was remarkable to find that this old tome is still a relevant and useful reference for researchers today. To frame the perspective of the authors, it is notable that they opined (in chapter 6) that "These remarks explain why the study of proteins [dilute solutions] offers one of the best applications on this method. As a matter of fact, a large number of investigations have already been carried out on proteins, as is shown in the bibliography at the end of the text. We believe that it is in this field that small-angle scattering can give the most valuable and important results from a general point of view." We are celebrating the 50th anniversary of the publication of *Structure of Hæmoglobin: A Three-Dimensional Fourier Synthesis at 5.5-Å. Resolution, Obtained by X-Ray Analysis*, [*Nature* 185, 416-422 (1960)] by Perutz, Rossmann, Cullis, Muirhead, Will and North. Guinier and Fournet did not foresee the explosion in protein structure that would start five years later after the publication of their reference. Yet, it is quite interesting that, 55 years after the publication, structural biologists have come back to SAXS as a tool for understanding the solution structure of proteins - that stage before crystallography takes over. Chapter 1 provides a very basic introduction to the scattering process, while Chapter 2 explains the theory in detail. Readers should be forewarned: Chapter 2 provides an in depth overview of the mathematical background behind the calculation of the radius of gyration, pair distribution function and even the second virial coefficient. Chapter 3 provides a detailed discussion of the three pinhole SAXS camera. The only detectors available then were Geiger counters and film so the reader must keep in mind that there has been 55 years of instrument development in the interim. Nevertheless, the discussion is useful in understanding modern SAXS cameras. Chapter 4 introduces readers to the interpretation of results. Chapter 5 compares the SAXS method with other, then state-of-the-art techniques to validate the results from Chapter 4. Chapter 6 goes through a number of applications, with the first part of the chapter devoted to the study of proteins in dilute solutions. Finally, an extensive bibliography is provided, that is obviously only current to 1955.

There are more modern textbooks and reviews on this subject, and the tools for collecting data and generating results have changed in the intervening 55 years, but anyone who is seriously interested in learning about SAXS would benefit from reading this classic text.

Game Change: Obama and the Clintons, McCain and Palin and the Race of a Lifetime by John Heilemann and Mark Halperin (2010) Harper, 448 pp, ISBN: 9780061733635

I had first heard about this book on NPR's *Left, Right and Center*. I bought a copy and thoroughly enjoyed it. One of the more enjoyable facets is that our politicians use the F-bomb as often (or more) than does the general population.

This book covers a lot of ground, not just the title characters' 2008 bid for the presidency, but the entire cast of characters including John Edwards, Mitt Romney and Rudy Giuliani to name a few. The authors provide a detailed analysis of the meltdown of the Clinton and McCain campaigns. The text is so generously populated with quotes from the sources, that it is hard to believe the authors weren't recording this as the campaign transpired. My last comment is that the book is sufficiently current that the details are not yet a dim memory and the lessons can be applied to the mid-term elections in 2010 and beyond. If you are a fan of US politics or a registered voter in the US you should read this book for posterity's sake.

On a completely different topic, for those of you with young children, you might take a listen to They Might be Giants' new studio album titled "Here Comes Science". It is series of short ditties designed to teach science to youngsters. The songs are scientifically sound and fun. I particularly liked "*My Brother the Ape*".

All reviews by Joe Ferrera

Editor's Note: An excellent review of Rupp's *Biomolecular Crystallography* written by Manfred Weiss appeared in *Acta Crystallographica D* in the May 2010 issue. This brings me to the first of what I am sure will be many errata. In thespring 2010 *RefleXions*, Katherine Kantardjieff was erreonsly listed as a co-author of *Biomolecular Crystallography*. She is not a coauthor and we apologize for any confusion the error might have caused.g

$$\begin{bmatrix} \cos 90^\circ & \sin 90^\circ \\ -\sin 90^\circ & \cos 90^\circ \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} a_2 \\ -a_1 \end{bmatrix}$$

Alexander Zdanov (1952-2010)

Alexander (Sasha) Zdanov, Staff Scientist in the Macromolecular Crystallography Laboratory, National Cancer Institute, Frederick, MD, passed away on May 19, 2010 at the age of 58. Sasha was born in Murmansk, Russia and obtained his training in protein crystallography with Natalia Andreeva at the Engelhardt Institute of Molecular Biology in Moscow, Russia. After spending two years as a Research Officer in the Biotechnology Research Institute in Ottawa, Canada, he joined NCI in 1993. His extensive early experience in crystallographic studies of aspartic proteases such as pepsin and chymosin led to subsequent work on retroviral proteases and on plant enzyme, prophytepsin. Sasha led the NCI efforts to investigate structural properties of a number of cytokines, such as IL-4, IL-10, IL-19, and IL-29, as well as their complexes with the extracellular parts of receptors. He published almost a hundred scientific papers, trained a number of scientists who are now independent investigators in the US and Canada, and collaborated with many postdoctoral investigators. He will be missed by all his colleagues and friends.

Dick van der Helm (1933-2010)

Dick was born in Velsen in the Netherlands on March 13, 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. In 1955 he joined C.H. Macgillavry's lab as an assistant. In 1957 he came to the U.S. to work with L.L. Merritt at the University of Indiana and two years later moved to the Philadelphia to work with A.L.(Lindo) Patterson at the Institute for Cancer Research. In 1962 he began his 38 year career with the University of Oklahoma during which he became a Full Professor of Chemistry in 1969 and was appointed George Lynn Cross Research Professor in 1977. He was the recipient of the Oklahoma Scientist Award in 1980 and the Oklahoma Chemist Award in 1985.

During his time with both Merritt and Patterson, Dick was writing computer code to solve the 3-dimensional structures of molecules. His endeavors soon resulted in the creation of programs that were shared with many other labs. A significant portion of Dick's later work was focused on molecules of biological interest, natural products from marine organisms and synthetic compounds with anticancer activity, cyclic peptides and lactams. In 1973, he received a grant for siderophore research, iron transport compounds in bacteria and fungi. He retained this NIH grant continuously for 29 years. In the middle eighties he and his collaborators started work on the outer membrane proteins in gram-negative bacteria which transport the ferric siderophores.

Dick was a highly respected scientist and a passionate learner. He had 336 peer-reviewed publications. He taught undergraduate physical chemistry and valued the time that he spent teaching students and post docs in his research lab. As an active member of the ACA he held several positions of leadership. He was a much sought after reviewer of grants by the NIH. He was thankful to all his collaborators, students, and postdocs.

He was an enthusiastic golfer and fisherman. He thoroughly enjoyed spending time with his grandchildren. He had a lot of fun traveling with his wife Louise and was an avid soccer fan.

He is survived by his wife Louise, his 6 children, and his 9 grandchildren. Dick will be missed by all he interacted with both professionally and personally.

Editors notes: *We learned of Dick's passing as we were about to go to press. A more complete appreciation of his life will appear in the fall issue of RefleXions.*

We also just heard the sad news that within months of losing Lieselotte we have also lost ***David Templeton (1920 -2010)****. An appreciation of David's life will also appear in the fall issue of RefleXions.*

Any friends and colleagues of either Dick or David who want to contribute should contact the editors.

2011 Art in Crystallography Contest

As too few submissions were received in response to the 2010 call for entries we have reschedules it as the ***2011 Art in Crystallography Contest*** and extended the deadline for entries to April 1st, 2011.

Entries in the form of images emailed to either editor (***connie-chidester@earthlink.net or acareflexions@gmail.com***) 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.

Jobs Board on the ACA website

Employers: Post open positions by downloading the Job Request Form and returning it to ***aca@hwi.buffalo.edu*** or by the board can be kept as up-to-date as possible.

Job Seekers: Find available employment positions in crystallography and related disciplines. Look for jobs based upon location, job description, hiring company.

Browse Job Categories: Faculty Positions; Post-Doctoral Research Fellowships (academic and industrial); Industrial and Commercial Positions (permanent); Other Positions

It is not required that you be an ACA member to use this job board ***www.amercrystalassn.org/content/pages/main-job-board***.

The World Directory of Crystallographers

During the IUCr Congress and General Assembly in Osaka, the Executive Committee invited me to succeed Yves Epelboin as General Editor of the WDC. I accepted the appointment because I have some ideas for its future development; but I must also admit that I have been very much attached to the editorial effort involved in the WDC, which I have been involved with for almost half of its lengthy history.

Last year, in a short visit to Chester, I met and discussed some ideas with the operational staff. The problem of keeping the information updated is of primary importance. But what makes it different from the regular databases and search engines existing today in the world wide web? We all agreed that it is not a simple 'mailing-list'. The *World Directory of Crystallographers* is a list of professionals engaged in very specific research areas related to x-ray crystallography. It was created to establish new links, open new perspectives, create interaction between students and researchers and promote sharing of technical resources worldwide. It is up to the scientific community itself to bring to the directory that 'something else' that makes it so particularly useful. In an era of fast communication, we must follow new trends, but cannot disregard the importance of the contents of the information. It is essential that the entries are updated periodically. The mobility of registered members is greater than in olden times; but this is offset by current fast communication tools. Updating biographical information is as easy as ever; but we need more than an e-mail address. We need to know about the academic status and research interests for each entry.

As it is now, with the latest tools in the search engine of the IUCr WDC site one can find a registered crystallographer from any country in the world in a snap by searching on a family name. You can even see their pictures! When a Journal requests authors to appoint reviewers for the papers being submitted, just knowing the names of the specialists in a certain area is not enough. Consulting the WDC database can readily provide all the necessary details (institution, position, addresses). Moreover, If you want to find information about groups of crystallographers in other countries you can obtain the information in several formats, according to your needs, by just one touch, pressing the control key and selecting the country. More interesting tools are being developed, and will be implemented after the general up-dating of the data during 2010.

We count on the community to improve and update our World Directory of Crystallographers. We will be trying hard during 2010 contacting National Committees from all countries listed. And for those who will attend the XXII International Congress in 2011 in Madrid, we will have a WDC 11 'up-dating station' at the IUCr booth. You will be able to access your entry and check your data for corrections and additions. I'll make sure to be there to help !

Iris L. Torriani - torriani@ifi.unicamp.br

Bridging the Sciences Program Launches

The NIH and NSF jointly announced two new research grant programs to bridge the sciences: (1) *New Biomedical Frontiers at the Interface of the Life and Physical Sciences* and (2) *Transforming Biomedicine at the Interface of the Life and Physical Sciences* (R01) PAR-10-141. The former focuses on basic research and the latter on clinical and translational research.

These two new programs are part of the Bridging the Sciences Demonstration Program, advocated by the Bridging the Sciences Coalition, of which the ACA is a member. The purpose of that program, and the Coalition's advocacy, was to provide a dedicated source of funding to cross-disciplinary and upstream research that often falls between the cracks of the basic research funded at NSF and DOE and the biomedical research funded at NIH. Breakthroughs such as x-ray crystallography, CAT scans, and magnetic resonance imaging have had an enormous and important effect on biology. These discoveries were funded by sources, such as the Bell Labs, which are no longer in existence. Thus, it is very difficult for researchers to work on similar breakthrough technologies today.

The program announcements indicate that many of the specific items advocated by the coalition were included. Both programs will provide grants of varying sizes and lengths to accommodate a variety of research, encourage young investigators with novel ideas to apply, and will be reviewed by special review panels that include reviewers from the physical, mathematical, and computational sciences selected by NSF. Applications will be accepted once a year in May through 2012. The first deadline was May 18, 2010.

