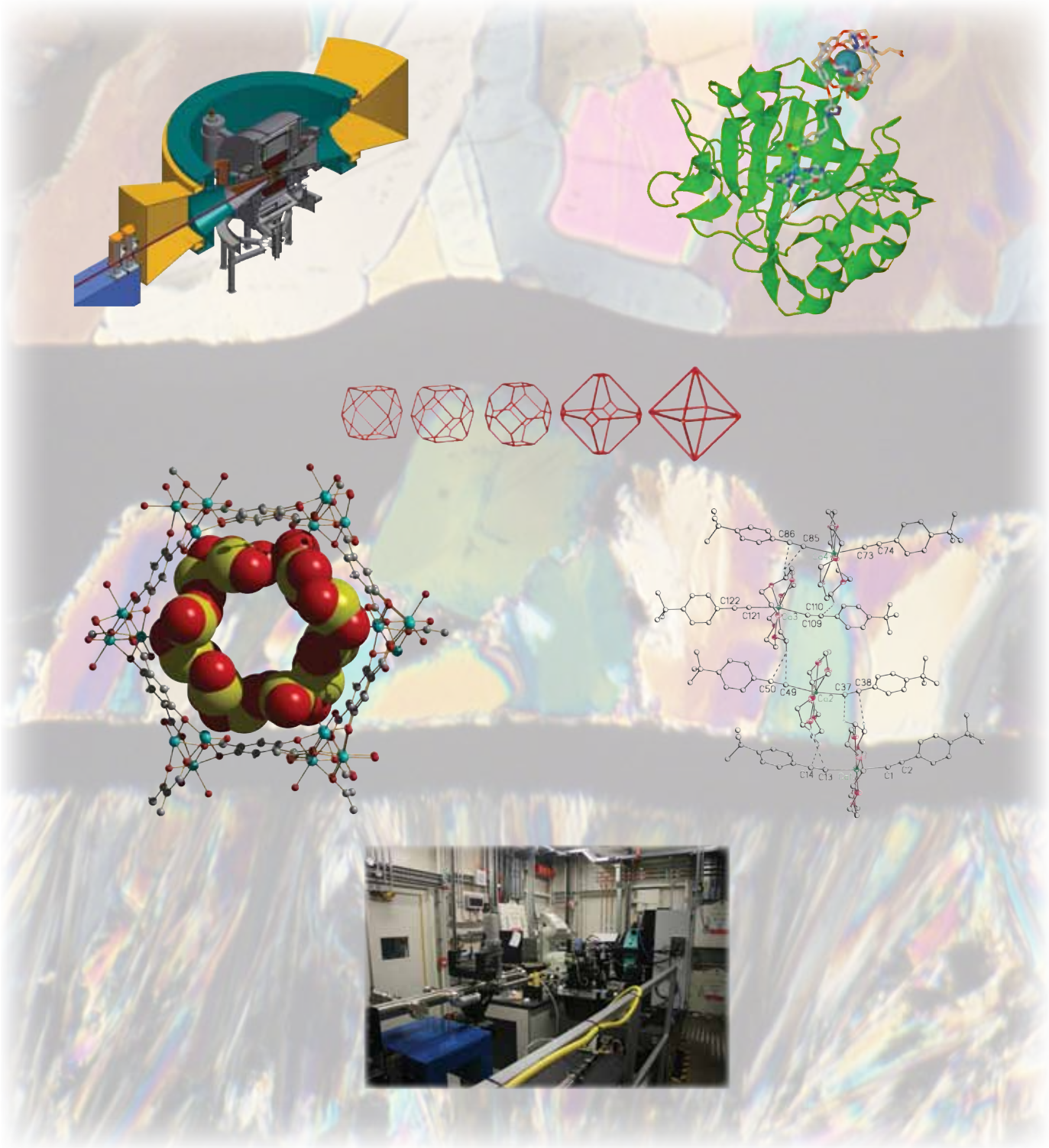
ACA RefleXions

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION

Number 2

Summer 2009



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President's Column

Recently I had the privilege of attending the semiannual meeting of the Council of Scientific Society Presidents (CSSP) in Washington, DC, at the American Chemical Society (ACS) headquarters - a very impressive place. The CSSP represents the views of the presidents, president-elects and past-presidents of some 60 scientific societies with a combined membership of 1.4 million scientists and science educators. This meeting had some 40-50 attendees representing organizations ranging from the ACS to the North American Benthological Society (you can look that one up as homework!). We heard from folks in a wide range of disciplines including talks by two Nobel Prize winners.

One of the more thought provoking presentations was by ***John Sterman*** from MIT who talked about "Adjustable Climate Models for Policy Thinking". He described the pitfalls of thinking that by "stabilizing" CO_2 emissions, we can stabilize the climate; he gave the analogy of a bathtub that is filled faster than water drains out. It overflows anyway! During his talk he demonstrated a new computer program, "Climate Rapid Overview And Decision-support Simulator" (C-ROADS) which rapidly simulates the effects of various policy choices for reducing green house gas emissions over a 100 year period. He anticipated that it will be available for download sometime later this year - you can Google "C-ROADS" to find it if you are interested. By the way, the modeling suggests for those folks who live at the ocean that it might be a good idea to move inland and gain at least a couple of meters of elevation above sea level almost no matter what policies are adopted!

Another fascinating talk was given by ***Todd Sacktor*** of SUNY Downstate Medical Center. He described his work in finding that a single protein, PKM-ζ, is responsible for retaining long-term memory (at least in rats!). Localized inhibition of PKM-ζ results in "erasure" of those long term memories residing in that location. These memories are permanently deleted; they do not recover even after the inhibitor is removed. Very thought provoking. Googling *PKMZ memory* will get you to a copy of his paper on this subject.

Several talks were aimed at organizational development, leadership and creativity. A take home message for me was that vital organizations that survive and grow constantly change to adapt to changing times. We, the ACA, are no different; our science has changed from being very esoteric and difficult to being a technique that is employed by many scientists to get structural results on their materials with perhaps little understanding on their part of the inner workings of the black boxes we have developed over the years. Our challenge is to find ways to change and to keep our validity and vitality. There are risks of change but as one speaker noted "the greatest risk is to stop taking risks!"

On this note, we are exploring the possibility of meeting with the Denver X-ray Conference (DXC) in Denver for our summer 2013 meeting. Some of you may recall that we have done this before. More than 30 years ago the ACA and DXC held a combined meeting in Snowmass, CO. By all accounts, this was a success and even featured a mountain thunderstorm! This time we're anticipating perhaps as many as 1200 attendees (the sum of the two meetings minus overlaps) and having perhaps 5-6 simultaneous sessions on a much expanded range of crystallographic and diffraction science; it would also include some sessions on x-ray fluorescence and possibly an expanded set of workshops. There could also be a broader range of exhibitors as well. The ACA Council and DXC organizing committee have endorsed this move; details are now being worked on. Needless to say, I'm very excited about this. There will be more on this later as our plans evolve.

Part of the CSSP meeting also featured nine committee meetings (actually *ad hoc* gatherings of the attendees) on a wide variety of issues ranging from "Diversity & Employment" to "Science Ethics". I chose to participate in "Environment & Energy" and "Scholarly Publication & Information Technology". In the latter we wondered what the library of the future would look like given the trend toward more electronic forms of publishing. All sorts of questions were raised. Would papers be posted on the web and folks could then post review them? How does peer review work with this open-ended form of electronic publishing? How can the journal publishers change to respond to this trend? (The President Elect of the ACS, ***Joseph Francisco*** was keenly interested in this question). How should promotion and retention evaluations at universities change to reflect the new modes of publication? How does electronic delivery of teaching change the business plans of America's universities? Our committee asked that for the next CSSP (December, 2009), a speaker be invited to talk on these kinds of issues for "The Library of the Future".

If you are interested in details about the CSSP and what it does, the web site is ***cssp.us***.

As we go to press the ACA Meeting in Toronto is just around the corner. All indications point to a very full and successful meeting. Jim Britten reports that over 600 abstracts for talks and posters have been submitted; he even commented that some of the posters (400+) may have to be displayed on Queen Street out in front of the hotel! You will notice that the meeting format is a little different from previous years. Each day begins with a plenary lecture for all to attend and then breaks out to the individual microsymposia. Be warned that current plans may have the opening session starting at 7:30AM on Sunday beginning with the Warren Award and lecture by ***Shih-Lin Chang***. The following morning is the Etter Early Career Award and lecture by ***Svilen Bobev.*** Tuesday and Wednesday begin with plenary lectures by ***Ted Baker*** and ***Phillip Coppens***. Finally on Thursday the morning begins with Buerger Award and lecture by ***Mike James.*** I'm looking forward to all of these and as many of the sessions as I can get to during the meeting. I hope to see you all there.

Best Wishes,

Bob Von Dreele

Meeting Costs I: Telecommunications

As Treasurer, I oversee the budget of the annual national meeting. As noted in the business meeting a year ago, we have sorted the expenses for the meeting into two main categories: fixed and variable. Fixed costs vary little from year-to-year or site-to-site, and we try to economize in that category as best we can. Variable costs offer the greatest challenge in maintaining a low registration fee and providing our attendees with the resources necessary for a great meeting. "Telecommunications" falls in the latter category, and to better inform the membership, I'll be highlighting specific expenses and options in a series of short articles for *RefleXions*. In this issue, we focus on "Telecommunications" as part of meeting expenses.

A decade ago, expenses in this "Telecommunications" category might have included costs related to setting up the telephone and FAX for the registration desk at the meeting, and providing network access to exhibitors, and for use by the "internet Corral" and special sessions. At that time the costs to the meeting were roughly $2000. We include internet access, if required, in determining workshop registration fees. In recent years, the office staff uses cell phones for communication, and "wi-fi" for an internet access for the laptop computer at the registration desk. Wireless internet connectivity is now common in the session and exhibits hall areas, but at a cost. Most recently, we have paid $5500-9300 for wi-fi access in the session and exhibitor hall areas, though in some venues, like Chicago 2004, cable and wi-fi were offered without any additional charge.

The costs for wi-fi have become excessive, ***even when*** we are charged a (supposedly reduced) rate of roughly $25 per connection per day. We have spent roughly $6000 for wi-fi at recent meetings and this number could easily rise to $25000 in Toronto if we offer 200 connections per day. This would have required an additional $25 increase in registration fees (based on close to 1000 projected attendees). Therefore, as a trial for the Toronto meeting, we will *not* offer wi-fi in the session halls. We have negotiated a reduced rate for wi-fi in your rooms ***at the hotel*** that is co-located with the conference site. Free wi-fi will also be available in the hotel lobby, coffee shops, and other areas close to the meeting site.

Will this decision significantly hamper your use of the internet such that you would you favor an increase the registration fee to support greater wi-fi coverage? Do you need network access in the session areas, and if so, what would you be willing to pay for it? I welcome your feedback on this issue, ***bds@uic.edu***.

Bernie Santarsiero

News from Canada

Welcome to Toronto: The Toronto ACA meeting is shaping up to be a great one. The program is varied and includes about 40% contributed lectures. There will be an international flavor to the meeting, and we are fortunate to have several members of the Executive Council of the IUCr presenting their work. Our local chair, ***David Rose,*** and his team, have been working very hard to make sure that everything runs smoothly and everyone enjoys the meeting and the city. The Swine or 'H1N1' flu has not lived up to its billing, and seems to be less serious than most seasonal influenzas, with the fewer cases reported each month. Information is available on the conference website, including the description of an Inuit greeting, 'Chimo', which does not involve handshaking!

Planning for IUCr 2014: A preliminary committee has been put together for the organization of the 23rd IUCr meeting in Montreal (August 5-12, 2014). It will be chaired by ***Louis Delbaere***, our leader in the Habs sweater in Osaka. ***Mirek Cygler*** will be the local chair (as he was for the Montreal ACA meeting). ***Joe Schrag*** will be Secretary, ***Lachlan Cranswick*** and ***Jim Britten*** will head the scientific program committee, with help from ***Pam Whitfield*** and ***Lee Groat***. ***Nancy Dufour*** will be in charge of fundraising; Louis will also be the IUCr representative; ***Laurier Forget*** and ***Rob Hart*** of the National Research Council of Canada will chair the Management Office; and ***Marie-France Polidori*** will represent the Palais des Congres. A June meeting will outline the timeline and duties of the group, as well as prepare for discussions with the IUCr EC in Toronto. There will also be a joint meeting of the US National Committee for Crystallography and the Canadian National Committee for Crystallography in Toronto this summer.

The 2009 Canadian Chemical Crystallography Workshop: The first Canadian Chemical Crystallography workshop was held May 28-30 at the MAX Diffraction Facility at McMaster University in Hamilton, Ontario. It was run as a satellite to the 92nd Canadian Chemistry Conference and Exhibition in downtown Hamilton, and followed the Joint Assembly Geology Meeting in Toronto. The workshop was organized by the MAX staff: ***Jim Britten, Hilary Jenkins***, and ***Vicky Jarvis***, with help from ***Anne Reynolds*** of the Brockhouse Institute of Materials Research.

The workshop was geared toward graduate students who wanted to improve their understanding and skills in single crystal structure determination. Fourteen eager participants took part, and were given a glimpse into reciprocal space, a space group teaser, links to great web sites, and lots of practice in solving and refining using WinGX. They worked on practice data sets, and on the data sets from hell that their supervisors sent along. They had hands-on demos of crystal mounting and data collecting. They learned to master, not fear, CIF's. Some students had no previous experience, while others were more advanced.

The computing sessions benefitted from the help of ***Jacques Barbier, Yurij Mozharivskij***, and ***Anthony Cozzolino***. We were also happy to have ***Jeanne Paquette*** of McGill's Earth and Planetary Sciences department as a participant. She did her initial training as an undergraduate crystallographer under the guidance of ***Gabrielle Donnay***. The students directed the program of the meeting with a constant stream of pointed questions, knowing that two and a half days is not much time for a crystallography course.

Back: Brad Herndon, Jess Priem, Vicky Jarvis, Po-Heng Lin, Christine Caputo, Ian Mallov, Darren Mercer, Nick Vukotic, Jim Britten

Center: Liz Strong, Aneta Borecki, Jeanne Paquette, Kalpana Maheria (visiting from India), Hilary Jenkins

Front: Qiang Wang, Chhatra Khadka, Varina Smith

We had a lot of fun, learned a lot of science, and were treated to a great meal at a British style pub by ***Sue Byram*** and Bruker AXS. We will try to offer this workshop at future Canadian Society for Chemistry meetings, enlisting the help of crystallographers in the host city. Be prepared for a knock on your door!

Jim Britten

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BALANCE SHEET - December 31, 2008 and 2007

	CURRENT FUNDS (2008)		TOTAL	
	Unrestricted	Restricted*	All Funds	
			2008	2007
ASSETS				
Current Assets:				
Cash	232,191		232,191	283,297
Investments	339,444	372,873	712,317	705,296
Inventory	2,225		2,225	5,600
Accounts Receivable	32,579		32,579	
Total Current Assets	606,439	372,873	979,312	994,193
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	612,2337	372,873	985,210	1,000,091
Liabilities:				
Unearned Dues	78,024		78,024	82,772
Credit Card Liabilities	556		556	
Total Liabilities	78,580		78,580	82,772
Fund Balance:				
Unrestricted	533,757		533,757	538,566
Restricted		372,873	372,873	378,753
Total Fund Balance	533,757	372,873	906,630	917,310
TOTAL LIABILITIES & FUND BALANCE	621,337	372,873	985,210	1,000,091

*** Current Balances in individual restricted funds - as of December 31, 2008**

Buerger Award	38,740
Etter Award	63,965
Fankuchen Award	67,594
Patterson Award	41,219
Pauling Award	33,317
Supper Award	11,402
Trueblood Award	33,737
Warren Award	31,276
Wood Science Writing Award	51,623

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.

Wayne Hendrickson Receives the "Kaj Linderstrøm-Lang Goldmedal"

At a ceremony held December 5, 2008 at the Carlsberg Laboratory in Copenhagen ***Wayne A. Hendrickson*** received the Kaj Linderstrøm-Lang Goldmedal. Carlsberg is a Danish brewery founded in 1847. Its visionary founder decided that the surplus generated by the brewery should benefit Danish science and in 1875 he established the well known Carlsberg research laboratory. Kaj Linderstrøm-Lang (1896-1959) was professor of chemistry and head of the Carlsberg Laboratory from 1938-1959. He was a pioneer in protein chemistry and enzymology and known for his use of deuterium exchange to study protein dynamics and for the classification of protein structure into primary, secondary and tertiary. Approximately every three years a gold medal is awarded to an outstanding scientist who has made major contributions within the research areas studied by Kaj Linderstrøm-Lang.

Ole Hindsgaul (Chair of the Committee of Trustees overseeing the award) presents the gold medal to Wayne

Wayne Hendrickson is the 15th recipient of the gold medal which was awarded "In appreciation of his outstanding pioneering work within structural biology, covering both development of methods and scientific results of important complex biological systems". The ceremony was followed by a dinner held at the beautiful old domicile of the Carlsberg founder, which provided a unique setting for the meal accompanied by different types of beer.

Gautam Desiraju Elected Fellow of the AAAS

Gautam R. Desiraju, a member of the ACA and of the IUCr Executive Committee, was recently elected a fellow of the AAAS. After a 30 year stay at the University of Hyderabad he has joined the Solid State and Structural Chemistry Unit of the Indian Institute of Science, Bangalore, India.

