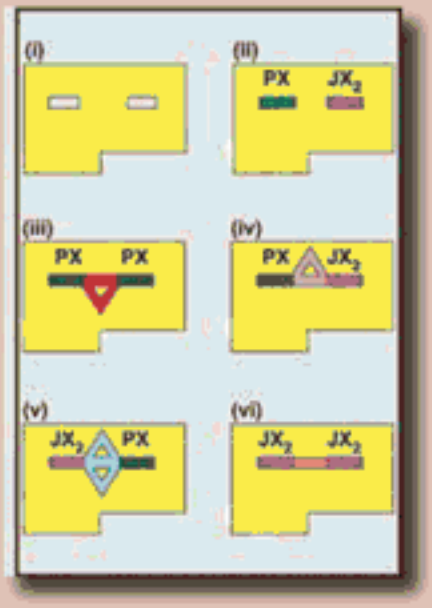
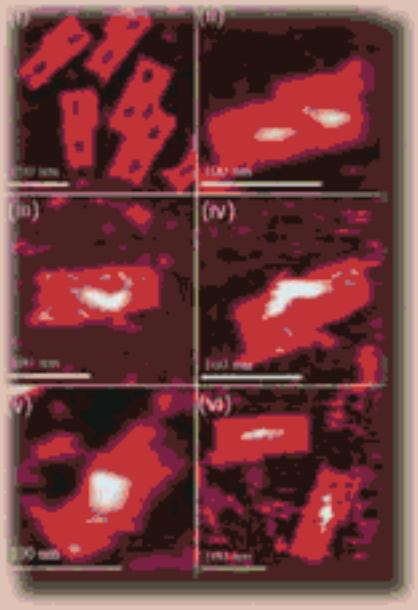
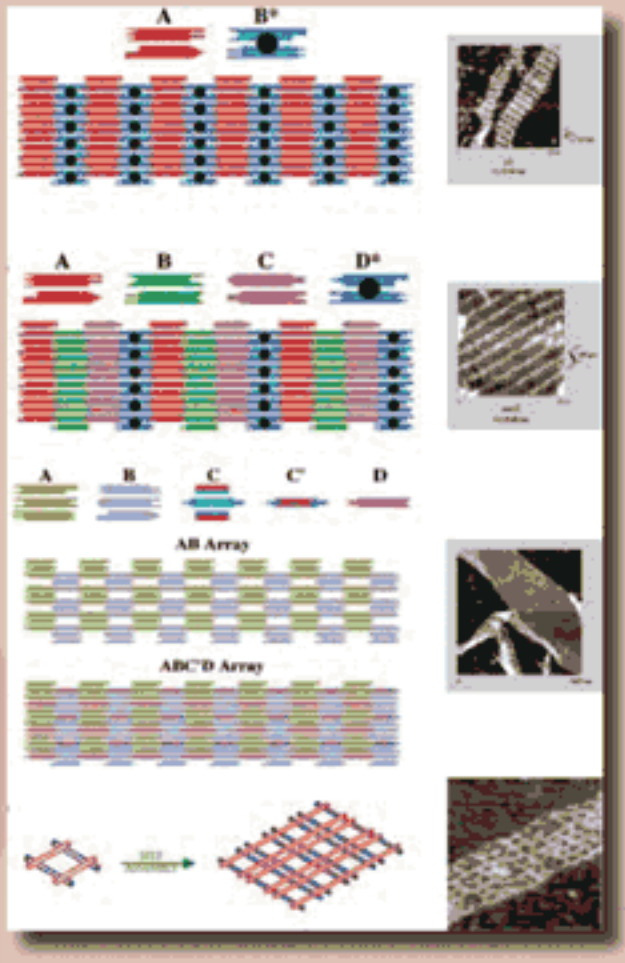
ACA RefleXions

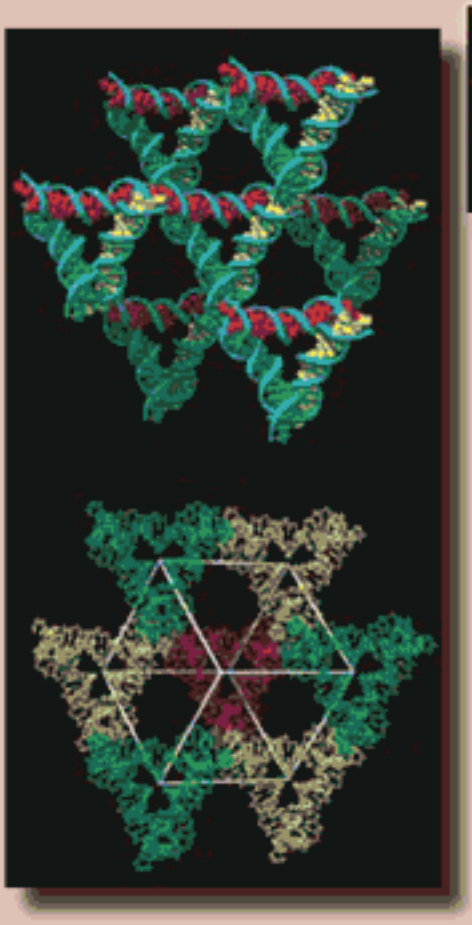
AMERICAN CRYSTALLOGRAPHIC ASSOCIATION

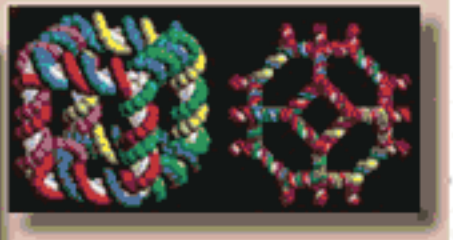
Number 2 Summer 2011

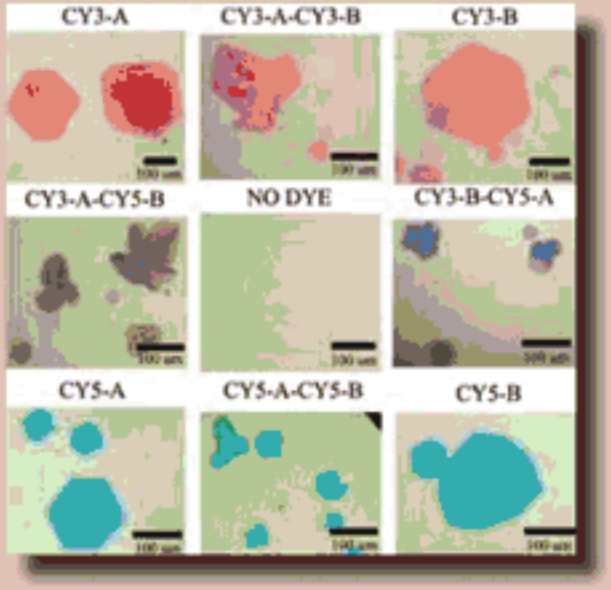












DNA & Nanotechnology

ACA RefleXions

American Crystallographic Association

ACA HOME PAGE: www.amercrystalassn.org

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Presidents Column:

As I write, beautiful spring weather has at long last arrived in New York and my thoughts are turning to ACA's annual meeting in New Orleans at the end of May. By the time that this summer issue of *Reflexions* hits your desks, many of you will have had the opportunity to enjoy the exciting scientific program organized for New Orleans by Program Chair Chris Cahill. We are greatly indebted to Chris and to our Local Chairs Ed Stevens and Cheryl Klein, along with the members of their respective committees, for all of their hard work to ensure a successful meeting.

One of the privileges that I have as your President is the opportunity to represent the ACA at meetings bringing together the leadership teams of our sister scientific societies. On March 30, I visited the American Institute of Physics in College Park, MD, where I attended the AIP's annual Assembly of Society Officers. I was joined at the Assembly by *RefleXions* Co-editor and member of the AIP Executive Committee, Judy Flippen-Anderson. The day's discussion highlighted a number of topics of mutual interest to AIP's member and affiliated societies including strategies for effective public communication, never more important than in today's extremely challenging budgetary environment. In talking with officers of other societies, I learned that a number of them have taken steps comparable to our initiative at ACA to encourage the involvement of our younger members, under which the chair of the Young Scientist SIG, Jamaine Davis, has joined the ACA Council as an *ex officio*, non-voting member.

On May 5-7 I participated in the semi-annual Council of Scientific Society Presidents (CSSP) in Washington, DC. ACA Past President Judy Kelly, who currently serves on the CSSP Board, also attended. The Council provides a unique forum for discussing issues of concern with a broad spectrum of leaders in the scientific community and also serves as a focal point for providing advice on science policy to members of the US Congress and of the Executive Branch. Topics discussed this year included visa and immigration policy, innovative techniques in Science, Technology, Engineering, and Mathematics (STEM) education, and initiatives at the US Patent and Trademark Office in response to the changing 21st century intellectual property landscape.

As *Reflexions* goes to press, Crystal Towns and Marcia Colquhoun are reporting that the number of advance registrations for New Orleanshas passed the 600 mark. We are looking forward to a dynamic meeting. In my column for the fall issue, I will feature news from the ACA Council's activities in New Orleans.

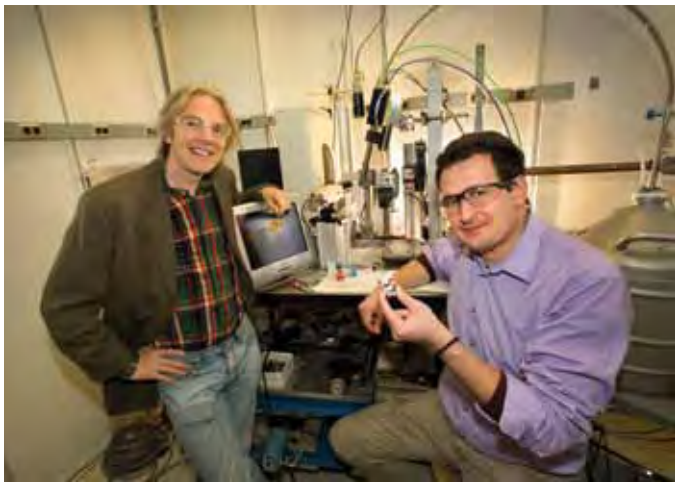
Have a great summer!

Tom Koetzle

In the past *RefleXions* has featured *Opinion* articles on Intelligent Design/the Evolution Debates and on Global Warming. It seems appropriate to include New Energy Materials as a topic as well.

Local Structure and New Energy Materials: in a 2006 *Nature* paper,[1] and a review article in the same issue by John Rehr,[2] the method of PDF analysis was introduced to the study of nanostructures. In a 2007 *Science* review article,[3] Simon Billinge and co-authors addressed what they called the "nanostructure problem" – that traditional crystallography works pretty well down to around 10 nm (1Å), but below that the Bragg peaks are too broad and diffuse and Bragg scattering is no longer the right starting point.

Then in December 2010, Simon, along with co-authors Emil Božin, Christos Malliakas, Petros Souvatzis, Thomas Proffen, Nicola Spaldin & Mercouri Kanatzidas, published a paper in *Science*[4] about their study of lead chalcogenides (lead paired with tellurium, selenium or sulfur), using atomic pair distribution functions (PDFs) to give a "local" view, (i.e. the distance from each atom to all its neighbors – rather than just the periodically averaged structure) that caught the attention of *ScienceDaily* editors. *ScienceDaily* published the photo of Simon and Emil below and noted that their discovery heralded a new "opposite-direction" phase transition that helps explain the strong thermo-electric response of these materials. Such an "opposite-direction" phase transition could be used to harness the energy lost as heat, for example in automotive and factory exhausts.



In their *Science* paper, the scientists described how the lead materials were made at Northwestern University in a purified powder form (Malliakas & Kanatzidis) and then subjected to neutron beams at the Lujan Neutron Scattering Center at Los Alamos (Božin, Proffen). Computer programs developed at Brookhaven and Columbia enabled modeling and interpretation of atomic level events over a range of temperatures. Emil Božin was the first to notice the odd behavior in the data and worked tenaciously to prove it was something new and not a data artifact. "If we had just looked at the average structure, we never would have observed this effect. Our analysis of atomic pair distribution functions gives us a much more local view – the distance from one particular atom to its nearest neighbors – rather than just the average," he said. The PDF analysis revealed that as the materials warmed, the atom-to-nearest-neighboring-atoms distances were changing on a quarter-Å scale indicating that individual atoms were becoming displaced. Simon Billinge explained that to understand the phase transition one should just think of a gas like steam cooling to form liquid water, and then freezing to form ice. In each case the atoms undergo some structural rearrangement, and "sometimes, further cooling will lead to further structural transitions: atoms in the crystal rearrange or become displaced to lower the overall symmetry." The behavior of such localized atomic distortions upon cooling is normal, but "what we discovered in lead chalcogenides is the opposite behavior: at the very lowest temperature, there were no atomic displacements, nothing – but on warming, displacements appear!"

In an extension of this work to small molecule systems, a *Cryst Eng. Comm.* paper by Billinge, Božin, Shankland & co-authors,[5] showed that a high-energy XRPD (X-ray Pair Distribution) method known as "total scattering" together with PDF analysis (TSPDF) produced unique structural fingerprints from amorphous and nanostrucural phases of the pharmaceuticals carbamezapine and indomethacin. Combining high energy (synchrotron x-rays) with imaging plate detectors resulted in accurate PDFs across a wide range of distances and showed that the melt-quenched drugs were not amorphous but nanocrystalline in a known metastable form or packing arrangement. Materials for energy and other applications that we have known about and used for many years, such as PbTe, are revealing new secrets when we go beyond crystallography and study structure at the nanoscale.

Connie Rajnak

1. *Ab Initio Determination of Solid-State Nanostructure* by P. Juhás, D.M. Cherba, P.M. Duxbury, W.F. Punch & S.J.L. Billinge, *Nature,* **440**, 655-58, (2006).

2. *Nanostructures in a New League* by John J. Rehr, *Nature* **440**, 618-19, (2006).

3. *The Problem with Determining Atomic Structure at the Nanoscale* by Simon J.L. Billinge and Igor Levin, *Science*, **316**, 561-65, (2007).

4. *Entropically Stabilized Local Dipole Formation in Lead Chalcogenides* by Emil S. Božin, Christos D. Malliakas, Petros Souvatzis, Thomas Proffen, Nicola A. Spaldin, Mercouri G. Kanatzidis, and Simon J.L. Billinge, *Science* **330**, (2010)

5. *Characterisation of Amorphous and Nanocrystalline Molecular Materials by Total Scattering*, by Simon J.L. Billinge, Timur Dykhne, Pavol Juhas, Emil Božin, Ryan Taylor, Alastair J. Florence & Kenneth Shankland, *Cryst. Eng. Comm.* **12**, 1366-68, (2010).

Editor's note: Simon and Emil, with their coauthors, are preparing a follow-up manuscript to the December 2010 Science paper in which they studied phonons in PbTe. They see a new phonon mode (which implies a local symmetry breaking) appearing with the same temperature dependence as the effects seen in the PDF which lends support to the picture of emerging structural distortions.