To read the announcements in full, go to ***http://grants.nih.gov/grants/guide/pa-files/PAR-10-142.html and http://grants.nih.gov/grants/guide/pa-files/PAR-10-141.html.***

Ellen Weiss

Tenure Track Position Available:

Applications are being accepted for a tenure track position at the Assistant or Associate Professor level in the Department of Biology, Faculty of Science, University of Waterloo. Applicants should have a PhD and postdoctoral experience with a research record in **Macromolecular X-ray Crystallography**. Duties of the position include establishment of an independent research program, teaching and supervision at the undergraduate and graduate levels, and participation in the running of the Department and University. The University has instrumentation for macromolecular crystallography, including a Rigaku Micromax/R-Axis 4++ diffractometer system. Inquiries and applications, consisting of a full *curriculum vitae* with publication record, statement of research interest and teaching experience, and names of three references, should be sent electronically to David R. Rose, Chair, Department of Biology, University of Waterloo, c/o Gini Kennings, ***givan@uwaterloo.ca***. The closing date for applications will be ***September 1, 2010***, with a starting date on or after January 1, 2011. All qualified candidates are encouraged to apply; however Canadians and permanent residents will be given priority. The University of Waterloo encourages applications from all qualified individuals

House Reauthorizes America COMPETES Bill

"Mr. Speaker, I demand a division of the question on the adoption of the amendment to enable the separate votes" declared House Science and Committee Chairman Bart Gordon (D-TN) on May 28th. For the third time, the America COMPETES reauthorization bill was before the House. About an hour after Gordon made his demand, H.R. 5116 passed the House by a vote of 262 to 150.

The procedure that Gordon called for essentially untied the package of proposed changes that House Science and Technology Committee Ranking Republican Member Ralph Hall (TX) had used to stop the legislation when the House first considered it on May 13. Just before the House was to vote on the bill, Hall used a House procedure to send the legislation back to the Science Committee with instructions on how it should be rewritten. Hall's package of changes included a three-year freeze in the authorization levels for the NSF, the DOE Office of Science, and the NIST. It also reduced the authorization period from five years to three years, eliminated the authorization for several new programs in the bill, and added a new veterans' benefit. Hall's package also included a provision to prohibit the payment of salaries to employees of the Executive Branch for viewing, downloading, or exchanging pornography on a Federal Government computer or "while performing official Federal Government duties." In describing the pending vote on Hall's motion, Rep. Lynn Jenkins (R-KS) described the choice facing Members: "If you think a couple of days of suspension, a reprimand, a transfer is the right response when someone uses government computers to spread pornography, then vote against this motion. But if you think spreading pornography with a government computer is an act that should lead to dismissal, then vote for this motion. I urge a vote for this motion." Hall's motion passed by a vote of 292 to 126.

A new version of the bill went back before the House using a streamlined procedure on May 19. The bill's price tag was reduced by 50 percent by changing the authorization period from five years to three years. It also included a pornography provision. This procedure required a 2/3 majority vote to pass. While the vote was 261 to 148, the bill failed to secure enough votes for passage.

On May 24th the House met at 9:00 A.M., and completed its consideration of the FY2011 National Defense Authorization Act. Just before 2:00 P.M., it was announced that the House would resume its proceedings on H.R. 5116 – the original bill with the five-year authorization period. Following brief floor procedures, Gordon moved what is called "a division of the question." This procedure allowed House Members to vote on each part of the amendment contained in Hall's May 13 Motion to Recommit. A division of the question has been part of the House Rules since 1789 and has been used during consideration of authorization and appropriations measures and in impeachment proceedings.

There was no debate when the House resumed its proceedings on H.R. 5116. Gordon's move divided Hall's amendment in the Motion to Recommit into nine portions. On three of these, the House voted to retain the original bill language regarding federal loan guarantees, regional innovation clusters, and Energy Innovation Hubs.

Roll call votes were demanded on the other portions, as follows:

Roll call vote 326 was to strike a new National Science Foundation prize award. The House voted 175 yes to 243 no, resulting in the retention of the prize award in the bill.

Roll call vote 327 was to remove a provision in the bill authorizing an Innovative Services Initiative at the National Institute of Standards and Technology. This failed by a vote of 163 to 244.

Roll call vote 328 was to provide special consideration for disabled veterans. This portion failed by a vote of 197 to 215.

Roll call vote 329 was approved unanimously to prohibit the payment of salaries to federal employees who view pornography while performing official government duties.

Roll call vote 330 would prohibit federal funding to institutions of higher learning if they deny or restrict campus access to ROTC or military recruiting. The House agreed to add this portion to the bill by a vote of 348 to 68.

The next roll call vote, 331, encapsulated much of the discussion there had been about future science spending in the Science Committee and on the House floor. This portion would have reduced the authorization period from five years to three years. Of note, it would have frozen the authorization levels for NSF, NIST, and the DOE Office of Science at current levels for FY 2011, 2012, and 2013. The House rejected this by a vote of 181 to 234. There were 181 Members voting for this portion, twelve of whom were Democrats and the rest of which were Republicans. A total of 234 Members voted against this portion: 233 Democrats and one Republican - Rep. Vern Ehlers (MI).

The final roll call vote, 332, was to pass the bill. There were 150 Members voting against passage of the bill, all of whom were Republicans. Seventeen Republicans joined 245 Democrats in voting to pass the bill.

The Republican and Democratic sides of the House Science and Technology Committee issued press releases after the passage of H.R. 5116. Ranking Member Hall commented "I am disappointed that my Democratic colleagues resorted to using a procedural tactic to defeat Republican changes that would have saved over $40 billion and restored the original COMPETES priority of basic research. While I am glad we were finally able to reauthorize many of the important research and education program in this bill, the bill that passed today spends too much money, authorizes duplicative programs, and shifts focus away from the bill's original intent."

Chairman Gordon stated: "As I've said before, this bill is too important to let fall by the wayside. Today, we took the action necessary to see consideration of this bill completed. And we allowed the Members of the House to be on record voting on provisions gutting funding for our science agencies, voting on whether we should eliminate programs that will help create jobs, voting on whether to eliminate programs that will make us more energy independent, voting in opposition to federal employees watching pornography, and voting on whether universities that ban military recruiters should receive federal research dollars. We have provided all Members, in a reasonable manner, with the ability to vote on each of these items separately instead of all together."

Richard M. Jones - AIP

Scientists Take to Capitol Hill for CVD

Over 270 scientists, engineers, and educators convened on Capitol Hill for the 15th Annual Science-Engineering-Technology Congressional Visits Day (CVD) on April 28 and 29.

CVD participants come from across the US to Washington, DC each year to emphasize the importance of consistent research and development (R&D) investments in science and technology (S&T), urge further investments in R&D and science education, and to thank Members of Congress for landmark legislation like the American Recovery and Reinvestment Act and the America COMPETES Reauthorization Act of 2010.

On the first day, CVD participants are given a lesson in Government 101—learning how the appropriations cycle works, how to speak with Members of Congress and their staff, and how to stay involved in the policy process when they return home.

This year, Representatives David Wu (D-OR) and Ralph Hall (R-TX) received the George E. Brown Jr. Science-Engineering-Technology Leadership Award at a reception put on by CVD organizers which highlighted 2010 as the 50th anniversary of the invention of the laser. That anniversary was later recognized by H. Res. 1310 which passed the House on May 4.

The second day of CVD began with a breakfast reception at which retiring Rep. Vern Ehlers (R-MI), himself a previous Brown Jr. Award recipient, thanked CVD participants for educating his colleagues about the importance of investments in S&T R&D. Afterwards, CVD volunteers dispersed to their respective Representatives' and Senators' offices to represent their professional community.

CVD participants are usually divided into groups by state. These groups will travel together between House office buildings and across the Capitol to Senate offices. Meetings generally follow a simple 15-minute format wherein CVD participants introduce themselves, discuss their work, deliver prepared talking points, and thank the staff for their support of S&T R&D. Participants frequently meet with Legislative Assistants—staff who handle multiple subject areas, like science issues, and provide policy advice to their Members. Some CVD groups will have the opportunity to meet with their Representatives and Senators.

Physics was particularly well represented with participation from organizations like AVS: The Science and Technology of Materials, Interfaces, and Processing; the American Astronomical Society (AAS); the American Geophysical Union (AGU); the American Physical Society (APS); and the Optical Society of America (OSA).

A record number of AAS and AGU members—16 and 29 respectively—traveled to Capitol Hill this year. Thirty-six physicists from APS, representing 19 states made 85 visits to offices. Likewise, 22 OSA members visited more than 30 offices.

CVD occurs in spring each year.. For more information, including how you can get involved with future visits to the Hill see ***www.agiweb.org/gap/cvd/cvd2010/index.html***

Rob Boisseau - AIP

2011 ACA Patterson Award to Keith Moffat

Keith Moffat (University of Chicago) has been selected as the recipient of the 2011 ACA Patterson Award. The Award, established in 1980 to honor A. Lindo Patterson, recognizes and encourages outstanding research in the structure of matter by diffraction methods, including significant contributions to the methodology of structure determination and/or innovative application of diffraction methods and/or elucidation of biological, chemical, geological or physical phenomena using new structural information. Moffat will be honored for his work in pioneering ultrafast time resolved x-ray diffraction using synchrotron radiation to capture the function of fundamental protein processes at atomic resolution.

Keith obtained his BSc in 1965 from the University of Edinburgh in Physics and his PhD in protein crystallography in 1970 from the University of Cambridge with Max Perutz. Following a short post-doc with Quentin Gibson at Cornell University he was appointed an assistant professor and quickly moved up to the rank of full professor of Biochemistry, Molecular and Cell Biology. During that time, he was fundamental in the construction of the Cornell High Energy Synchrotron Source (CHESS) in 1981 and in establishing its macromolecular crystallography arm (MacCHESS) in 1982. In 1990, he moved to the University of Chicago where he is currently Louis Block Professor in Biochemistry and Molecular Biology, a founding member of the university's Institute of Biophysical Dynamics, and Director of BioCARS, the structural biology component of the interdisciplinary Consortium for Advanced Radiation Sources.

Arriving in America at the tail end of 1969, he soon realized that his proposal to develop time-resolved crystallography was not yet possible given the then limitations in x-ray and laser sources, but he didn't give up. By 1983-84, Moffat was able to show that a naturally polychromatic synchrotron source such as CHESS yielded gorgeous Laue diffraction patterns with very short x-ray exposures, and that the Laue technique was thus well suited to fast time-resolved approaches. He progressively extended the time resolution from minutes to milliseconds and ultimately to picoseconds. In 1996, he published the first film of a protein at work (the photolysis of CO-myoglobin) at atomic resolution (2.0 Å). Thus, in just over 25 years since his initial proposal, Moffat has succeeded in demonstrating how short-lived structural changes that accompany all chemical and biochemical reactions can be observed by time-resolved crystallography through the application of synchrotron radiation.