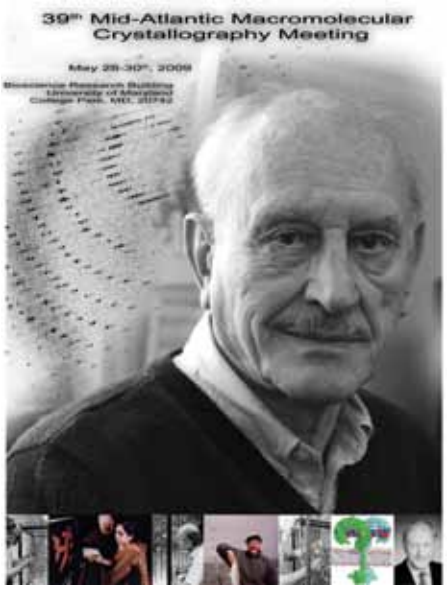
2009- Ohio State University – Distinguished Scholar Award to Michael Chan

The Distinguished Scholar Award, established in 1978, recognizes exceptional scholarly accomplishments by senior professors who have compiled a substantial body of research, as well as the work of younger faculty members who have demonstrated great scholarly potential.

ACA member ***Michael K. Chan*** (Departments of Biochemistry and Chemistry) has been named as the 2009 recipient of this prestigious award. He is an internationally recognized structural biologist whose co-discovery of a new, 22nd genetically encoded amino acid has been called a "true tour de force." He also was first to define the structure of a metalloenzyme that serves a major role in the pathway that is responsible for most of the world's natural production of the greenhouse gas, methane.

Among his many honors, he has received a CAREER Award from the NSF and a research fellowship from the Alfred P. Sloan Foundation. His research is funded by the NIH.

David Davies Symposium



A highlight of the 39th Mid-Atlantic Protein Meeting held May 28-30, 2009 at the University of Maryland was a symposium honoring ***David Davies*** (NIH) for his five decades long career in crystallography. Speakers included: ***Brian Matthews*** (U. Oregon) "Holey proteins and holy people", ***Alexander Wlodawer*** (NCI / NIH) "Back to the future: or, how I finally decided to follow in David's footsteps by studying antibodies", and ***Robert Stroud*** (UCSF) "Maxwell's Demons and 'r Breniniaethau chan Cymru". The symposium concluded with David's presentation on "Fifty years of protein structure: from myoglobin to the innate immune system".

Leslie Lessinger (1943 – 2009)

Leslie Lessinger, AB 1964, Ph.D. in Chemistry 1971, died peacefully at home in Brooklyn, NY March 13, after a 3-year battle with pancreatic cancer.

Les was an x-ray crystallographer from his early years in graduate school. After graduation from Harvard he spent 18 months with R. Srinivasan at the Centre for Advanced Study of Physics at the University of Madras, where he developed an abiding love for India and particularly for Madras City (now Chennai). He spent 3 years as a postdoctoral fellow in the Physics Department of the University of York with M.M. Woolfson. He then spent one year as research fellow with T. N. Margulis, in Boston. In 1977 he was hired to teach in the Chemistry Department of Barnard College in New York City and remained there until his retirement as Professor Emeritus in June 2008. At Barnard he was known both for his dedication to students and for his wide-ranging intellectual interests outside chemistry.

He carried out research on the fundamental methods of x-ray crystallography and he contributed to the solution of the crystal structure of several compounds of bio-pharmacological importance. He was an invited speaker at the international direct methods schools in Erice (Italy, 1974), York (England, 1975) and Sao Carlo (Brazil, 1976).

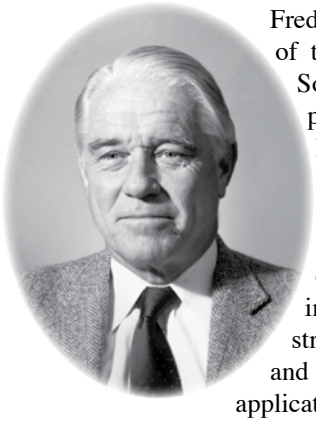
When I received from Hanna the news that Les had passed away I was gripped by a sense of loss. I had seen him for the last time in Seattle in 1996 and then we lost contact, but Les has always remained an unforgettable friend. Despite our different backgrounds, I felt we had many things in common, and not just because we both were left-wing non-practicing Jews.

During our common exciting experience in Michael Woolfson's group in York in 1974-75, I had the privilege of sharing with him many ideas and conversations, not only on science, but on the most different aspects of life. I admired his gentle but firm attitude of preferring the world of actual facts to that of arrogant appearance. This attitude can be appreciated by reading again his classical paper on "MULTAN Failures" (*Acta Cryst. (1976)* **A32**, 538-550).

We then met at a number of meetings, Hanna showed me and Carmelo Giacovazzo around Boston in 1976 and in 1985 Les and Hanna visited us in Torino on the occasion of the 9th European Crystallographic Meeting. When in 2007 I attended the meeting of the American Crystallographic Association in Salt Lake City, I was surprised not to see Les, but now I know the sad reason: he was fighting against pancreatic cancer.

Davide Viterbo

Frederic M. Richards (1925-2009)



Frederic M. Richards, former president of the ASBMB and the Biophysical Society was a towering figure in protein chemistry, having played a key role in moving the concept of proteins from amorphous colloids to discrete molecular structures. His contributions to protein science ranged from his central role in founding what is now known as structural biology (both experimental and computational) - to the design and application of new chemical reagents for probing protein structure and function.

Richards was born in New York City. After his graduation from Phillips Exeter Academy, he matriculated at MIT. Military service intervened toward the end of WWII, but he returned to MIT after his discharge and received a BS. degree in 1948. For his graduate study, he moved to E. J. Cohn's department at Harvard Medical School, where he worked with Barbara Low and received a PhD in 1952. He stayed at Harvard for a year as a research fellow with Cohn and then moved to the Carlsberg Laboratory in Denmark, where, with Kaj Linderstrøm-Lang and others, he began working with ribonuclease. After a short stint at Cambridge University as a NSF postdoctoral fellow, Richards joined the faculty of the Dept. of Biochemistry at Yale University in 1955 as an assistant professor. He rose rapidly through the ranks, becoming professor in 1963.

In 1963, Richards was appointed chairman of the Dept. of Molecular Biology and Biophysics at Yale. He spent a sabbatical at Oxford University from 1967 to 1968, for which Richards and his wife Sally sailed their own boat with a small crew across the Atlantic Ocean. Following this break, when Yale merged the Medical School Dept. of Biochemistry and the Yale College Dept. of Molecular Biology and Biophysics to form a new university-wide Dept. of Molecular Biophysics & Biochemistry, Richards became its founding chair (1969–1973).

Summarizing Richards' contributions to protein science is difficult because of the breadth that he covered. Much of the early work in Richards' laboratory focused on bovine pancreatic ribonuclease, and in particular a preparation that he discovered while in Linderstrøm-Lang's laboratory, dubbed ribonuclease-S (RNaseS). Richards and co-workers purified and characterized RNaseS, separated it into S-peptide (residues 1–20) and S-protein (residues 21–124), both enzymatically inactive, and showed that S-peptide did not retain an ordered structure in solution but could be reconstituted with S-protein into enzymatically active RNaseS. They crystallized RNaseS and showed that RNaseS was enzymatically active in the crystal, putting to rest the widely held view (at that time) that protein crystal structures were irrelevant to the conformation and behavior of enzymes in solution. In collaboration with the late H. W. Wyckoff, they solved the structure to atomic resolution (a tie for the third protein structure ever solved to atomic resolution) with and without bound nucleoside monophosphate. While on sabbatical at Oxford, Richards designed and built the Richards Optical Comparator, better known in the

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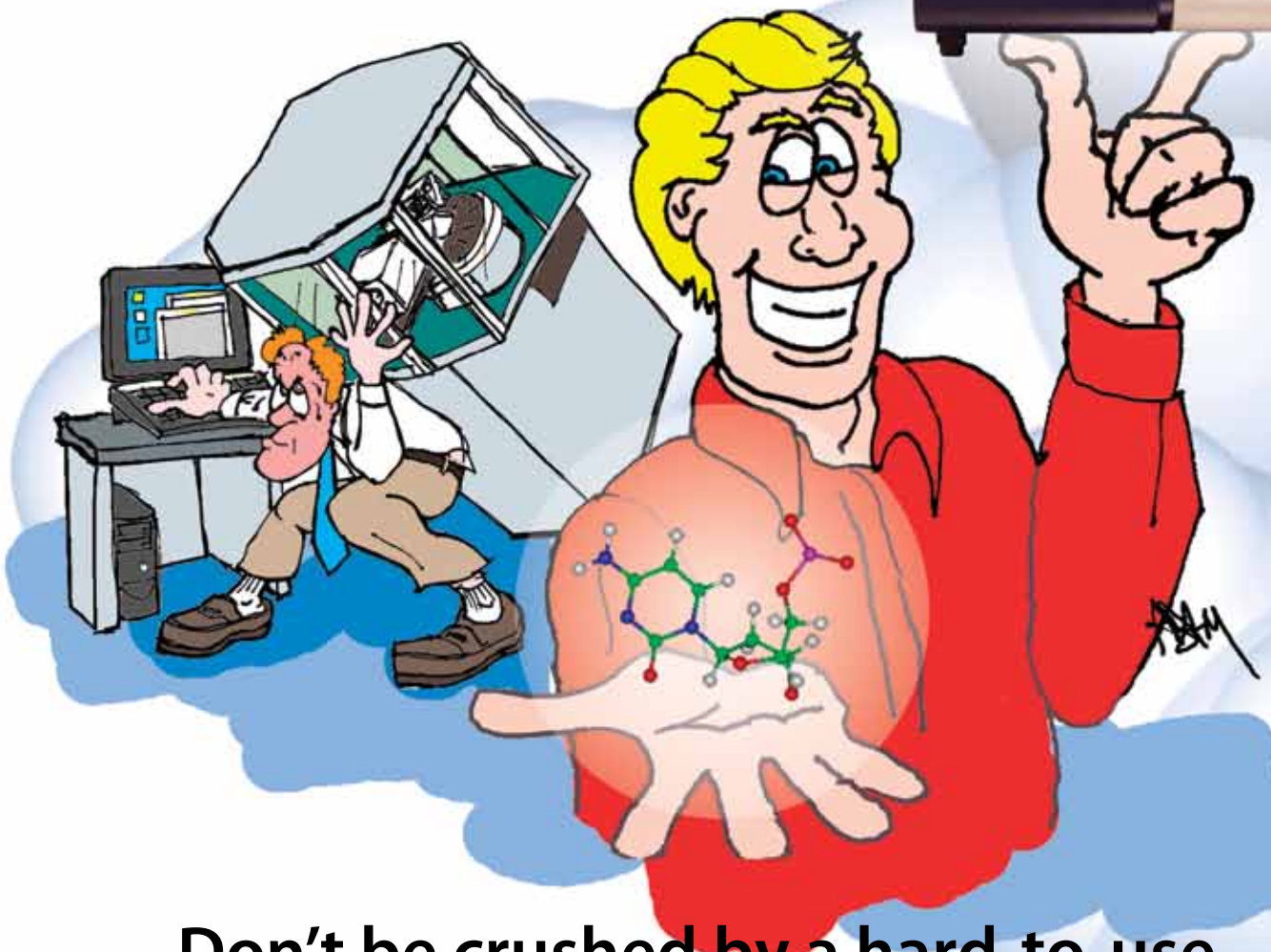

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field as "Fred's Folly," or simply "the Folly," which remained the method of choice for converting electron density maps to models, until it was supplanted by computer graphics.

The Richards Lab always included a "wet" component focused on the properties of proteins in solution and on the design and application of new chemical reagents for modifying proteins in ways that reported on the proteins' structure and/or function. Types of reagents pioneered in the Richards laboratory included hydrophilic and hydrophobic photoactive reagents for studying membrane protein topology, cleavable cross-linking reagents for studying protein quaternary structure, and reagents that exploited the remarkably strong binding between ferritin and avidin for use in localizing target proteins within cellular structures.

Richards received many honors for his scientific achievements, including the Pfizer-Paul Lewis Award in Enzyme Chemistry (1965), a Guggenheim Fellowship (1967-1968), election as Fellow of the American Academy of Arts and Sciences (1968), election to the National Academy of Sciences (1971), the Kai Linderstrøm-Lang Prize in Protein Chemistry (1978), the AS-BMB Merck Award (1988), the Stein and Moore Award of the Protein Society (1988), and the State of Connecticut Medal of Science (1995).

What should not be overlooked in reviewing Richards' science is that the Richards Lab was a wonderful place to develop as a scientist, whether one's experience there was as an undergraduate student, graduate student, postdoctoral fellow, or sabbatical visitor.

James V. Staros

Editors note: The Richards memoriam was reprinted by permission from ASBMB Today, April, 2009.

Robert Everest Newnham (1929 – 2009)

Robert Everest Newnhamn was a graduate of four universities. Bob studied math at Hartwick College (BS, 1950), physics at Colorado State (MS, 1952), physics and mineralogy at Penn State (PhD, 1956) and crystallography at Cambridge University (PhD, 1960). Prior to joining the Penn State faculty in 1966, he was an I.C.I. Fellow at the Cavendish Lab of Cambridge Univ. He also taught in the Electrical Engineering Dept. of MIT. for 10 years.

At Penn State, Bob taught courses on crystal physics, crystal chemistry, electroceramics, mineralogy, gem minerals, biomaterials, x-ray diffraction, and crystal structure analysis. Widely known for his enthusiastic lectures and colorful illustrations, Bob was honored with the Outstanding Educator Award of the Ceramic Education Council, and the Wilson Teaching Prize of the College of Earth and Mineral Sciences. During his career, he delivered the Dow Lectures at Northwestern University, the Wolff Lecture at M.I.T., the McMahon Lecture at Alfred University, the Pond Lectures at Johns Hopkins, the Maddin Lecture at the University of Pennsylvania, and the Byron Short Lecture at the University of Texas. After retirement, Bob taught for two years at the Hong Kong Polytechnic University and the Georgia Institute of Technology.

Bob was active in several professional societies, serving as Editor of the *Journal of the American Ceramic Society*, Secretary of the Materials Research Soc., ***President of the ACA (1985),*** and Distinguished Lecturer for the Institute of Electrical and Electronic Engineers. Among his many awards was the Jeppson Medal, the E.C. Henry Award, the Bleininger Award, the David Kingery Award of the American Ceramic Soc., the third Millennium Medal and Ultrasonics Achievement Award of the IEEE, the Centennial Award of the Japan Ceramics Soc., the Turnbull Lecturer Award of the Materials Research Soc., the Adaptive Structures Prize of the American Soc. of Mechanical Engineers, the Benjamin Franklin Medal for Electrical Engineering from the Franklin Inst., and the Basic Research Award of the World Academy of Ceramics.

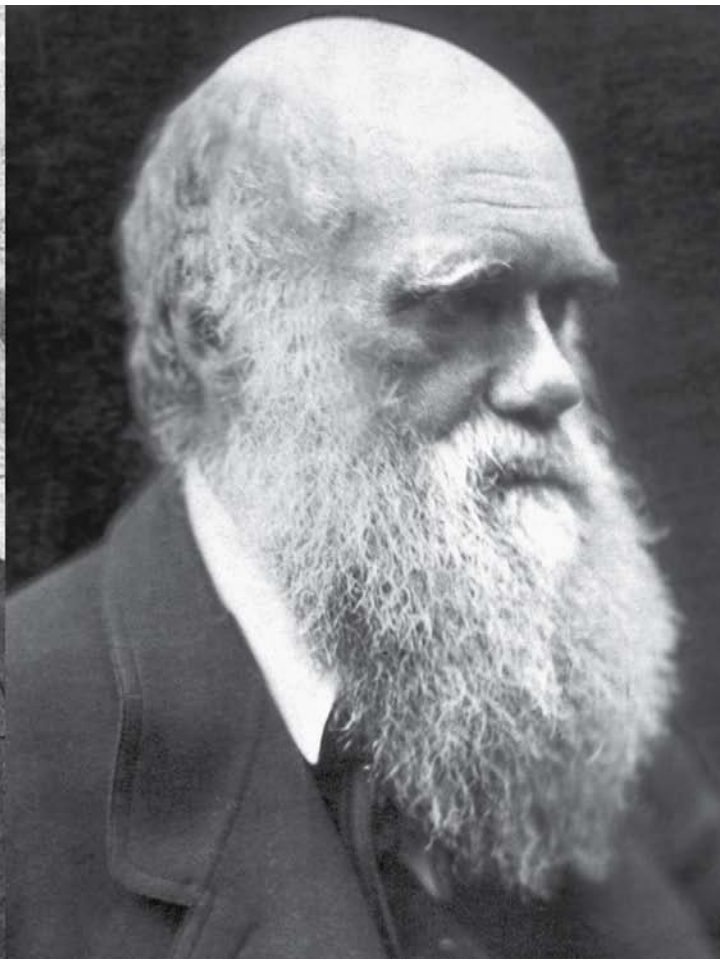
A member of the National Academy of Engineering, Bob Newnham wrote five books, more that 500 research papers and 20 patents on electroceramics and composite materials for electronic and acoustic applications. His early career revolved around crystallography and understanding structure-property relations. He performed structure refinements of several important minerals, including ruby, some feldspars, fresnoite, and some bismuth layer structure ferroelectrics.

During the past forty years, Bob and his long-time colleague Eric Cross, built up one of the largest ferroelectrics research programs in the world. Together they pioneered a number of new piezoelectric and electrostrictive materials for use as sensors, actuators, and capacitors. They were the first to carry out a complete classification of primary and secondary ferroics with examples of each. The composite piezoelectric transducers developed in his laboratory revolutionized the quality of ultrasound images in cardiology, obstetrics, and underwater sonar. Every major ultrasonics manufacturer in the world including several in central Pennsylvania use composite transducers based on his designs. His miniature flextensional transducers for hydrophone towed arrays is one Penn State's most successful patents. They are widely used in underwater oil explorations and geophysical research.

He retired from Penn State in 1999 as Alcoa Prof. Emeritus after serving eight years as Assoc. Director of the Materials Research Lab and 18 years as Director of the Intercollege Program on Solid State Science. Bob is remembered with great love by friends, former students, and scientific colleagues around the globe.