News from Canada, May, 2011

The Canadian National Committee has awarded ***Larry Calvert Memorial Travel studentships*** for the IUCr Congress to ***Konstantin Popovic, Stephen Campbell*** and ***Carle Protsko***. Current membership of the CNC is: ***Jim Britten*** (Chair), ***Pam Whitfield*** (Vice-Chair), ***Joe Schrag*** (Secretary), ***Marie Fraser*** (Treasurer), ***Stan Cameron, Lee Groat,*** and ***David Rose*** (ex-officio).

The Canadian Light Source in Saskatoon has reported that there are now 2 beamlines in operation for macromolecular crystallography. Joining its sister line CMCF-BM, the CMCF-ID beamline is set up especially to handle large unit cells. From the CLS website (***www.lightsource.ca***): the beamline is equipped with a Röntek Spectrometer System XFLASH 101A to perform x-ray spectroscopy for MAD and x-ray absorption near edge structure (XANES) on the same crystals, and x-ray fluorescence (XRF) for metal tracing on protein derivative crystals. There are ongoing efforts to equip the beamline with a cryogenic sample changer to facilitate remote access to the facility."

The Website for the 2014 IUCr Congress in Montreal is due to be launched in July, 2011 at ***www.iucr2014.com/***. For those who like to plan ahead, the dates are August 5-12, 2014.

In other news… on May 2nd, we held a federal election. For an election that "no-one wanted" in the words of the ruling Conservative Party, it sure generated a lot of interest. Unfortunately that did not convert to voter participation, which, at about 60%, was an improvement over previous elections, but still disappointing. The Conservative Party again captured the most votes, just under 40% (all results from the Elections Canada website, ***enr.elections.ca/National_e.aspx***), but that was sufficient (due to the nature of a parliamentary system) to win a majority of the seats in the House of Commons (167 out of 304) and the right to form the government. The more surprising results were those of the other parties, the traditional opposition, the centrist Liberal Party, ended up in third place, while the leftist New Democratic Party (NDP) will form the new official opposition with 102 seats. Much of the NDP gain resulted from a major collapse in the separatist Bloc Quebecois, which was reduced to only 4 seats. The political pundits are still floating hypotheses to explain the unexpected results but the prevailing opinion seems to be that, rather than a ringing endorsement of the Conservatives, they reflect a frustration with the Liberal and BQ parties.

What does this mean for support for crystallographic research through either NSERC or CIHR, both of which have reached record lows in success rates? As elsewhere, the trend recently has been the targeting of government research funding to specific outcomes (such as partnerships with companies), to big science projects, to infrastructure, or to elite personnel programs at all levels (student, post-doc and faculty). As there is no longer any scientific advisor to the Prime Minister, input from the funding bodies, the scientific societies and grass-roots scientists is very limited. With a continued Conservative government, these policies are likely to continue. However, we can only hope that, with a majority in parliament, the government might be more open to a longer-term outlook towards understanding the role of basic research in the future economic development and international stature of the country.

David Rose

Synchrotron funding problems are not unique to Canada

The US: Since early February, scientists supported by the Department of Energy (DOE) Office of Science had been bracing for massive layoffs at the department's 10 national laboratories and the temporary closure of many of their large user facilities. The culprit was vicious budget hacking by a congress seemingly bent on reducing the federal deficit. Instead, the agency will see its annual budget for science clipped by a mere $30 million from the 2010 level, or 0.6%, to $4.874 billion.

That number is part of the final continuing resolution to fund the federal government through the end of the fiscal year (September 30) and is a welcome relief to an agency that just a few months ago was looking at an 18% cut to its budget.

The surprising budget compromise means that DOE can keep running its synchrotron x-ray sources, neutron sources, nanotech facilities, and other "user facilities". There may have to be adjustments in how the centers are operated but they will not have to be shut down.

With the relatively modest cut, the national labs won't have to make the huge layoffs they'd been planning. However, the final budget is still 4.8% short of the original request for 2011. So some belt-tightening will be required, and there are no guarantees that there will be no layoffs.

The news comes as a particular relief to researchers supported by DOE's biological and environmental research (BER) program. The original continuing resolution would have BER funding reduced from $558 million in fiscal 2010 to $302 million in 2011. And coming halfway through the current fiscal year in which researchers were spending at 2010 levels, it would have effectively left the program with nothing for the rest of the year. The overall reaction of this community is relief but much concern remains for the future.

Concerns for the future of funding for basic scientific research are not limited to the DOE community. The message from congress is clear in that they continue to question the value of basic research. It is up to all of us to educate them on just how wrong headed such a policy would be.

Australia: The $200 million Australian Synchrotron could be shut down next year after the Baillieu government failed to commit to ongoing funding for this research facility which is at the center of Melbourne's thriving scientific community. With funds due to run out in June (2012) the synchrotron's board is making contingency plans for its closure, just five years after it opened.

"There's a great sense of unease in the community," said one synchrotron scientist. ''People are just holding their heads in their hands."

Letter to the Editors:

I just wanted to point out that in the last two issues of *Reflexions* (Page 34, Winter 2010 and Page 24, Spring 2011) my name has been misspelled next to my picture. Just thought I'd let you know so if my photo comes up again perhaps it can be assigned to me, ***Krystle McLaughlin*** Have a nice day!

Krystle

From the Editor's Desk

Paul Ewald was the first president of the IUCr in 1946 and since then only two women have held that office: ***Dorothy Hodgkin*** (1972) and ***Sine Larsen*** (2008). Two women have been vice-president: ***Dame Kathleen Lonsdale*** (1960 and 1963) and ***Iris Torriani*** (2005). The 9th Ewald Prize will be awarded this year (2011) at the IUCr Congress in Madrid and ***Eleanor Dodson*** will be the first woman to share the prize.

The ACA has done better with the top position on council. ***Elizabeth Wood*** was the first woman president (1957) after which there was a 19 year hiatus until ***Isabella Karle*** served in 1976. ***Jenny Glusker*** followed 3 years later (1979) and then ***Helen Berman*** occupied the top spot in 1988 (an 8 year gap). However, since 1991 seven of 21 (33%) have been women: ***Judy Flippen-Anderson*** (1991), ***Elinor Adman*** (1994), ***Carol Huber*** (1996), ***Penny Codding*** (1998), ***Connie Chidester*** (2000), ***Fran Jurnak*** (2004) and ***Judy Kelly*** (2010). Six the 17 crystallographers that have served as ACA Secretary (35%) have been women and all 6 are among the most recent 8 (75%). Only two women have served as treasurer (2 of 14 = 14%). Photos of the presidents (names highlighted in ***maroon)*** are included in this article - can you match the names with the faces?

The list of winners for the ACA awards does not paint a pretty picture: No women have ever been selected for the Warren or Trueblood Award; one for the Patterson, ***Lieselotte Templeton*** shared the award with her husband David (1987); one for the Buerger, ***Helen Berman*** (2006); and three for the Fankuchen, ***Dorothy Hodgkin*** (1977), ***Jenny Glusker*** (1995), and ***Eleanor, Dodson*** (1998). My math says this comes out to 8.6% (5 out of a total of 58).

On the other hand, the 9 Etter Early Career Awardees includes 4 women (44%): ***Julian Chan*** was the first ever winner in 2003 followed by ***Jennifer Swift*** (2005), ***Carrie Wilmot*** (2006) and ***Cora Lind*** (2007). Does this bode well for our future or does it say that the young women are moving out of crystallography before they 'mature' into the other awards? Comments are welcome.

Nominations for the Etter Early Career Award are accepted all year long. Criteria for selection and nomination forms can be obtained from the ACA website (www.amercrystalassn.org) under the awards button.

AIP Center for the History of Physics

History can be important to AIP Member Societies in as many ways as those societies can imagine. The AIP supports two distinct history programs: the Center for History of Physics and the Niels Bohr Library and Archives. Why two? Simply put, it's because of the importance of history to physicists. Among the many functions of the library and archives is the preservation of important records for all member societies. It is also an information clearinghouse and constantly expands the International Catalog of Sources (ICOS), a worldwide union catalog of individual physicists' manuscript collections: their letters, notebooks, and other important papers. (Looking for Richard Feynman's letters to colleagues? Check ICOS: They're at Caltech). In addition, the library cares for a growing collection of 18,000 titles, focused on the physical sciences of the 19th and 20th centuries—as well as 30,000 photographs, more than 1,000 oral history interviews, a number of institutional histories, and more. In 2010, the Center for History of Physics online exhibits received more than 1,100,000 visits. The Center for History of Physics will work with any member society to explore its ideas regarding activities and projects having to do with history.

Greg Good

ACA History Archive

The ACA is working with the AIP to archive material on the history of crystallography. As part of this effort, we invite crystallographers to recount their own personal history. Shortened versions of these personal histories will be featured in *RefleXions*, and the full-length accounts will be deposited in the archive. The AIP History Center already has information on a number of crystallographers (***www.aip.org/history/*** – keyword crystallography). The series is being developed by Virginia Pett. The first one to appear was contributed by Jim Stewart (summer 2010) and the second by David Sayre (winter 2010). This issue has contributions from Sidney Abrahams and Bill Busing. If you would like to deposit your own history, please contact Virginia (***pett@wooster.edu)*** for some very flexible guidelines. If you are interested in helping with the history of crystallography project, please also contact Virginia.

In addition, one of the services the AIP provides to its member societies is the storage of other historical documents. Thanks to Frances Bernstein our collection has been significantly expanded. We are still missing copies of early ACA *Newsletters* edited by Jenny Glusker (anything pre 1957, 1961-1968, 1978 and 1979). We are also missing the *Call for Papers* for ACA meetings prior to 1997. If you have any of these items please contact Judy (***acareflexions@gmail.com***) and she will let you know how to get it to the AIP.

NOTE to all ACA Past Presidents: The AIP will also archive any papers you have tucked away that detail your years on ACA Council.

Crystallography on Stage and Screen

The compelling story behind the 1953 discovery of the structure of DNA has found new audiences through a surprising venue--the theater.

Anna Ziegler's *Photograph 51* recently completed runs at Theatre J in Washington DC (March 23 - April 24, 2011 - ***washingtondcjcc.org/center-for-arts/theater-j/on-stage/10-11Season/photograph-51/***) and the Ensemble Studio Theatre in New York City (October 27-November 21, 2010 - ***ensemblestudiotheatre.org/about/past-productions/2010-2011/photograph-51/***)). The play examines Rosalind Franklin's life, focusing on her time at King's College London. It contrasts her fierce independence with the relationships among James Watson, Francis Crick, and Maurice Wilkins. The science underlying the work is woven into explorations of how sexism, ambition, and personalities affected the race to discovery.

Photograph 51 was developed and produced by The Ensemble Studio Theatre/Alfred P. Sloan Foundation Science & Technology Project to promote public understanding. The performances have been well reviewed and attended.

Naturally, this portrayal of the race for the double helix provided opportunities to discuss the relationships and controversies that surrounded it. A panel that accompanied the New York run in November featured the RCSB PDB's Helen Berman; California State University professor and Franklin scholar Lynne Osman Elkin; New York Times science journalist Nicholas Wade; playwright Anna Ziegler; and Columbia University's Stuart Firestein as moderator. The discussion, available online, touched on the issues of gender and attribution as represented in the play (***www.scientificamerican.com/blog/post.cfm?id=rosalind-franklin-and-dna-how-wrong-2010-11-03)***.

The Ann Loeb Bronfman Gallery's exhibition *What Was There to Be Seen* featured art by Carolyn Bernstein and Kindra Crick (granddaughter of Francis) in partnership with the DC production of the play. Several panel discussions and a guided educational activity were also held in support of the play.

The Ensemble Studio Theatre production will return to the New York stage as part of the World Science Festival in June (***worldsciencefestival.com/events/photograph_51_Friday***). One of the performances will include a discussion with James Watson and emeritus professor of biology Don Caspar, two of the men portrayed in *Photograph 51*.

A film adaptation of this play was just awarded financial and creative support from the Tribecca Film Insitute Sloan Filmmaker Fund, provided by the Alfred P. Sloan Foundation. Ziegler's script has filmakers Ari Handel, Darren Aronofsky, and Rachel Weisz attached as producers.

Christine Zadecki

A Special Symposium Celebrating the 40th Anniversary of the PROTEIN DATA BANK

October 28 - 30, 2011
Cold Spring Harbor Laboratory

WORLDWIDE PDB
PROTEIN DATA BANK

In October 2011, the Worldwide Protein Data Bank (wwPDB) will host a scientific symposium celebrating the 40th anniversary of the inception of the PDB, and the many scientific contributions it archives.

The program will showcase the scientific impact made by structural biology during the past 40 years with a distinguished panel of scientists who have been instrumental in the development of the PDB and structural biology.

The meeting will begin with an evening reception and plenary session on Friday, and conclude with lunch on Sunday.

Confirmed Speakers:

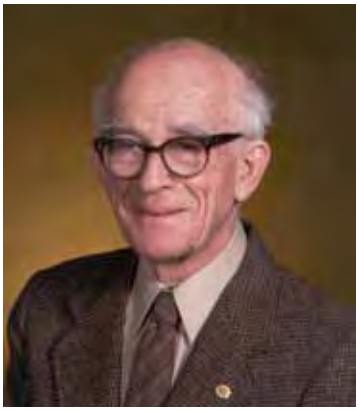
- Cheryl Arrowsmith, University of Toronto, Canada
- David Baker, University of Washington
- Ad Bax, NIH/DHHS/NIDDK/LCP
- Axel Brunger, Stanford University/HHMI
- Stephen K. Burley, Eli Lilly & Co.
- Wah Chiu, Baylor College of Medicine
- Angela Gronenborn, University of Pittsburgh
- Richard Henderson, MRC Laboratory of Molecular Biology, United Kingdom
- Wayne Hendrickson, Columbia University
- Mei Hong, Iowa State University
- So Iwata, Imperial College London, United Kingdom
- Louise Johnson, University of Oxford, United Kingdom
- T. Alwyn Jones, University of Uppsala, Sweden
- Brian Matthews, University of Oregon
- Jane Richardson, Duke University Medical Center
- Michael Rossmann, Purdue University
- Andrej Sali, University of California, San Francisco
- David Searls, Independent Consultant
- Susan Taylor, University of California, San Diego
- Janet Thornton, EMBL, Hinxton, United Kingdom
- Soichi Wakatsuki, Institute of Materials Structure Science, Japan
- Kurt Wüthrich, The Scripps Research Institute, ETH Zürich
- Ada Yonath, Weizmann Institute, Israel

Organizers:

Helen Berman, RCSB PDB, Rutgers University, United States
Stephen K. Burley, Eli Lilly & Co., United States
Gerard Kleywegt, PDBe, EMBL-EBI, United Kingdom
John Markley, BMRB, University of Wisconsin, United States
Haruki Nakamura, PDBj, Osaka University, Japan

meetings.cshl.edu/meetings/pdb40.shtml

Sidney Cyril Abrahams was a crystallographer at Bell Labs for 31 years, a charter member of the ACA and its president in 1968. As part of the ACA History Project, he describes here his career as a crystallographer, also as editor of Acta Crystallographica. Sidney's full narrative will be deposited at the Center for the History of Physics (AIP). This article is part of an ongoing series by individual crystallographers. If you would like to contribute your story, contact Virginia Pett, pett@wooster.edu.