Arthur Lindo Patterson, for whom this award is named, is also the eponym for the Patterson Function, which represents perhaps the most important single development in crystal-structure analysis since the discovery of x-ray diffraction itself. Keith Moffat's pioneering work in time-resolved crystallography is another huge advancement in macromolecular crystallography that is well deserving of the Patterson Award. Previous winners wereB.C. Wang (2008), Alwyn Jones (2005), Douglas Dorset (2002), Gerard Bricogne (1999), Christer E. Nordman (1997), George Sheldrick (1993), Michael M. Woolfson (1990), David and Lieselotte Templeton (1987), Jerome Karle and Herbert Hauptman (1984), and Wayne A. Hendrickson (1981). The ACA will present Keith Moffat with the award at the 2011 ACA Meeting in New Orleans. A historical sketch of Patterson can be found in the Summer 2008 issue of *RefleXions*.

2011 ACA Wood Award to Daniel Nocera

In 1997, the ACA established the Wood Science Writing Award to honor Elizabeth A. Wood, President of the ACA in 1957 and author of science books for lay readers. The purpose of the award is to recognize and honor the authors of outstanding publications that bring science to the attention of the general public. Successful nominees need not be crystallographers or scientists and 'publications' is not limited to written work but could include such things as artistic efforts or museum displays. The award is presented every three years. This year the ACA Council is proud to announce ***Daniel G. Nocera*** (MIT) as the 2011 winner.

Nocera obtained his BS in Chemistry from Rutgers University in 1979 and his PhD in Chemistry from the California Institute of Technology in 1984. He then joined the faculty of Michigan State University as an assistant professor, becoming full professor in 1990. He moved to MIT in 1997 where he is presently the Henry Dreyfus Professor of Energy and Professor of Chemistry. The Nocera group focuses on basic mechanisms of energy conversion in biology and chemistry. He is most famous for his work on renewable energy sources. Mimicking plants' photosynthetic ability to use sunlight to split water, he has developed

INCOATEC
innovative coating technologies gmbh

Protein Crystallography

Small Molecule Crystallography

IμS Incoatec Microfocus Source

30 W

air-cooled

Quazar multilayer optics

for Cu and Mo
Ag and Cr

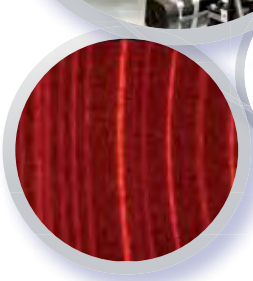
unprecedented
flux density

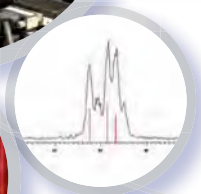
low maintenance

2D focusing or collimating

3 years warranty

XRD





High Brilliance Sealed Tube

SAXS

www.incoatec.de

an inexpensive and efficient, nontoxic way for converting solar energy to chemical fuel. Nocera's ultimate goal is to provide a personalized energy source for every home such that each home becomes its own solar power and gas station. With his technology, just over a gallon of water would be needed to power a whole house.

Not only does he bring science to the general public by wanting to incorporate it into their homes, but also by his frequent guest appearances on TV (*ABC Nightline*, *PBS*, *NOVA*, *Discovery Channel*, and *Explora* in Europe) and radio (*NPR*). He developed the pilot that was used to begin the new PBS science program *ScienceNow*, and has also helped develop a *National Geographic* five part series on *The Lifestyle of Carbon*. His success in communicating science to a wider audience was made most evident in 2009 when he was named one of *Time* magazine's Top 100 most influential people. Other names listed were Barack and Michelle Obama, Hillary Clinton, Ted Kennedy, and Oprah Winfrey.

When asked in an interview by *Wicked Local* in his hometown of Winchester, MA if there was anything he would like to add about his discoveries or the environment, Nocera replied, "… I will make myself available to give a general energy talk (town hall, high school, you name it). The talk isn't super technical. It is designed to get the scale of the problem across to the public and give them the correct numbers. And then we can have a genuine Q&A session. I give talks like this all over the world. … I can paint the energy picture for the future, so that residents in Winchester can be informed about how they might best contribute in their own way to addressing the energy challenge." It is this genuine desire to inform the public and make a global environmental change that makes him a laudable recipient of the ***Elizabeth A. Wood Science Writing Award***.

The ACA will present Nocera with the award at the 2011 ACA Meeting in New Orleans. Previous winners are Lisa Randall (2007), Oliver Sacks (2004), Ira Flatow (2002), K.C. Cole (2001), Robert Weinberg (1999), Robert M. Hazen (1998), and Roald Hoffmann (1997). A biographical sketch of Elizabeth Wood can be found in the summer 2006 issue of *RefleXions*.

2011 ACA Etter Early Career Award to Yurij Mozharizskyj

To honor the memory of Margaret C. Etter (1943-1992), the ***Etter Early Career Award*** was established to recognize outstanding achievement and future potential in crystallographic research demonstrated by a scientist at an early stage of their independent career. The ACA is proud to announce ***Yurij Mozharivskyj*** (McMaster University) as the 2011 recipient. Mozharivskyj is being honored for having applied the techniques and theory of crystallography at a high level in his exploration of the structure property relationships in complex functional materials through the detailed study of phenomena such as phase transitions, structural disorder, twinning and diffuse scattering. He has also made important contributions towards the development of the technique of high temperature, single crystal x-ray diffraction on a laboratory source and has addressed other important problems in a wide class of materials of intense current interest including magnetocaloric, thermoelectric, and superconducting systems.

Mozarivskyj earned his BSc in Chemistry at Lviv State University in the Ukraine in 1993 and his PhD in Chemistry at Iowa State University in 2002. He stayed in Iowa to do a postdoc with

Gordon Miller until 2005, when he moved to McMaster, where he is currently assistant professor of chemistry and Tier II Canada Research Chair. Throughout all stages of his career, crystallography and structural chemistry have been key elements in of his research. As an expert synthetic solid-state chemist and crystallographer, Yurij has substantially advanced our understanding of structure-property relationships in responsive materials. His success can be seen in the 57 peer-reviewed papers that have been published during his short career, all of which reveal a consistent set of structural challenges which have been cleverly solved and interpreted. It is his combination of talents for synthesis, structural characterization, and detailed physical and theoretical understanding that sets Yurij apart from his peers and that has earned him the ***Etter Early Career Award.***

Bomina Yu

Four ACA members elected as 2009 AAAS Fellows: In November, the American Association for the Advancement of Science (AAAS) Council elected 531 members as Fellows of AAAS. Among them were ACA members ***H. Frederick Dylla***, Executive Director and CEO of the American Institute of Physics, ***Martin Egli***, professor of biochemistry at Vanderbilt University, ***Liang Tong***, professor and co-director of graduate studies in the Department of Biological Science at Columbia University, and ***Cynthia Wolberger***, professor of biophysics and biophysical chemistry at Johns Hopkins University School of Medicine and a Howard Hughes Medical Institute investigator. Election as a Fellow of AAAS is an honor recognizing exceptional contributions to science and technology. The new Fellows received a certificate and a blue and gold rosette as a symbol of their distinguished accomplishments at the Fellows Forum held in February during the 2010 AAAS annual meeting.

Knox Inducted into Missouri Academy of Chemists and Biochemists: ***James R. Knox*** (professor emeritus of molecular and cell biology at the University of Connecticut) is one of seven scientists recently inducted into the Missouri University of Science and Technology Academy of Chemistry and Biochemistry. Members of the academy are scientists with ties to the university who have made outstanding contributions to their profession. His most recent research focused on the structural characterization of cell-wall synthesizing enzymes and of the penicillinase enymes. Knox has published more than 100 journal articles or book chapters and has given more than 120 invited lectures and talks on his work in characterizing the tertiary structures and enzymatic mechanisms of several other bacterial drug targets.

The NSSA awards Craig Brown the 2010 Science Prize: The Neutron Scattering Society of America (NSSA) established the ***Science Prize*** to recognize a major scientific accomplishment or important scientific contribution within the last 5 years using neutron scattering techniques. Nominees were to have been within 12 years of receiving their PhD and preference was given to applicants whose work was carried out predominantly in North America. ***Craig M. Brown*** (NIST Center for Neutron Research) is the 2010 recipient of the biennial award is for his "outstanding neutron scattering studies of hydrogen-framework interactions in metal-organic frameworks". Brown is an instrument scientist for the Disk Chopper Spectrometer at the Center where he has been responsible for the operations of several spectrometers over the past decade. He is the leader of the NCNR effort within the Hydrogen Sorption Center of Excellence, funded by the US Department of Energy. Research in the Brown lab focuses on the structure and dynamics of novel materials, such as fullerenes, nanotubes, and inorganic polymers. His work highlighting the importance of coordinatively unsaturated metal centers in enhancing the binding of hydrogen molecules in these sorbent materials aims at developing hydrogen storage systems that operate efficiently at room temperature. Hydrogen fuel cells present a promising alternative to the internal combustion engine. However, one key obstacle to their use is the need to store hydrogen in a safe, affordable, and convenient manner at high storage densities. Brown's discoveries on the various forms of hydrogen related to storage has provided new insights into how hydrogen molecules interact with metal organic frameworks. His research has greatly influenced how chemists tailor new materials to achieve enhanced hydrogen storage properties. His accomplishments have established him as a leading expert in the field of hydrogen storage.

Brown's outstanding scientific contributions have also been recognized with a 2008 Presidential Early Career Award for Scientists and Engineers (PECASE), the highest honor bestowed by the United States government on young professionals in the early stages of their independent research careers. He will be awarded the NSSA Science Prize and a $2500 honorarium at the 2010 American Conference on Neutron Scattering in Ottawa, Canada this June.

Polish Academy of Sciences Award to Zbigniew Dauter

On March 9, 2010, Michal Kleiber, the President of the Polish Academy of Sciences, presented Zbigniew Dauter with the ***Nicolaus Copernicus Medal***, the highest distinction awarded by the Polish Academy of Sciences. The award recognizes his contribution to the development of protein crystallographic methodology, in particular in the areas of phasing methods and macromolecular structure at ultimate resolution. Zbyszek (as he is known to his friends and colleagues) has been associated for many years with several synchrotrons and developed a number of methods that are in wide use. Of particular importance is the technique of quick halide soaks ("dauterization" of protein crystals), as well as exploitation of weak anomalous signal (for example, of phosphorus in nucleic acid structures). Zbyszek is an expert experimenter, widely known for his skills in getting the best possible diffraction data from macromolecular crystals. A native of Poland, he graduated from the Gdansk University of Technology and later obtained a PhD for crystallographic work on small-molecule drugs done under supervision of Zofia Kosturkiewicz in Poznan. He later worked as a postdoctoral fellow with Michael Woolfson (Univ. of York), and ultimately settled in synchrotron centers (DESY, Hamburg; NSLS, Brookhaven; APS, Argonne), helping external users of macromolecular crystal-

lography beamlines and conducting his own structural biological research. The stations that he has supervised are among the most successful beamlines in protein crystallography. He has had a stunning number of collaborations, mostly because of his expertise in synchrotron data collection and structure determination. Currently, he is Principal Investigator in the Macromolecular Crystallography Laboratory of the National Cancer Institute at Frederick, and facilitator for the NIH users of the SER-CAT beamline operating at the APS synchrotron in Argonne.

Majkrzak among 14 scientists elected as NSSA Fellows*.** Through their Fellowship Program, the NSSA recognizes members who have made significant contributions to the neutron scattering community in North America in one or more of the following areas: advances in knowledge through original research and publication; innovative contributions in the application of neutron scattering; contributions to the promotion or development of neutron scattering techniques; and service and participation in the activities of the NSSA or neutron community. This year, fourteen members were elected as NSSA Fellows. Among them is ACA member ***Charles F. Majkrzak (NIST - NCNR) for his "fundamental contributions to the development of neutron reflectivity."