In private life, Bob was an unabashed liberal in politics and religion. He and his wife, Pat, were strong supporters of the peace movement, the Unitarian-Universalist Fellowship of Centre County, and numerous liberal charities. In his spare time, he was an ardent mineral collector and model airplane builder. He loved the smell of airplane glue. The family encourages friends to honor his memory by attending local peace vigils.

Susan Trolier-McKinstry



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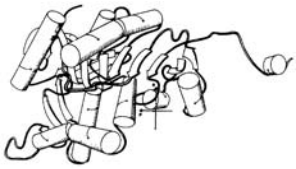
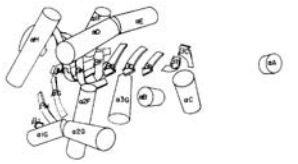
Audrey Rossmann (1928-2009): A Personal Tribute

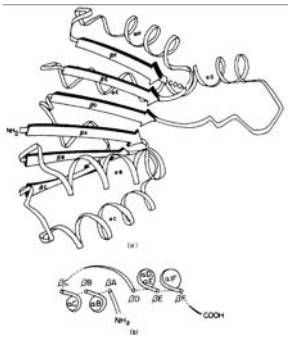
Historically, little attention has been paid to the spouses of high profile scientists and the role that they have played in the accomplishments of their companions. I can refer to Mme Lavoisier, less known as Marie-Anne Pierrette Paulze, who diligently worked with her husband (the illustrious chemist) in writing experimental protocols, illustrating his chemical apparatus and so many other contributions; yet she remains an unknown contributor to the history of science. I can also mention Marie Laurent, who became Mme. Louis Pasteur, another woman devoted to the absorbing science of her husband and probably known by very few. I do hope that some scholarly research is done on this area to enrich our lives and change our perception of famous scientists as laboring alone in the laboratory, their companions providing only the domestic support.

Audrey Rossmann contributed and was devoted to Michael's work in many different ways. She provided an artistic balance and complement to the gallery of structures that he and his colleagues unveiled over the years at the Department of Biological Sciences at Purdue University. In doing so, she had her own tangible 'structures' to present to the world.

Older generations of protein crystallographers may remember the first 'cartoon' sketches of the meanderings of the polypeptide chain in lactic dehydrogenase (LDH) and the Rossmann fold. These classic representations (shown here) were drawn by Audrey Rossmann at the suggestion of Anders Liljas (at that time a Swedish postdoc in the lab). Similar renderings of the different protein folds were popularized by Jane Richardson in her own unique style. Nowadays, computers do the drawings in a more timely and efficient manner, but certainly with very different artistry.







After the milestone of the LDH structure in Michael's lab, the structures of viruses began to appear. First Southern Beam Mosaic Virus (SBMV), a humble plant virus, and later Rhino (HRV), the first human virus to be solved at atomic resolution. The theme of virus structure and symmetry was quickly picked up by Audrey in her pottery work, clothes and other artistic creations. I still treasure in our own yearly Christmas tree decoration ritual, hanging the virus-like adornment that Audrey gave us in 1982.

Members of the laboratory often received a pottery memento of their stay in the lab. A most precious gift is the 'virus-within-a-virus' ceramic piece that Michael and Audrey gave Victoria and me as a goodbye present when we departed from the lab in 1985. It is decorated on the outer shell with the signatures of people in the lab at the time, the projects I worked on and the triangular faces were painted with brown and black earthly colors. Floating inside is another full sphere triangulated with the faces of an icosahedron. I remember Audrey bringing the pieces to the lab in a tray for the people to sign, with the inside sphere wrapped inside a newspaper, ready to be fired in the kiln. I never thought that this piece would become a treasured memory of her.

All around the world in the houses of family, friends, colleagues and collaborators, there are many other Audrey structures - ceramic art masterpieces. Her creations were always unique in concept and design with soft contours, forms and designs, always exhibiting superb craftsmanship. Some of them were shown most recently (Fall 2008) at the Art Museum of Greater Lafayette in a two month long exhibition entitled "A Tribute to Audrey Rossmann: Realizing Excellence" (***www.lafayette-online.com/artsentertainment/exhibits/2008/08/audrey-rossmann-exhibition/***)

There is another way in which Audrey graciously supported Michael's science as only she could do. She tirelessly hosted students, postdocs, colleagues and collaborators and their families at dinners, lunches, and brunches in their home and in spring, summer and fall at seasonal barbecues at various park venues around Lafayette and its surrounding areas in the outdoors that both Audrey and Michael always loved so much. Audrey has left an indelible mark on a multitude of people that were fortunate enough to meet her.

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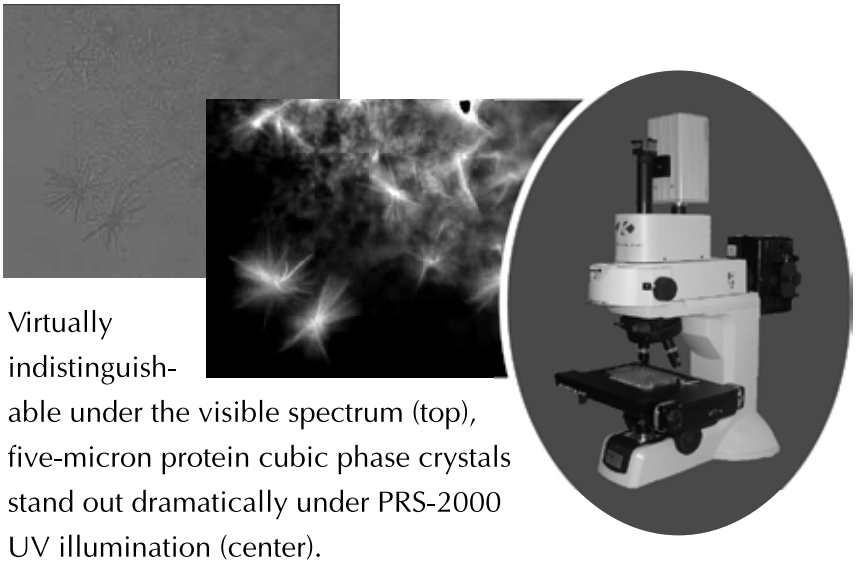

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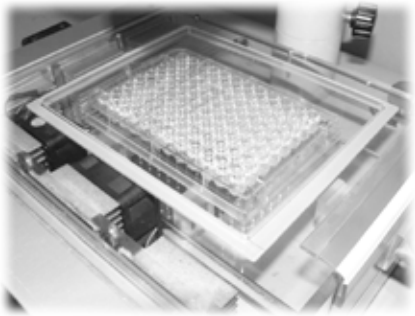

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Margaret C. Etter (1943 - 1992)

Margaret C. Etter, Professor of Chemistry at the University of Minnesota and one of the coordinating editors of *Molecular Engineering,* died June 10, 1992 of cancer. She was a charming person, an excellent lecturer, and an outstanding scientist. No one knew her for more than five minutes without calling her Peggy. She was the kind of person who made a lasting impression on virtually everyone who made her acquaintance.

Peggy had a wonderful sense of humor. Her students, colleagues, and friends knew her streak of fun loving, characterized by a singular laugh that easily echoed across the room or down the hall. A few of us will remember the scented smiley stickers or the giant-sized $100 bills we received to reward some research results, a well-presented seminar, or a truly original idea. She was a very down-to-earth person, who did not take herself too seriously. After an excess of sexist verbal transgressions during one of her group meetings, her old friend Joel Bernstein was awarded "The Book on Nonsexist Writing."

She was a *Phi Beta Kappa* graduate of the University of Pennsylvania and received a master's degree in chemistry from the University of Delaware prior to beginning graduate studies at the University of Minnesota, where she received a Ph.D. in chemistry for her work on topotactic reactions under the direction of Jack Gougoutas. Upon leaving the chemistry department in 1975, Peggy taught organic chemistry at Augsburg College in Minneapolis during one year, after which she joined the 3M Company's Central Research Laboratory in St. Paul as a research chemist.

At 3M she was involved in projects ranging from polymer chemistry to hydrogen bonding in organic solids. Peggy set about establishing an organic solid-state chemistry group which ultimately included Ruth Kress Johnson and William (Bill) Gleason. Peggy didn't just talk, she did things: things that were not necessarily popular at the time. She helped to establish the 3M Visiting Women's Scientist program, the purpose of which was to encourage female students to consider science as a career. She was also a director and instructor in the STEP program, directed at encouraging minority students to become scientists.

A belated postdoctoral stint in solid-state NMR provided the final intellectual ingredient and catalyzed the extraordinary burst of creativity and productivity that characterized Peggy's academic career. She returned to the chemistry department at the University of Minnesota in 1983, where she made rapid progress from assistant to full professor in 1990. There she received a Sloan Foundation award and obtained research support from the NSF, the NIH, and the Office of Naval Research.

Peggy's intelligence, elegant presentation, enthusiasm, and radiant personality did not change from the early seventies, when she was a graduate student at the University of Minnesota. To those who had the opportunity to work with Peggy she demonstrated what it meant to show respect and compassion for everyone, irrespective of status or behavior. In important matters she always did what she considered to be the right thing. In several cases this cost her a great deal- and she knew that it would. Her rapid rise to professor, her outstanding students, publications, research support and awards, all these were wonderful for old friends to watch. She really deserved these things; after all she had gone through. Often succeeding against very long odds, Peggy persevered in an academic career, which will serve as a model to many aspiring women scientists. It is remarkable that this career spanned a mere seven years, during which she built a world-renowned group in organic solid-state chemistry (usually hovering around ten people, including post-docs and sabbatical visitors), that made major contributions in applications of solid-state NMR, organic non-linear optical materials, and understanding and utilizing hydrogen-bonding interactions in crystals. In all these subjects she was in constant demand as a plenary lecturer at international meetings, as in Bordeaux in 1990, and authored landmark reviews. Her output during that brief sparkling career exceeded eighty significant publications.

Bill Gleason, Peggy Etter and Ian Paul

Peggy was very active in the ACA. She served as chair of the Small Molecule Special Interest Group, and edited the 1988 *Transactions* volume entitled: *NMR and X-ray Crystallography: Interfaces and Challenges*. She was the program chair for the 1991 national meeting in Toledo, and helped to organize a session on chiral recognition at the 1992 meeting in Pittsburgh.

A warm, sincere, supremely competent person, with uncompromising scientific standards in thinking and in writing, she was an active and trusted member of the communities of crystallographers and of organic chemists. Within the limits of ever increasing demands on her time, she tried never to refuse to serve on a committee, help to organize a meeting, or edit a book or a special issue of a journal. In the fall of 1990 she became the only female co-editor of the newly launched *Molecular Engineering*. Always a champion of organic solid-state chemistry in its broadest sense, she organized special sections on the subject for ACA, ACS, and IUPAC meetings, actively served on the international advisory boards of other meetings, and initiated the Midwest Symposium on Organic Solid-State Chemistry to serve as a forum for researchers and graduate students from different institutions.

Second Mid-West Meeting - University of Minnesota - June 1989

When Peggy was diagnosed with kidney cancer in April of 1991, all who knew her were devastated. Characteristically, she took it upon herself to cheer her friends, take care of her students, and get her house in order. No matter how bad things were during the ensuing year, she always found the positive side of it all, the silver lining. This last February she visited Israel, finally realizing a dream of more than a decade. Although she was weakened by her illness, her commitment to and excitement for the science she loved gave her the strength to deliver three brilliant lectures, the third one being the main lecture of the Israel Chemical Society's annual meeting. Not a soul in that audience of 500, save her closet friends and her sister who accompanied her, was aware of the supreme effort and inner strength that she summoned to present that stellar talk. It was to be her last.

For all whose lives were touched by Peggy Etter, she was one of those individuals gone too soon, to be sorely missed, but always to be remembered.

Editors note: *The preceding was gathered by Jean Naruani from tributes written in September 1992 by former students, colleagues, and close friends including Dan Adsmond, Gayle Frankenback, Alojos Kalman, Meir Lahav, William Gleason, and Joel Bernstein. It was published in Molecular Engineering (1992) 2, 213-214. It is reprinted here with the kind permission of Springer Science and Business Media. Thanks also to Joel Bernstein for the photos.*

This article is another in the RefleXions series on the people for whom ACA awards have been named. The ACA Student Travel Fund was started in 1987 and named after Peggy when she passed away. While that fund still bears her name the awards have not been called Etter travel awards since 2001 mainly because student travel to ACA meeting is now funded from a variety of sources. In 2002 the Etter Early Career Award was established and the Etter Student Lecturer Awards (one awarded by each SIG) was started in 2003. As of this writing the winner of the 2010 had yet to be selected. Carrie Wilmont touched on Peggy's life and involvement with students in her "where are they now" article on previous winners (ACA RefleXions Spring 2009, pp 4-6.) In that article Svilen Bobev was incorrectly listed as the 2008 winner. The correct list follows:

ACA Etter Early Career Award Winners and Lecture Titles:

2009 Svilen Bobev

Rare Earth Intermetallics - How Far Does One Need to Go Searaching for New Structures and Properties.

2008 Radu Custelcean

Manipulating Hydrogen Bonds in Crystalline Solids: From Etter's Rules for Anion Recognition

2007 Cora Lind

Negative Thermal Expansion Materials: X-ray and Neutron Diffraction Adventures under Non-ambient Conditions

2006 Carrie Wilmot

X-rays, Action, Camera! The Joys and Heartaches of Making Movies of Redox Enzymes in Motion

2005 Jennifer A. Swift

Growth and Dissolution of Cholesterol Crystals

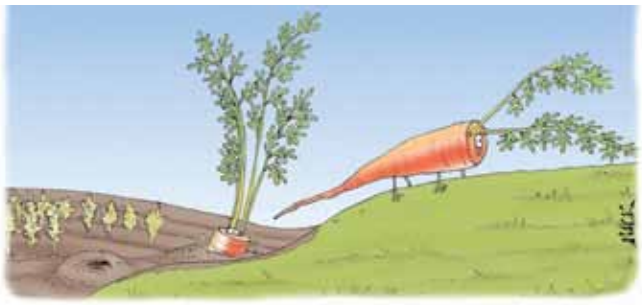
2004 Leonard MacGillivray

Linear templates: Tools for Constructing Molecules in the Solid State

2003 Julia Chan

Structure-Property Relationships of Superconducting and Heavy Fermion Intermettalics

The winners of 2009 Etter SIG Student Lecture Awards for ACA Toronto are listed on page (43) of this issue of *RefleXions*.



The next great step in carrot evolution.

New Texas Standards Question Evolution, Fossil Record

New science standards for Texas schools strike a major blow to the teaching of evolution, say scientists and educators who last week tried unsuccessfully to block the adoption of last-minute amendments aimed at providing an opening for the teaching of creationism. The standards incorporate talking points from the intelligent design literature, including doubt that the fossil record provides convincing evidence of evolution. Supporters of the new standards, which prevailed by a vote of 13 to 2, say the next step will be to press publishers to modify biology textbooks.

"I think the new standards are wonderful," says Don McLeroy, chair of the Texas Board of Education and a dentist who claims that "dogmatism about evolution" has sapped "America's scientific soul." He believes that biology texts should include "an evaluation of the sudden appearance of fossils" and "an explanation of stasis or how certain organisms stay the same over time." He also wants the textbooks to declare there is no "scientific explanation for the origin of life" and that "unguided natural processes cannot account for the complexity of the cell."

He anticipates that in 2 years the state will adopt new biology textbooks. Because Texas is the second-largest textbook market in the US, publishers have a strong incentive to be certified by the board as "conforming 100% to the state's standards," says Dan Quinn of the Texas Freedom Network in Austin, which has campaigned to keep creationism out of the science classroom.

Quinn and his colleagues thought they had won a major victory earlier in the 3-day meeting when the board voted to strike from the existing standards the requirement that teachers present the "strengths and weaknesses" of evolutionary theory. But the next day, conservatives won support for a similar phrase that calls on teachers to "analyze, evaluate, and critique scientific explanations in all fields of science by using empirical evidence, logical reasoning, and experimental and observational testing, including examining all sides of scientific evidence of those scientific explanations so as to encourage critical thinking by the student."

The new language covers two hot-button topics. Teachers will now be required to have their students "analyze and evaluate scientific explanations concerning the complexity of the cell" and "analyze and evaluate the evidence regarding formation of simple organic molecules and their organization into long complex molecules having information such as the DNA molecule for self-replicating life." Students will also be expected to "analyze and evaluate a variety of fossil types such as transitional fossils, proposed transitional fossils, significant fossil deposits with regard to their appearance, completeness, and alignments with scientific explanations in light of this fossil data."

The creationists were "dogged," says Eugenie Scott of NCSE. "It was like you put the stake in the heart of the vampire and it comes back." Moderates on the board may have failed to recognize the final amendments as intelligent design talking points, she added, because they were focused on the "strengths and weaknesses" clause.

From the News of the Week feature in Science (2009) 234,25 reported by Yudhijit Bhattacharjee.

Anti-evolution Bills Die in Texas, June 1st, 2009

Two antievolution bills died when the Texas legislature adjourned on June 1, 2009. One would have exempted institutions such as the Institute for Creation Research's graduate school from Texas's regulations governing degree-granting institutions, thus freeing the ICR to offer a master's degree in science education despite the Texas Higher Education Coordination Board's 2008 decision to deny the ICR's request for a state certification of authority to offer the degree. The ICR is currently suing THECB in federal court over its decision. The other bill would have required the Texas state board of education to restore the controversial "strengths and weaknesses" language in the Texas state science standards. Although creationists on the board were unsuccessful in restoring the "strengths and weaknesses" language, they successfully introduced a requirement that students examine "all sides of scientific evidence." Partly due to his attempts to undermine the treatment of evolution in the state science standards, the senate voted not to confirm Don McLeroy in his position as chair of the board; the Fort Worth Star-Telegram (May 31, 2009) editorially commented, "It is overly optimistic to say the Senate's rejection of Don McLeroy as chairman of the State Board of Education will end the missteps and arguments that have plagued the board during the past two years. Still, we can hope."