Born May 28, 1924 in London, England and educated at Ilford County High School 1935-1938 and Greenock Academy 1938-1942, the present writer graduated BSc with first class honors in chemistry from the University of Glasgow in 1946, where J. Monteath Robertson was Gardiner Professor of Chemistry. Entering graduate school under the supervision of JM, a pioneer of x-ray crystallography, was a "no brainer". Working at the Royal Institution with such major figures as W. H. Bragg, W. T. Astbury, J. D. Bernal and K. Lonsdale, JM had become a founder of organic crystallography, an area in which he played a major role by his development of heavy-atom and isomorphous-replacement methods for solving the phase problem.

JM's research group in 1946 included Jack D. Dunitz, A. (Sandy) McL. Mathieson and John G. White, each of whom subsequently made valuable contributions to structural crystallography. In 1948, the summer before completing his PhD thesis, the writer received an invitation to participate in Massachusetts Institute of Technology's coming summer term as one of 62 graduate students from 18 different European countries, four of whom were from the United Kingdom. Entirely fortuitously, the first Congress of the International Union of Crystallography with its 310 participants was due to convene that summer at nearby Harvard University, presenting the opportunity for meeting such major figures as Lawrence Bragg, Desmond Bernal, Dorothy Hodgkin and Kathleen Lonsdale.

The writer received his PhD in early 1949 and, soon after, an invitation from Bill Lipscomb to join him in Minnesota as a post-doc, with a view to setting up a low temperature crystallographic laboratory. A day or so after disembarking in New York, it proved possible to visit I. Fankuchen's low temperature laboratory in Brooklyn Polytechnic. In Minnesota, we built on and extended Fan's excellent techniques that allowed a liquid at ambience within a capillary mounted on a precession camera to be cooled below its melting point and grown into a single crystal, the diffraction pattern of which could then be visually estimated. A single crystal of H_2O_2 and, later, one of thiophene could thus be grown and each structure determined relatively efficiently; these techniques were later extended by Bill and his students in their exploration of the boron hydride (borane) structures, leading to his Nobel Prize award in 1976.

Bill and the writer proved part of the large majority, at the 1949 summer business meeting of the Crystallographic Society of America in Ann Arbor MI, that voted enthusiastically in favor of merging the CSA and the American Society for X-ray and Electron Diffraction, ASXRED, a result leading directly to formation of the ACA. Both also participated in the first ACA meeting the following year, held in State College, PA where members' enthusiasm for the new society was palpable. This enthusiasm was likely enhanced by the new and exciting computational possibilities offered by Ray Pepinsky, the meeting's chairman, from use of his x-ray analog computer (XRAC). Many members present brought enough structural data to let them experiment with XRAC and achieve useful results. During that meeting, Emmanuel Grison unexpectedly invited the writer to visit MIT's Laboratory for Insulation Research (LIR) as a candidate for the position he was leaving in order to return to France.

Arthur von Hippel, director of the LIR, offered the open position as member of MIT staff to the writer during his visit some weeks later. Among the primary interests of the LIR were the physical, particularly the dielectric, properties of condensed matter; as such properties relate to structure, they also became major interests of the writer. He investigated the structure of such materials as the polysulfides, magnetite, the alkali borohydrides, several peroxides and elemental sulfur at MIT, some jointly with Emmanuel Grison before the latter returned to the Service de Radiométallurgie du Commissariat à l'Énergie Atomique, France. His interest in instrumental improvements, such as adapting commercial powder diffractometers for use below liquid nitrogen temperatures, thereby allowing relatively high-accuracy lattice constants to be measured over wider thermal ranges, increased further over that period. He also adapted such devices for comparable use in single crystal diffraction measurement. Soon after Emmanuel left, Judith Grenville-Wells, who had just received her PhD under Kathleen Lonsdale, joined the writer as his first post-doc.

Accepting the offer of a Research Fellowship in Glasgow funded by Imperial Chemical Industries, he returned to the UK in 1954 with every intention of remaining in his native country. However, although he completed a series of successful structural investigations, capped by the award of a DSc in 1957, the economically stringent conditions in the UK during the mid-50's made the offer of an appointment at Bell Telephone Laboratories too good to pass.

Bell Labs in Murray Hill, N.J. was home to many distinguished scientists with interests close to crystallography including Clinton (Clint) Davisson, co-winner with George Thomson of the 1937 Nobel Prize for the discovery of electron diffraction who, although retired some years earlier, still visited Bell Labs and Lester Germer, president of ASXRED in 1944; the Davisson-Germer experiment of 1927 unambiguously demonstrated the wave nature of the electron. Also still at Bell Labs were Richard Bozorth, likely in 1923 to have been the first Bell Labs member to solve a crystal structure; Walter Bond, who designed and built an automatic recording x-ray diffractometer and a high temperature powder diffraction camera; and Betty Wood, president of ACA in 1957, whose interests ranged from the growth of single crystals having useful and unusual properties to their crystallographic investigation.

Soon after the writer's arrival at Bell Labs, and spurred by the discovery of ferrimagnetism in rare earth-iron garnets, Seymour Geller and he determined and refined the structure of a grossularite garnet. A few months later, the writer moved to Brookhaven National Laboratory where Bell Labs maintained a neutron diffraction facility run by Edward (Ted) Prince. The measurement of neutrons diffracted by a single crystal was, at that time, largely a manual operation, hence rather slow. In jointly revising the paper tape system that Ted had initiated for controlling the system, the Bell Labs diffractometer became one of the first such systems to be automated. We subsequently incorporated a goniometer-mounted liquid-helium cryostat into our system, thereby significantly extending the available thermal range of measurement. The writer returned permanently to Murray Hill in 1960 where he set up a new automated x-ray diffraction laboratory while remaining responsible for the neutron facility.

He participated in the 4th IUCr Congress held in Montreal on his return to the US in 1957 and, thereafter, in each succeeding Congress until the 18th in Glasgow, except for the 16th in Beijing. Similar participatory patterns were not uncommon among his contemporaries. His crystallographic and related investigations over the following decades continued vigorously, ably assisted by his long term assistant Joel Bernstein and, later, Phil Marsh together with a sequence of post docs and visiting scientists including Peter Jamieson, Tom Keve, Rune Liminga, Jörgen Albertsson, François Lissalde, Christer Svensson, Jean Ravez, Åke Kvick and Jörg Ihringer. The results that followed included a further increase in the accessible thermal range for structure determination, contributions to automated instrumental measurement, estimation and reduction of both systematic and random measurement error, and relationships between physical properties and structure, including the prediction of some properties.

During the 11th IUCr Congress in Warsaw, the IUCr Executive Committee invited him to succeed Arthur Wilson as Editor of *Acta Crystallographica*. Willingly accepting this responsibility, one of his most satisfying early editorial actions led to the decision that journal production would henceforth be undertaken within the IUCr offices in Chester, thereby achieving a major increase in efficiency at about the same time it was announced that *Acta Cryst*. B would be split into two Sections. *Crystal Structure Communications*, independently founded in 1972 by Mario Nardelli and edited by him since that date would be absorbed, with Mario's enthusiastic agreement, into a new and identically named Section C of *Acta Cryst*. The boundaries between Sections would be drawn more clearly in the future. *Acta Cryst*. A, *Foundations of Crystallography*, would continue to be devoted to crystal physics, diffraction, theoretical and general crystallography; submissions to the new *Acta Cryst*. B, *Structural Science*, would be expected to advance our level of scientific understanding not only structurally but *also* in related areas of science; as noted "The purpose of this new section is to provide a showcase for exciting papers on all aspects of structural science, in which they can be published only in the company of similar papers." Offerings to *Acta Cryst*. C, *Crystal Structure Communications*, were expected to be concise, resembling the "Short Structural Papers" formerly submitted to *Acta Cryst*. *B*.

A charter member of the ACA, he was elected President in 1968. He was Founding Editor of the *Transactions of the American Crystallographic Association* with the publication of volume 1 in 1965. He was a member of the USA National Committee for Crystallography from 1966-1980 and its chairman 1970-1972. He served as IUCr representative on the International Union of Pure & Applied Chemistry's Interdivisional Committee on Terminology, Nomenclature and Symbols from 1984-2004.

Sidney Abrahams in 1969 flanked by then ACA President Walter Hamilton and the 1967 President John Kasper, both good personal friends of his but alas now both departed.

He was named "distinguished member of technical staff" at Bell Labs in 1982. After he retired in 1988, he was appointed Adjunct Professor of Physics at Southern Oregon University in 1991. He was elected Fellow of the American Association for the Advancement of Science in 1980, the American Physical Society in 1981 and IUPAC in 2004.

Sidney Abrahams and Robert E. Newnham, ACA President in 1985. (1982 ACA meeting in San Diego)

Crystallographic methods have been applied, intermittently, to newer fields of science as the full value of understanding the detailed atomic distribution of materials with increasing complexity and importance became increasingly recognized. With the growing accessibility of high flux sources for investigating the structural dynamics of phase transitions and chemical reactions,

crystallographic applications are expected to lead to a rapid increase in time-resolved experimental evidence that is likely to enhance and enlighten current theory. The resulting specialized information and terminology expected to develop in these fields, as in other crystallographic areas of rapid growth, is generally best tested initially by collegial discussion at ACA or IUCr meetings followed by submittal of resulting manuscripts to *Acta Cryst*. and the consequent acceptance of new models and terminology.

ACA Past-Presidents at the 50th Anniversary meeting in St. Paul (2000): Elizabeth Wood, David Templeton, Robinson Burbank and Sidney Abrahams. Bill Busing and Carroll Johnson in the background.

The crystallographic community has always warmly encouraged its younger members, as the writer found during the first meeting of both the ACA and the IUCr Congress, with similar encouragement clearly evident at subsequent meetings. The continuing rise in attendance, however, with 963 registrants at the recent Chicago meeting of the ACA and 2,477 at the 21st Congress, makes such interactions increasingly difficult although, potentially, of even greater value. Such encouragement can be most valuable for personal development and, although many years have now passed since his last ACA meeting and IUCr Congress so personal observation is lacking, he has confidence that neophytes will continue to receive such encouragement.

It is a pleasure to thank Peter Strickland, IUCr Managing Editor, Mike Dacombe, IUCr Executive Secretary, Chip Calhoun, AIP Niels Bohr Library, Cora Lind, Secretary-Treasurer USNCCr, Terry A. Renner, Executive Director IUPAC and Crystal Towns, ACA Membership Secretary for providing or confirming institutional assignment information

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The Puzzle Corner

This issue of the Puzzle Corner has responses to the *names into adjectives* discussion as well as answers to the questions posed in the spring 2011 issue of *RefleXions* and some new questions posed by one of our careful readers.

Historical artifacts: Jim Silverton writes: "At a recent performance of the play, *Photograph 51*, by Anna Ziegler, which is concerned with the work of Rosalind Franklin on the DNA structure and the use of her data by Watson, Crick and Wilkins, Franklin is shown manipulating a piece of realistic looking apparatus. Although the x-ray generator was only suggested, I wonder if anyone who has seen the play can confirm that the apparatus is a real fiber diffraction camera? I don't think I have ever seen one". Perhaps some answers can be found in the article *Crystallography on Stage and Screen* on page 6.

Jim continues: "A related question arises as I wonder how many examples of classical apparatus for x-ray diffraction, like rotation cameras and Weissenberg and precession cameras, actually remain in working condition or even in use. More elaborate crystallographic data collection equipment like the Ladell and Arndt-Willis analog diffractometers may also already have disappeared. I would be glad to know of examples of apparatus that still remain in working condition and, if it seems suitable, I might prepare a listing that could be published in *RefleXions"*. (***jim.silverton@sigmaxi.net)***

Crystallography in the movies: We asked if anyone could name the last crystallographer to appear in a Hollywood movie (answer: Ryonosuke Shiono, George Jeffrey's group at U. of Pittsburgh played a symposium doctor in *Lorenzo's Oil*) and which science fiction book references Martin Buerger's *X-Ray Crystallography* (answer: A *Clockwork Orange* by Anthony Burgess).

New movie puzzler: Which Jimmy Stewart movie mentions crystallography ? Who was his co-star? In what circumstances was crystallography mentioned?

Crystallographic adjectives: Virginia Pett suggested that Wooster *ish,* Wodehouse-style GBR, could become Wooster *ite* a person from Ohio USA.

Jack Dunitz writes: "The background to your puzzle is interesting and deserves further study. Indeed, -ian and -ic enjoyed wide application in converting proper names to adjectives. Your scientific and mathematical examples are mainly pre-1900. In addition to these mathematical examples, one can think of Gaussian, Hermitian, Eulerian, Euclidian, ... but not Pascalian or Poissonian. Why is this? Both crystallographic and post-1900 examples from physics and chemistry are hard to find because, from then on, the proper noun is simply used as an adjective: e.g. Schrödinger equation, Bose-Einstein statistics, Dirac function, de Broglie relation from physics; Pauling electronegativity, Cope rearrangement, Fischer convention, Lewis acid, Woodward-Hoffmann rules from chemistry and Bijvoet pairs, Patterson function, Sayre equation, Weissenberg camera, Bernal chart (who remembers that now?) from crystallography, as well as innumerable others. In each example, the proper name is used as an adjective, without the -ian or -ic. Sometimes there is a possessive — Planck's constant, Bragg's Law but, more often, not. The primary question seems to be: why did the -ian or -ic ending, formerly used to convert a noun into an adjective, disappear? Who has an answer to this?"

Who is in the photo and when was it taken: We have identified everyone in the photo but still do not know when and where..

Back row: David Sayre, Bob Newnham, David Shoemaker, Ken Trueblood. Middle row: Ray Young, Jerry Karle, Phil Coppens, Bill Busing, Bill Duax, John Kasper. Front row: Isabella Karle, Sidney Abrahams, David Harker, Hal Wykoff.

ACA meeting, Spring 2002, San Antonio, TX: Who are the gentlemen at the banquet (top) and the members of the Data Committee (middle)? The images below the photos are from a poster illustrating the teaching of crystallography - who presented the poster?

*Sidney Abrahams (**sca@mind.net**)*

Networking Yesterday and Tomorrow

Point, click, swish: the computer in your palm, lap, desktop is an instant link to the world. Horizions, the borders of your imagination, recede and even vanish. While only a fraction of the Internet is used for scientific purposes, crystallographers have always been at the forefront in creating or using available technology to advance scientific knowledge. The seniors among us will remember punching holes in tapes or cards for computer input/output – only 40-50 years ago. Who could have predicted then the vistas provided by networking and the internet? What links and tools are emerging to stretch and deepen our scientific insights: Networking yesterday and tomorrow.