Majkrzak is currently the leader of the Surfaces and Interfacial Science team at the NCNR where he has employed his technical and scientific creativity to profoundly advance the field of neutron reflectometry. His design to integrate supermirror polarizers into neutron instruments resulted in very low backgrounds and consequently the highest signal-to-noise achieved anywhere, providing the most detailed and reliable structural information available. Majkrzak and collaborators have also developed a solution to the phase problem for neutron reflectivity that allows the direct inversion of the reflection amplitude to obtain the scattering length density profile uniquely within the dynamical theory of diffraction, which is of immense importance for neutron reflectivity studies of unknown structures. He will be honored for his extraordinary contributions with the other new Fellows at the 2010 American Conference on Neutron Scattering to be held in Ottawa, Canada this June.

Majkrzak was also the 2006 winner of the ***ACA Warren Award***, which recognizes an important contribution to the physics of solids or liquids using x-ray, neutron, or electron diffraction techniques

Robert Fletterick elected into the National Academy of Sciences: The NAS recently announced the election of 72 new members and 18 foreign associates in recognition of their distinguished and continuing achievements in original research. Among the new members is ***Robert J. Fletterick***. Fletterick is a Professor of Biochemistry at the University of California San Francisco where he studies hormone receptors that regulate neurodevelopment, embryogenesis, steroid metabolism and prostate development and cancer. His laboratory solved the first structure of a nuclear receptor bound to its hormone and the first structure of the molecular motor kinesin found in nerve cells. The NAS is a private organization of scientists and engineers dedicated to the furtherance of science and its use for the general welfare. With the newly elected, the total number of active members comes to 2,097 and the total number of foreign associates to 409.

.

Calls for Nominations for Future Awards

ACA Awards for 2012

B. E. Warren Award: To recognize an important recent contribution to the physics of solids or liquids using x-ray, neutron, or electron diffraction techniques. Works published within a six-year period ending June 30 of the year preceding the Award may be nominated. A monetary award of $1,500, up to $1,500 in travel expenses to accept the award, and a certificate are awarded every third year. Established in 1970 by students and friends of Bertram E. Warren on the occasion of his retirement from the Massachusetts Institute of Technology.

M. J. Buerger Award: To recognize mature scientists who have made contributions of exceptional distinction in areas of interest to the ACA. There are no restrictions as to nationality, race, sex, religion, or membership in the ACA. Awarded triennially in memory of Martin J. Buerger, Institute Professor Emeritus of M.I.T. and University Professor Emeritus of the University of Connecticut, a mineralogist who made major contributions to many areas of crystallography. Established in 1983. The first award was made in 1985. A monetary award of $1,500, up to $1,500 in travel expenses to accept the award, and a certificate are awarded every third year.

Nominations for both awards are due by April 1, 2011 and should be sent to Marcia Colquhoun (***marcia@hwi.buffalo.edu***). Nomination form are available on the ACA website (***www.amercrystalassn.org***).

IUCr - Ninth Ewald Prize

The IUCr is pleased to invite nominations for the ***Ewald Prize*** for outstanding contributions to the science of crystallography. The Prize is named after Paul P. Ewald, in recognition of his significant contributions to the foundations of crystallography and to the founding of the IUCr. Ewald was the President of the Provisional International Crystallographic Committee from 1946 to 1948, the first Editor of *Acta Crystallographica* from 1948 to 1959 and the President of the IUCr from 1960 to 1963.

The ninth Prize, for which nominations are now being invited, will be presented at the Madrid Congress in August 2011.

Scientists who have made contributions of exceptional distinction to the science of crystallography are eligible, irrespective of nationality, age or experience. The Selection Committee will give careful attention to the nominations of outstanding scientists who have not yet won a Nobel Prize. Either an exceptionally distinguished scientific career or a major scientific accomplishment may be recognized. No restrictions are placed on the time or the means of publication of the nominee's contributions. The Prize may be shared by more than one contributor, but not more than three, to the same scientific achievement.

Nominations should be submitted in writing to the Executive Secretary of the IUCr, 2 Abbey Square, Chester CH1 2HU, England. ***The closing date for nominations is 31 August 2010***.

The Prize consists of a medal, a certificate and a financial award, and is presented once every three years during the triennial International Congresses of Crystallography.The recipients to date are as follows:

1987	Perth, Aust.	J.M. Cowley and A.F. Moodie
1990	Bordeaux, Fr	B.K. Vainshtein
1993	Beijing, China	N. Kato
1996	Seattle, USA	M.G. Rossmann
1999	Glasgow, UK	G.N. Ramachadran
2002	Geneva, Switz.	M.M. Woolfson
2005	Florence, Italy	P. Coppens
2008	Osaka, Japan	D. Sayre

ASBMB Announces Diversity in Science Award:

The American Society for Biochemistry and Molecular Biology (ASBMB) has announced the creation of a ***Diversity in Science Award*** for 2011. The award was established to honor an outstanding scientist who has shown a strong commitment to the encouragement of under-represented minorities to enter the scientific enterprise and/or to the effective mentorship of those within it. Candidates need not be an ASBMB member but must be nominated by Society members. The award consists of a plaque, $3,000, and transportation expenses to present a lecture at the annual ASBMB meeting. Although the recipient can be from any racial or ethnic background, it is hoped that many candidates and future recipients will be from backgrounds underrepresented in the science, technology, engineering and mathematics fields, so that they will serve as role models to young scientists. "As we enter the new millennium and appreciate the abundance of scientific progress made during the last century, we must take heed that the extent of participation in the scientific enterprise by certain groups is regrettably far below the level commensurate with their representation in the general population," the ASBMB Minority Affairs Committee said in a statement. "This lack of representation, of course, is unhealthy for the prosperity and best interests of our country, as well as for science in general." Engaging this underrepresented sector of our work force will require, among other interventions, proper mentorship, particularly by those with whom this sector shares close ethnic or cultural ties."

Science Prize for Young Life Scientists

GE Healthcare and Science/AAAS seek to foster visionary thought and research by supporting scientists at the onset of their careers by awarding ***Young Life Scientists Prizes***. To be eligible, entrants must have received their PhD in 2009. Their thesis work must be in the field of molecular biology, which is defined as "that part of biology which attempts to interpret biological events in terms of the physico-chemical properties of molecules in a cell" Four regional winners (US $5000). and one grand prize ($25,000 and a trip to Stockholm, to participate in the Nobel Prize seminar), will be awarded. See ***www.gescience-prize.org/*** for more information. ***Applications are due no later than August 1, 2010.***

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION, INC.
BALANCE SHEET - December 31, 2009 and 2008

	CURRENT FUNDS (2009)		TOTAL	
	Unrestricted	Restricted*	All Funds	
			2009	2008
ASSETS				
Current Assets:				
Cash	291,991		291,991	232,191
Investments	336,159	371,653	707,812	712,317
Inventory	2,225		2,225	2,225
Accounts Receivable	1,740		1,740	32,579
Total Current Assets	632,115	371,653	1,003,768	979,312
Fixed Assets:				
Computers and Printers	4,598		4,598	4,598
Office Equipment	1,300		1,300	1,300
Accumulated Depreciation	0		0	0
Total Fixed Assets	5,898		5,898	5,898
TOTAL ASSETS	638,013	371,653	1,009,666	985,210
Liabilities:				
Unearned Dues	93,019		93,019	78,024
Credit Card Liabilities	(186)		(186)	556
Total Liabilities	92,833		92,833	78,580
Fund Balance:				
Unrestricted	545,180		545,180	533,757
Restricted		371,653	371,653	372,873
Total Fund Balance	545,180	371,653	916,833	906,630
TOTAL LIABILITIES & FUND BALANCE	638,013	371,653	1,009,666	985,210

*** Current Balances in individual restricted funds - as of December 31, 2009**

Buerger Award	36,470
Etter Award	62,709
Fankuchen Award	68,364
Patterson Award	42,739
Pauling Award	33,492
Supper Award	11,892
Trueblood Award	35,052
Warren Award	28,617
Wood Science Writing Award	52,318

A more detailed report on the ACA finances may be obtained by sending a written request to the ACA office in Buffalo, PO Box 96, Ellicott Station, Buffalo, NY 14205-0096.

We gratefully acknowledge the continued support of our ACA CORPORATE MEMBERS

Alliance Analytical
www.aaisolutions.com

Area Detector Systems Corp.
www.adsc-xray.com

Anachem Instruments, Ltd.
www.anachem-instruments.co.uk

Art Robbins Instruments
www.artrobbinstruments.com

ATPS Inc.
www.atpsinc.com

Axygen Biosciences
www.axygenbio.com

Blake Industries, Inc.
blake4xray@worldnet.att.net

Bruker/AXS
www.bruker-axs.com

Cambridge Crystallographic Data Centre
www.ccdc.cam.ac.uk

Charles Supper Company, Inc.
www.charles-supper.com

Cryo Industries of America, Inc.
www.cryoindustries.com

Dectris Ltd
www.dectris.com.

Douglas Instruments Limited
www.douglas.co.uk

Emerald Biosystems
www.emeraldbiostructures.com

FMP Products
www.fmpharma.com

Formulatrix
www.formulatrix.com

Hampton Research
www.hamptonresearch.com

Hecus X-ray Systems GmbH
www.hecus.at

Incoatec GmbH
www.incoatec.de

Jena Bioscience GmbH
www.jenabioscience.com

Korima, Inc.
www.korimainc.com

MiTeGen LLC
www.mitegen.com

Molecular Dimensions, Inc.
www.moleculardimensions.com

Oxford Cryosystems
www.oxfordcryosystems.com

Oxford Diffraction Ltd.
www.oxford-diffraction.com

Rayonix LLC
www.mar-usa.com

RCSB-Protein Data Bank
www.rcsb.org/pdb

Rigaku Americas, Inc.
www.Rigaku.com

West Bond, Inc.
www.westbond.com

Wyatt Technology
www.wyatt.com

Xenocs **SA**
www.xenocs.com

We are especially grateful to our Sponsors of the 2010 ACA Meeting

Candidates for ACA Offices in 2011

The Nominating Committee has proposed the following candidates for the 2010 elections for ACA offices in 2011

Officers:

Vice-President: **Jim Kaduk and George Phillips**

Canadian Representative to Council: **Emil Pai and David Rose**

Committees:

Communicatons: **Gloria Borgstahl and Stephan Ginell**

Data, Standards & Computing: **Ilia Guzei and Joe Reibenspies**

Continuing Education: **Jeanette Krause and Joel Harp**

To nominate write-in candidates for any of these offices, write to the ACA Secretary: Carrie Wilmot, Department of Biochemistry, Molecular Biology & Biophysics, 6-155 Jackson Hall, 321 Church St SE, Minneapolis, MN 55455-0215. (***wilmo004@umn.edu***). Letters must be received by September 15, 2010 and must be signed by 5 supporting ACA members and include a signed statement by the candidate describing his or her qualifications. Statements from all candidates will be included with the ballots which will be sent to all members in ***October 2010***.