Texas Creationist Board Chair Out, May 28th, 2009

The Texas Senate voted not to confirm Don McLeroy in his post as chair of the Texas state board of education on May 28, 2009. Although the vote to confirm him was 19-11, a two-thirds approval was required. The *San Antonio Express-News* (May 28, 2009) explained, "The Senate seldom rejects gubernatorial appointments. Their blocking of McLeroy will force Gov. Rick Perry to appoint a new board leader. McLeroy will keep his spot as a board member."

McLeroy's confirmation was editorially opposed by a number of Texas newspapers, including the *San Antonio Express-News* (May 3, 2009), which wrote, "McLeroy has demonstrated he is unfit to lead a body that crafts public education policy for this great state," and the *Austin American-Statesman* (May 8, 2009), which described his tenure as chair as "disastrous," while cautioning, "Simply removing McLeroy, a dentist, from the chairmanship won't be enough to bring sanity" to the board.

A major concern of the senators voting against McLeroy's confirmation was his attempts to undermine the treatment of evolution in the state science standards. Eliot Shapleigh (D-District 29), for example, questioned his endorsement of a book that describes parents who want their kids to learn about evolution as "monsters," scientists as "atheists," and clergy who see no conflict between science and faith as "morons." McLeroy is, notoriously, a creationist himself, as the *Austin American-Statesman* (March 8, 2009) described in detail.

In a statement dated May 28, 2009, Kathy Miller of the Texas Freedom Network commented, "We had hoped that the Legislature would take more action to put this train back on the tracks, but clearly new leadership on the board was a needed first step. The governor should know that parents will be watching closely to see whether he chooses a new chairman who puts the education of their children ahead of personal and political agendas."

The Federal University of Minas Gerais (UFMG) is well known for its experimental research in different areas, many of which are greatly dependent on structural studies. For this reason, the creation of a new Center for the Structural Characterization of Materials and Molecules (CCEM&M) was very exciting for crystallographers in Brazil. One facility within the CCEM&M will be the *Laboratório de Cristalografia* (LabCri). To complete this facility new diffractometers dedicated to small molecule studies have already and a rotating anode dedicated to the studies of protein structures for the biochemistry department have been acquired.

To commemorate this occasion a crystallography school was held at UFMG in March, 2009. The school was organized by four members of the UFMG faculty: ***Carlos Basílio Pinheiro***, coordinator and ***Nivaldo Lúcio Speziali*** (physics), ***Nelson Gonçalves Fernandes*** (chemistry) and ***Ronaldo Alves Pinto Nagem*** (biochemistry).

Carlos Basílio Pinheiro and Nivaldo Lúcio Speziali

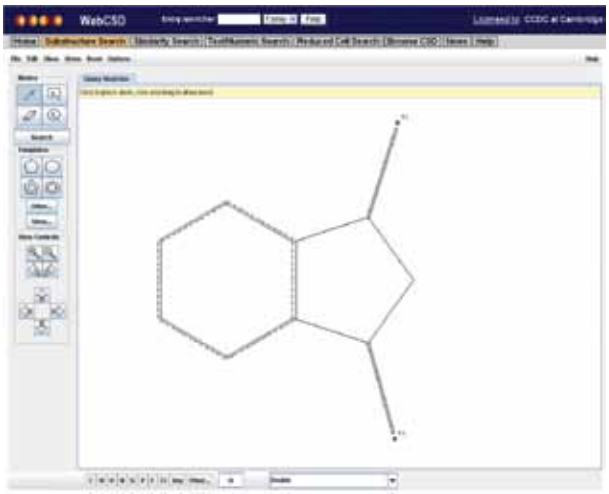
The lectures presented were preceded by an introduction on the multidisciplinary nature of crystallography (***I.L. Torriani***), followed by presentations on a variety of topics: structural crystallography at the UFMG (***N.L. Speziali***), characterization of supra-molecular compounds (***R. Diniz***), protein crystallography (***J.A. Barbosa***), study of thin films (***M. Fantini***), applications of XRD in metalurgy (***V. Buono***), applications of XRD in industry (***F. Costa***), polymorphism (***J.Ellena***) and XRD in nanocrystalline matrials (***S.R. Teixeira***).

This was a very successful meeting. The organizers reached the right audience, and a lot of activity is expected from both the UFMG experienced researchers and young students in the near future.

Iris L. Torriani

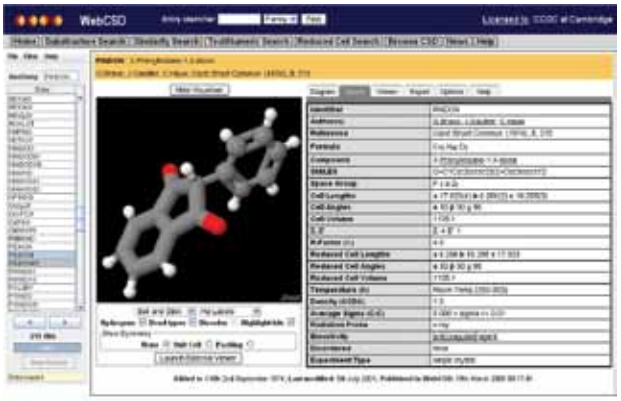
WebCSD: A New Generation Crystallographic Resource

The CCDC is pleased to announce that internet access to the Cambridge Structural Database (CSD) will soon be available. This new resource, WebCSD, has been developed using CCDC's C++ toolkit and enhances the search, analysis, exploration and validation tools already provided with the CSD, known as the CSD System. The software searches on a relational SQL version of the CSD. Users with an unlimited licence to the CSD System will be able to freely access WebCSD without the need for a local installation of the software. Further details are provided on the CCDC website: ***www.ccdc.cam.ac.uk/webcsd/***.



A substructure search defined in WebCSD's sketcher.

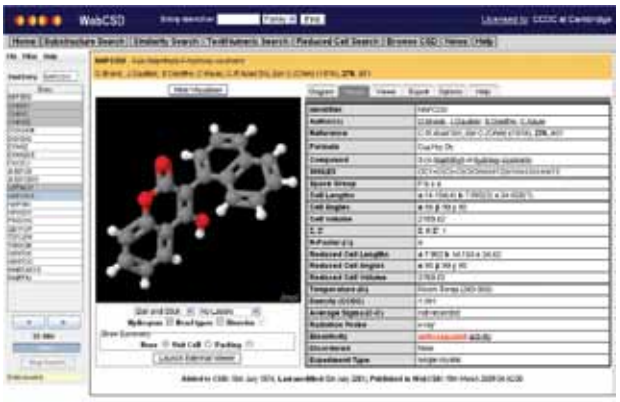
WebCSD will initially be hosted from servers at the CCDC. If you are interested in using this version of WebCSD please contact ***admin@ccdc.cam.ac.uk*** for further information. Later this year, an on-site (intranet) version will also become available that will allow organizations to make the CSD available on their own internal webs.



Results of the substructure search using the fragrment shown above. One of the hits, PINDON, is an anticoagulant agent .

WebCSD offers a range of search functionality, the focus of which is on speed, convenience and ease of access and use. Match 2D substructures, search for a specific refcode of interest, perform a reduced cell search or retrieve similar molecules to a query structure. Make use of a full range of text, numeric and bibliographic search options, with rapid retrieval of results for keyword searches e.g. *phase transition*, *activity*. Search results are displayed in 3D with a choice of embedded 3D visualizer: JMol or AstexViewer. Additional information stored with each entry, including a 2D connectivity diagram, is easily accessible via a tabbed view. Selected text fields are hyperlinked in the search results window for near instantaneous retrieval of all CSD entries containing that keyword e.g. *plate*, *cyclopentadienyl*, *Allen*.

Because WebCSD is a web application there is scope for applying automatic software and database updates. This would mean that new features could be available as soon as they are programmed, and the database could be more regularly updated e.g. weekly.



Results of clicking on the anticoagulant hyperlink in PINDON; all CSD entries with the keyword anticoagulant are returned.

With WebCSD comes much easier access to the wealth of crystallographic and structural knowledge contained in the CSD. In particular teachers obtain a tool that will have great value in the classroom: the teaching of the theory behind important chemical concepts supported by real structural data that can be visualised and inspected. Further information and teaching examples are provided on the CCDC website: ***www.ccdc.cam.ac.uk/free_services/teaching/.***

WebCSD is still being developed: if you are a WebCSD user and have feedback or comments please let CCDC know by contacting ***support@ccdc.cam.ac.uk*** or by filling in the web form provided via the Help menu in WebCSD's interface!

Susan Henderson

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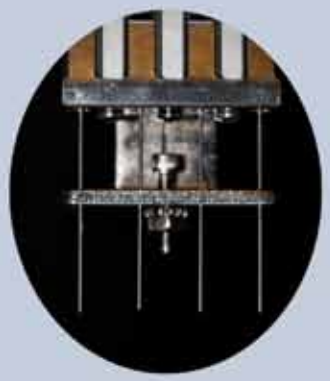

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PSI-Nature Structural Genomics Knowledgebase – a portal to structures, models, methods, and more

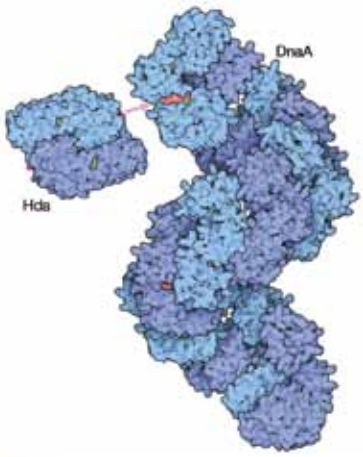
As we continue to expand our knowledge of protein space, it is becoming increasingly possible to understand the relationships between protein sequence, structure, and function. To help identify these relationships, a free, online resource, the Structural Genomics Knowledgebase (SGKB, ***kb.psi-structuralgenomics.org***) has been created. The SGKB allows a user to connect ***pro***tein sequence and three-dimensional structure to biological annotations. In addition, the SGKB enhances these results with experimental information obtained from the Protein Structure Initiative (PSI), such as current work status, protocols, DNA materials, and technologies used for protein production and structure determination. Used together, this "one-stop shop" provides comprehensive information that can enable research.

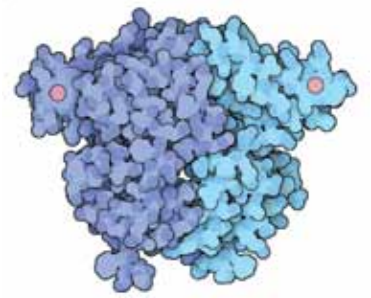
There are several ways that the SGKB can be used:

Search the SGKB by sequence/PDB ID: To search for information on individual protein sequences, the SGKB combines the resources of 6 databases to deliver one aggregate report. These include: structures from the ***Protein Data Bank (www.pdb.org);*** biological and structural annotations from the SGKB database with links to over 200 external biological resources; computational models from the ***Protein Models Portal (www.proteinmodelportal.org)***; target information - status of similar sequences from the SG target registration database ***TargetDB (targetdb.pdb.org)***; corresponding protocols from the Protein Expression, Purification, and Crystallization Database ***pepcDB (pepcdb.pdb.org)***; and availability of DNA clones from the ***PSI Material Repository (www.hip.harvard.edu/PSIMR/)***.

Browse the Research Library and Technology Portals: The ***Research Library***, updated monthly, provides a collection of articles selected by the Nature and SGKB editors that focus on structural biology, structural genomics, and metagenomics. The articles range from structural publications to methods developments. The ***Technology Portal*** presents solutions developed by the PSI centers to many laboratory bottlenecks ***(technology.lbl.gov/portal/home)***. Organized by steps in the experimental "pipeline" from cloning to annotation, the PSI ***Technology Portal*** introduces methods and technologies that can be used by non-structural specialists and structural biologists alike. Both portals can also be searched by performing a text search from the SGKB homepage.

Browse the editorial content: Each month, the Nature Publishing Group provides the ***Structural Genomics Update***, a general collection of editorials, news, and an events calendar to help keep you apprised of the latest research and technology highlights. David Goodsell (Scripps Research Institute) also writes a monthly feature, similar to the RCSB PDB's Molecule of the Month, which gives a detailed portrait of a biological molecule solved by PSI efforts. Recent articles include an illustrated description for the Hda protein. PDBID 2hcb (DnaA) and PDBID 3bos (Hda) (seen at the right), which plays an essential role in the activation of bacterial DNA replication, and CBS Domain Protein TA0289 (PDBID 2qh1 seen at the left), a protein of unknown function with an interesting history.





Services provided by the PSI and PSI SGKB:

Submitting sequences for study: *I'm interested in how structure denotes function, but what if there is no structural representative of my sequence yet?* If no similar experimental structures or computational models exist for your sequence, consider submitting your sequence for study by the PSI centers and resources for free. A community-nominated targets proposal system ***(kb.psi-structuralgenomics.org/KB/targetlogin.jsp)*** allows investigators to submit target nominations for structural determination by the 10 PSI Large-Scale and Specialized Centers. Targets that are <30% similar to sequences already in the Protein Data Bank are given priority, and authors can suggest which center to send their sequence to (see ***kb.psi-structuralgenomics.org/KB/psi_centers.html)***.

Interactive modeling service: The ***Protein Model Portal (PMP)*** also offers an interactive modeling service (see 'modeling service' option in the left menu) to create a homology model of your protein sequence using up to three modeling services. Certain restrictions apply – see the PMP site for more details.

Data for Structural Bioinformatics Methods Development: The SGKB provides two collections of data that structural bioinformaticists can use for assessing the accuracy of new methods. First, the Functional Sleuth area is a gallery of all structures solved by the PSI center whose functions have yet to be experimentally confirmed. This feature is offered as a challenge to the biological community to explore these structures and provide further insights into their possible functions. Interestingly, this subset of structures can also be used as a test set for functional prediction methods. Users can obtain this dataset by following the instructions provided on our new web services page (*kb-beta.psi-structuralgenomics.org/KB/WebServices*). In addition, the PSI recognizes that certain technology development projects could benefit from "blind test" data for assessing the accuracy of new methods before the corresponding structures are released to the public. For further information regarding currently available data (updated weekly), please visit the SGKB's See Latest Structures page at *kb.psi-structuralgenomics.org/KB/search.do?SSIDSearch=whatsnew.*

The SGKB has been created by the PSI in collaboration with Nature Publishing Group, and is updated on the 3rd Thursday of each month. You can receive notice of new editorial content (monthly) or newly released PSI structures (weekly) by subscribing to Really Simple Syndication (RSS) feeds or Nature's E-alert system, available from the KB homepage. Questions and comments regarding the SGKB can be sent to *comments@psi-structuralgenomics.org*. To learn more about the SGKB and other Nature Gateways, please visit *www.nature.com/databases* .

Margaret Gabanyi

The 6th Annual SER-CAT Symposium, University of Alabama in Huntsville, March 20-21,2009

The Symposium was hosted by the University of Alabama in Huntsville (UAH) and held at the Shelby Center for Science and Technology on the UAH Campus. ***Joseph Ng*** (UAH) was the primary organizer and coordinator for this symposium; we are very grateful for his efforts in organizing this meeting. 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. This symposium showcases the diverse and often outstanding science emanating from the use of the SER-CAT facility, and this year's meeting was no exception.

After welcoming remarks by ***Joseph Ng*** and UAH President ***David Williams***, the morning program began with a presentation by ***B. C. Wang*** (University of Georgia) who emphasized developments at SER-CAT in sulfur-SAD phase determination. In particular, SER-CAT has embarked on a program of longer wavelength ($\lambda > 1.5$Å) beamline optimization, as well as software development for data collection with an enhanced signal-to-noise ratio. B. C.'s presentation was followed by ***Liqing Chen*** (UAH) who spoke about a successful S-SAD phasing of *Penicillium expansum* lipase using 1.9Å wavelength data collected at the SER-CAT 22ID beamline. The next presentation by ***Stephen Tomanicek*** (Neutron Scattering Sciences Division, ORNL) presented structural insights into substrate recognition by the FEN-1 family of enzymes. The final talk in this session was by ***Ying Zhang*** (Georgia State University) on the structural perspectives on HIV-1 protease drug resistance, a major problem in the development of HIV/AIDS treatments.

The keynote speaker, ***Richard Myers*** (Hudson-Alpha Institute for Biotechnology, Huntsville, AL), provided a very interesting discussion of his institute's efforts directed towards a global genomic approach to human biology and disease. The next talk by ***Zhi-Jie Liu*** (Institute of Biophysics, Chinese Academy of Sciences, Beijing, China) discussed methylation-assisted crystallization of protein molecules. Methylation of lysine residues in a nuclease protein resulted in the successful production of crystals which diffracted to 1.2Å resolution. The last speaker in the morning session, ***Marc Pusey*** (Extremozyme Inc., Huntsville, AL), discussed protein crystallization screening using fluorescence anisotropy. An instrument has been assembled to test Fluorescence-based Analytical Crystallization Technologies (FACT); a high success rate was reported from studies thus far.

Guoxing Fu (Georgia State University) receives the SER-CAT Young Investigator Award from B. C. Wang

Participants at the Sixth Annual SER-CAT Symposium at the University of Alabama at Huntsville

Following lunch, eight poster presentations, primarily by students, were held in the lunch room lobby. These posters were judged, and two poster prize winners were announced at the dinner reception held that evening. The winners were ***Miranda L. Byrne-Steele*** (UAH) and ***Rosanna Robertson*** (MUSC).

James Hurley (NIDDK) was selected for the SER-CAT Outstanding Science Award. Hyung Ho Lee (NIDDK), is shown accepting the award for Hurley (inset in the lower left) from B. C. Wang"

The afternoon session began with the presentation of the Young Investigator Award to ***Guoxing Fu*** (Georgia State University) from Irene Weber's laboratory. Mr. Fu's award presentation described his work on the structural basis for substrate specificity of executioner caspases. The Outstanding Science Award was presented to ***James Hurley*** (Laboratory of Molecular Biology, NIDDK). Dr. Hurley was unable to attend the symposium, but fortunately his associate at NIDDK, ***Hyung Ho Lee***, attended and accepted the award on his behalf and presented a talk on the selected work. The lecture discussed mid-body targeting of the ESCRT machinery by a non-canonical coiled coil in CEP55.