September 6, 1971, marks the beginning of networking in the life sciences and arguably in the chemical sciences as well (*A Brief History of Networking in the US,* E. F. Meyer and N. F. Funkhouser *J. Chem. Infor. & Comp. Sci.* (1998) **38**:951-955). Within a year several laboratories were part of CRYSNET, a star-type network with the main computer at Brookhaven National Laboratory and dial-up telephone lines the physical links. The seminal event on this auspicious day was the first remote access to and retrieval from the nascent Protein Data Bank (PDB) by Walter Hamilton and myself (EM). Although the PDB contained only a handful of structures in 1971, then-current network searches had been limited to 1-D text queries (titles, authors, etc.). Novel software permitting 3-D searches of the PDB using geometric or biological descriptors were executed at 110 baud over a distance of 2800 km, marking the dawn of remote searches and the inauguration of the PDB.

1973 CRYSNET software team: David Klunk, Tom Koetzle, Edgar Meyer, Herb Bernstein, Tom Willoughby (missing: Larry Andrews, Carl Morimoto)

Even as the PDB grew, other labs joined CRYSNET, enhanced by computer graphics and interactive computing programs to increase the power of database searches. 40 years ago, the four cornerstones of our science of computational crystallography were set in place: structure analysis -> data bases (PDB, CCDC, ICSD) -> networking -> interactive graphics -> structure analysis. In parallel, the Cambridge Crystallographic Data Centre (CCDC) released small-molecule structural data on magnetic tape starting in 1972; structure-based search tools became available in 1978. For the Inorganic Crystal Structure Database (ICSD), remote access became available about the same time and Dayhoff's Atlas of Protein Sequence and Structure was published in 1965.

Initially, progress was slow and the impact on the life sciences limited. Few had access to computers, even fewer to interactive graphics. Remember, until virtual memory addressing became available in the late 1970s, computer systems, programs, and data were memory-bound to 32k words – total. From such modest beginnings, as hardware and software advanced with time, network access grew: TCP/IP, packet switching, the internet, the world wide web – these were giant steps toward today's capabilities: e-books, remote robotic surgery, planetary probes, social networking, streaming video of daytime soaps operas and yes, clever, insidious hackers, all are now part of everyday experiences. So, what does the future hold?

Walter Gilbert, the Nobel Laureate and a pioneer in biology said 2 decades ago that biology is fast becoming an information science. The "genome" revolution would never have been possible without the dramatic advances in informatics and thousands of biologists would never had made such dramatic progress without strong networking tools. The bandwidth, the speed of communication and the advances in information technology spanning databases, query and processing engines all have led to a paradigm shift in biology research.

The role of informatics in genome sequence-driven biology began in Los Alamos with VAX computers, where researchers manually typed the 1-D sequences of proteins obtained by painstaking procedures. The data were stored as a spread sheet and accessed through an arcane query system which led to a traditional ascii text search process. This was the forerunner of the GenBank.

Today, sequence data, even with the vast annotations associated, form only a minuscule part of the total data publicly available. Sequence data comprises 1-D strings of alphabetic characters and the storage requirements of strings are small. However, experimental innovations now yield vast amounts of high throughput data in the form of images - such as 2-D optical imaging and radiological imaging, gene expression data – in the form of intensities or tables, but the sheer volume is daunting, proteomics and metabolomics data – a combination of mass spectrometric imaging, western blots and NMR measurements, and a host of clinical data whose volume is ever increasing. A large effort is being invested in developing ontologies for the myriad types of data in biology so that these can be organized and structured in 3-D to n-D databases. The era of 1-D flat files and 2-D excel spread sheets to store vast amounts of data is almost over. Such spread sheets cannot be cross-queried and this challenge notwithstanding several other formats are forcing biologists to consider database technologies that are completely alien to biology and other sciences.

Relational and object-relational databases are now commonplace in biology. Genbank and ENSEMBL are now databased in Oracle or as are some protein structure databases. Gene expression datasets can be downloaded as tab-limited files, but significantly processed data are also available in the form of stored heatmaps, clustergrams and in other n-D representations. With the advent of next generation sequencing, vast amounts of genomic and epigenomic data will be available, although the primary images from sequencing are not stored given that each query cycle produces a terabyte of data.

While database technology has become pervasive in biology, the usefulness to biology is in our ability to query and analyze these data. As a result biological data are present in multi-tier n-D information architectures. The back end tier is always the database that contains data in the form of tables based on well-defined schema which in turn are founded on a defined ontology. The development of the schema is the most challenging first step that requires strong collaboration between computer and information scientists and biologists. The assembly of the data tables can be automated through scripts. The interface tier is almost always designed as a web interface with a few exceptions where customized user interfaces are built. Examples of the former include in addition to ENSEMBL and GenBank, GEO, the Signaling Gateway, RCSB (PDB), and EcoCyc, to name a few. The latter includes several pathway and image data interfaces. The middle-tiers involve significant software engineering. These include the query and analysis framework for the data infrastructure and are often invoked by commands from user-friendly interfaces. Structured Query Language (SQL) forms the foundation for all relational database queries. However, experimental biologists are not trained in SQL and it would be a challenging task to introduce mandatory training. Fortunately, there are an increasing number of automated tools that translate standard web interface queries into SQL and the results are presented in graphical or easily readable formats. Analysis queries are often more complicated and involve an additional layer. For instance, if the query involves correlation between gene expression and proteomic data then a statistical tool is invoked following fetching of data from the databases through a sequel query. Such concatenation between a query and analysis is achieved through back-end software in the infrastructure. For the crystallographer, this provides the link back to the 3-D structure.

We are witnessing the tip of the iceberg in the biology data revolution. The expected rate of data increase will outpace Moore's law. However, the challenge will be in the ability to access, process and use these data. Significant development of ontologies and data representations, query and visualization methodologies and most importantly a large number of analysis tools is essential for next generation biology. This requires a different generation of scientists and researchers who are highly proficient in biology, information and computational sciences and statistics. Further developments in web and database technologies are essential for this growth, challenging the current structure of college curricula in mathematics and the natural sciences.

The age-old dimensional challenge, linking information – knowledge – wisdom, is recast as databases are linked - queried - mined and resulting hypotheses must be tested, novel experiments designed, and multi-dimensional concepts distilled for our limited, human 3-D perceptions.

Edgar Meyer, co-initiator of the Protein Data Bank
Shankar Subramaniam, creator of The Biology Workbench

Crystallographic Computing at Oak Ridge National Laboratory 1954 to 1968

ACA President (1971) and winner of the ACA Buerger Award (1985) William R. Busing is known for his many contributions to the computing side of x-ray and neutron diffraction. The computer program ORFLS (Oak Ridge Structure Factor Least Squares) that he and Levy originated at Oak Ridge National Laboratory was widely used by a generation of crystallographers. In this narrative Bill describes the programming challenges in the early days of crystallographic computing. This article, complete with references, can be found in the IUCr Commission on Crystallographic Computing Newsletter No. 8, available at http://iucrcomputing.ccp14.ac.uk/iucr-top/comm/ccom/newsletters/2007nov/

The ORACLE (Oak Ridge Automatic Computer and Logical Engine)

I arrived at Oak Ridge National Laboratory (ORNL) in September, 1954, and joined the neutron crystallography group headed by Henri A. Levy. My previous work had been in Raman and infrared spectroscopy and I was interested in structures, but I had very little knowledge of crystallography. I was certainly aware of the pioneering work that had been done by Henri together with Selmer W. Peterson, who was on sabbatical for the year. I started out by trying to grow millimeter-sized crystals of various hydroxides.

Henri Levy and Bill Busing

I knew that Henri had been learning to program for the ORACLE and when I expressed some interest in this, he offered to teach me all about it while I waited for crystals to grow. According to Henri, the first step in writing a program is to make a flow chart, a procedure that I have found useful in all my subsequent work. We started out by writing a simple program to calculate Bragg angles and put out an ordered list. The ORACLE, a vacuum-tube computer that occupied a large room, had been built at Argonne National Laboratory by ORNL personnel and installed here during the previous year. Its cathode-ray-tube (CRT) memory consisted of 1024 40-bit words. Each word can be described as ten hexadecimal characters, using the symbols 0 to 9 and A to F. A word could be treated as one fixed-point number or as two five-character commands. Each command used two characters for the command and three for an address ranging from 000 to 3FF.

Fixed-point additions and subtractions were done in a 41-bit accumulator, or A register, and multiplications and divisions used a 40-bit Q, or quotient register. Numbers in these registers could be shifted left or right, using either one or both registers. There were no index registers or indirect addressing. To step through a loop, we would set a counter initially and then increment it and test it on each pass through the loop. To step through an array, we would set an initial address in a command. Then after each pass we would pick it up, increment it, and put it back.

Input and output were done with five-hole teletype tape. Four hole positions were used for the characters 0 to F and the fifth was a parity check. Input tapes were prepared by typing on teletype machines, and output tapes were printed on these same machines.

Programs were prepared in hexadecimal and temporary storage locations were assigned. If π or other constants were needed, they would be manually converted to hexadecimal and included in the program. Then the program would be manually typed onto tape so that it could be loaded into the ORACLE, starting at a specified location. Input and output subroutines were available so that decimal data could be read by a program and output could be converted to decimal, punched, and later printed off line.

At the console of the ORACLE was a cathode-ray tube that displayed the 32 x 32 grid representing one bit of the 40-bit words in the memory. One could follow the course of a program by watching where the spots brightened momentarily. A speaker also produced an audio signal as the commands were executed, and one could get to know what a particular program sounded like. Our Bragg-angle program was finally ready for its initial tests just before the December holidays. The program was loaded and started, but shortly thereafter the speaker started emitting a continuous tone and one area of the memory lit up brightly indicating that the program was in an unending loop. We followed the usual procedure of punching out and printing a dump of the memory contents. Overnight I found what I hoped was the single bug, and the next day I went back to get another shot at the ORACLE. But it was Christmas Eve, the mathematics party was in full swing, and the ORACLE was playing Christmas carols! I had to wait till after the holidays to get my first list of ordered Bragg angles.

Absorption-correction software for the ORACLE

The first crystals that I was able to grow were calcium hydroxide. The heavy-atom positions were known from the early x-ray work of Bernal and Megaw, who also postulated the hydrogen positions. In previous neutron diffraction studies by Levy and Peterson the practice had been to grind the samples to a cylindrical shape, so that tabulated absorption corrections could be applied. This had been done by putting the oriented crystal on a sandblasting lathe and grinding the edges off. But calcium hydroxide is a layer structure that cleaves like mica, and the sandblaster immediately caused the crystals to open up like the pages of a book. This led Henri and me to consider whether we could use the ORACLE to calculate the absorption correction for a crystal whose shape had been carefully measured.

In the first version of this absorption program, we integrated the correction over a few hundred equally spaced scattering points within the crystal volume. Later a consultation with mathematicians showed us that we could get better accuracy by selecting the points and weighting the contributions according to the rules of Gaussian integration. This program and a later Fortran version were used for all our neutron-diffraction studies after that.

Structure-factor data for fifty-three *h0l* reflections from calcium hydroxide were measured at two temperatures, and Henri suggested that we should make a Fourier projection. He had commissioned the ORNL Math Panel to prepare a Fourier program for us, but our first tries at using that program showed that it would be very tedious to use. This led us to prepare a new two-

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dimensional Fourier program more suitable for crystallographic purposes. This program initially calculated a look-up table with all the values of the sines and cosines that would be needed. Most of the rest of the memory was allocated to the map that would be produced. The indices and structure factor were read from paper tape one reflection at a time, and its contribution was added to each point of the map. After all the reflections had been included an output tape was punched so the map would be printed in a suitable format to be contoured by hand

Least-squares software written for the ORACLE

To get more precise coordinates and interatomic distances, Henri suggested that we could use the method of least squares. My knowledge of least-squares refinement was based on Margenau and Murphy. I was not even aware of the pioneering crystallographic least-squares refinement work of Hughes. The parameters for calcium hydroxide included two coordinates, six anisotropic temperature-factor coefficients, and a scale factor, for a total of nine parameters. The ORACLE program that we wrote was probably designed for this particular problem. The appropriate derivatives were used to set up the full matrix, and a subroutine was available to solve the nine simultaneous equations. The four cycles of least-squares adjustments needed for convergence took about twenty minutes of ORACLE time.

In order to calculate the standard errors of the distances and angles, we needed the variance-covariance matrix that could be derived from the inverse of the least-squares matrix; but no matrix inverter was available for the ORACLE at that time. Instead, we inverted the matrix by solving nine simultaneous equations a total of nine times, using as the nine column vectors (1,0,0,0,0,0,0,0,0), (0,1,0,0,0,0,0,0,0), etc. The nine solution vectors then formed the columns of the inverse matrix.

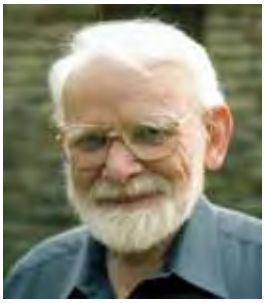
At about this time Henri and I realized the desirability of writing a generalized least-squares program that could be used to adjust the parameters defining any arbitrary function. The function would be provided by the user, who would need only to write a subroutine to evaluate the function based on the parameters and the values of one or more independent variables for which experimental values had been obtained. For example, we refined the lattice parameters of diaspore using observations of the Bragg angles from an x-ray powder pattern. Here the independent variables were the indices, along with an indicator as to whether the wavelength for an $\alpha 1$, an $\alpha 2$, or an unresolved line should be used.

A unique feature of this general least-squares program was that the user had the option of calculating the required derivatives of the function with respect to the parameters or letting the program calculate derivatives numerically. In the latter case the user would just provide a list of increments to be added to one parameter at a time. The function was recalculated with the incremented parameter, and the derivative was taken as the ratio of the change in the function to the parameter increment. This program and its successors were so easy to use that other groups at ORNL and elsewhere used it routinely to analyze thermodynamic data, spectral patterns, and other complicated functions.

Crystallographic least-squares refinement on the IBM 704

About 1958 an IBM 704 computer became available at the gaseous diffusion plant in Oak Ridge. Although this required a drive of about seven miles, the advantages over the ORACLE were considerable. These included a memory of 8,192 36-bit words, hardware floating-point arithmetic, index registers, removable magnetic tapes, and punched card input and output. An assembler was available to facilitate writing programs that would be automatically converted to binary form.

Henri and I decided to write a least-squares program that could be used for the refinement of any crystal structure based on x-ray or neutron-diffraction data. Whenever we couldn't decide how to do something we left it as an option for the user. Thus the program could refine a structure based on either F or F^2. An overall temperature factor or individual isotropic or anisotropic temperature factors could be used. Symmetry cards were included to allow for the refinement of any centrosymmetric or noncentrosymmetric structure. Atom multipliers were provided to correctly weight atoms in special positions or to treat disordered structures. Anomalous scattering factors could be included. Different scale factors could be applied to data from different samples. Henri and I wrote a program to invert a symmetric matrix in the space required to store only its unique upper-triangular elements. Although this program was later shown to be rather inefficient, it allowed for the adjustment of up to 120 parameters in the 8,192-word memory. When Carroll Johnson joined our group in 1962, he and Henri wrote an improved matrix inverter that made use of the Choleski method of factoring a symmetric matrix.