James Kaduk, Vice-President

President, Poly Crystallography Inc, 423 East Chicago Avenue, Naperville IL 60540

Education: PhD Northwestern U. (1977) in Inorganic Chemistry

Professional Activities: My experience in non-profit management includes serving as Chair of the Board of Directors of the ICCD (the Powder Diffraction File) and Chair of the USNCCr, as well as many other positions in both organizations. I have also served as President of the Naperville (IL) Chorus, and serve on the Northwestern University Library Board of Governors. I am currently Vice Chair of the Materials SIG, chair the Powder/Single Crystal Crystallography Proposal Oversight Panel at NSLS, and serve on the X-ray Powder Diffraction Beamline Advisory Team at NSLS-II, the Structural Characterization Advisory Subcommittee at APS, and the Neutron Scattering Science Review Committee at ORNL. I am a Co-Editor of *Acta Crystallographica Sect B*, *Powder Diffraction*, and *Advances in X-ray Analysis*. I serve on the IUCr Commission on Powder Diffraction as a consultant and ICDD Representative and on the Denver X-ray Conference organizing committee.

Research Interests: I am a crystallographer. There, I've said it, and I'm proud of it. The crystallography is in the genes. My father (though he was a chemical engineer) did phosphor chemistry at GE in Cleveland, and was essentially a solid state inorganic chemist. He needed x-ray diffraction analyses to characterize his materials. My mother was a technician in the analytical labs under Jeanette Cooper (whom I met at my first ACA meeting in 1974), and that's how they met.

My high school and early undergraduate chemistry courses convinced me that I really wanted to know "where the atoms are". I learned crystallography as an undergrad with Bob Scheidt at Notre Dame, and as a graduate student with Jim Ibers at Northwestern. I never dreamed that I could make a living as a crystallographer, so worked in catalyst R&D at Amoco Chemicals for 8 years. During that time I learned that I really was more interested in figuring out what I had made than in actually making it. When the opportunity came to get back into crystallography, the time to say "yes" was measured in nanoseconds.

My work during 32 years at Amoco/BP/Innovene/Ineos involved what I like to call powder crystallography. The challenge was to obtain the necessary structural information from polycrystalline real materials, and grow single crystals when possible (though it often wasn't). Working for a large company, I worked on many different systems, including catalysts, corrosion deposits, organic small molecules, coordination complexes, and polymers. I even dabbled in powder diffraction of proteins and computational studies of biomolecules, and maintain interest in current developments in structural biology. Mainly I used x-rays, but did significant amounts of neutron diffraction, and relied on colleagues for electron diffraction data.

I retired in 2009, and formed a consulting company, Poly Crystallography Inc. I have joined Illinois Institute of Technology as an adjunct professor, and am setting up a powder diffraction laboratory there. As a recent retiree (though I cannot imagine not doing crystallography), I have the time to devote to serving on the ACA Council.

Statement: The ACA is a well-run organization. An obvious (but often unspoken) job of the Council is to ensure it stays well-run, and pass it on to our successors in better shape than we found it. I believe in complete transparency, and hope to publish an annual report to summarize and advertise the accomplishments of the ACA.

The ACA is in a period of gradual (not revolutionary) change. There has been staff turnover recently, and some long-time ACA stalwarts are starting to retire. We need to ensure that the institutional memory is preserved, and that ACA adapts to new challenges and opportunities. It is sobering that I have been an ACA member for over half of the organization's existence!

A challenge for the ACA is to increase the number of members. Why should someone join the ACA? I join a scien-

tific society for the science (meetings and journals) and for the networking; in other words, because membership is useful to me professionally. So, the challenge for the Council is to make ACA membership so incredibly useful that joining becomes a "no-brainer". I certainly intend to work through the SIGs to increase the breadth and depth of the science at ACA meetings, and to keep the cost of attending them affordable.

Crystallographic expertise is such a basic part of the scientific infrastructure that it is generally taken for granted. Both the ACA and the USNCCr know that the general state of crystallographic education is pretty bad; it's up to the crystallographers themselves to correct that situation. Even as an industrial crystallographer, I have for many years spent 3-4 weeks per year teaching crystallography at ACA summer courses, ICDD Clinics, and short courses and workshops around the world. Crystallographic education is something I'm passionate about! Now that I will have students at IIT, I look forward to developing crystallographic education resources. I hope to make the ACA web site not only a pointer to (evaluated) crystallographic resources on the Web, but to be a place for crystallography education content.

As crystallographers, we rely on specialized instrumentation and ionizing radiation to do our science. The result is that it is not as familiar to many students as other measurement sciences. I would like to see the ACA become involved in broadening access to crystallographic experimentation efforts such as the STaRBURSTT consortium. Because so many of the pictures used to entice students into science come from crystallography, I would like to see the ACA participate in K-12 outreach activities, particular for junior high/middle school students in grades 5-8.

Crystallography is a relatively small field, and the ACA is a medium-sized scientific society. We therefore need to look both internally and externally to achieve our aims. Even the internal interactions become complicated. The ACA is the "American Crystallographic Association", not the "U.S. Crystallographic Association". I take that distinction seriously. I have been to Latin America several times though I still don't speak much Spanish. I'll try to fix that. I believe I speak Canadian fairly well, but probably won't attempt Portugese. I want the ACA to be as helpful as it can be to meeting the individual and varied needs of Latin American crystallographers, being always mindful of cultural sensitivities. The interactions need to be two-way. The ACA can learn a lot from Mexican crystallographers about crystallographic education, and we can imagine north-south and south-north movements of both students and experts.

If elected, my time on the Council would be 2011-2013. This would not include the IUCr meeting in Montreal, but the time leading up to it. I'll try to ensure that the ACA is as helpful as it can be to the organizers of the Montreal Congress.

The ACA is a Regional Associate of the IUCr. Relations between US crystallographers and the Union are not as smooth as they might be. Having been sensitized to the cultural differences between US, European, and Asian crystallographers (and developing more political skills than I had the last time I ran for Council 10 years ago), I expect to work to overcome them, and ensure that the US has the appropriate influence within the Union.

Almost all scientists use crystallographic information at some time or other, so the opportunities for "external" interactions are almost limitless. While we will always welcome non-crystallographers at ACA meetings, the most productive way of interacting with other societies may be to offer joint crystallography workshops, so that non-crystallographers know enough to interpret crystallographic results and to generate them when they need to, even though they may not wish to become crystallographers. It is easy to imagine working with the powder diffraction community (despite the recent failed attempt to organize a combined ACA meeting/ Denver X-ray Conference), the Materials Research Society, the various mineralogical societies, and even the American Chemical Society (even though it has removed mention of crystallography from the recent curriculum recommendations). I personally would have to work harder to interact with biological societies, but given the importance of structural biology to the life sciences, see it as essential. I know I can count on the help of ACA members to do so.

In this statement I have envisioned more than any one person could hope to achieve in three years on the Council. If elected, I promise to try to make progress in at least some of these areas. I write these words so that you know the directions in which I'd like to head, so that you are clear about what you'd be getting. While not exactly the last of the Jedi, it is the time of life to pass on what I have learned, and give back both to my science and my society.

George Phillips, Vice-President

Professor of Biochemistry and of Computer Sciences, University of Wisconsin-Madison.

Education: BS Chemistry and Biochemistry (1974) and PhD Biochemistry (1976), Rice University; advisor F. Quiocho. Postdoctoral, Structural Biology, Brandeis University (1977-1982) with Carolyn Cohen.

Professional Activities: Before moving to UW-Madison in 2000, I was a professor of Biochemistry and Cell Biology back at my alma mater, Rice University (1987 to 2000). I was also on the faculty at the University of Illinois (1982 to 1987), in the departments of Physiology and Biophysics and also Biochemistry. I have served on seemingly innumerable committees relating to structural science over the years including NSF, NIH and international grant reviews, and committees involved with x-ray synchrotron facilities, x-ray crystallography, computational biology, and electron microscopy centers. I have been active in the construction of x-ray synchrotron beamlines at the CAMDr at Louisiana State and at the APS at Argonne National Laboratory.

Research Interests: I remember the day I first learned about crystallography. I was a goofy sophomore in college and was going around on a Rice University Chemistry department open house tour. I entered a room (in the laboratory of Ronald Sass) with a large table that was covered with sheets of paper with strange markings on them. I was told by a student there that these sheets were used to determine atomic structures, they were call Patterson maps, and that solving atomic structures was akin to solving puzzles. Being a puzzle nut, I thought to myself, "you mean there are jobs out there where you can be paid to solve puzzles?" As a senior, with help from members of the Sass laboratory, I solved my first small molecule structure, a heavy-atom labeled sterol produced in George Schroepfer's laboratory in the Biochemistry Department. After that I was hooked. I have turned to larger molecules, but am still very interested in atomic and molecular structure and dynamics.

My interests in atomic and molecular structures have expanded to include many more uses of scattering for imaging and other purposes, including macromolecular crystallography, diffuse x-ray scattering, methods for imaging using the new x-ray lasers just coming on line, and solution x-ray scattering. I am involved in not only using these methods, but also interested in contributing new methods.

More recently, I have been involved in structural genomics and high-throughput structural biology, and have been fortunate enough to work with fine colleagues over the years to put a total of about 300 coordinate depositions into the Protein Data Bank. Current topics of interest also include enzymes involved in natural product biosynthesis, connections between protein dynamics and function, the role of heme in protein function, and the understanding of cellulase enzymes in the production of biofuels.

Statement: Like others before me, I am both honored and flattered to be nominated to help lead the ACA. I have attended ACA meetings (not all) since my graduate school days, and have always found them to be quite stimulating, as I consider myself to be both a crystallographer and a structural biologist. Some of my colleagues don't understand the difference but, by my book, the former is interested in the science of crystallography for its own sake, and the latter is motivated by biological questions. Because of my broader interests in diffraction, I think I can appreciate the whole range of activities that the ACA supports, and would endeavor to promote them all.

I also have a keen interest in teaching crystallography, and education is the basis for future development of our field. I have written a broadly used piece of software called XrayView that illustrates the Ewald construction graphically, and have contributed a Pymol software plug-in for printing physical models of the packing of protein crystals in various space groups. I teach a full semester course on protein crystallography, including homework exercises to grow crystals, collect data, solve, and refine a protein structure.

As for particular goals I think the ACA should work on in the immediate future, I would listen to others, as I have not been on the ACA council, but would eagerly catch up on areas that need work and pitch in enthusiastically. One area that I KNOW needs work is validation of coordinates that come from the crystallographic community, both small molecules and macromolecules. The recent exposure of fraudulent or seriously mistaken structures of both types creates disproportional damage to our field. There are ways we can work with journal editors and the data repositories to reduce the chances of these events from recurring, and at the same time enhance the value of these growing informatics resources.

Crystallography, like all fields, evolves over time. I am proud to be a part of the maturation of the technology and its widespread usage and dissemination. Those who worry that crystallography is dying because some experiments can now be done by non-specialists should not grieve for the olden days, but push ahead to new frontiers. There are many puzzles waiting to be solved, new x-ray sources on the horizon, and new methods ripe for development. Let our diverse backgrounds and interests push to new heights!

Emil Pai, Canadian Representative

Canada Research Chair in Structural Biology and Professor, Departments of Biochemistry, Medical Biophysics, and Molecular Genetics, University of Toronto; Senior Scientist, Division of Cancer Genomics & Proteomics, Ontario Cancer Institute/Princess Margaret Hospital, Toronto.