Next, ***Alena Fedarovich*** (MUSC) discussed the challenges in the structure determination of the penicillin binding protein A from *Mycobacterium tuberculosis*. Then, ***Zhi-Qing (Albert) Fu*** (University of Georgia / SER-CAT) described the rewsults of some control tests that were run on data collected at random times at SER-CAT 22ID to search for a diagnosis of higher-than-expected HKL2000 spatial X^2's. ***John Chrzas*** (University of Georgia / SER-CAT) then described efforts to provide "Light When YOU Need It" to the SER-CAT membership by designing and implementing a virtual synchrotron. After approximately two years of work, the goal of providing a completely automated remote access beamline is very near realization. Next, ***Richard Walter*** (Shamrock Structures LLC) addressed beamline efficiency. In his opinion, based on his experiences, SER-CAT automated crystal mounting and screening implementations are some of the best that he has encountered. Lastly, ***Mark Beno*** (APS) described new opportunities for macromolecular research from the planned APS renewal. Innovations at APS in instrumentation, x-ray optics, and x-ray sources could generate orders-of-magnitude improvements in sensitivity and precision, as well as deliver new capabilities for enabling experiments that may not be performed today.

In the evening, an excellent dinner reception held inside the NASA Space and Science Rocket Center was enjoyed by all who attended. Participants were allowed to wander throughout the space center to view the various excellent rocket and space exhibits on display. After dinner, former astronaut ***Owen Garriott***, gave us a very entertaining and informative talk about his (and his son's) adventures in space. He was one of six scientist-astronauts selected by NASA in 1965. He set a world record for duration of 60 days aborad Skylab in 1973 and later was aboard Spacelab-1 in 1983. He has also held several positions at the Johnson Space Center. In 1986, after leaving NASA, he has held various important consulting and space industry positions and has received many honors and awards.

Gary Newton

It was on a short-cut through the hospital kitchens that Albert was first approached by a member of the Antibiotic Resistance.

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Diffuse Scattering and Defect Structure Simulations A Cook Book Using the Program DISCUS by Reinhard B. Neder and Thomas Proffen - December, 2008, Oxford University Press : ISBN13: 9780199233694; ISBN10: 0199233691. Hardback, 240 pages

Compared to structural analysis via diffraction methods, which has thousands of practitioners world wide, the use of diffuse scattering techniques to characterize crystal defects has stayed largely within an experts-only domain. But this new book by Reinhard Neder and Thomas Proffen will help to bring diffuse scattering into the scientific mainstream. The book is a unique contribution to the scattering literature that aims to make diffuse-scattering practitioners out of entry-level researchers (e.g. graduate students) who have only a basic knowledge of diffraction techniques and reasonably good computer skills. Given the profound impact that structural anomalies have on macroscopic material properties, and the ready access to diffuse scattering data provided by modern area detectors, the materials-characterization community has been waiting for something like this for some time. At 240 hard-bound pages, with a companion CD in the back cover, the price is not unreasonable.

Because there are already a number of outstanding books on the experimental, theoretical and computational aspects of diffuse scattering, Neder and Proffen do not focus heavily on any one of these areas. Rather, their book is a guided tour of step-by-wstep examples that utilize the DISCUS software package. Readers who work through each example and exercise as they go will walk away confident in their ability to build their own defect models and to simulate diffuse scattering patterns for comparison against experimental data, even for complicated structures where analytic descriptions would be next to impossible to derive.

The two primary applications of DISCUS are model building (*chapter 3*) and the simulation of diffuse scattering patterns (*chapter 4*). The authors highlight a variety of features for importing, exporting, assembling, modifying, querying and characterizing a model (i.e. a list of atom types, positions and occupancies), in addition to features for calculating single-crystal diffuse scattering, powder diffuse scattering and powder pair-distribution-function (PDF) patterns. These calculations are highly optimized, but still take time when operating on large models with many atoms. The central portion of the book provides well-illustrated descriptions and examples of several common defect structures, including short-range-order (*chapter 5*), occupancy and displacement waves (*chapter 6*), stacking faults (*chapter 7*) and domain structures (*chapter 8*), as well as an introduction to nanoparticle models in the context of powder PDF analysis (*chapter 9*). After explaining how to both quantitatively and visually evaluate the correlations hiding within a disordered-structure model (*chapter 10*), the book ends with an ambitious discussion of disorder-model refinement against experimental diffuse-scattering data (single-crystal or powder), and introduces an evolutionary refinement program called DIFFEV, the newest member of the DISCUS software suite (*chapter 11*).

Fundamentally, DISCUS is a command-line macro language, such that each command available to the user is a simple program. Inside the terminal window (e.g. Unix "bash" shell or Windows "cmd" shell), one can either interactively execute these commands one at a time and check results along the way, or place a sequence of commands into a macro (.mac file) and run the whole macro at once. This language provides for the naming and assignment of real and integer variables, and for numerous intrinsic math functions, logic functions and control structures. Readers will quickly discover that a macro-language is the ideal tool for generating realistic defect models. While a point-and-click GUI might allow for variations of a very specific type of model, e.g. a point defect, it wouldn't begin to cover the range of ingenuity required to handle the structures encountered in real materials. The DISCUS macro language does have some obvious limitations, though it is easy to learn and use. The fact that every macro command has been listed and described in a two-page appendix is evidence of its simplicity. An advanced user who wants additional functionality can always customize the source code, or else use home-grown software to further manipulate a model stored in a DISCUS .stru file.

In order to use the book effectively, one must first install the DISCUS software, which is available on the CD inside the book cover and also freely downloadable via the internet. When I recently installed the latest version of DISCUS on three different platforms (Windows XP, Ubuntu Linux and Mac OSX 10.4), the Windows installation was by far the easiest, only taking about 5 seconds. For the Linux and Mac platforms, I had to compile the software suite from source code (about 4 minutes on each machine) and set one environment variable to enable the online help functionality. On the Windows platform, I found it helpful to customize the DISCUS experience by modifying the .bat file invoked by the DISCUS desktop icon. A few changes allowed me to open the terminal window to the working directory of my choice, and to manually start or exit the "discus" or "kuplot" programs without closing the window, making it much easier to navigate back and forth amongst the example macros that came with the book.

The worked examples provided on the CD are so easy to read and execute that an inexperienced reader might inadvertently become proficient at simulating complicated diffuse scattering patterns without knowing very much about them. For this reason, I highly recommend reading this book in conjunction with other books such as *Diffuse X-ray Scattering and Models of Disorder* by T. R. Welberry, *Diffuse Neutron Scattering from Crystalline Materials* by V. M. Nield and D. A. Keen, *Underneath the Bragg Peaks* by T. Egami and S. J. L. Billinge, *X-Ray Diffraction in Crystals, Imperfect Crystals and Amorphous Bodies* by A. Guinier, or *Diffuse X-ray Reflections from Crystals* by W. A. Wooster. The new DISCUS "cook book" is a valuable addition to this literature and a must-have for those entering the diffuse scattering arena for the first time.

Branton J. Campbell

Synchrotron Radiation (Production and Properties). by Philip John Duke. (2009) *Oxford Science Publications*, Paperback. ISBN 0198517580.

Undoubtedly, synchrotron radiation has become a major structural research tool across the world in numerous scientific areas. As a consequence, the number of users of this unique type of radiation has increased considerably, attracting researchers from A(rcheometry) to Z(oology). Certainly, many of these will not dare to throw light on this black box; however, those who do wonder about the origins of synchrotron radiation will find in P. J. Duke's book a valuable and thorough source of facts describing its physical basis from first principles. From a single free electron to a beam of electrons in a storage ring; from Maxwell's description of electromagnetic radiation to Einstein's special theory of relativity; and from square waves to wiggles, all unfolded within merely 251 pages and 15 chapters.

More than 40 years of experience in the field qualify Duke to thoroughly cover this topic. Chapters 1-7 deal with the theoretical aspects of radiation emission from accelerated electrons while chapters 8-15 describe the practical features of electron accelerators. These are highly relevant to the general properties of the radiation beams which are ultimately produced for research applications, and they are recommended reading for those intending to pursue such applications. These later chapters also provide useful material for those wishing to extend their understanding of modern accelerators for synchrotron radiation.

However, the information that radiates from this book cannot be captured without the appropriate mathematical background and - as one immediately notices - there are plenty of formulae. This may perhaps present an obstacle or even deterrent for the enthusiast with modest mathematical ambitions. A typical synchrotron radiation user without a background in physics is likely to find it hard going. On the other hand, the author attempts to derive most of the equations within the consecutive chapters of the book (i.e. one reason why the first chapter introduces the mathematical picture of electromagnetic waves) and hence the reader is guided without having to resort to much ink and paper or specialized literature. The first four chapters provide a good introduction for physics undergraduates and the rest of the book would be of more interest to graduates aiming to become specialists in synchrotron radiation.

Bearing in mind this specialist viewpoint, it is questionable whether this volume of the series will end up in the top ten list of books for the typical synchrotron radiation user. Certainly, advanced physics students and those involved in beamline design for new synchrotron radiation sources will greatly benefit from the detailed discussions of the concepts and properties of x-ray and electron beams. Without doubt, it ought to be available on bookshelves of science libraries.

J. G. Grossmann, R. W. Strangea and V. P. Sullera,

Editors note: This review appeared when the hardcover version of the book was published (J. Synchrotron Rad. (2001). 8, 38) . Reprinted with permission of the IUCr

Remarks of President Barack Obama - National Academy of Sciences, Washington, DC, April 27, 2009

It is my privilege to address the distinguished members of the National Academy of Sciences, as well as the leaders of the National Academy of Engineering and the Institute of Medicine who have gathered here this morning.

I'd like to begin today with a story of a previous visitor who also addressed this august body.

In April of 1921, Albert Einstein visited the United States for the first time. His international celebrity was growing as scientists around the world began to understand and accept the vast implications of his theories of special and general relativity. He attended this annual meeting, and after sitting through a series of long speeches by others, he reportedly said, "I have just got a new theory of eternity." I'll do my best to heed this cautionary tale.

The very founding of this institution stands as a testament to the restless curiosity and boundless hope so essential not just to the scientific enterprise, but to this experiment we call America.

A few months after a devastating defeat at Fredericksburg, before Gettysburg would be won and Richmond would fall, before the fate of the Union would be at all certain, President Lincoln signed into law an act creating the National Academy of Sciences.

Lincoln refused to accept that our nation's sole purpose was merely to survive. He created this academy, founded the land grant colleges, and began the work of the transcontinental railroad, believing that we must add "the fuel of interest to the fire of genius in the discovery... of new and useful things."

This is America's story. Even in the hardest times, and against the toughest odds, we have never given in to pessimism; we have never surrendered our fates to chance; we have endured; we have worked hard; we have sought out new frontiers.

Today, of course, we face a more complex set of challenges than we ever have before: a medical system that holds the promise of unlocking new cures and treatments - attached to a health care system that holds the potential to bankrupt families and businesses. A system of energy that powers our economy - but also endangers our planet. Threats to our security that seek to exploit the very interconnectedness and openness so essential to our prosperity. And challenges in a global marketplace which links the derivative trader on Wall Street to the homeowner on Main Street, the office worker in America to the factory worker in China - a marketplace in which we all share in opportunity, but also in crisis.

At such a difficult moment, there are those who say we cannot afford to invest in science. That support for research is somehow a luxury at a moment defined by necessities. I fundamentally disagree. Science is more essential for our prosperity, our security, our health, our environment, and our quality of life than it has ever been. And if there was ever a day that reminded us of our shared stake in science and research, it's today.

We are closely monitoring the emerging cases of swine flu in the United States. This is obviously a cause for concern and requires a heightened state of alert. But it is not a cause for alarm. The Department of Health and Human Services has declared a Public Health Emergency as a precautionary tool to ensure that we have the resources we need at our disposal to respond quickly and effectively. I'm getting regular updates on the situation from the responsible agencies, and the Department of Health and Human Services as well as the Centers for Disease Control will be offering regular updates to the American people so that they know what steps are being taken and what steps they may need to take. But one thing is clear - our capacity to deal with a public health challenge of this sort rests heavily on the work of our scientific and medical community. And this is one more example of why we cannot allow our nation to fall behind.

Unfortunately, that is exactly what has happened.

Federal funding in the physical sciences as a portion of our gross domestic product has fallen by nearly half over the past quarter century. Time and again we've allowed the research and experimentation tax credit, which helps businesses grow and innovate, to lapse.

Our schools continue to trail. Our students are outperformed in math and science by their peers in Singapore, Japan, England, the Netherlands, Hong Kong, and Korea, among others. Another assessment shows American fifteen year olds ranked 25th in math and 21st in science when compared to nations around the world.

And we have watched as scientific integrity has been undermined and scientific research politicized in an effort to advance predetermined ideological agendas.

We know that our country is better than this.

A half century ago, this nation made a commitment to lead the world in scientific and technological innovation; to invest in education, in research, in engineering; to set a goal of reaching space and engaging every citizen in that historic mission. That was the high water mark of America's investment in research and development. Since then our investments have steadily declined as a share of our national income - our GDP. As a result, other countries are now beginning to pull ahead in the pursuit of this generation's great discoveries.

I believe it is not in our American character to follow - but to lead. And it is time for us to lead once again. I am here today to set this goal: we will devote more than three percent of our GDP to research and development. We will not just meet, but we will exceed the level achieved at the height of the Space Race, through policies that invest in basic and applied research, create new incentives for private innovation, promote breakthroughs in energy and medicine, and improve education in math and science. This represents the largest commitment to scientific research and innovation in American history.

Just think what this will allow us to accomplish: solar cells as cheap as paint, and green buildings that produce all of the energy they consume; learning software as effective as a personal tutor;

prosthetics so advanced that you could play the piano again; an expansion of the frontiers of human knowledge about ourselves and world the around us. We can do this.

The pursuit of discovery half a century ago fueled our prosperity and our success as a nation in the half century that followed. The commitment I am making today will fuel our success for another fifty years. That is how we will ensure that our children and their children will look back on this generation's work as that which defined the progress and delivered the prosperity of the 21st century.

This work begins with a historic commitment to basic science and applied research, from the labs of renowned universities to the proving grounds of innovative companies.

Through the American Recovery and Reinvestment Act and with the support of Congress, my administration is already providing the largest single boost to investment in basic research in American history.

This is important right now, as public and private colleges and universities across the country reckon with shrinking endowments and tightening budgets. But this is also incredibly important for our future. As Vannevar Bush, who served as scientific advisor to President Franklin Roosevelt, famously said: "Basic scientific research is scientific capital."

The fact is, an investigation into a particular physical, chemical, or biological process might not pay off for a year, or a decade, or at all. And when it does, the rewards are often broadly shared, enjoyed by those who bore its costs but also by those who did not.

That's why the private sector under-invests in basic science - and why the public sector must invest in this kind of research. Because while the risks may be large, so are the rewards for our economy and our society.

No one can predict what new applications will be born of basic research: new treatments in our hospitals; new sources of efficient energy; new building materials; new kinds of crops more resistant to heat and drought.

It was basic research in the photoelectric effect that would one day lead to solar panels. It was basic research in physics that would eventually produce the CAT scan. The calculations of today's GPS satellites are based on the equations that Einstein put to paper more than a century ago.

In addition to the investments in the Recovery Act, the budget I've proposed - and versions have now passed both the House and Senate - builds on the historic investments in research contained in the recovery plan.

We double the budget of key agencies, including the National Science Foundation, a primary source of funding for academic research, and the National Institute of Standards and Technology, which supports a wide range of pursuits - from improving health information technology to measuring carbon pollution, from testing "smart grid" designs to developing advanced manufacturing processes. And my budget doubles funding for the Department of Energy's Office of Science which builds and operates accelerators, colliders, supercomputers, high-energy light sources, and facilities for making nano-materials. Because we know that a nation's potential for scientific discovery is defined by the tools it makes available to its researchers.

But the renewed commitment of our nation will not be driven by government investment alone. It is a commitment that extends from the laboratory to the marketplace.

That is why my budget makes the research and experimentation tax credit permanent. This is a tax credit that returns two dollars to the economy for every dollar we spend, by helping companies afford the often high costs of developing new ideas, new technologies, and new products. Yet at times we've allowed it to lapse or only renewed it year to year. I've heard this time and again from entrepreneurs across this country: by making this credit permanent, we make it possible for businesses to plan the kinds of projects that create jobs and economic growth.

Second, in no area will innovation be more important than in the development of new technologies to produce, use, and save energy - which is why my administration has made an unprecedented commitment to developing a 21st century clean energy economy.

Our future on this planet depends upon our willingness to address the challenge posed by carbon pollution. And our future as a nation depends upon our willingness to embrace this challenge as an opportunity to lead the world in pursuit of new discovery.

When the Soviet Union launched Sputnik a little more than a half century ago, Americans were stunned: the Russians had beaten us to space. We had a choice to make: we could accept defeat - or we could accept the challenge. And as always, we chose to accept the challenge.

President Eisenhower signed legislation to create NASA and to invest in science and math education, from grade school to graduate school. And just a few years later, a month after his address to the 1961 Annual Meeting of the National Academy of Sciences, President Kennedy boldly declared before a joint session of Congress that the United States would send a man to the moon and return him safely to the earth.

The scientific community rallied behind this goal and set about achieving it. And it would lead not just to those first steps on the moon, but also to giant leaps in our understanding here at home. The Apollo program itself produced technologies that have improved kidney dialysis and water purification systems; sensors to test for hazardous gasses; energy-saving building materials; and fire-resistant fabrics used byfirefighters and soldiers. And, more broadly, the enormous investment of that era -in science and technology, in education and research funding - produced a great outpouring of curiosity and creativity, the benefits of which have been incalculable.