Carroll Johnson

We wanted to distribute this program to anyone who requested it. However, with instructions punched one per card, the source program consisted of over 4,000 cards. We considered that this would be too expensive to copy and ship. Instead, we distributed copies of the binary card decks that were produced by the assembler. A handbook was available that gave detailed instructions on how to use the program.

In 1961 Kay Martin of the ORNL Math Panel joined our group to help with computer programming. Her first job was to convert the structure-factor least-squares program to Fortran. This made it easier for us to distribute the source program either on punched cards or via magnetic tape. When the ORACLE was replaced by the Control Data 1604 and later by the IBM 360, the Fortran program was easily adapted to the new computers.

Availability of the Fortran source code also allowed others to make changes in the program. Jim Ibers and Walter Hamilton of BNL improved the form for input of the symmetry information. Methods of correcting for extinction were introduced. Carroll added the ability to refine more complicated forms of thermal motion. No further printed reports were written, but the instructions included with the distributed program were kept up to date. The latest version lists nine persons as contributing authors. In 1982 *Current Contents* listed the 1962 report as a *Citation Classic* that had been cited more than 3000 times.

The primary purpose of most crystallographic investigations is to obtain detailed information about the chemical structures of the molecules or ions involved. After the lattice parameters, atomic coordinates, and temperature factor coefficients have been obtained, it is desirable to calculate bond distances, bond angles, torsion angles, and other quantities, some of which depend on the observed thermal motion. It certainly is useful to obtain the standard errors of the calculated quantities, and these can be calculated in a straightforward way from the variance-covariance matrix that is proportional to the inverse matrix of the normal equations.

After completing the first version of our crystallographic least-squares program Henri and I proceeded to write a Fortran program to calculate some fifteen different kinds of functions together with their standard errors. The functions calculated included bond distances, bond angles, torsion angles, the difference between two bond distances or angles, the sum of several bond angles, and nine more functions involving thermal motion.

The calculation of standard errors requires the values of the derivative of the function with respect to each parameter involved. A unique feature of this program is that, instead of deriving expressions for these derivatives, we decided to determine them numerically by adding an increment to a parameter, recalculating the function, and computing the derivative as the ratio of the change in the function to the parameter increment. This method produces a correct result, even when certain parameters are constrained by symmetry or for some other reason, provided that the constraint is reapplied each time a parameter is incremented.

Provision was made for the user to write subroutines defining any new functions desired. Available for this purpose were subroutines for picking up atomic coordinates and temperature factor coefficients, manipulating matrices and vectors, and calculating angles. Other mathematical routines could also be used. This program was later modified by Kay Martin to conform to the Fortran version of the least-squares program. It has been kept up to date with a few improvements and has been generally distributed on request together with the least-squares program.

Three-circle neutron diffractometer control using paper tape

Shown in Fig. 1 is the three-circle neutron diffractometer that we installed in 1960 at the newly operational Oak Ridge Research Reactor. A crystal monochromator centered in a concrete shield reflected the neutrons to produce a vertical beam. A General Electric diffractometer was mounted on its side to support the appropriately counter-weighted neutron counter. Centered on this instrument was a ring to provide the chi-angle orientation and support the phi-angle drive.

Fig. 1: The three-circle paper-tape controlled neutron diffractometer. (Photograph courtesy of ORNL).

This instrument was controlled by electronics that read the desired two theta, chi, and phi angles from paper tape. Motors would drive each shaft until the encoders registered the desired angles. It was arranged that the final adjustment of each angle would always be made slowly in the same direction to avoid backlash problems.

With this then-new type of instrument we no longer needed to orient a crystal sample. We only had to center it and determine its orientation by observing the angles for two or more reflections. ORACLE programs were written to use this angle information to refine the orientation and prepare a tape with the angles for data collection. It was arranged that after the electronics had set the initial angles it would make a theta-two-theta step scan through the reflection, punching the observed counts on an output paper tape. This tape was then carried back to the ORACLE for further data processing to obtain the integrated count and the peak position in two-theta. Assuming that the counter has a large aperture, this peak maximum occurs when the reflecting plane best satisfies the Bragg condition. Deviations from the calculated two-theta were then used to further refine the orientation and lattice parameters.

After the ORACLE was replaced by the Control Data 1604 computer the three-circle data collection programs were rewritten for that machine. The Control Data 160A auxiliary computer was used to convert from magnetic tape to paper tape and vice-versa.

Four-circle x-ray diffractometer control using a DEC PDP-5

In the fall of 1962 I went to England to spend a year on sabbatical working with Owen Mills at the University of Manchester. There the computer engineers were in the process of installing the Ferranti Atlas supercomputer, a state-of-the-art machine that was to run several programs at a time, switching them in and out of memory from an auxiliary storage drum. Owen was having a four-circle x-ray diffractometer built by Hilger-Watts, and he intended to use the Atlas computer to control this instrument. Working in this time-sharing mode, the diffractometer would use only a small fraction of the computer's resources.

I wrote computer programs to calculate instrument angles, drive motors, center reflections, calculate orientation, and collect intensity data. All these programs were written without the presence of the diffractometer that was not delivered until April of 1963. After the diffractometer was interfaced to the computer, we were only permitted to test it on Saturday mornings, times set aside for computer maintenance. After we got started it seemed as though the Atlas would never run for more than about fifteen minutes before it crashed. Then we would spend the rest of the morning arguing with the engineers as to whether the problem was with our software or with the computer hardware. I had to leave Manchester before these problems were solved.

When I returned to Oak Ridge we wanted to install an automatic four-circle x-ray diffractometer, but I was sure that we didn't want to interface it to a large time-sharing computer. Cole, Okaya, & Chambers had recently described a diffractometer controlled by a dedicated IBM 1620 computer, but that computer, at about $100,000, was too expensive for our budget. Then we learned of the DEC PDP-5 computer that was available for about $20,000.

We also knew that Tom Furnas of the Picker X-ray Corporation had recently designed and built a four-circle diffractometer

that Picker intended to market for use with paper-tape control. It didn't take long for us to realize that we could easily control this diffractometer with the PDP-5 computer. In 1965 we produced the system shown in Fig 2.

Fig. 2: The four-circle Picker x-ray diffractometer and the PDP-5 computer that was programmed to control it (Photographs courtesy of ORNL)

The PDP-5 (a predecessor of the PDP-8) had a core memory of 4096 12-bit words divided into 32 pages of 128 words each. An instruction occupied one word and the type of instruction was defined by the first three bits so there were only eight different kinds of commands. Six of these instructions used seven bits to define an address that could be either on the same page or on page zero, but it could also refer to any location in the memory by indirect addressing. Hardware arithmetic was limited to addition, but a complete package of subroutines to perform floating point arithmetic was available.

Input or output was accomplished by a teletype interfaced directly to the computer. Input could be typed or loaded from punched-paper tape. Output could be printed or punched on tape.

We decided to use Slo-Syn stepping motors that took one hundred steps to make a revolution. The angles of the Picker diffractometer were geared to change one degree for each turn of a drive shaft. Thus, with a motor on each shaft, the angles two-theta, omega, chi, and phi could be set to the nearest 0.01 degree without the use of encoders. To provide a check on the angles ORNL engineers designed an optical detector to signal the computer at each even degree.

A feature of the PDP-5 that was new to us was the availability of a hardware interrupt. Thus any external action, such as the typing of a teletype key or the closing of a limit switch, could interrupt the program that was operating and jump to a special interrupt program. We knew that the Slo-Syn motors could run smoothly at 300 pulses per second, so we arranged for a crystal-controlled oscillator to interrupt the computer 300 times each second. An interrupt program would check to see which motors should be running and send a single pulse to step that motor forward or backward. Every 30th clock interrupt was treated as a tenth-of-a-second interrupt and used for timing counts or any required delays.

At about the time the PDP-5 was delivered, Sharron King of the ORNL Mathematics Division joined our group to help with the diffractometer programming. Although an assembler program was available for the PDP-5, we found it useful to create an assembler program, written in Fortran, to run on the CDC 1604 and 160A computers. We put our instructions on punched cards, and the assembler produced a binary tape that could be loaded into the PDP-5.

The subroutines for floating point arithmetic, trigonometric functions, and matrix operations took up about half of the memory. The other half would be loaded with programs for the particular operations we were performing. A setup program would be used to search for reflections, center them, and establish initial lattice parameters and sample orientation. Then a least-squares program could be loaded to refine this information. Finally, a data collection program would measure the reflections systematically, making step scans and punching the results on paper tape. This output tape would be processed further by the CDC computers.

This data collection system remained in operation for almost twenty years. When it was acquired, the PDP-5 was one of the first minicomputers at ORNL. When it was finally decommissioned it was the oldest computer at the laboratory.

This has been the story of one group's experiences in the early uses of computers for crystallography. Everything seemed new and exciting at the time we were working on it. We certainly never envisioned the days when similar things could be done on a laptop computer at unimagined speeds. But that seems to be the way science works.

Bill Busing

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION, INC.
BALANCE SHEET - December 31, 2010 and 2009

	CURRENT FUNDS (2010)		TOTAL	
	Unrestricted	Restricted*	All Funds	
			2010	2009
ASSETS				
Current Assets:				
Cash	208,659		208,659	291,991
Investments	301,650	407,683	709,288	707,812
Inventory	2,225		2,225	2,225
Accounts Receivable	10,500		10,500	1,740
Total Current Assets	522,989	407,683	930,672	1,003,768
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	528,887	407,683	936,570	1,009,666
Liabilities:				
Unearned Dues	30,752		30,752	93,019
Credit Card Liabilities	(134)		(134)	(186)
Total Liabilities	30,618		30,618	92,833
Fund Balance:				
Unrestricted	498,269		498,269	545,180
Restricted		407,683	407,683	371,653
Total Fund Balance	498,269	407,683	905,952	916,833
TOTAL LIABILITIES & FUND BALANCE	498,269	407,683	936,570	1,009,666

*** Current Balances in individual restricted funds - as of December 31, 2010**

Buerger Award	36,500
Etter Award	63,089
Fankuchen Award	68,404
Patterson Award	42,899
Pauling Award	33,732
Supper Award	11,912
Trueblood Award	35,182
Warren Award	28,637
Wood Science Writing Award	52,328
Bau Neutron Award	35,000

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 14203-0906.

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See Page 39 for a full list of meeting sponsors

What's on the Cover - (all images provided by Kavli Prize winner Ned Seeman who gave a plenary lecture at ACA New Orleans)

Upper Left: *Dynamic Patterning Programmed by DNA Tiles Captured on a DNA Origami Substrate* - Schematics (left) and atomic force micrographs (right) of the origami arrays and capture molecules. ***Panels i*** (left) illustrates the origami array containing slots for the cassettes and a notch to enable recognition of orientation; the slots and notches are visible in the AFM on the right. *Panels ii* show the cassettes in place; the color coding used throughout the schematics is green for the PX state and violet for the JX2 state; the presence of the cassettes is evident in the AFM image. *Panels iii* illustrate the PX-PX state which captures a triangle pointing toward the notch in the schematic and in the AFM image. *Panels iv* illustrate the PX--JX2 state, containing a triangle that points away from the notch, which is evident in the corresponding AFM image. *Panels v* illustrate the JX2-PX state which captures a diamond-shaped molecule; its shape is visible in the AFM image. *Panels vi* show the linear molecule captured by the JX2-JX2 state, both schematically (left) and in the AFM image (right). (*Nature Nanotechnology* (2009) **4**, 245-248))

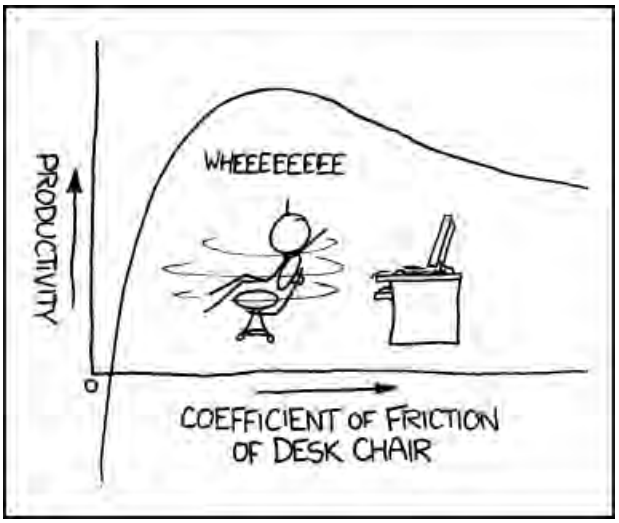
Upper Right: *At the Crossroads of Chemistry, Biology, and Materials: Structural DNA Nanotechnology*: *2D DNA Crystalline Arrays*. *From top to bottom (a-d): (a) Two DX Molecules Tile the Plane*. A conventional DX molecule, A, and a DX+J molecule, B*, are seen to tile the plane. The extra domain on B* leads to stripes. The molecules are 4 x 16 nm, so the stripes are ~32 nm apart, as seen in the AFM image at the right. Sticky ends are shown as geometrical features. *(b) Four DX Molecules Tile the Plane*. This arrangement is similar to *(a)*, but there is only one DX+J molecule, D*, so the stripes are separated by ~64 nm, as seen on the right. *(c) A TX Array*. Two TX tiles, A and B are connected by complementarity between their first and third double helical domains, resulting in spaces between the tiles. D is a linear duplex that fits in the yellow rows, and C is a TX re-phased by three nucleotide pairs; it fits into the gray rows and extends helices beyond the AB plane in both directions, as shown in the micrograph at the right. *(d) A DNA Parallelogram Array*. Four Holliday junction analogs form a parallelogram that is extended to produce a periodic array. The sizes of the cavities in the array may be tuned. Those in the array on the right are ~13 nm x ~20 nm (*Chemistry and Biology* (2003) **10**, 1151-1159).

Lower Right: *A DNA Crystal Designed to Contain Two Molecules per Asymmetric Unit* – Covalent attachment of dyes to the independent molecules in the crystal. The way in which the components of each crystal drop were prepared is indicated above each image of crystals. In the top row, from left to right, Cy3 has been attached to the A molecule, to both molecules, and to the B molecule. Crystals in all three drops are pink. The bottom row has a similar arrangement of molecules to which Cy5 has been attached: left, A; center, both; and right, B. Crystals in all three drops are blue-green. The center row contains drops with both arrangements of molecules containing both dyes, Cy3 on molecule A and Cy5 on molecule B in the drop on the left, and the opposite arrangement on the right. Both drops are purple in color. The center drop contains a control whose molecules have neither dye attached to them. (*JACS Communications* (2010) **132**, 15471-1573).