***Education*:** Diploma (1976) and Dr. rer. nat. (1978) Chemistry, Heidelberg University and Max-Planck-Institute for Medical Research (MPIMR), Heidelberg; postdoc, MPIMR, Heidelberg (1978-1980)

Professional Activities: Group Leader MPIMR, Heidelberg (1980-1982 and 1983-1991); visiting scientist with T.C. Bruice, Dept. of Chemistry, UCSB (1982-1983); NSERC Industrial Research Chair in Protein Crystallography (1991-2001), University of Toronto; Division Head, Ontario Cancer Institute (1996-2005); University representative, Ontario Synchrotron Consortium (since 2001); member Board of Trustees, Canadian Institute for Synchrotron Radiation (since 1995); President, Canadian Institute for Synchrotron Radiation (since 2005). Member; Board of Directors, Canadian Light Source, Inc. (since 2002), Beamline Team, Canadian Macromolecular Crystallography Facility (since 1998), various Scientific Advisory Committees, Canadian Space Agency (1999-2007), several NIH, NCI, and NSF review and site visit committees (2001-2006), and NIH-BioCARS Advisory Committee (since 2001). Editor, Section on Catalysis and Regulation, *Current Opinion in Structural Biology* (1995, 1997, 1999). Member; Editorial Boards of ABB

Reproducible. Accurate. Compact.

Desktop Alchemist™ - Fine Screen Maker

Leading With Innovation

Go from one fine screen to the next
in under 3 minutes!

Rigaku's Desktop Alchemist

With our patented BirdFeeder™ technology
there are no tubes or pumps to clean
when changing stock solutions.

www.DTAlchemist.com

Rigaku

Rigaku Americas Corporation phone: 281-362-2300 e-mail: info@rigaku.com
Rigaku Europe phone: +[44] 1732 763367

(1992-1994), *Protein & Peptide Letters*, *Current Proteomics*, and *Research Letters in Biochemistry*, AAAS, ACA, ASBMB, CSBMCB, and CISR.

Use of macromolecular crystallography to define the structural framework of molecular interactions of biomedical relevance. My interest in the structural basis of enzymatic activity, the question that caused a 'hard-core' chemist to take a look at crystallography, has never waned although I am now more focused on enzymes as targets of anti-malarials and anti-cancer drugs. Further areas of research are: broadly neutralizing anti-HIV-1 antibodies, the structural transitions of prion proteins, membrane ion channels, and the breaking of the stable carbon-fluorine bonds (linked to use and refinement of time-resolved crystallography techniques; a collaboration with Zhong Ren and Keith Moffat at BioCARS.

***Statement*:** I regard it an honor to be nominated as candidate for Canadian Representative to the ACA Council. Soon after moving to Canada in 1991, I became involved in various aspects of Canadian crystallography through membership in the ACA, as organizer, invited expert, or speaker at various synchrotron-related meetings and workshops in Canada and internationally, and a session organizer at the 2009 ACA meeting in Toronto being the latest example. As a member of boards and consortia, I took on more administrative duties, especially in support of Canada's one and only synchrotron source, the CLS. Especially the position on its Board of Directors has educated me about the considerable successes achieved but also the multitude of problems faced by Canadian crystallographers that are not in my own field of macromolecular crystallography. This experience, if elected, would make it easier for me to speak for all crystallographers from the Northern Regional Affiliate. I intend to not only make the voice of the Canadian community heard but also try to increase participation of the Canadian membership in the work of the ACA.

David Rose, Canadian Representative

Currently: Professor and Chair, Department of Biology, University of Waterloo. Previously: Senior Scientist, Ontario Cancer Institute, Professor, Department of Medical Biophysics, University of Toronto.

Education: BA University of Pennsylvania; D. Phil., Oxford University (D.C. Phillips); Postdoc, MIT (G.A. Petsko)

Professional Activities: Structure/function studies of glycosidases by macromolecular crystallography. Roles of glycosidases in human health and in nature.

Research Interests: With ACA: Canadian Representative on Council; Chair, Canadian Division; Local Chair, 2009 annual meeting in Toronto. IUCr: *ad hoc* attendee, Canadian National Committee; participated in the bid committee for the Montreal IUCr Congres

Statement: As the official organization supporting research in all aspects of crystallography in the Americas, the ACA has been my professional home for over 25 years. At ACA meetings, I have met colleagues ranging from undergraduate students to Nobel Laureates. I have learned more about technical advances in our discipline and recent research results from ACA meetings than from any other single source.

My formal service to the ACA (beyond being a member) began almost 10 years ago. I was inspired to take part in order to promote the organization to colleagues at all levels, but particularly at the trainee level. ACA meetings are unusually welcoming to young scientists, helping them to make the connections that will be so important in establishing their careers. However, the meetings are only as good as the participants; a goal of mine is to encourage and facilitate attendance by my senior colleagues.

As Canada has no regular national meeting for crystallographers, the ACA has traditionally filled this void. Canadians are represented in disproportional numbers among past ACA Presidents, and among ACA meeting attendees. The ACA has recognized this status by establishing a special seat on Council for a representative from Canada. I was fortunate to have occupied that seat from 2002-2005, during which time I worked to increase Canadian visibility, for example by promoting a special Canadian Pauling Poster Prize. I had the pleasure of working with Louis Delbaere to improve communication across our community, and to increase interactions between the ACA and the Canadian National Committee of the IUCr. More recently, as Chair of the Canadian Division of ACA, I have tried to facilitate Canadian representation among session speakers, by negotiating with SIGs for Canadian co-Chairs of selected sessions. I have also worked with the Canadian Light Source to increase their visibility at Canadian Division and ACA meetings. In 2009, I served as Local Chair of the ACA meeting in Toronto, an experience I will always remember fondly. In addition to overseeing a fabulous group of volunteers supporting the ACA staff at the meeting, we took steps to revitalize the tradition of events for accompanying persons. The ACA family is truly that: a family.

It would be an honor and great pleasure to continue my participation in the ACA as Canadian Representative on Council. Jim Britten has raised the Canadian presence on Council to new heights and leaves huge shoes to fill. However, I hope that my experience with the organization in several capacities and my commitment to the ACA as a focus and advocate for national and international crystallographic research, will equip me to serve the community well in this position.

Gloria Borgstahl, Communications

Professor, Eppley Institute for Cancer Research and Allied Diseases, 987696 Nebraska Medical Center, 10732A Lied Transplant Center, Omaha, NE 68198-7696.

Education: BSE (1985) Biomedical Engineering; PhD (1992) Biochemistry, The University of Iowa.

Professional Activities (last 5 years): 2010: Member USNCCr), 2008: *Ad hoc* reviewer, American Institute of Biological Sciences; New York State Department of Health peer review for NYSTEM Program; American Cancer Society Genetic Mechanisms in Cancer (GMC) Peer Review Committee. 2007: Nominated by the UNMC Student Senate for the Alvin M. Earle Outstanding Health Sciences Educator Award. 2006: Selected and served the American Cancer Society Celebration on the Hill Ambassador for the High Plains Division. 2005: Chair, NIGMS Specialized Centers for Protein Structure Initiative Special Emphasis Panel; member ACA Continuing Education Committee; reviewer for Young Scientist travel awards to ACA annual meeting; participated in USNCCr."Education Summit"

Research Interests: The application of protein crystallography and other biophysical methods to the cancer problem. My current personal research interests are two-fold: (1) in the area of DNA Metabolism with a focus on DNA double-strand break repair; (2) in developing crystallographic methods to solve incommensurately modulated crystals of profilin:actin.

Statement: I have an interdisciplinary approach to scientific research and would like to continue to promote this point of view. One of my major research interests in incommensurately modulated protein crystallography sits on the cutting edge of crystallography and is a challenging marriage between protein and small molecule approaches to crystallography. I have enjoyed my past service to our community through my involvement with the ACA and USNCCr and I would like to think I contributed to the field and helped others through this and other service. I would enjoy serving on the Communications Committee and I would help promote and advertise the outreach activities and research results of the community.

Stephan L. Ginell, Communications

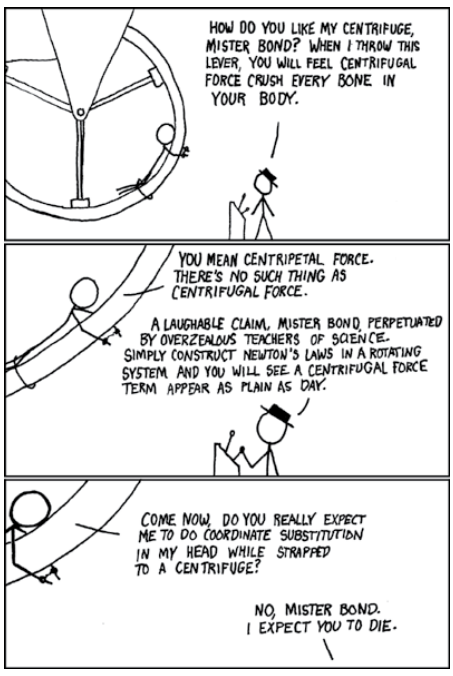
Biophysicist/Crystallographer, Biosciences, Argonne National Laboratory, Argonne, IL 60439.

Education: PhD Biophysics (1980) and MS (1975), Roswell Park Memorial Institute, SUNY at Buffalo; AB Physics (1971), Kansas Wesleyan University.

Professional Activities: NIH Grant review committees (2007-present), Argonne National Lab Risk Management Council (2009- present). ANL Institutional Biosafety Committee (IBC) (2005-present), ACA Macromolecular SIG Chair and member (2004-2006), ACA program committee (2005), Advanced Photon Source User Organization Steering Committee member (APSUO) (2003-6), NSLS UEC member (1995-1996) , organizer for "Workshop on Multiplewavelength Anomalous Dispersion (MAD) in Protein Crystallography " NSLS Annual Users Meeting (1996), Lecturer at the Cold Spring Harbor Laboratory workshop on crystallographic methods (1993-1998); local committee member, ACA, Philadelphia (1988). Member of ACA, AAAS, Sigma Xi.

Research Interests: Macromolecular crystallography; radiation damage within macromolecular systems; development of cryo-crystallographic technique; development of high-throughput user-friendly synchrotron beamlines for the macromolecular crystallographic community.

Statement: Communications is our life! Be it publishing scientific results, presenting at meetings, teaching, or casual discussions with colleagues. There is, however, the venue of communications with the general public that is often overlooked. Communicating our scientific results and agendas (why we do structures) to the general public is critical in gaining approval for larger funding initiatives, such as synchrotron and neutron radiation facilities and structural and functional genomics as well as for the general success of our society. In order for the general public and our legislative leaders to strongly support science they need the information on why. A strong and focused PR presentation by the ACA in support of its member's research is essential. Additional areas that I would like to see supported more are the communications between the different disciplines of crystallography and communications between the crystallography community and other areas of science. If elected, I will strive to make communications amongst the members of our scientific community and with the general public a high priority.



Ilia Guzei, Data Committee

Senior Scientist, Molecular Structure Laboratory, University of Wisconsin-Madison.

Education: MS, Chemistry, Lomonosov Moscow State University, USSR (1992), PhD, Chemistry, Wayne State University (1996), Postdoc, University of Delaware (1998).

Professional Activities. Co-editor for *Acta Cryst. C* (2005-present), reviewer for a number of chemistry and crystallography journals, administrator of the Bruker crystallographic on-line discussion forum, coordinator of the Bruker Users Meeting in the USA (every other year since 2001.