The fact is, there will be no single Sputnik moment for this generation's challenge to break our dependence on fossil fuels. In many ways, this makes the challenge even tougher to solve - and makes it all the more important to keep our eyes fixed on the work ahead.

That is why I have set as a goal for our nation that we will reduce our carbon pollution by more than 80 percent by 2050. And that is why I am pursuing, in concert with Congress, the policies that will help us meet this goal.

My recovery plan provides the incentives to double our nation's capacity to generate renewable energy over the next few years - extending the production tax credit, providing loan guarantees, and offering grants to spur investment. For example, federally funded research and development has dropped the cost of solar panels by ten-fold over the last three decades. Our renewed efforts will ensure that solar and other clean energy technologies will be competitive.

My budget includes $150 billion over ten years to invest in sources of renewable energy as well as energy efficiency; it supports efforts at NASA, recommended as a priority by the National Research Council, to develop new space-based capabilities to help us better understand our changing climate.

And today, I am also announcing that for the first time, we are funding an initiative - recommended by this organization - called the Advanced Research Projects Agency for Energy, or ARPA-E.

This is based on the Defense Advanced Research Projects Agency, known as DARPA, which was created during the Eisenhower administration in response to Sputnik. It has been charged throughout its history with conducting high-risk, high-reward research. The precursor to the internet, known as ARPANET, stealth technology, and the Global Positioning System all owe a debt to the work of DARPA.

ARPA-E seeks to do this same kind of high-risk, high-reward research. My administration will also pursue comprehensive legislation to place a market-based cap on carbon emissions. We will make renewable energy the profitable kind of energy in America. And I am confident that we will find a wellspring of creativity just waiting to be tapped by researchers in this room and entrepreneurs across our country.

The nation that leads the world in 21st century clean energy will be the nation that leads in the 21st century global economy. America can and must be that nation.

Third, in order to lead in the global economy - and ensure that our businesses can grow and innovate, and our families can thrive - we must address the shortcomings of our health care system.

The Recovery Act will support the long overdue step of computerizing America's medical records, to reduce the duplication, waste, and errors that cost billions of dollars and thousands of lives.

But it's important to note: these records also hold the potential of offering patients the chance to be more active participants in prevention and treatment. We must maintain patient control over these records and respect their privacy. At the same time, however, we have the opportunity to offer billions and billions of anonymous data points to medical researchers who may find in this information evidence that can help us better understand disease.

History also teaches us the greatest advances in medicine have come from scientific breakthroughs: the discovery of antibiotics; improved public health practices; vaccines for smallpox, polio, and many other infectious diseases; anti-retroviral drugs that can return AIDS patients to productive lives; pills that can control certain types of blood cancers; and so many others.

And because of recent progress - not just in biology, genetics and medicine, but also in physics, chemistry, computer science, and engineering - we have the potential to make enormous progress against diseases in the coming decades. That is why my Administration is committed to increasing funding for the National Institutes of Health, including $6 billion to support cancer research, part of a sustained, multi-year plan to double cancer research in our country.

Fourth, we are restoring science to its rightful place.

On March 9th, I signed an executive memorandum with a clear message: Under my administration, the days of science taking a back seat to ideology are over. Our progress as a nation - and our values as a nation - are rooted in free and open inquiry. To undermine scientific integrity is to undermine our democracy.

That is why I have charged the White House Office of Science and Technology Policy with leading a new effort to ensure that federal policies are based on the best and most unbiased scientific information. I want to be sure that facts are driving scientific decisions - and not the other way around.

As part of this effort, we've already launched a website that allows individuals to not only make recommendations to achieve this goal, but to collaborate on those recommendations; it is a small step, but one that is creating a more transparent, participatory and democratic government.

We also need to engage the scientific community directly in the work of public policy. That is why, today, I am announcing the appointment of the President's Council of Advisors on Science and Technology, known as PCAST, with which I plan to work closely.

This council represents leaders from many scientific disciplines who will bring a diversity of experiences and views. I will charge PCAST with advising me about national strategies to nurture and sustain a culture of scientific innovation. It will be co-chaired by John Holdren, my top science advisor; Eric Lander, one of the principal leaders of the Human Genome Project; and Harold Varmus, former head of the National Institutes of Health and a Nobel laureate.

In biomedicine, for example, this will include harnessing the historic convergence between life sciences and physical sciences that is underway today; undertaking public projects - in the spirit of the Human Genome Project - to create data and capabilities that fuel discoveries in tens of thousands of laboratories; and identifying and overcoming scientific and bureaucratic barriers to rapidly translating scientific breakthroughs into diagnostics and therapeutics that serve patients.

In environmental science, it will require strengthening our weather forecasting, our earth observation from space, the management of our nation's land, water and forests, and the stewardship of our coastal zones and ocean fisheries.

We also need to work with our friends around the world. Science, technology, and innovation proceed more rapidly and more cost-effectively when insights, costs, and risks are shared; and so many of the challenges that science and technology will help us meet are global in character. This is true of our dependence on oil, the consequences of climate change, the threat of epidemic disease, and the spread of nuclear weapons, among other examples.

That is why my administration is ramping up participation in - and our commitment to - international science and technology cooperation across the many areas where it is clearly in our interest to do so. In fact, this week, my administration is gathering the leaders of the world's major economies to begin the work of addressing our common energy challenges together.

Fifth, since we know that the progress and prosperity of future generations will depend on what we do now to educate the next generation, today I am announcing a renewed commitment to education in mathematics and science.

Through this commitment, American students will move from the middle to the top of the pack in science and math over the next decade. For we know that the nation that out-educates us today - will out-compete us tomorrow.

We cannot start soon enough. We know that the quality of math and science teachers is the most influential single factor in determining whether a student will succeed or fail in these subjects. Yet, in high school, more than twenty percent of students in math and more than sixty percent of students in chemistry and physics are taught by teachers without expertise in these fields. And this problem is only going to get worse; there is a projected shortfall of more than 280,000 math and science teachers across the country by 2015.

That is why I am announcing today that states making strong commitments and progress in math and science education will be eligible to compete later this fall for additional funds under the Secretary of Education's $5 billion Race to the Top program.

I am challenging states to dramatically improve achievement in math and science by raising standards, modernizing science labs, upgrading curriculum, and forging partnerships to improve the use of science and technology in our classrooms. And I am challenging states to enhance teacher preparation and training, and to attract new and qualified math and science teachers to better engage students and reinvigorate these subjects in our schools.

In this endeavor, and others, we will work to support inventive approaches. Let's create systems that retain and reward effective teachers, and let's create new pathways for experienced professionals to enter the classroom. There are, right now, chemists who could teach chemistry; physicists who could teach physics; statisticians who could teach mathematics. But we need to create a way to bring the expertise and the enthusiasm of these folks - folks like you - into the classroom.

There are states, for example, doing innovative work. I am pleased to announce that Governor Ed Rendell (PA) will lead an effort with the National Governors Association to increase the number of states that are making science, technology, engineering and mathematics education a top priority. Six states are currently participating in the initiative, including Pennsylvania, which has launched an effective program to ensure that his state has the skilled workforce in place to draw the jobs of the 21st century. I'd want every state participate.

But our work does not end with a high school diploma. For decades, we led the world in educational attainment, and as a consequence we led the world in economic growth. The G.I. Bill, for example, helped send a generation to college. But in this new economy, we've come to trail other nations in graduation rates, in educational achievement, and in the production of scientists and engineers.

That's why my administration has set a goal that will greatly enhance our ability to compete for the high-wage, high-tech jobs of the 21st century - and to foster the next generation of scientists and engineers. In the next decade - by 2020 - America will once again have the highest proportion of college graduates in the world. And we've provided tax credits and grants to make a college education more affordable.

My budget also triples the number of National Science Foundation graduate research fellowships. This program was created as part of the Space Race five decades ago. In the decades since, it's remained largely the same size - even as the numbers of students who seek these fellowships has skyrocketed. We ought to be supporting these young people who are pursuing scientific careers, not putting obstacles in their path.

This is how we will lead the world in new discoveries in this new century. But it will take far more than the work of government. It will take all of us. It will take all of you.

And so today I want to challenge you to use your love and knowledge of science to spark the same sense of wonder and excitement in a new generation.

America's young people will rise to the challenge if given the opportunity - if called upon to join a cause larger than themselves. And we've got evidence. The average age in NASA's mission control during the Apollo 17 mission was just 26. I know that young people today are ready to tackle the grand challenges of this century

So I want to persuade you to spend time in the classroom, talking - and showing -young people what it is that your work can mean, and what it means to you. Encourage your university to participate in programs to allow students to get a degree in scientific fields and a teaching certificate at the same time. Think about new and creative ways to engage young people in science and engineering, like science festivals, robotics competitions, and fairs that encourage young people to create, build, and invent - to be makers of things.

And I want you to know that I'm going to be working along side you. I'm going to participate in a public awareness and outreach campaign to encourage students to consider careers in science, mathematics, and engineering - because our future depends on it.

And the DOE and the NSF will be launching a joint initiative to inspire tens of thousands of American students to pursue careers in science, engineering and entrepreneurship related to clean energy.

It will support an educational campaign to capture the imagination of young people who can help us meet the energy challenge. It will create research opportunities for undergraduates and educational opportunities for women and minorities who too often have been underrepresented in scientific and technological fields - but are no less capable of inventing the solutions that will help us grow our economy and save our planet. And it will support fellowships, interdisciplinary graduate programs, and partnerships between academic institutions and innovative companies to prepare a generation of Americans to meet this generational challenge.

For we must always remember that somewhere in America there's an entrepreneur seeking a loan to start a business that could transform an industry - but she hasn't secured it yet. There's a researcher with an idea for an experiment that might offer a new cancer treatment - but he hasn't found the funding yet. There is a child with an inquisitive mind staring up at the night sky. Maybe she has the potential to change our world - but she just doesn't know it yet.

As you know, scientific discovery takes far more than the occasional flash of brilliance - as important as that can be. Usually, it takes time, hard work, patience; it takes training; often, it requires the support of a nation.

But it holds a promise like no other area of human endeavor.

In 1968, a year defined by loss and conflict, Apollo 8 carried into space the first human beings ever to slip beyond the earth's gravity. The ship would circle the moon ten times before returning home. But on its fourth orbit, the capsule rotated and for the first time earth became visible through the windows.

Bill Anders, one of the astronauts aboard Apollo 8, could not believe what he saw. He scrambled for a camera. He took a photo that showed the earth coming up over the moon's horizon. It was the first ever taken from so distant a vantage point, soon to become known as "Earthrise."

Anders would say that the moment forever changed him, to see our world - this pale blue sphere - without borders, without divisions, at once so tranquil and beautiful and alone.

"We came all this way to explore the moon," he said, "and the most important thing is that we discovered the Earth."

Yes, scientific innovation offers us the chance to achieve prosperity. It has offered us benefits that have improved our health and our lives - often improvements we take too easily for granted. But it also gives us something more.

At root, science forces us to reckon with the truth as best as we can ascertain it. Some truths fill us with awe. Others force us to question long held views. Science cannot answer every question; indeed, it seems at times the more we plumb the mysteries of the physical world, the more humble we must be. Science cannot supplant our ethics, our values, our principles, or our faith, but science can inform those things, and help put these values, these moral sentiments, that faith, to work - to feed a child, to heal the sick, to be good stewards of this earth.

We are reminded that with each new discovery and the new power it brings, comes new responsibility; that the fragility and the sheer specialness of life requires us to move past our differences, to address our common problems, to endure and continue humanity's strivings for a better world.

As President Kennedy said when he addressed the National Academy of Sciences more than 45 years ago: "The challenge, in short, may be our salvation."

Thank you all for your past, present, and future discoveries. God bless bless you and may God bless the United States of America.

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See page 43 for a full list of current sponsors of the 2009 ACA Meeting in Toronto and the meeting website (www.cins.ca/aca2009/) for anything added after we went to press.

Candidates for ACA offices in 2010

The Nominating Committee has proposed the following candidates for the 2009 elections for ACA offices in 2010:

Vice-President: **Jim Britten and Tom Koetzle**

Treasurer: **Bernie Santarsiero**

***Committees*:**

Communicatons: **Ross Angel and Stephan Ginell**

Data, Standards & Computing: **Ilia Guzei and Cora Lind**

Continuing Education: **Frank Fronczek and Charles Lake**

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, 2009 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 2009.

Jim Britten-Vice-President

Manager, MAX Diffraction Facility, Department of Chemistry and Brockhouse Institute for Materials Research, McMaster University, Hamilton, ON, Canada

Education: BSc, Saintt.Francis.Xavier U. (1977); PhD, McMaster U. (1984); NSERC PDF, U. de Montreal (1984, 1985); Killam PDF, Dalhousie U. (1986)

Professional Activities: Program Co-chair for 2014 IUCr Congress, Montreal; Program Chair, ACA2009, Toronto; Organized First Canadian Chemical Crystallography Workshop (Hamilton, ON, May 2009); Co-organizer of 'Frontiers in Materials Characterization with X-Rays, Neutrons and Electrons' session for 2009 CSC, Hamilton, ON; Invited Speaker, Advanced Crystallography Workshop, ChemMatCARS, APS, (Dec.3-5, 2008); Canadian Representative to ACA Council (2008-2010), Vice-Chair, Canadian National Committee for Crystallography (2007-present); Member of Beamline Advisory Committee, CLS; Reviewer for Journal of Chemical Crystallography; Chair, Canadian Division of ACA (2003-2006); Invited Speaker in ACA2007 *Transactions* Symposium on 'Diffuse Scattering'; Co-organizer of 'Laboratory X-Ray and Neutron Diffraction for Materials Chemistry' session for 2007 CSC, Winnipeg, MN; Co-organizer of session 'Canadian Light Source' at 2006 ACA Meeting; Member of ACA; Chair, ACA Service SIG, 1997; Secretary, ACA Canadian Division 1998, 1999; Organizer of session on 'Service Crystallography at Synchrotrons', ACA Meeting, 2000; Advisory Committee member for McMaster's Research and High Performance Computing Support Group; Member of Canadian Institute for Synchrotron Radiation; Principal Investigator for Small Molecule Crystallography Beamline Proposal (approved) at the CLS; Member of the Beamline Team for the Brockhouse Scattering and Diffraction Sector at the CLS.

Research Interests: Molecular and solid state crystallography; reciprocal space volumes; diffuse scattering; 2D and 3D powder diffraction of alloys, films, and polymers; synchrotron crystallography; crystallographic education; charge density. I am first and foremost a service crystallographer. Most of my clients are graduate students – chemists, physicists, and engineers. There are two SOP's in my lab which we always follow. First, we will try to tackle any problem posed by the student at least once, even if it means pushing the diffractometer in directions that were not originally in the manual. Second, the student must teach us something about the material in question. This approach to characterization keeps the job interesting, keeps the students involved in the analyses, and continuously expands our repertoire. In order to carefully examine the variety of diffraction patterns we are measuring, we have developed a software package to display the full 3D diffraction volume resulting from area detector scans. This has turned out to be an invaluable tool for screening crystals, examining diffuse scattering, monitoring phase changes, studying the polycrystalline texture of alloys, polymers or thin films, and explaining to students exactly what we (or they) were observing. For the tougher problems, we and others are building a small molecule diffraction beamline at the Canadian Light Source.

Statement: It is an honor to have been nominated as a candidate for Vice-President of the ACA. My previous experience on council has shown me that the cornerstones which keep the organization stable are Marcia Colquhoun, Bill Duax, Narasinga Rao, and Bernie Santarsiero. The remaining council members are given the opportunity to make things better, but not worse.

This is an invaluable organization for crystallographers, and the atmosphere of mutual respect without formalities has put many young scientists in direct contact with the leaders in the field.

There are several important initiatives in progress that we need to reinforce. The

ACA is a regional organization representing the Americas. Efforts are being made to encourage and assist in the participation of more South American countries and their crystallographers. We need to continue supporting the international development of crystallography, and find ways to overcome the financial and political barriers to the growth of our community. The high percentage of international abstracts for the Toronto meeting demonstrates the widespread interest in the ACA.

The efforts of our current President to bring the powder diffraction community (ICDD/DXC) and the ACA together under the same roof will eventually lead to larger, more cost effective meetings, new possibilities for scientific sessions, less travel for our members, and a more attractive venue for the exhibitors. This initiative will succeed, but it will require continued cooperation, negotiation and refinement over the years.

A number of our members have been trying to get more crystallography into high schools and undergraduate programs, and to get more students out to ACA meetings. Increased funding for student travel and more opportunities for graduate students to give oral presentations at our meetings will help sustain an interest in our science and in ACA participation. In this internet age, with so many authoring tools at our disposal, we should be able to set up a web page that gets younger as we get older and wiser. Council should work closely with our Continuing Education Committee and provide them with resources to improve our web offerings and support our teaching resource contributors. We should be adding to, and benefiting from, the resources available through the IUCr. Not only do we need to develop the skills of our young crystallographers, but we must be able to explain the usefulness of crystallography to the public (including high school teachers and students) as well as provide some theory and tools to graduate students who would rather become chemists, biochemists, physicists, material scientists, engineers, etc.

Another area that needs a bit of a tune-up is the relationship between the ACA and the IUCr. We have a former ACA President, Louis Delbaere, on the IUCr Executive Council (EC) and representing the IUCr at ACA Council meetings. We have several of our members chairing or participating in IUCr Commissions and we have excellent participation from the EC in the scientific program for the Toronto meeting. We could do more. Bringing the JANA workshop to our members exposes us directly to recent advances in crystallography in Europe. The ACA should have a mechanism to formally sponsor presentations by our members at crystallographic meetings around the world. The IUCr congress will be held in Montreal in 2014, and we should be strengthening our international scientific ties in the meantime.

It all boils down to tracking down the financial resources required. If elected to the VP office, I will work with my colleagues towards achieving these goals. If the membership chooses to elect my worthy opponent, you will still find me working with my colleagues towards achieving these goals.