Lower Left (and middle): *From Molecular to Macroscopic via the Rational Design of a Self-assembled 3D DNA Crystal*: *Lattice Formed by the Tensegrity Triangles*. *Top*: Surroundings of a triangle. This image distinguishes three independent directions by base-pair colour. The central triangle is flanked by six other triangles. *Bottom:* Rhombohedral cavity formed by tensegrity triangles. This image shows seven of the eight triangles that comprise the rhombohedron's corners. The cavity outline is drawn in white. The rear red triangle connects through one edge each to the three yellow triangles in a plane closer to the viewer. The yellow triangles are connected through two edges to the green triangles in a plane yet closer (*Nature* (2009) **461**, 74-77).

Lower Middle: Schematic design, sequence, and crystal pictures. *Top*: Schematic of the tensegrity triangle. The three unique strands are shown in magenta (strands restricted to a single junction), green (strands that extend over each edge of the tensegrity triangle) and dark blue (one unique nicked strand at the center passing through all three junctions). Arrowheads indicate the 39 ends of strands. Nucleotides with A-DNA-like characteristics are written in bright blue. Cohesive ends are shown in red letters. *Bottom:* An optical image of crystals of the tensegrity triangle. The rhombohedral shape of the crystals and the scale are visible.

Middle: *Early topological constructs built from DNA*: *Left*: A cube-like molecule. This molecule is a hexacatenane; each edge corresponds to two double helical turns of DNA. Each backbone strand is drawn in a different color, and each one corresponds to a given face of the cube. Each is linked twice to each of the four strands that flank it, owing to the two-turn lengths of the edges (*The Synthesis from DNA of a Molecule with the Connectivity of a Cube*, *Nature* **350**, 631-633 (1991)). *Right*: A DNA-truncated octahedron. This molecule is a 14 catenane, again with each edge consisting of two turns of double helical DNA. Although the truncated octahedron has three edges flanking each vertex (i.e., it is "three connected"), it has been built using four-arm junctions. (*The Construction of a DNA Truncated Octahedron*, *Journal of the American Chemical Society* (1994) **116**, 1661-1669).



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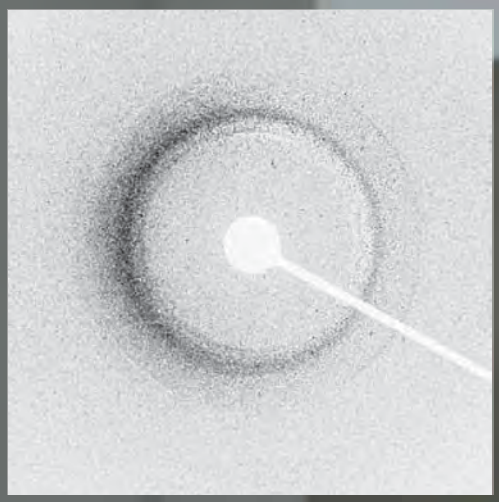

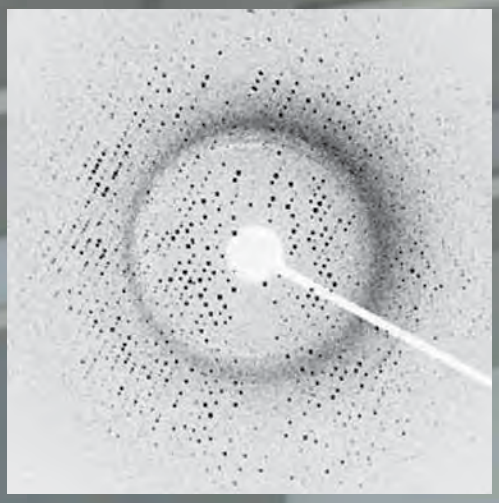

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Ed Collins - Vice President

Department of Microbiology and Immunology, Department of Biochemistry and Biophysics, Lineberger Comprehensive Cancer Center, University of North Carolina at Chapel Hill.

Education: University of Connecticut BS (1983); University of Texas at Austin PhD (1990) with Jon Robertus; Harvard University Postdoc with Don Wiley; John Radcliffe Hospital, Oxford, UK Visiting Fellow (1995) with Alan Townsend and Vincenzo Cerundolo.

Professional Activities: *ACA*: BIOMAC SIG Chair (2010), Program Chair ACA Orlando (2005), Poster Judging Committee Organizer, Hawaii (2006), Session Chair (2007-current); *NIH*: Cellular and Molecular Immunology Study Section (2010-2012), *Ad Hoc* CMB; AED, NSF: Graduate Student Fellowship Review (2008-2010); *Societies*: American Association of Immunologists, American Society for Biochemistry and Molecular Biology; *Regional*: Development and oversight of Southeastern Regional Collaborative Access Team, Mid-Atlantic Crystallography Meeting Program Chair.

Research Interests: I found protein crystallography accidentally. While I was a rotation student in Jon Robertus' lab at UT Austin doing molecular biology, another student was fitting an electron density map of ricin using an Evans and Southerland graphics station running FRODO. Although the display was black and white, I was green with envy because of the sophistication of the technique and sense of discovery. I wanted to be fitting that electron density that no one had seen before. In that moment, my focus switched to protein crystallography and I have never looked back. At the time, I was working on ribosome-inhibiting proteins (pokeweed antiviral protein and ricin). I bet I still have a good titer of anti-ricin antibodies. The idea was to conjugate these toxins to antibodies as magic bullets to treat cancer. After graduating, I went to Don Wiley's lab to work on major histocompatibility complex proteins where I was introduced to the wonderful world of synchrotron radiation at CHESS. The collaboration with Don and Jack Strominger stimulated my interest in immunology and the delicate and destructive interplay between host and pathogen that continues today. Currently, my lab studies molecular recognition of the Major Histocompatibility Complex by T cell receptor which is the first directed induction of the adaptive immune response; mechanisms of bacterial survival inside macrophages by *Francisella tularensis* focusing on how the bacteria escapes from the phagolysosome, two-component signaling proteins in a variety of bacteria, but mostly *E. coli* and iron thievery from hemoglobin by *Hemophilus ducreyi* and *Neisseria gonorrhoeae*.

Statement: It is a great honor to be nominated as a candidate for the Office of Vice-President of the ACA. My interactions with the ACA council have been uniformly positive. They are a dedicated and hard-working group of people. My first professional meeting was an ACA meeting in Austin, TX, (1987), and the ACA has played a large role in my professional life ever since. I can remember meeting people at ACA meetings that I greatly admired and found them to not only be approachable but sincere in their interest in students. This had no small influence on my research, because I had found a place where I felt welcomed and appreciated. I had found a home.

The role of the ACA, as I see it, is to provide an environment for scientists who are working with, and training in the use of, x-ray-based methods. That broad scope is important. It is very easy to imagine a near future where all of structural biology is relegated to the small print in the supplemental data. However, the great buzz on structural biology listservs shows that the community still debates central issues important to proper structural biology. In spite of this, many non-structural biologists in decision-making positions are unaware that these issues are still not well defined. It is in our hands to educate

Candidates for ACA Offices in 2012

The Nominating Committee (Stephan Ginell, Gerald Stubbs, and Bob Von Dreele) has proposed the following candidates for the 2011 elections for ACA offices in 2012

Officers:

Vice-President: **Edward Collins and Cheryl Klein Stevens**

Secretary: **Patrick J. Loll and John Tanner**

***Committees*:**

Communicatons: **Edward Snell and Ashfia Huq**

Data, Standards & Computing: **Howard Robinson and John Westbrook**

Continuing Education: **Angela Criswell and Amy Sarjeant**

To nominate write-in candidates for any office, write to the ACA Secretary: Carrie Wilmot, Dept of Biochem, Molecular Biol & Biophys, 6-155 Jackson Hall, 321 Church St SE, Minneapolis, MN 55455. (***wilmo004@umn.edu***). Letters must be received by September 15, 2011 and must be signed by 5 ACA members and include a signed statement by the candidate describing his or her qualifications. Voting will be by electronic ballot. Statements from all candidates will be available on the eclection site. The voting window will be open in ***October 2011***.

those people in the real issues associated with structural biology and to foster support for funding the science associated with these approaches. In addition, it is critical to give the next generations of structural biologists strong foundations in the techniques. Where else are they going to get it? My belief in this role for the ACA has led to my helping to organize many of the methods sessions for the ACA national meetings in the past ~10 years. If elected, I will serve with enthusiasm and dedication. I do not want to see my home fall into disrepair.

I am fond of telling my students that I follow the question, not the technique. Therefore, protein crystallography is a smaller fraction of the science in my lab than in my mentor's lab. That puts me in the large group of the up-coming generation of crystallographers that visualizes protein crystallography as a useful tool, but not primarily the focus of the research. However, it also puts me in the past generation where it was critical to know vector algebra to set up a precession photograph properly. The first crystallography class I took was designed for small molecule crystallographers. This allows me to see that the problems small molecule and material science crystallographers face now are harbingers of those we macromolecular crystallographers may face soon. If elected, I am looking forward to working with the structural biology community in bridging the exchange of ideas with the larger biological community and in assisting to foster the next generation of structural biologists.

Cheryl Stevens -Vice-President

Margaret W. Kelly Endowed Professor of Chemistry, Associate Dean for Research, Xavier University of Louisiana, New Orleans, LA 70125

Education: BS Chemistry, University of Tampa (1978); PhD Physical Chemistry, University of New Orleans (1982) with Louis Trefonas.

Professional Activities: Local Co-chair, ACA New Orleans (1990 and 2011). US National Committee for Crystallography (2002-2008); Department Chair (2005-2011) Department of Chemistry, Xavier University of Louisiana; Adjunct Professor (2008-) Tulane University Health Sciences Center; Adjunct Professor (1982-) University of New Orleans; Member of the Xavier Advisory Committee for the Louisiana Cancer Research Consortium (2008-); Director of the RCMI Molecular Structure and Modeling Core facility (2009-) Xavier University of Louisiana;

Research Interests: My research focuses on the use of x-ray crystallography for determination of the structures and charge densities of inhibitors of cancer growth and initiation (P450 and tyrosine kinase). I am also interested in QSAR, substrate docking, and database mining of these enzymes/substrate systems. My research projects have been funded by the NIH, Department of Defense, Board of Regents, and the Petroleum Research Fund.

Statement: It is an honor to have been nominated as a candidate for Vice-President of the ACA. I attended my first ACA meeting in Columbia, Missouri (spring, 1983) when the ACA had two meetings each year and hosted them on college campuses. I was fortunate enough to be able to serve as a local co-chair for the annual meeting in New Orleans in 1990. It was the first meeting that the ACA held entirely at a hotel. We certainly have grown in both membership and diversity of scientific interest since my early days. I was impressed then by the tight knit community of crystallographers and still believe that type of community exists. I look forward to the possibility of being involved, as Vice-President and then President, as the ACA plans for the future of our organization and community.

I believe that as a professional society, it is our responsibility to:

Organize intellectually stimulating and relevant conferences. This is especially important for engaging young crystallographers as they develop their research programs and their careers.

Advocate for the ACA in the larger scientific community, especially with respect to the importance of x-ray diffraction in an expanding group of scientific disciplines.

Educate crystallographers, other scientists, and the general public about crystallographic concepts, tools, and applications.

Provide leadership to the Special Interest Groups as they provide programming at annual meetings

Secure funding for our programs and initiatives so that we can be as strong as possible.

My positions as chair of a large and diverse department at a small liberal arts college, Associate Dean for Research, member of the Advisory Committee of the Louisiana Cancer Research Consortium, Director of the Molecular Structure and Modeling Core facility, researcher in crystallography, and teacher have given me the experience necessary to serve on the ACA Council. I am confident that my past accomplishments, experiences, and suite of transferrable skills make me a viable candidate for this position. If given this opportunity, I believe that I would be an excellent Vice-President / President of the ACA. It is such an honor to be considered.

Patrick J. Loll - Secretary

Professor of Biochemistry and Molecular Biology, Drexel University College of Medicine, Philadelphia, PA, USA

Education: BChE Chemical Engineering, Catholic University of America (1981); PhD Biophysics, Johns Hopkins University (1989); Postdoc, University of Chicago (1989-1995).

Professional Activities: Member ACA since 1988; Past Secretary, BioMac SIG; Co-editor, *Acta Cryst. F, (*2004-2010); ACA Pauling Prize committee (1998, 2002); Member, Protein Society, Biophysical Society, and American Chemical Society; Instructor and advisory panel member, NSLS Workshop on Membrane Protein Crystallization.

Research Interests: Structural basis of antibiotic activity; anesthetic recognition by proteins; deubiquitinating enzymes; macromolecular crystallization.

Statement: The ACA has been a fantastic resource for me over the last two decades, and I would be delighted to support its continued success by discharging the duties of the Secretary. In addition to acting in an organizational support role, the Secretary is a member of Council, and as such can influence the ACA's future direction. I feel prepared for this role, since: 1) my own research places me within the burgeoning structural biology "wing" of the ACA, and I have developed a keen appreciation for the tremendous new challenges facing structural biology in the post-genomic era; and 2) during my career I have also been lucky enough to be exposed to many other aspects of diffraction, including chemical crystallography, methods development, solution scattering, and crystallographic education. These experiences have given me an appreciation for the extraordinary diversity and scope of the disciplines falling under the ACA's umbrella, and I believe it is critical that the ACA continue to represent the broadest possible spectrum of interests. As Secretary, I would be honored to work conscientiously toward this goal.