Research Interests: Crystallographic software development and documentation, small molecule structural determination, phase transitions, steric interactions among ligands in organometallic complexes.

Statement: The appeal of serving on the Data Committee is multifaceted. I am interested in developing and supporting publication/deposition standards for reporting routine and especially non-routine crystallographic results, such as from twinned crystals and incommensurate structures. I would work on modernizing the required content of the CIF file to reflect more refinement details, such as constraints and restraints. I have participated in the creation of many CIF dictionary entries and handled over 150 manuscripts submitted to *Acta Cryst. C* and have a unique perspective of what constitutes challenges in the presentation of structural information. Maintaining a high level of quality and availability of structural results is crucial. I will participate in creating, supporting, and publicizing databases with idealized molecular geometries that can be used for structural refinement; these will be beneficial to everyone working with challenging structures. If elected, I would work with software and database developers to achieve these goals and encourage the ACA to organize workshops promoting crystallographic software and to advance structural informatics as an important area in the fields of small and macromolecular crystallography.

Joseph H. Reibenspies, Data Committee

Senior Research Instrument Specialist, Texas A & M University, College Station, Texas 77843.

Education: PhD (1987), Chemistry, Colorado State University with Oren Anderson. MS (1982) and BS (1980), Chemistry, Wichita State University.

Professional activities: Research Instrument Specialist, Texas A&M, (1987-). Member: ACA, Texas A&M Radiological Safety Committee (1994-1997), the President's task force for Staff Council Formation (2007), the National Science and Engineering Research Council of Canada, and the National Committee for Crystallography (2010-). MRS review committee (2008), Editor/Author of "Principles and Practice of Powder Diffraction", Wiley (2008), Editor of the *Journal of Arabian Science and Engineering* (1998-1999),

Research Interests: I have a particular interest in single-crystal and powder diffraction with emphasis on structural chemistry and well as small angle x-ray scattering of waxes and polymers. I have extensively studied crystal engineering, in particular, polymorphism of pharmaceutical compounds. I study the practical side of crystallographic research with interest in instrument design and sample mounting methodology. I study the uses of crystallographic instrumentation with the goal of developing new techniques of analysis. I have written many crystallographic programs and integrated them into the practical aspects of crystallographic science.

Statement: I am honored to accept this nomination to the Data, Standards and Computing Committee. As an old programming hack I have written and debugged thousands of lines of crystallographic code over last twenty-five years. I understand the importance of crystallographic software to our community and how that software interacts with the average scientist.

As a laboratory manager and director I know the importance of standards to the operation of a crystallographic facility. I have personally written dozens of Standard Operating Procedures (SOP) and Standard Administrative Procedures (SAP) for my laboratory to fulfill the requirements of the Good Laboratory Practices as well as numerous training manuals, laboratory notes and technical manuscripts. I have also written and edited a power diffraction book and co-authored hundreds of scientific papers. Documentation is a critical link in the crystallographic chain of information and is the one that is most often overlooked.

As a working professional crystallographer I have solved literally thousands of structures, collected thousands of data sets and sorted many hundreds of gigabytes of crystallographic information. With so much information to process it is important that the community set standards and recommendations to process and disseminate this information to other scientists and to ourselves.

It is in this light that we must maintain and support the various databases that we rely on to gather and disseminate this information. These databases must be available in a format that all scientists can readily access. This is also true for the crystallographic software that is available now and will be in the future. As a programmer I realize that coding the program is the easy part, explaining it to others is the real task.

The aging of our present programs is another serious concern we as a community will face in the next ten years. Many of the programs that we rely on were written by individual scientists or groups for

their own personal use. These programs were distributed to others and have now become the standard for our community. The programs do not have a commercial base and as such are generally free and open to the public. The question that we face is what will become of these programs when their authors have retired and their groups disbanded.

To these ends I support various initiatives.:

1) Software stewardship: Popular software that is now freely available must be supported and the stewardship of the software must be established for long term stability.

2) Expanded access of crystallographic databases: Access to the crystallographic databases should be at the institutional level. All scientists and engineers would benefit from structural information if that information is readily available on a web based system. This initiative would involve well documented web based search engines and institutional licenses.

3) Standardization of data formats: Software and instrument vendors should be given incentives to produce or export their data in a standard format.

4) Broader appeal for the crystallographic sciences: In particular the proper use of crystallographic software. I believe that this can be accomplished at the local level, if the established crystallographic laboratories would share their knowledge and experience with their neighbors. The established laboratories would need incentives and compensation to undertake this task as it would be a drain on their resources; however the rewards would be a larger well informed community and a source for future graduate students and trained employees.

5) "White papers" from selected symposia (ACA conferences) on subjects related to Data, Standards and Computing. The "white papers" would be written by the symposia chair from material presented at the ACA sponsored symposia and reviewed by the committee and the ACA. Selected "white papers" would then be made available on-line for use and reference by various funding, academic and industrial institutions. For example a researcher could support their funding proposal by referencing a "white paper" that was the end result of an ACA symposia or a department could employ the ACA "white paper" as a mechanism to forward a crystallographic agenda. In any case the "white papers" would be welcome documentation of ACA promoted initiatives and a source of information for researchers and administrators.

If elected, I would work with the Data, Standards and Computing Committee and the ACA to advance these and other initiatives that would best fit the Committee's and ACA's mission. In this race for science we have been handed a golden baton, it is up to us to hold it, improve our position in the race and eventually pass it on to the next runner or we may drop it. The choice is ours

.

Joel Harp- Continuing Education

Director of Operations, Biomolecular Crystallography, Vanderbilt University Center for Structural Biology and Research Assistant Professor, Biochemistry, Vanderbilt University School of Medicine, Nashville, TN.

Education: PhD (2000). The University of Tennessee/ Oak Ridge National Laboratory (UT/ORNL) Graduate School of Biomedical Sciences (2000), MS (1975) and BS (1973), Biology, West Texas A&M.

Professional Activities: As a Research Associate at The UT/ORNL Graduate School of Biomedical Sciences (1985-2001) I won an Oxford Poster Prize and an ORNL Technical Achievement Award for work on macromolecular crystal annealing and an ORNL Technical Achievement Award for work on microgravity crystallization of nucleosome core particles. Assistant Professor of Research, University of Virginia (2001-2003). Oxford Poster Prize Chair ACA meeting, Chicago, 2004.

Research Interests: As Director of Operations for Biomolecular Crystallography in the Vanderbilt University Center for Structural Biology (2003-present) I have been involved in the installation, operation, and maintenance of x-ray equipment from three different manufacturers as well as robotics for liquid handling and automated imaging in addition to training, teaching and advisory function. I am involved in macromolecular structure projects in collaboration with a number of laboratories across the Vanderbilt campus. These projects currently involve drug targets and computationally designed macromolecules. In these collaborations, I have the opportunity to work with an unusually broad variety of structural problems. I have recently begun a limited program for small molecule determination within the facility.

My current research interests include structure determination of nucleic acids using in-house data and direct method and SAD phasing. I will be collecting single-crystal neutron diffraction data later this year using the Spallation Neutron Source at ORNL.

Statement: I am pleased to have an opportunity to contribute to the work of the ACA. It is especially gratifying to have been nominated for the Continuing Education Committee.

Crystallography as a set of techniques for probing the structure of matter at the atomic/molecular level is a non-linear process requiring training and skill in a number of disciplines that one might not otherwise consider related. Crystallographers are by necessity jacks-of-many-trades and professional development often means adding yet another trade as well as continuously polishing and sharpening the tools of those we already practice. This is perhaps the primary challenge of training in crystallography as well as one of the field's most endearing characteristics.

I see the challenges for continuing education in a number of categories: training of non-crystallographers who are consumers of crystallographic results; primary training of new crystallographers; providing experienced crystallographers

with a channel of information about the latest developments; and finally, cross-talk between subdisciplines within and with related disciplines outside the crystallographic community. The Continuing Education committee should address each category while working with the IUCr and other entities to maximize impact. Given recent unfortunate experiences, a special outreach to journal editors (excepting the IUCr editors of course) may be appropriate to help prevent fraud and encourage high standards in reporting crystallographic results. I am also interested in providing emphasis on complementary techniques such as cryo-electron microscopy and small-angle scattering.

Workshops and special sessions at meetings are invaluable but it also seems that the ACA could make greater use of internet resources to continue the work of education beyond annual gatherings. I would like to encourage the use of webinars and multimedia presentations in particular for communicating developments such as refinement using the invariom model or dealing with radiation damage to protein crystals or electron-impact liquid-gallium-jet x-ray sources. Having authoritative voices explaining such topics can add greatly to the advancement and excitement of crystallography.

Jeanette A. Krause, Continuing Education

Director & Sr. Research Associate, Richard C. Elder X-ray Crystallography Facility, Department of Chemistry, University of Cincinnati, Cincinnati, OH 45221.

***Education*:** BS, Chemistry & Cellular-Molecular Biology, University of Michigan (1982); MS (1987) and PhD (1989), Inorganic Chemistry, Ohio State University; Postdoctoral, SmithKline Beecham Pharmaceuticals (1989-1991).

***Professional Activities**: ACA*: Program Chair, ACA'03 Conference; Member, ACA Nominating Committee (2007-2008), Communications (2001-2004, Chair 2004) Committee, Continuing Education (1997-1999, Chair 1999) Committe, Publications (1995-1997, Chair 1997) Committee, conference organizing committee/session organizer (1993-1999, 2001, 2004-2009); workshop chair, ACA'99; Chair (2009, 1997), Chair-elect (2008, 1996), Secretary (2004-2005, 1994-1995) Small Molecule SIG; Secretary/Treasurer (2007-2008), Chair (2005), Chair-elect (2004) GIG; Chair (2006), Chair-elect (2005), Secretary (1995-1996) Service Crystallography SIG. *Pittsburgh Diffraction Society:* Past-President (2003); President (2001-2002); Chair, Nominating Committee (2004); Member, Program Committee (2002-2003); Conference Chair, 59th PDC(2001); PDC Conference Webmaster (2001-2002). *IUCr:* US Sub-editor, World Directory, 10th edition (1996); symposium co-chair, 17th IUCr GA (1996). *American Chemical Society:* 2nd Vice Chair of the Cincinnati Section; (2008/09); program chair, 39th Central Regional Meeting (CERMACS2007)— the winner of the ACS ChemLuminary Award (2008) for Outstanding Regional Meeting; conference webmaster - CERMACS2007; program committee member CMACS2000 and CMACS1992.

***Research Interests*:** Current research interests include chemical crystallography, methods of crystal growth, and application of synchrotron radiation techniques to chemical crystallography.

***Statement*:** It is an honor to be nominated to serve on the Continuing Education committee. I first served on this committee from 1997-1999 and, as mentioned in my statement so many years ago, and which is still true today - the world of crystallography is alive and continually evolving. Thus, we are constantly in a process of continuing our crystallographic education whether it is on our first day or after many years in the field. There is much to be learned from our colleagues regardless of specific crystallographic sub-discipline. If elected to serve, I would strive to continue the legacy of high-quality workshops and tutorials that has become the norm of the ACA.