Thomas F. Koetzle -Vice-President

Senior Chemist, Brookhaven National Laboratory (Retired); Special Term Appointee, Argonne National Laboratory; Scientific Secretary, Instrument Development Team for the TOPAZ Single-Crystal Diffractometer at Oak Ridge National Laboratory's Spallation Neutron Source (SNS).

Education: Harvard University, Chemistry, AB (1964), AM (1965), PhD (1970), with William Lipscomb; Brookhaven National Laboratory, AEC and NIH postdoctoral fellow, 1970-1973, with Walter Hamilton.

Professional Activities: Scientific Staff Member, Brookhaven National Laboratory, 1973-1998; Head, Protein Data Bank (PDB), 1973-1993. Guest and Special Term Appointment-Senior Scientist, Argonne National Laboratory Intense Pulsed Neutron Source (IPNS), 1999-2008. Science and Technology Agency Fellow, Japan Atomic Energy Research Institute, 2000. Member, USA National Committee for Crystallography, 1984-1986, 1988-1990. President, Pittsburgh Diffraction Society, 2006. ACA Activities: Committee on Crystallographic Data, 1974-1976 (Chair, 1976); Neutron Scattering SIG (Founding Chair, 1983-1984), Synchrotron Radiation SIG (Chair, 1999), Biological Macromolecules SIG; ACA *Transactions* Symposium Co-Chair (1980, 2006). IUCr: Commission on Crystallographic Data, 1984-1993. Member, Program Advisory Committee, Los Alamos Neutron Science Center, 1998-2002, and CCLRC Rutherford Appleton Laboratory ISIS Facility Access Panel, 2004-2007. SNUG (Synchrotron and Neutron Users Group) representative, 2005-2008. General Editor, *Molecular Structures in Biology*, Oxford University Press, 1991.

Research Interests: I was introduced to crystallography at Harvard when I joined the Lipscomb research group as a second-year graduate student and began to work on the structures of polyhedral carboranes. The year was 1965, a fascinating time, and direct methods were just coming into use. I remember carrying out symbolic addition by hand and being excited and amazed when the structure fell out of my first E-map. Crystallography surely has come a long way since then!

After my PhD, I moved to Brookhaven to postdoc with Walter Hamilton. During this time we carried out a series of neutron diffraction studies at the High Flux Beam Reactor (HFBR) including structure determinations of most of the common, naturally occurring amino acids. The ability of neutrons to 'see' hydrogen atoms and to accurately determine their positional and thermal parameters was opening up many exciting possibilities, and I decided to make the application of single-crystal neutron diffraction to problems in structural chemistry a central theme of my career. Also at Brookhaven, following Hamilton's untimely death in 1973, I became the first head of the PDB.

Working with many dedicated Brookhaven colleagues, and in collaboration with Helen Berman and Edgar Meyer, I guided the PDB resource for two decades from its inception through the start of a period of explosive growth that has brought the number of structures in the database from well over 1000 in 1993 to over 57000 as of this writing.

Highlights of our neutron diffraction research at the HFBR include our studies of metal hydrides and molecular dihydrogen complexes, where we systematically explored the principles for bonding between hydrogen and transition metals with many collaborators, including the late Robert Bau and his students, and Alberto Albinati. More recently, working with Arthur Schultz and collaborators at the IPNS at Argonne, I participated in investigations of covalent bond activation in transition metal sigma complexes, in which two electrons in an X–H sigma-bond form a dative bond with a transition metal, and which are of great relevance in catalysis.

Going forward, pulsed neutron sources are making increasingly important contributions especially now that the SNS has come on line at Oak Ridge. Since 2002 I have had a leadership role in the development of the SNS TOPAZ single-crystal diffractometer, which is scheduled to begin operation later this year and which is expected to greatly advance the capabilities of neutron diffraction. Surely, there will be an explosion of new applications of neutrons in crystallography, and the community of users will grow dramatically, much as has occurred over the years with x-rays at synchrotron radiation sources.

Statement: It is a great honor to be nominated as a candidate for the office of Vice-President. Ever since I joined the ACA as a fresh postdoc, I have thought of the ACA as my professional home. I have received so much from the ACA during my career and, if I am elected, it would be a privilege to have the opportunity to serve and to give back a small measure of what I have received.

Many times over the years I have heard members express their feelings for the ACA as a unique community. Looking back to the first meeting I attended, in 1970 in New Orleans, I can still remember the warmth and friendliness of a number of eminent, senior crystallographers in attendance who showed genuine interest in me and in answering my questions. As the ACA has grown, I feel it is truly remarkable that this community atmosphere has endured and, indeed, has strengthened. It is a testament to the efforts of our many colleagues who have served on the ACA Council, and of our incredible dedicated staff in the Buffalo Office, that each year when we convene at our annual meeting we can enjoy the unique 'small town' atmosphere that is the ACA. We can, and indeed we must, leverage our strength as a cohesive community to maximize our effectiveness going forward.

This is a time of exciting opportunities with the significant new support for science in the U.S. Federal Government's economic stimulus package. From the perspective of the crystallographic community, a significant portion of new funding is likely to be channeled through user facilities and shared resources. The ACA should continue to play a central role in informing the community on the resources that are available, and in coordinating education and outreach activities with those of the user facilities. For example, we should foster increased interaction of the ACA Small Molecule and Macromolecular Summer Schools with schools and workshops sponsored by the neutron and synchrotron radiation facilities. I feel that it also would be useful for the ACA to establish a formal presence at the facilities' annual user meetings so that, in particular, young scientists who are users of crystallography at the facilities will be encouraged to join the ACA. Years back, the formation of Special Interest Groups helped the ACA to attract to our meetings those who may identify themselves primarily as biologists, chemists, or materials scientists. Today, by reaching out to the synchrotron and neutron user facilities and other shared resources, the ACA can participate fully in the growth stimulated by these facilities. Outreach activities such as this will help ensure that the ACA retains its place at the center of gravity of our community. At our own annual meetings, I would encourage the program chairs to arrange more sessions with joint sponsorships in order to further our interactions with societies having shared interests with the ACA.

The person elected to serve as ACA Vice-President, and then as President, has the responsibility to be a spokesperson for our community. I believe that my varied background working at user facilities and at the PDB, where I have had the privilege of interacting with a broad cross-section of the ACA membership, together with my experience serving as President of the Pittsburgh Diffraction Society, would be valuable in this role. The relationships that I have formed through the ACA have always been a source of tremendous satisfaction to me, and I would welcome the chance to be of service to our community.

Bernard D. Santarsiero - Treasurer

Research Professor, Center for Pharmaceutical Biotechnology (CPB); Adjunct Research Professor, Department of Medicinal Chemistry and Pharmacognosy, University of Illinois at Chicago, Chicago, IL
Education: BS, Chemistry, Harvey Mudd College (1975). PhD, Physical Chemistry, University of Washington (1980).

Professional Activities: Member: ACS, ACA, American Society for Pharmacognosy, Protein Society; ACA Apparatus and Standards Committee (1997-1999); Structural Biology Review Board, NASA (1998-2002); SER-CAT Automation Committee (2002-present); Co-founder and consultant, Syrrx (1996-2002); Local co-chair, ACA Annual Meeting (2004, 2010); Instructor, ACA Crystallography Summer Course (2002-2004); Manager, Information Technology, CPB (2003-present); Manager, Small Molecule X-ray Diffraction Facility (2003-present); Co-Manager, Macromolecular Structure Facility (2004-present); Science Advisory Board, Shamrock Structures (2003-present); Secy, Gerber-Hart Library (2005-

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think forward

Crystallography

2008); USNCCr (2006-2009); Member, Ed. Advisory Board, *Journal of Natural Products* (2007-present).

Research Interests: My research spans four major themes: structure-based drug design of therapeutics against disease, identification of natural products as chemopreventative, anti-cancer, and anti-infectious agents, the analysis and redesign of enzymes to modify specificity, stability, and reactivity, and the development of enabling technologies in biological and chemical crystallography, including variable temperature and pressure, solution, powder and neutron diffraction.

Statement: The ACA Treasurer serves the membership by overseeing the financial commitments of the organization, and as a representative of the council to the American Institute of Physics and the US National Committee for Crystallography. The ACA is in excellent financial shape after a decade of strong leadership. We continue to keep membership dues and conference costs low while still providing the resources necessary to host interesting annual meetings by choosing wisely in meeting sites and organizing excellent scientific programs. The council continues to do a good job in broadening the appeal of membership in the ACA, and in fostering the education of physical, chemical, and biological crystallography on a national and international scale. I am a strong advocate for education, sustained government support of our research, and the continuing vision of molecular structure as a unique portal towards the understanding of function, reactivity, and energetics of physical, chemical, and biological systems. On a personal level, I have been a member of the ACA for nearly thirty years and I continue to marvel at the continuing improvement and expansive use of our craft, and thoroughly enjoy attending the annual meetings with old colleagues and new acquaintances. It would be an honor to serve again as your Treasurer and Council member, and I appreciate the opportunity to "give back" something to the organization. I hope that you will seek me out to voice concerns and offer suggestions about the ACA: ***bds@uic.edu.***

Editors note: *The ACA-Bylaws allow for the nomination of a single candidate only in the case of a treasurer running for a second term. All other offices must have a minimum of two candidates.*

Ross J. Angel – Communications

Research Professor, Dept of Geological Science, Virginia Tech, Blacksburg, VA

Education: MA (1972) and PhD (1985) University of Cambridge, England. Postdocs at SUNY Stony Brook, Carnegie Institution of Washington, University College, London.

Professional Activities: Associate Editor, *European Journal of Mineralogy,* (1994-present), Member, Mineral and Rock Physics Committee of AGU (2002-present), Councillor, and meetings coordinator, Mineralogical Society of America (2005-2007) Member, Facilities Access Panel, ISIS spallation neutron source, UK (2004 – 2007), Program Chair ACA Meeting, 2010.

Research Interests: The characterization of compression mechanisms, structural phase transitions, crossovers, and compression mechanism changes in minerals by high-pressure diffraction in order to understand the crystal-chemical factors that determine the evolution of crystal structures with pressure. The main method I employ is single-crystal high-pressure diffraction, for which I am continuing to develop software for diffractometer control and data reduction.

Statement: If elected to serve on the Communications Committee of the ACA I would work with my colleagues to develop a better understanding of crystallography both within and without the ACA. Within the ACA it is important not to let the great breadth of crystallography become a barrier to communication and exchange of ideas; all of us would benefit from greater integration of the scientific program at our annual meetings by the promotion of more interdisciplinary sessions. Outside of our organization, we should take the opportunity of our annual meetings to advertise our science to the general public. We must also work with our scientific colleagues to overcome the common impression that crystallography now only has a service role. We must regain the respect that the profession of crystallography used to receive. Perhaps the ACA could take one step towards this goal by initiating an ACA lecture tour to universities and colleges.

Stephan L. Ginell - Communications

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

Education: PhD Biophysics (1980), 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 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) , workshop and program organizer for numerous NSLS and APS users meetings (1995 to present), lecturer at the Cold Spring Harbor Laboratory workshop

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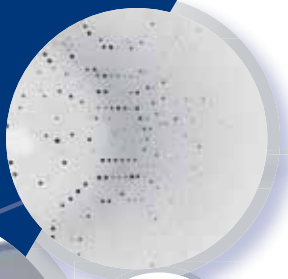

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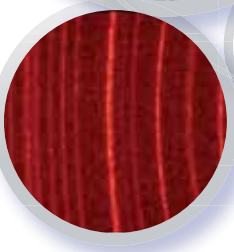

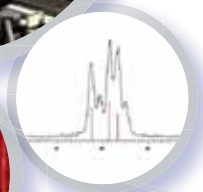

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on crystallographic methods (1993-1998), Local committee member, ACA, Philadelphia meeting (1988), Member of ACA, AAAS, Sigma Xi.

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. Clearly communicating our scientific results and agendas 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, and for the general success of our society. A strong and focused PR presentation by the ACA in support of our member's research is essential. Additional areas that I would like to see have more support are communication between the different disciplines of crystallography and between the crystallographic community and other areas of science. If elected, I will strive to make communication amongst the members of our scientific community and with the general public a priority of the utmost importance

Reminder: You must be a member in good standing to cast your ballot in October. Please check to be sure that your 2009 dues have been paid so that you can have a voice in charting the future of the ACA

Cora Lind - Data Committee

Associate Professor, Dept. of Chemistry, University of Toledo, Toledo, OH.

Education: Prediploma, Chemistry, University of Wuppertal (1996), MS, PhD, Chemistry, Georgia Institute of Technology (1999, 2001)

Professional Activities: Member ACA, ACS, MRS, PDS; Symposium Organizer, Pittsburgh Diffraction Society Meeting (2004); USNCCr (2007-2009); Chair, ACA Powder Diffraction SIG (2008); Instructor, ACA Crystallography Summer Course (2008, 2009); Vice Chair, SHUG (2009)

Research Interests: Structure-property relationships in solid-state materials, x-ray and neutron powder diffraction, Rietveld analysis, structure determination from powder data, non-ambient diffraction (low and high temperature, high pressure), phase transformations as a function of temperature, pressure and composition.

Statement: Crystallography has been transformed from an "experts only" field to a tool open to many researchers. A major driving force of this change has been the incredible increase in computing power over the past decades, which makes characterization of simple structures a routine task that can often be accomplished by simply "pushing buttons". With this increase in user base and computing power comes the responsibility for our community to provide databases and standards that allow users of crystallography to ensure the soundness of their data even if they are not "experts in crystallography" in the traditional sense. This requires easy access to data and standard procedures.

Databases play an important role both in user education and evaluation of experiments. Knowledge of and access to databases is therefore crucial. If elected, I would like to work with the committee and the ACA to encourage database and software companies to explore new options that allow broader access to the data and education of users. This would include agreements about frameworks for educational use like granting short-term educational licenses for crystallography classes or summer schools. At the same time, these opportunities will need to be advertised to the community so that instructors are aware of these options, which are already considered by some companies. Another area that needs work is the definition of site licensing, which has traditionally been restricted to the physical location of a single building. This is obviously not feasible in many universities and companies. The move towards using cyber-based license keys may open up possibilities for redefining sites based on entities/IP identification, which would allow a useful redefinition of site licenses.

In addition to databases, standards are often necessary to properly evaluate experimental conditions, instruments and thus data quality. Diffraction standards for diffractometer alignment under ambient conditions are readily available through NIST and other vendors. However, standards for non-ambient experiments are little explored, and knowledge about standards and appropriate calibration procedures is less widespread. Many users of variable temperature options on in-house diffractometers rely on thermocouple readout for their non-ambient experiments, which can lead to significant errors in temperature estimates. "Standard procedures" are rare to non-existent. The user community would benefit from suggestions for standardized procedures (including *in situ* temperature standards) for non-ambient experiments for different types of variable temperature stages.

Ilia Guzei -Data Committee

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

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

Professional Activities: Co-editor for *Acta Cryst. C* (2005-present), reviewer for a number of chemistry and crystallography journals, coordinator of the Bruker Users Meeting in the USA (every other year since 2001), coordinator of the Struchkov Prize Society Meeting (2007).

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. Disordered and twinned structures ought to be considered routine, because crystallographers routinely deal with problematic structures. 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 on 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 and could be beneficial to everyone working with challenging structures. If elected, I would work with software and database developers to achieve the above 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.

Frank Fronczek - Continuing Ed

Research Associate; Director of X-ray Laboratory, Department of Chemistry, Louisiana State Univ., Baton Rouge, LA

Education: BS in Chemistry, LSU (1970); PhD Caltech (1975, with Bill Schaefer and Dick Marsh); Postdoc, U.C. Berkeley (1975-76 with Ken Raymond).

Professional Activities: ACA member since 1971; chairman Service Crystallography SIG, 1992-93; chair of Patterson Award Committee, 2007; member of Education Subcommittee, USNCCr, 2004-2006; organizing committee, USNCCr Education Summit, 2005; Coeditor, *Acta Cryst.*, Section B , 1996-1999; Coeditor, *Acta Cryst.*, Section C, 1996-2005; Adjunct Professor, Dept of Pharmacognosy, School of Pharmacy, U. of Mississippi, 2003-present.

Research Interests: Structure and absolute configuration of natural products having medicinal potential, derived from terrestrial plants and marine organisms; macrocycles; heterocycles; cryocrystallography; polymorphism; service crystallography.

Statement: Continuing education is arguably the most important function of the ACA. This is because, despite the central importance of crystal structure determination in so many fields of science, there is currently little formal teaching of crystallography in many (most?) departments, as compared to a generation ago. ACA summer courses and workshops have become critically important in educating researchers doing practical crystallography, and they should be supported, encouraged, and expanded. We should also be paying more attention to what happens *after* summer courses and workshops. In many cases, relatively inexperienced cystallographers find themselves alone in trying to deal with non-routine problems. Web resources and discussion boards can be helpful, but it can still get pretty lonely out there under such circumstances. Having someone more experienced to talk to is invaluable. The ACA should assist by continuing to encourage the mentor-mentee concept, helping to pair young people with more seasoned crystallographers with whom they can feel comfortable in asking for regular guidance. Much more can be learned from such encounters than from textbooks and websites. Ideally, such pairings would be geographically close enough to allow eyeball-to-eyeball meetings when advantageous. The ACA should also actively encourage universities with a wealth of data-collection resources to provide help to those who are capable of determining their own structures, but who are at institutions without diffractometers. I was on the receiving end of such arrangements early in my career and was greatly appreciative. I have been on the giving end ever since. It is an excellent way of continuing crystallographic education, puts instruments to good use at times when they might otherwise lie idle, and embodies the cooperative spirit of our association. I am honored to be nominated to stand for election to the Cont. Ed Committee. While I am primarily a "service" crystallographer, crystallographic education is one of my primary interests and concerns.

Charles H. Lake, Continuing Ed

Associate Professor, Department of Chemistry, Indiana University of Pennsylvania, Indiana, PA

Education: BS Geology-Chemistry, State Univ. College at Fredonia (1989), PhD Chemistry, State Univ. of New York at Buffalo (1995).