Jack Tanner - Secretary

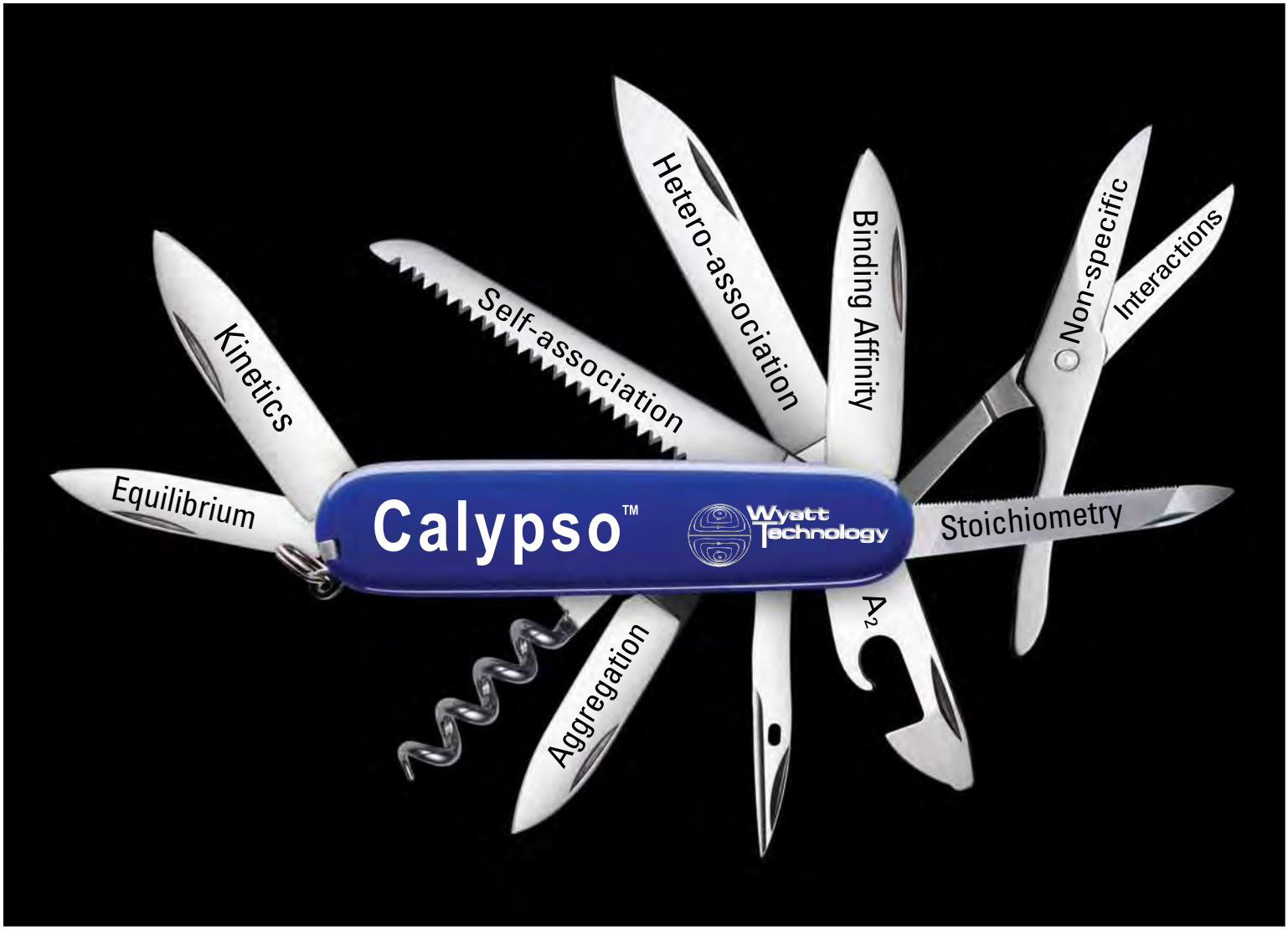
Professor of Chemistry and Biochemistry, University of Missouri-Columbia, Columbia, MO

Education: BS, Chemistry, University of Missouri-Columbia (1983): PhD, Physical Chemistry, Brown University (1988); postdoc in computational biology with J. Andrew McCammon, University of Houston (1988-1990); postdoc in protein crystallography with Kurt L. Krause, University of Houston (1990-1997).

Professional Activities: Co-Host, Midwest Crystallography Workshop, Columbia, MO (2000); Chair, Session on Computational Crystallography, Southwest Macromolecular Symposium, Houston, TX (2003); participant, American Chemical Society (ACS) Leadership Conference (2003); Secretary-Treasurer and Chair-Elect, University of Missouri ACS Local Section (2000-2003); Co-Chair, New Structures Session, and poster prize judge ACA meeting, Orlando (2005); contributor, ACA *Newsletter* (2004-2005); Secretary-Treasurer, BIOMAC SIG (2006-2008); Selection Committee for the ACA Etter Student Lecturer Award (2007); ALS beamline 4.2.2 operations committee (2004-present); Editorial Board, *Enzymes Research* (2010-present); *Ad hoc* panel member: NIH BBCB (2004), NIH Biophysical and Chemical Sciences IRG Postdoctoral Fellowships study sections (2004, 2006, 2008, 2009; chair 2006, 2008), NIH SEP on Macromolecular Structure and Function (2005), NIH study section on National Centers for Biomedical Computing (2005), NSF Molecular Biochemistry Advisory Panel (2006), NIH MSFC study section (2009), NIH MSFE study section (2010); NCI site visit review committee (2010); Co-Organizer, Third International Proline Symposium, Lincoln, NE (2010).

Research Interests: Structural biology of proline metabolic enzymes, phosphatases, parvalbumins, and UDP-galactopyranose mutases using single crystal x-ray diffraction, SAXS, and various biophysical techniques.

Statement: I am honored to stand for the position of ACA Secretary. I became an ACA member in the early 1990s when I joined Kurt Krause's nascent protein crystallography group at the University of Houston. At that time, I knew nothing about crystallography, having earned a PhD in gas phase scattering theory and done postdoctoral research in protein molecular dynamics simulations. Kurt encouraged me to attend ACA meetings as part of my education. I recall, in particular, the isomorphous replacement workshop at the 1994 Atlanta meeting. Greg Petsko gave a talk about preparing heavy atom derivatives. Bill Furey lectured about the mathematical basis of MIR and anomalous scattering. I would use what I learned from that workshop to solve my first structure using a *trimethyl lead acetate* derivative whose Patterson map I could solve by hand. I still use the workshop booklet to teach my students about experimental phasing. As a PI, I now attend ACA meetings with my students, and I value the educational mission of the ACA. As Secretary, I will support the tradition of high quality workshops as well as sessions at the national meeting on fundamental and practical aspects of crystallography. I would appreciate the opportunity to give back to the crystallographic community by serving as ACA Secretary.



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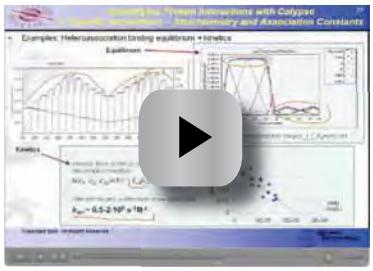

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Ashfia Huq - Communications

Instrument Scientist, powder diffractometer POWGEN, Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge TN 37831

Education: PhD Physics (2003) SUNY Stony Brook; AB Physics and Computer Science (1996) Mount Holyoke College.

Professional Activities: ACA Powder SIG chair (2009); Organizer of Workshop "Combined Use of X-rays and Neutrons", Denver X-ray Conference (2008); Co-organizer of workshop "Frontiers of Structure Analysis using Powders," Argonne National Laboratory User Meeting, Argonne, IL (2007).

Research Interests: Neutron and x-ray powder diffraction of condensed matter systems. Topics include solid oxide fuel cell materials; battery materials; catalysis; magnetic and structural properties of strongly correlated electron systems such as geometrically frustrated magnets; and *ab initio* structure solutions from powder data.

Statement: While I am a physicist by training, crystallography has been the principal tool I use to answer the questions that interest me: materials chemistry and solid state physics. I work at a Department of Energy (DOE)-owned, contractor operated, national laboratory facility which was built and is operated by tax payers' money; one of the questions I am often faced with from the general public is "why should the tax payer support your work?" This clearly identifies how crucial the role of communication is. I also find that if spoken on the right level, it is not at all hard to get people excited about the kind of work all ACA members are engaged in, since so many of our research interests have direct links to day-to-day life. Last year I had the chance to participate as a mentor to four high school science teachers chosen to attend the *Siemens Teachers as Researchers* (STAR) program. I also participated in the USA science festival held on the mall in Washington, DC doing outreach activities for students of all ages as well as for their parents. These were wonderful opportunities to reach out, especially to the younger audiences and get them excited about science in general and crystallography specifically. If elected I will strive to create better communication channels among the different SIGs within ACA and make communications with the general public a high priority.

Edward Snell - Communications

Senior scientist, Hauptman-Woodward Medical Research Institute, Buffalo NY.

Education: PhD The University of Manchester, England, BSc (Hons 1st) Applied Physics, John Moore University, Liverpool. Postdoc, National Research Council Resident Research Associate at NASA's Laboratory for Structural Biology, Huntsville Alabama.

Professional activities: Council member, International Organization for Biological Crystallization; Referee for numerous journals and several funding agencies.

Research Interests: Macromolecular crystallization, metalloproteins and complexes, radiation damage, technique development and complementary structural methods, e.g. small angle solution scattering.

Statement: Beware of Greeks bearing gifts (especially if they are large and wooden). I was reminded of that saying on receiving a phone call with a polite query on whether I might consider running for the ACA Communications Standing Committee. After putting the coffee cup down the first question I asked was what do they do? After some further conversation and a little research on the ACA website, I found that they "*meet annually to plan the work of the Committee, coordinate electronic and printed publications of the ACA, organize a press conference at the annual meetings and prepare reviews of crystallographic research*". I'm probably the worst person to be involved with this as I still have lapses putting the 'u' in color and talk about aluminium quite a lot. However, I noted that the description of the committee used a capital 'C' therefore it must be important. Sometimes it's easy to make decisions with an appropriate coffee deficit in the morning. I said yes and found I had to write a description of what I'd do should anyone be foolish enough to elect me. I'm a physicist who took a right instead of a left and ended up looking at proteins instead of particles. I found many of them to be difficult to crystallize (both the proteins and particles) so I've gradually drifted toward resolving this and in cases where I can't, staying with the solutions. This has given me a background in many of the areas that the ACA represents. I'm equally capable of communicating with a biologist or beamline scientist and of stepping outside my comfort zone in protein crystallography to look at a broader view of the field.

Jesting aside, I'm fascinated by crystallography - the ability to see the world on an atomic scale. At every level it offers richness to those who take a closer glance - the key for the Communications Committee is encouraging that more detailed glance. Beyond the science that each of us is interested in, we see crystals produced that are as beautiful as the most precious gemstones (and to their growers just as valuable). From the biological perspective the structures that result reveal fascinating images of life and these images provide the landmarks for a landscape that reveals the very living process.

I'd like to use the Communications Committee to bring this perspective to the general public, the decision makers and our colleagues in other disciplines. I'd like to raise the awareness of the diversity of research encompassed by the ACA and the importance of that research in advancing our knowledge of the world

around us. My area of interest is biological crystallography but it's important that the Communications Committee encompass all the areas exemplified by the membership and show the importance of crystallographic research and why it should be strongly supported. I've been a member of the ACA since crossing the pond in 1996 and have been to every ACA meeting since then. The ACA has helped me by bringing together a scientific family (and the uncle you don't talk about in the cupboard) with common interests. I feel it's important to give something back to the ACA. My way of doing it is to stand for this Committee. That way I'll feel less guilty when I vote for the other candidate.

Angela Criswell – Continuing Education

VP, Life Sciences X-ray, Rigaku Americas Corp, 9009 New Trails Drive, The Woodlands, TX 77381

Education: BS (1998) University of Houston; PhD (2002) Rice University, Houston, TX.

Research Interests: Macromolecular crystallography; protein crystallography, small angle x-ray scattering

Statement: I am honored to be nominated to the Continuing Education Committee. ACA workshops and meetings provide an important avenue for both beginning and continuing education. This is especially important today, when reduced attention is given to teaching crystallographic theory, because most laboratories must utilize a number of different methodologies and techniques to answer or complement structural questions. In a sense, the structure solution process is increasingly looked upon as a 'black box' technique. It's essential to remember that the need to know many techniques doesn't diminish our obligation to provide comprehensive crystallographic education to the next generation of crystallographers or to maintain our own knowledgebase of current and emerging crystallographic techniques. If elected, I will work to support the vital educational efforts of the ACA and to facilitate the expansion of educational resources for the crystallographic community

Amy Sarjeant Continuing Education

Senior Research Associate, X-Ray Crystallography, Department of Chemistry, Northwestern University, Evanston IL.

Education: BS (1995) Chemistry, The College of William and Mary; PhD (1999), Northwestern University, with Jim Ibers.

Professional Activities: ACA member since 2000; Chair, Service SIG (2010-2011); member, USNCCr (2011-2013).

Research Interests: Structure elucidation and compound identification of complex network materials via single crystal and powder diffraction.

Statement: As single crystal x-ray diffraction becomes a widespread tool for chemical analysis it is our job as crystallographers to ensure that each new generation of chemists understands the fundamentals of this technique. Modern instrumentation and advancements in software have allowed crystallographic experiments to become routine such that even those who have no formal training can solve structures. Consequently, the casual user may lack a full understanding of both the power and the limitations of the technique. It is imperative that those who use crystallography to support their research are able to do so wisely. To this end, the foundation of crystallographic education should begin within the undergraduate curriculum. In much the same way that techniques such as mass spectrometry and NMR are introduced and continually reinforced throughout undergraduate education, so should crystallography be an integral part of basic chemistry.

It has been noted that there is a lack of young crystallographers entering the field to pick up where retiring developers are leaving off. By demystifying crystallography for young chemists, we can spark an interest in the discipline that will carry over into graduate and post-graduate careers and help to fill this gap. By developing educational programs such as the ACA Summer School, we can reach scientists of all levels and encourage them not only to use crystallography to support their research, but also to continue to develop the technique.

In my current position at Northwestern, I have the opportunity to participate in undergraduate and graduate level classes where crystallography is incorporated in the coursework. It is inspiring to see undergraduate students elect to pursue crystallography for their independent research projects, and equally inspiring to help graduate students solve their own structures. I would bring this same enthusiasm for crystallography to the Continuing Education Committee should I be elected.

Have you paid your dues for 2011 ? You can do it online at www.amercrystalassn.org/content/pages/main_membership

Howard Robinson – Data, Standards and Computing

Biophysicist, Biology Department, Brookhaven National Lab, Upton, NY 11973

Education: PhD (1980) Cell and Molecular Biology, University of Michigan. BS (1974), Math and Botany, University of Michigan.

Professional Activities: ACA member; synchrotron beamline provider for the macromolecular x-ray crystallographic community.

Research Interests: Structures from x-ray crystallographic diffraction of large macromolecular assemblies.

Statement: As our available computing technologies expand, we are challenged to effectively apply them to improving the ability to pursue our scientific goals. We seek better visualization and analysis, but also better organization and management for our data. Although the crystallographic community has long been a leader in providing access to scientific data, we could benefit by simplifying the process for providing context for that data. I believe that the efforts of the DSC committee can be most effective in encouraging the development and dissemination of technology in these areas through promoting events at ACA meetings and other ACA activities.

John Westbrook – Data, Standards, and Computing

Research Assoc. Professor, Rutgers, The State University of New Jersey, Department of Chemistry and Chemical Biology, 610 Taylor Road, Piscataway, NJ 08854-8087

Education: PhD (1995) Chemistry, Rutgers University, MS (1985) Chemistry, Rochester Institute of Technology, MS/BS, (1984) Imaging Science, Rochester Institute of Technology.

Professional Activities: Co-editor ***Acta Cryst Section F*** (2005-2011); IUCr Committee for the Maintenance of the CIF Standard (COMCIFS) (1997- 2011); PDB Developer Representative Open Biomedical Investigation Ontology Project (2007-2011); International Scientific Advisory Board of the Protein Circular Dichroism Data Bank (PCDDB) (2010-); Protein Data Bank Lecturer, Cold Spring Harbor Laboratories Crystallography School, Cold Spring Harbor (2001-2010), NSF Advances in Biological Informatics Advisory Panels (2007-2009), Department of Energy review panels (2006-2008).