2010 Travel Award Winners

Brazil
Lorraine A. Malaspina
Federal Univ. of Goiás

Canada
Varin Gosein
McGill
Andrey Grishin
McGill
Vikash Jha
Manitoba
Kyra Jones
Waterloo
Kevin Kirouac
Western Ontario
Nobuhiko Watanabe
Alberta

China
Wen Yang
Nankai

France
Rita Giordano
ESRF

Germany
Andrew Stewart
Johannes Gutenberg-Univ Mainz

Hungary
Margit Fabian
Res Inst Solid St Phys And Optics

Peru
Chris Pacheco Rivera
U Peruana Cayerano Heredia

South Africa
Serah Kimani
Cape Town

Thailand
Nongnaphat Khosavithitkul
Suranaree Univ of Tech

United Kingdom
Peter Byrne
Edinburgh
Richard Gildea
Durham
Kyle Morris
Sussex
Craig Robertson
Durham

United States
Balendu Avvaru
Florida
Aaron Bart
Kansas
Donnie Berkholz
Mayo Clinic College of Med
Jennifer Cash
Cincinnati
Yuan Cheng
UNC Chapel Hill
Watchalee Chuenchor
Maryland
Nick Deifel
George Washington
Chris Farrow
Columbia
Aaron Finke
Illinois - Urbana-Champaign
Jennifer Gehret
Michigan
Sudipto Guha
Illinois - Urbana-Champaign
Ju He
Colorado - Denver
Hua He
Delaware
Bradley Hintze
Duke
Ryan Jackson
Utah State
Emmanuelle Laffly
Maryland - Baltimore County
Meytal Landau
UCLA
Yuzhou Liu
New York
Angeline Lyon
Michigan
Krystle McLaughlin
Rochester Medical Center
Brandon Q. Mercado
UC Davis
Tara Michels-Clark
Tennesee
Vector Naumov
Columbia
Yi Peng
Case Western Reserve
Jason Porta
Nebraska Medical Center
Li Qiu
Alabama Huntsville
Bryan Reynolds
Southeast Missouri State
Karthik Sathiyamoorthy
Michigan
Mette Schmoekel
SUNY Buffalo
Stacey Smith
Brigham Young
Amber Smith
Michigan
Michael Takase
MIT
Rodrigo Torres
UC Irvine
Jennifer Urban
The College Of NJ
Fernando J. Uribe-Romo
UCLA
Weina Wang
Duke
Sung-il Yoon
The Scripps Research Inst
Tae-Soo You
Delaware
Linda Yu
Columbia
Elena Zlateva
Dowling College

2010 Margaret Etter Awards

Etter Early Career Award

Ray Trievel
Michigan

Etter Student Lecturer Awards

Bio-Mac SIG
Krystle McLaughlin
Rochester

Fiber Diffraction SIG
William Wan
Vanderbilt

Industrial SIG
Wei Ke
Case Western Reserve

Materials Science SIG
Cathleen Hoel
Northwestern

Neutron SIG
Stacey Smith
Brigham Young

Powder Diffraction SIG
Fernando Uribe-Romo
UCLA

Service SIG
Jason Porta
Nebraska Medical Center

Small Angle Scattering SIG
Ramnath Ramachandran
Cincinnati

Small Molecule SIG
Brandon Mercado
UC Davis

Synchrotron SIG
Mark Hunter
Arizona State

Meeting Exhibitors

Advanced Photon Source - Argonne
Anachem Instruments, Ltd.
Anton Paar
Area Detector Systems Corp.
Art Robbins Instruments
Blake Industries, Inc.
Bruker AXS, Inc
Canadian Light Source
CCDC
CCP4
Centeo Biosciences Ltd
Cornell University
Cryo Industires of America, Inc.
Dectris Ltd.
Diamond Light Source
Douglas Instruments
Formulatrix, Inc.
Incoatec Gmbh
IUCr
JAN Scientific, Inc.
LS-CAT Northwestern University
Micro Photonics, Inc.
Microlytic
MiTeGen, LLC.
Molecular Dimensions, Inc.
NatX-ray / Irelec
Oak Ridge National Laboratory
Oxford Cryosystems
Oxford Diffraction, Inc.
Rayonix, LLC
RCSB Protein Data Bank
Rigaku Americas Corp.
SER-CAT
SSRL - Stanford Sync. Rad. Lab.
Stoe & Cie GmbH
TA Instruments
Thermo Scientific NanoDrop
TTP Lab Tech Ltd
West Bond, Inc.
Xenocs SA

Meeting Sponsors

DIAMOND
IUCr
Oak Ridge National Lab

EMERALD
Bristol-Myers Squib
Bruker AXS
Dectris, Ltd.
Genentech
Rigaku
Roche

SAPPHIRE
Hampton Research

QUARTZ
Oxford Diffraction
P212121

Diamond - $5000 - above (a)
Ruby - $2500-4999 (b)
Emerald - $1000-2499 (b)
Sapphire - $500-999 (b)
Quartz - $1-499

a - Sponsorship of a lecture plus (b)
b - Invitation to the President's Reception

ACA Corporate Members are highlighted in blue

ACA 2010 - Once Again an International Meeting

Australia
Brazil
Canada
China
Columbia
Denmark
France
Germany
Hungary
Israel
Italy
Japan
Mexico
New Zealand
Peru
Poland
South Africa
South Korea
Spain
Switzerland
Taiwan
Thailand
Turkey
The UK
Ukraine
USA

Index of Advertisers

AUGUST 2010

22-27 **XXIVth ICMRBS** (International Council on Magnetic Resonance in Biological Systems), Cairns, Australia. www.icmrbs.org.

29-2 **ECM26**, European Crystallographic Association Meeting in Darmstadt, Germany. www.ecm26.org/.

SEPTEMBER 2010

12-16 **13th ICCBM**, Crystallization Workshop, Trinity College, Dublin, Ireland. www.iccbm13.ie.

20-23 **XTOP2010,** Int Conf on High-resolution X-ray Diffraction and Imaging**,** University of Warwick, UK, **www2.warwick.ac.uk/go/XTOP2010.**

OCTOBER 2010

1-3 **AsCA2010**, Busan, Korea. **www.asca2010.org.**

NOVEMBER 2010

9-10 **APC2010, Adv in Protein Cryst,** Florence, Italy. **www.selectbiosciences.com/conferences/APC2010/**

MAY-JUNE 2011

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

AUGUST 2011

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

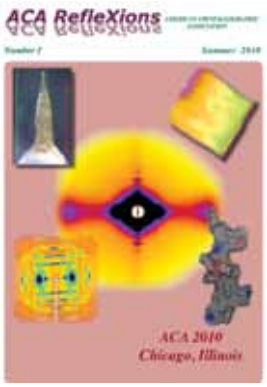
JULY 2012

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

AUGUST 2014

5-12 **ACA - XXIII Congress and General Assembly of the IUCr,** Montreal, Quebec, Canada: ***www.cins.ca/cncc/montreal/2014iucr***

What's on the Cover



Fiber diffraction blasts off at this summers ACA meeting in Chicago 2010 with sessions dedicated to amyloids and pathological fibril forming peptides (amyloid sample picture shown top left with numbers 1-9) and another session covering new developments in the field (remaining images). Technology and method development are critical drivers for any scientific discipline, at this years meeting we will hear how new advances in microdiffraction and cryo preservation methods have helped fiber diffraction advance in recent years. Representing this are example data, structures and samples: Center; micron scale x-rays delivered to lamprey notochord (cartilage-like tissue) allows the collection of crystalline data from sub-populations of fibers within the tissue, Bottom Left; as does the facility of scanning for the sample for the best diffracting portions of a Cellulose sample, Top Right; Whilst raster scanning the sample, the crystallite orientation can be detected in each diffraction pattern and used to map sample ultrastructure, Bottom right; using isomorphus replacement, the one-dimensional structure of lamprey notochord (see center image) was recently solved and used as a basis to model the structure of the telopeptides (here is shown the C-telopeptide), Top left, this is not a micron sized rocket, but a stretched dried sample of amyloid fibers which was then scanned (tiny blue box at sample base is relative beam size to sample and 1mm scale bar) to locate the most crystalline areas for optimum data collection.

School on Fundamental Crystallography and Workshop on Irreducible Representations of Space Groups,

The IUCr Commission on Mathematical and Theoretical Crystallography is organizing a school to be held in Uruguay in the fall of 2010. The school will be held at the *Facutad de Quimica of the Universidad de la Républica*, Montevideo, Uruguay, 29 November – 4 December 2010

It is aimed at researchers, young scientists and students of different fields with an average background in crystallography, who wish to widen their crystallographic knowledge. The program includes a detailed introduction to crystallography in both direct and reciprocal space with exercises on the use of the Volume A of the *International Tables for Crystallography*, as well aspractical sessions on the use of the *Bilbao Crystallographic Server*. The last day is devoted to a workshop on the *Irreducible Representations of Space Groups*.

Invited lecturers include Mois Aroyo (Bilbao), Massimo Nespolo (Nancy), Ernesto Estevez Rams (Havana), Leopoldo Suescun (Montevideo), Gustavo Echeverría (La Plata) and Eduardo Granado (Campinas).

Details about the scientific program and the organization, application for financial support and registration formalities can be found at ***www.crystallography.fr/mathcryst/montevideo2010.php*** and more detailed information about the local organization ***at cryssmat.fq.edu.uy/ISFC2010/isfc2010_home_EN.html.***

Contributors to this issue: Rob Boisseau, Gloria Borgstahl, Charlie Carter, Joe Ferrara, Stephan Ginell, Ilia Guzei, Joel Harp, Michael James, Mariusz Jaskolski. Richard Jones, Jim Kaduk, Judy Kelly, Jeanette Krause, Gary Newton, Emil Pai, Virginia Pett, George Phillips, S.N. Rao, Joe Reibenspies, John Rose, David Rose, James Stewart, Mark van der Helm, Ellen Weiss, Carrie Wilmot, Alex Wlodawer, Bomina Yu

Cover: Images / samples supplied by Paul Langan, Gerald Stubbs, Olga Antipova and Joseph Orgel. Thanks to NE-CAT and BioCAT. The images were collected and contributed by Joseph Orgel (supported by NSF grant #MCB-0644015 CAREER and NIH grant #RR08630).

Cartoons: Pages 2, 19 and 38 courtesy of Randall Munroe at ***xkcd.com***

Bruker AXS

X8 PROSPECTOR

High Performance, Low Maintenance

The X8 PROSPECTOR is an exceptionally low maintenance x-ray system designed to simplify crystal screening and data collection. The X8 PROSPECTOR has the reliability, speed and performance to make any structural biology lab more productive.

- Ultra-reliable IμS source with QUAZAR MX optics for a surprisingly high intensity
- Taperless CCD for ultimate detector sensitivity and speed
- Low maintenance, low cost of ownership - air-cooled source

SuperNova

The Fastest, Most Intense Dual Wavelength X-ray System

- Automatic wavelength switching between dual Mo and Cu X-ray micro-sources
- 50W X-ray sources provide up to 3x more intensity than a rotating anode*
- The fastest, highest performance CCD. Large area 135mm Atlas or highest sensitivity Eos with 330e⁻/X-ray Mo gain
- A full 4-circle kappa goniometer
- AutoChem, automatic structure solution and refinement software
- An extremely compact, low maintenance design

Agilent Technologies – formerly Oxford Diffraction. Visit us at the ACA meeting at booth #111

www.oxford-diffraction.com
sales@oxford-diffraction.com
Tel: 540-443-9272

*when compared to a 5kW rotating anode with optics

Agilent Technologies