Professional Activities: Member ACA since 1989, Co-organizer of the ACA Small Molecule Summer Course since 2003 (under contract until 2011). Board of Directors of the Pittsburgh Diffraction Soc. since 2001 (one term as Member at Large (2001 - 2002), 3 terms as Treasurer (2003 - present)), NSF Solid-State and Materials Science Program (1996), Staff Crystallographer, Univ. of Alabama at Birmingham (1995 - 1999), very active in promoting crystallography in Western PA through lectures/demonstrations at area museums, middle and high schools and adult continuing education programs.

Research Interests: Single crystal and powder x-ray diffraction, crystallographic education, solid-state chemistry. Current projects involve the synthesis and characterization of dilute magnetic semiconductor materials and the incorporation of crystallography into the existing curriculum of the natural sciences.

Statement: Crystallography is a very old science that is more than just single crystal structure elucidation. While the number of crystallographers is a small fraction of the scientific community, their contribution to research has made significant strides toward the advancement of all natural sciences. Over the past few decades, the demand for crystallographic information has rapidly increased. Unfortunately, over the same time frame, the opportunity to gain a scientific education in the basic principles of crystallography has steadily decreased. With modern crystallography addressing a wide range of new, exciting scientific problems the role of crystallographic education has become more important then ever. If the science of crystallography is to remain vibrant and growing, student participation must increase and the opportunity for a scientific education in the basic principles must remain accessible.

To achieve this goal, Bryan Craven and I began organizing the ACA Summer Small Molecule Course in 2003. For the course, we have brought together leading experts in the field to help educate students in the basic principles of powder and single crystal crystallography. Besides being taught the basic principals, students are shown a wide range of scientific problems which can be addressed. They are also taught to ask "why" crystallographic decisions are made. This is extremely important in the era of modern software. It also helps students critically evaluate the proposed models.

If elected to the Continuing Education Committee, I would explore ways to improve student involvement in the ACA as well as looking for outreach opportunities to the community. I would continue supporting the ACA summer courses and make them affordable and attractive to students. I would help predominantly undergraduate universities incorporate crystallography in their lectures and laboratories. Powder diffraction can be used to demonstrate a wide range of scientific topics and could easily be incorporated into existing physics, chemistry and geoscience laboratory courses. At IUP we have diffraction laboratories in experimental physics, physical chemistry, inorganic chemistry and analytical chemistry courses (we have also run XRD experiments in mineralogy and petrology). This gives the student a basic idea of the types of problems that can be addressed by crystallography. Personally, I feel that increased student participation is extremely important for the health of both the society and the science of crystallography.

2009 Travel Award Winners

Stefan Schmelz
Univ. of St Andrews, Scotland
Miha Andrejasic
Jozef Stefan Inst., Slovenia
Misty Balcewich
Univ. of Manitoba, CANADA
Matt Beekman
Univ. of South Florida
Jason Benedict
Univ. at Buffalo, SUNY
Horacio Botti
Inst. Pasteur of Montevideo, Uruguay
Dejan-Kresimir Bucar
Univ. of Iowa
Stacie Bulfer
Univ. of Michigan
Carina Buttner
Univ. of York, UK
Ivan Campeotto
Univ. of Leeds, UK
Diego Andres Campo Ceballos
Univ. of Cauca, Colombia
Paulo Junior Carvalho
Univ. Estadual de Goi·s, Brazil
Peder Cedervall
Univ. of Minnesota
Subhendu Chakraborti
Univ. of Delaware
Haiyan Chen
New Jersey Inst. of Tech.
Prashant Chopade
Kansas State Univ.
Haemi Chung
Univ. of Nebraska-Lincoln
Jonathan Coome
Univ. of Durham, UK
Sean Dalrymple
Univ. of Saskatchewan, Canada
Jamaine Davis
Natl. Cancer Inst. at Frederick
Nicholas Deifel
The George Washington Univ.
Richard Dowling
Univ. of Manchester, UK
Nicoleta Economou
Drexel Univ., College of Medicine
Safiyyah Forbes
Kansas State Univ.
Anna Gardberg
Oak Ridge National Lab.
Peter Gin
Stony Brook Univ.
Alister Gould
Univ. of Western Ontario, Canada
Jason Grigg
Univ. of British Columbia, Canada
Robert Gruninger
Univ. of Lethbridge, Canada
Ankit Gupta
Univ. of Rochester School of Med.
Michael Hast
Duke Univ. Medical Center
Jae-Hyuk Her
National Inst.of Standards and Tech.
Greg A. Hogan
Univ. of Missouri-St. Louis
Peter Horanyi
Univ. of Virginia
Ping-Yen Hsieh
Univ. of Maryland-College Park
Mark Hunter
Arizona State Univ.
Troy Johnson
Kansas Univ. Medical Center
Christopher Kimberlin
The Scripps Research Inst.
Graham King
The Ohio State Univ.
Valerie Klema
Univ. of Minnesota
Leonardus Koharudin
Univ. of Pittsburgh
Samroeng Krachodnok
Muang Nakhon Ratchasima, Thailand
Seungjoo Lee
Case Western Reserve Univ.
Jeffrey Lee
The Scripps Research Inst.
Andreas Lemmerer
Ben-Gurion Univ. of the Negev, Israel
Mitch Luna
The Scripps Research Inst.
Viivi Majava
Univ. of Oulu, Finland
Yogesh Manjare
National Chemical Lab., India
Colin McCrimmon
Univ. of Virginia
Ainsley McFarlane
Univ. of Manitoba, Canada
Brandon Mercado
Univ. of California at Davis
Scott Mottarella
Rochester Institute of Tech.
Mayasree Oottil
Univ. of Waterloo, Canada
Chuttree Phurat
Chulalongkorn, Thailand
Daniel Pohl
Univ. of Ottawa. Canada
Jason Porta
Univ. of Nebraska Med. Center
Janeth Presores
Georgetown Univ.
Nicholson Price II
Columbia Univ.
Arbin Rajbanshi
Kansas State Univ.
Craig Robertson
Durham Univ., UK
Navdeep Sidhu
Univ. of Saskatchew, Canada
Harkewal Singh
Univ. of Missouri - Columbia
Katherine Sippel
Univ. of Florida
Dhiraj Srivastava
Univ. of Missouri-Columbia
Paul Stonaha
Indiana Univ.
Tianjun Sun
Univ. of Calgary, Canada
Felipe Trajtenberg
Pasteur Inst. of Montevideo, Uruguay
Catherine Tupper
Los Alamos National Lab
Kristopher White
Stanford Univ.
Ardian Wibowo
Indiana Univ.
Tao Wu
New Jersey Inst. of Tech.
Zhen Xu
Cleveland Clinic Foundation
Juan Yu
Univ. of Virginia
Elena Zlateva
Dowling College

Contributors to this Issue:

Cele Abad Zapatero, Ross Angel, Joel Bernstein, Jim Britten, Branton Campbell, Frank Fronczek, Margaret Gabanyi, Stephan Ginell, Bill Gleason, Ilia Guzei, Susan Henderson, Tom Koetzle, Charles Lake, Sine Larsen, Cora Lind, Gary Newton, Bruce Noll, N. Rao, Bernie Santarsiero, James Staros, Iris Torriani, Susan Trolier-McKinstry, Davide Viterbo and Bob Von Dreele. *Nicholas Noinaj for the David Davies collage (page 7), and the cartoons on pages 15, 18, and 22 are courtesy of Nick D. Kim, an analytical environmental chemist who currently works for the Waikato Regional Council. He is an honorary lecturer at the University of Waikato in New Zealand.*

2009 Margaret Etter Awards

Etter Early Career Award

Svilen Bobev
University of Delaware

Etter Student Lecturer Awards

Bio-Mac SIG
Alaji Bah
Washington Univ. School of Med.

Materials Science SIG
Wen Jingshen
Brookhaven National Laboratory

Neutron SIG
Catherine Tupper
Los Alamos National Laboratory

Powder Diffraction SIG
Matt Beekman
University of South Florida

Service SIG
Partha Das
University ofZurich

Synchrotron SIG
Jesse Smith
University of Ottawa, Canada

Young Scientist
Ivan Cameotto
University of Leeds, UK

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The 2009 ACA Meeting in Toronto will truly be an 'international' meeting. The following countries will be represented:

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Portugal
Scotland
Serbia
Singapore
Slovenia
South Africa
Spain
Sweden
Switzerland
Taiwan
Thailand
The Netherlands
The United Kingdom
Uruguay
USA

JULY 2009

25-30 **ACA Annual Meeting - Toronto, Ontario - Canada** *www.cins.ca/aca2009*

AUGUST 2009

16-21 **XXV European Crystallographic Meeting.** Istanbul, Turkey. *www.ecm25.org/*

24-29 **International Summer School on Fundamentals and Basic Methods of Crystal Growth,** Brasov, Romania, *rocam.unibuc.ro/intschool/*

25-28 **Romanian Conference on Advanced Materials,** Brasov, Romania, *rocam.unibuc.ro/*

SEPTEMBER 2009

9-12 **Biannual Meeting of the Brazilian Crystallographic Association,** Federal University of Minas Gerais (UFMG), Belo Horizonte, Brazil, *torriani@ifi.unicamp.br*

24-25 **First International Symposium on Structural Systems Biology** Hamburg, Germany, *www.conventus.de/cssb2009*

OCTOBER 2009

22-25 **Joint Conference of the Asian Crystallographic Association and the Chinese Crystallographic Society,** Bejing, China: *www.ciccst.org.cn/asca09/*

JUNE 2010

24-29 **Gordon Research Conference in Crystal Engineering,** Waterville Valley Resort, Waterville Valley, NH *www.grc.org/programs.aspx?year=2010&program=crystaleng*

JULY 2010

6-11 **ACA - Chicago, IL. Local chair: Bernie Santarsiero** *(bds@uic.edu)***, Program chair: Ross Angel (rangel@vt.edu)**

18-23 **Gordon Conference on Diffraction Methods in Structural Biology,** Bates College, Lewiston, ME. *www.grc.org/programs.aspx?year=2010&program=diffrac*

MAY-JUNE 2011

28-2 **ACA - New Orleans, LA.**

AUGUST 2011

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

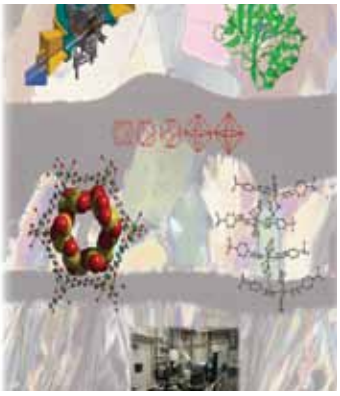
JULY 2012

21-26 **ACA - 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



The cover is illustrated with a small sampling of the 43 submissions for the General Interest Sessions of the 2009 ACA meeting in Toronto. *Credits (clockwise from upper left):* A. Savici *et al*. (ZEEMANS - A High Magnetic Field Neutron Scattering Instrument.), P. Carroll (Jmol - A Set of Open-Source Java Applets for Molecular and Crystallographic Visualization.), K. Ruhlandt-Senge *et al*. (Rationalizing the Unusual Geometry in Heavy Alkaline Earth Metal Acetylides.), W. Clegg *et al*. (Bringing the Power of Synchrotron Crystallography to the Chemical Community.), P. J. Byrne *et al*. (Utilizing X-ray Diffraction to Investigate the Storage Capabilities of Metal Organic Frameworks.) *Center:* B. Chakoumakos (Bubbles, Foam, and the Clathrate Connection.) *Background:* A. Lemmerer *et al*. (Pyrithyldion and Isopropylphenazone: Crystal Structures of their Polymorphs and their 1:1 Co-crystal.). Many thanks to ***Bruce Noll*** for collecting the images and designing the cover.

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First Announcement

The 67th Annual Pittsburgh Diffraction Conference will be held from October 28th - 31st, 2009 at the University of Georgia Center for Continuing Education.

Program topics this year include RNA Crystallography, Protein Small Angle X-ray Diffraction, Crystallization of Protein-Protein Complexes, Small Molecule Neutron Diffraction and X-ray diffraction in Material Science. In addition, a new feature of the conference is the Pittsburgh Diffraction Society Future Leaders Symposium, which will highlight outstanding research carried out by graduate and undergraduate students.

The conference will be preceded by a hands-on workshop on sulfur-SAD phasing organized by B.C. Wang on October 27th.

For more information: www.pittdifsoc.org/

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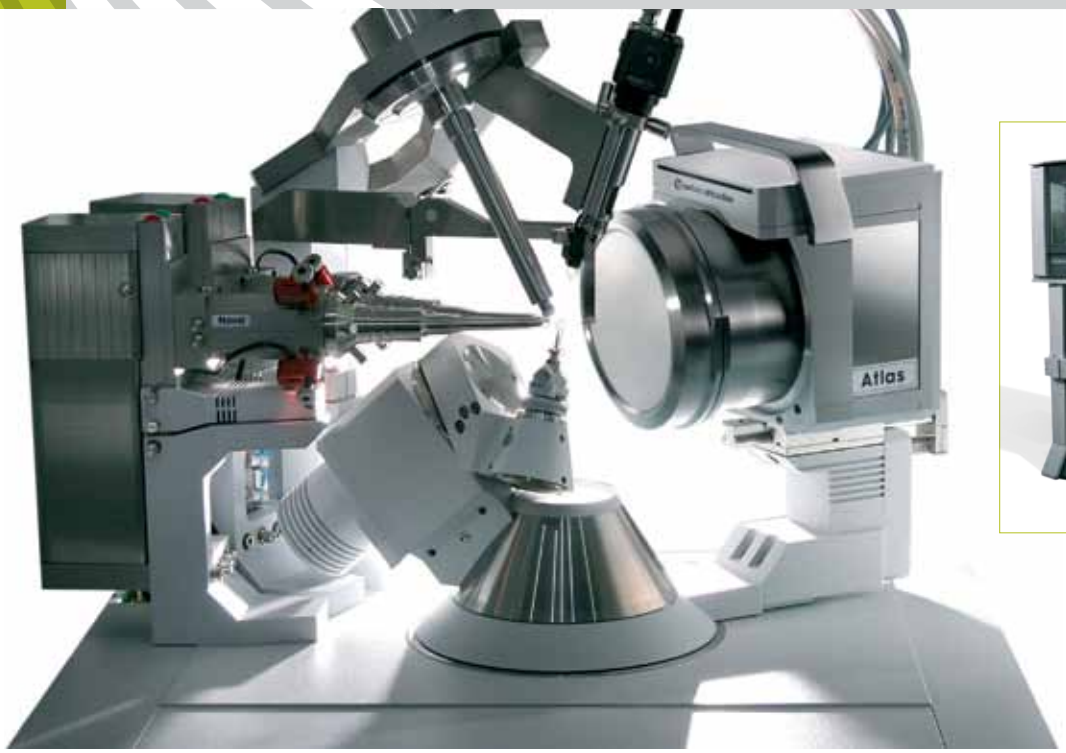

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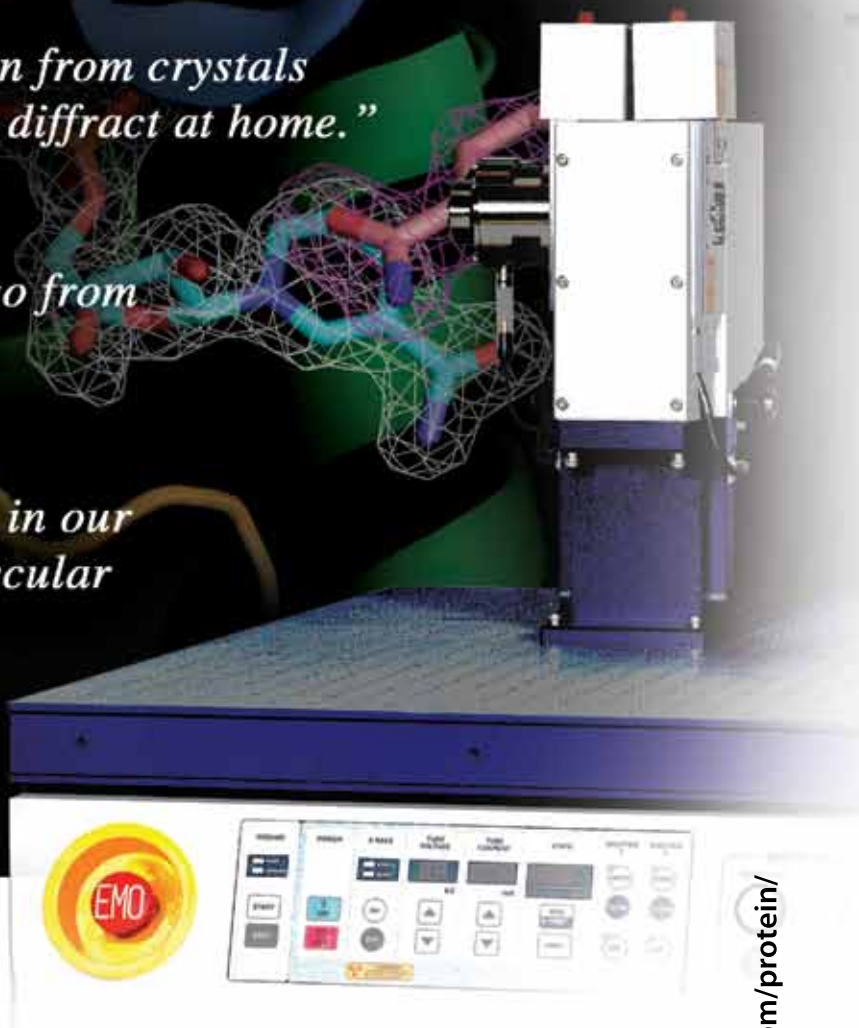
Dr. Paul Taylor
University of Edinburgh, Scotland



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