Research Interests: Developing new tools and infrastructure to support technical challenges in data acquisition, data validation and standardization, and data mining in the structural biology and life sciences domains. Current projects include: The RCSB PDB (***rcsb.pdb.org***), the Protein Structure Initiative Structural Biology Knowledgebase (***sbkb.org***), the Nucleic Acid Database (***ndbserver.rutgers.edu***), the 3D Electron Microscopy Database (***EMDatabank.org***), the mmCIF & PDBML Resource sites (***mmcif.pdb.org & pdbml.pdb.org***), and Ligand Expo (***ligand-expo.rutgers.edu***).

Statement: The crystallographic community has a distinguished history in developing standards for data representation and data quality. I believe the ACA Data Committee should continue to play an important role in supporting these activities as it is uniquely positioned to promote a broader understanding of existing and emerging data standards.

This could could be done in various ways. The committee can identify new ways to support and promote the activities of the public data repositories and open source software projects on which our community depends. For commercial database resources and software applications the committee could negotiate licensing incentives for ACA members, facilitate access to these resources for academic users, and promote the adoption of community data standards.

The committee can also sponsor educational outreach activities that take advantage of ACA resources such as *RefleXions*, annual meetings, and the ACA website. Some high priority educational activities include: introductory or tutorial programs for new and young investigators, programs focused on data integration, and programs targeting data issues with new and leading edge technologies.

Data standardization can also extend to providing unambiguous digital identifiers for individuals. A number of open standards are emerging which aim to provide this functionality. By selecting an open identifier standard and facilitating its adoption by the ACA, the DSC committee can help members establish secure and portable digital identities linked to their professional profiles and publication data.

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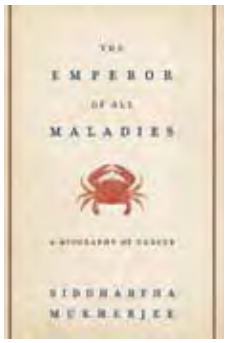
The Emperor of All Maladies: A Biography of Cancer by Siddhartha Mukherjee, Simon & Schuster, 2010, ISBN: 978-1439107959



I am asked where I get ideas for books to review. In this case, I listened to an interview with the author on NPR's Fresh Air. The author said he could not reply to the statement "I'm willing to go on, but before I go on, I need to know what I'm battling." He could not properly answer the question, so he set out to write this book in the summer of 2004. It is a fabulous book. Those of you who know me will understand it when I say this book is one of the hardest I've read in a long time.

The book follows a general timeline from the first recorded case of breast cancer and mastectomy in Atossa, a Persian princess, to modern day directed therapies. Along the way individual people for which the doctor and his team have provided care are outlined to give the reader examples and to personalize the text.

Mukherjee starts with the diagnosis of a Boston schoolteacher with acute lymphocytic leukemia, ALL, and the start of her treatment. We learn about the ancient descriptions of cancer by Hippocrates and Galen, following through to the middle ages and eventually the 20th century. Along the way we are introduced to a number of important characters, most notably Sydney Farber and Mary Lasker. It was Farber who first targeted ALL in children with dehydrofolate reductase inhibitors to induce remissions. Farber started with ALL because he wanted a cancer for which outcome and progress are easily measurable *via* blood count. We learn about the evolution of chemotherapy from short term remission to long term survival with multidrug therapy, radiation and surgery.

We also learn how Mary Lasker helped create the American Cancer Society and helped initiate the founding of the NIH and Nixon's War On Cancer. The author provides a view of the interaction of cancer and the system for providing care for cancer patients. Here we also learn about bone marrow transplants, and how they took so long to move from an experimental technique to standard treatment.

Next the author takes a look at the first cancer epidemic, lung cancer, and its cause, tobacco, as well as the legal wrangling to get cigarette ads off the air, and ends with the reimbursement of states for medical costs. The discovery of *H. pylori*, a cause of stomach cancer, is also described, as well as other preventable cancers.

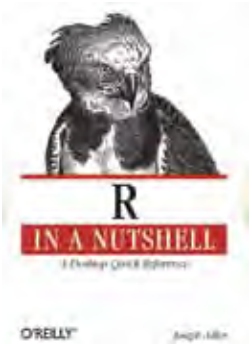
Readers are provided with more examples and learn about the genetic basis of cancer using the nuclear estrogen receptor and tamoxifen in breast cancer as one example and familial retinoblastoma as another.

The author explores the discovery of the HER receptor and development of herceptin by Genentech. The politics of drug discovery and citizen activism is also elucidated. Finally, he discusses the miracle of Gleevec developed by Ciba-Geigy before their merger with Sandoz.

A final chapter, "Atossa's war," summarizes the book exquisitely. Here the author traces the prognosis of Atossa's disease through the ages from mastectomy to chemotherapy and radiation, to today's directed therapies and a vision for 2050.

Since this review first appeared this year, the book has won the Pulitzer prize in the general nonfiction category.

R in a Nutshell, A Desktop Quick Reference by Joseph Adler, O'Reilly, 2011, ISBN: 978-0-596-80170-0



Three months ago I switched from a Dell with Windows and Linux to a MAC with a Windows virtual machine. I had been using wgnuplot for 13 years for most of my graphing but was determined to find an alternative native to the MAC. I hadn't had much luck until I came across Rupp's posting on CCP4 about R. I downloaded a copy and started playing with it. I was lost. I started looking at the online documentation but I needed something more. I went online and found this O'Reilly book.

This is the first O'Reilly book I've read cover-to-cover and the first programming book in more than a decade. R is a programming language for graphics and statistics. It is provides for interactive graphing and analysis. It is much more powerful than wgnuplot but with that comes more structure and perhaps pitfalls. It is maintained by CRAN and freely available and covered by the GNU General Public License. Adler provides many examples of data sets that can be downloaded from the Internet for analysis.

The author begins with the basics: how to get R, how to install R, how to drive the user interface and how get packages that extend the capabilities beyond the basics. In the second part Adler covers the R language with chapters on syntax, objects, symbols and environments, and functions. This part concludes with a chapter on the basics of object oriented programming as applied to R and making R high performance.

The next section of the book deals with data and data structures, and graphing. The default graphics are good but there is an implementation of Trellis graphics, called lattice, that really makes some interesting plots. Lattice is not loaded by default so you'll want to load that package.

Part III covers the analysis of data, statistical tests and regression. This was a fun section because I feel that I really learned something about the statistics. I am reading the *The Black Swan* by N. N. Taleb and am also unlearning things about statistics but that is anbother review (see page 34). Also covered are classification methods, survival methods and times series data. I was disappointed to find no Fourier transform in R since the very thing I do with time series data is an FT to analyze the components. The last chapter of Part III provides an example of the use of R in a bioinformatics study.

The remainder of the book, not quite 100 pages, is the R reference manual. If you are using R, you want this book. If you are doing statistics, there are certainly better references but this is a good primer.

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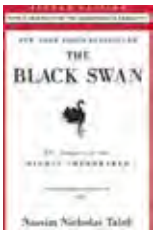
The Black Swan, The Impact of the Highly Improbable by Nassim Nicholas Taleb. Random House, 2007, ISBN: 978-1-4000-6351-2



I wish I had read this book when my brother-in-law, an economist, gave it to me three years ago. In hindsight, it presaged the 2008 financial collapse beautifully and has opened my eyes to the fallacy of a predictable life. This is really a book about realizing that no matter how good your models are, you can't predict the future and your best bet is to recognize that and prepare for it.

The title comes from the fact that for centuries all swans were thought to be white - then the unthinkable happened - black swans were found in Australia. A "black swan" is an event that it is unpredictable, has high impact, and requires some *ex post facto* explanation.

He begins with a short autobiography of his childhood in Lebanon, schooling at Wharton and his first job at Credit Suisse. This is a fascinating prelude to his first example of a black swan: the civil war in Lebanon, previously an area that had millennia of relative peace. The first part deals with the topic of validation and how it is important for humans to feel they have some measure of predictablity. He hints this is the start of religion. He also introduces a concept called the Ludic fallacy, in which simple game theory is used to predict real events, and does not work.

The second part deals with recognizing black swan events and how to deal with them. He reminds us that we need to look closely at the evidence presented "because no evidence of disease is not the same as evidence of no disease." The third part basically tears apart the idea that you can use the Gaussian distribution to predict the future. Taleb replaces this with the idea that Mandelbrot sets with fractal power laws provide a better modeling tool. You could subtitle this section "he who lives by the Gaussian shall die by the Gaussian". He finally concludes with some advice for hedging against black swan events in the purview of his specialty, the financial markets.

Alone Together: Why We Expect More From Technology and Less From Each Other, by Sherry Turkle, Basic Books, 2011, ISBN: 978-0465010219

A good friend recommended this book and, about halfway through reading it, I heard an interview with the author on Science Friday. The interview is worth a listen and the book, at least the second half, is worth reading. The author uses a number of case studies and personal interviews with subjects of all ages to substantiate her points.

Her book is divided into two parts, with a conclusion that synthesizes the discussion in each. The first part discusses the interaction of humans with computers and robots. She first looks at how people, mostly children and the elderly, interacted with fad items like Tamagotchis and Furbies. She then draws some conclusions about how these individuals might interact with robot caretakers replacing parents too busy to look after a child in the former case, and adults too busy to care for their infirm parents in the latter. She suggests that, at least for the very young and very old, the substitution of a robot for a human, emotionally, is possible since neither group knows better.

She then reviews our interactions with others through the technology of networks: the internet, cell phones, texting, MySpace, Twitter, and Facebook that we treat as distinctly different from direct, interactive communication. She suggests, for example, that we have forgotten how to pick up the phone and engage in real time conversation. She captures well our sense of loneliness when we can't access email or SMS. Is our failure to disconnect ruining our lives? Our children's?

She asks if we have we lost our sense of privacy. What does the future hold? At what point do we become so antisocial that we no longer care to see other humans? Is that the point at which a computer program or a robot is sufficient companionship for us? This is what ties the two parts of the book together. At what point does it no longer matter with whom we communicate, and at what point does a computer becomes sufficient to satisfy our need to be social?

Joseph D. Ferrara

Frank H. Herbstein (1926-2011)

Frank H. Herbstein, professor emeritus at Technion – Israel Institute of Technology, died March 23rd.

Frank was born in Cape Town in the Union of South Africa (as it then was) on 3 July 1926. He got his BSc degree from the University of Cape Town, came to Israel in 1948, received a PhD from the Hebrew University and later a DSc from the University of Cape Town. He went to MIT on a postdoc in 1953, returned to South Africa in 1956, and then returned (permanently) to Israel in 1965 as a Professor of Chemistry at Technion. In 1992 he was honored by election as a Foreign Associate of the Royal Society of South Africa. In 2007 he was honored by being chosen to receive the ACA Fankuchen Award.

As a PhD student Frank was involved in the crystal structures of overcrowded aromatic hydrocarbons and the three-dimensional structure of phenazine. At that time it took few months just to obtain a Fourier electron density map. Frank described himself as the third crystallographer in the science history of Israel (after Schmidt and Alexander). After 15 years abroad he based his career in Haifa after he was invited to add an x-ray diffraction facility to the Department of Chemistry at Technion. There he added much more sophisticated approaches to topics that he had only touched on earlier. Phase transitions was one of these. Second order transitions were the first to be developed; the simplest of these was the second order transition of naphthazarin C, studied in collaboration with Curtin and Paul in Urbana and Mogens Lehmann in Grenoble, which led to a study of the *cis*-enol system benzoylacetone over a temperature range of 9 to 300 K with Finn Larsen's group in Arhus. His interest in the second order phase transition at ~160 K in the charge transfer compound pyrene : pyromellitic dianhydride was greatly extended, including a structure determination at 19 K, during a sabbatical at Caltech with R. E. Marsh and Sten Samson. This led to a review of second order transitions published in *Crystallographic Reviews*, ((2000) **5**, 181-226). When Frank was asked what was his favorite among the various research projects with which he had been associated over the years, he would undoubtedly say that it was the "Spontaneous Deformation of Protochatechuic Acid (3,4-dihydroxybenzoic acid) Monohydrate ($PCA{\cdot}H_2O$) crystals: Crystallographic Aspects" (Agmon & Herbstein, *Proc. Coy. Soc. Lond.* (1983) **A387**, 311-336) despite its being one of the least cited papers in the crystallographic literature. When he was asked what were his favorite crystals, he answered that trimesic acid and the various polyiodides (and polyiodines) ran neck to neck.

Frank's willingness to write a review on "Crystalline Molecular Compounds: Chemistry, Spectroscopy and Crystallography" resulted, after a few years, in a two volume monograph entitled "Cryatalline Molecular Complexes and Compounds (Structures and Principles)". The book was enthusiastically accepted by the crystallographic community as can be seen by this quote from one of the book's reviewers (Israel Goldberg).

"…this publication is an invaluable resource of information on, and an excellent reference to, *Crystalline Molecular Complexes and Compounds*. It contains broad-scope coverage of the structural chemistry and physical properties of such materials, aiming at a wide academic audience. The well-organized text presents the scientific evidence and the author's perspective on the subject in an attractive manner and easy to read language, while avoiding as much as possible the use of too specific technical terms. Clear definitions and classification of the discussed compounds into sub-classes at the outset, accompanied by instructive introductory background sections on these groups in the respective chapters as well as by concise conclusion paragraphs, ease on the reader to grasp step by step the information wealth contained in this account. The nearly 600 illustrations and diagrams in the text are an excellent aid in this endeavor".

Frank held many important positions in the academic administration of Technion. Among them Dean of the Department of Chemistry, Dean of Graduate School, Vice President of Technion for Development. Frank was a dear person, honest, gentle, kind, and was always interested to hear the younger research scientists. He was a man of work and continued his involvement in crystallographic research for more than 16 years after his retirement.

His many friends and former students mourn his passing.

Manahem Kaftoury

William Nunn Lipscomb Jr., a Retrospectroscopy

He was born on December 9, 1919 in Cleveland, OH. A year later, his music teacher mother and physician father moved the family to Lexington, KY where he spent the rest of his childhood. Over the next century he would become husband, father, clarinetist, scientist, prankster, teacher, mentor, detective, friend, Kentucky Colonel and Nobel Laureate, until pneumonia and complications from a fall would take his life on April 14th, 2011 at the age of 91. He is survived by his wife Jean, three children, three grandchildren and four great-children.

How often do the accounts of today's scientists begin with a toy chemistry set at the age of 12? Probably too often. But how many of those child chemists build a whole laboratory in their bedroom, ordering apparatus and chemicals from suppliers and drugstores and then go on to win the Nobel Prize? Bill Lipscomb made stink bombs and fireworks and even tried to "isolate a large amount of urea from the natural product". By the time he graduated from high school, his home laboratory had grown so much that when he donated it to the school it more than doubled their equipment.

He went to college at the Univ. of Kentucky on a music scholarship, but graduated with a degree in chemistry. He then hitchhiked to Los Angeles to attend graduate school at Caltech. He studied under Linus Pauling and earned his doctorate in Chemistry in 1946. He served four years in the US Office of Scientific Research and Development during WWII. The parts of his PhD dissertation describing that work are still classified and confidential. However, he has disclosed in an interview that some of that research involved analyzing smoke particles to "cloud up LA so that the Japanese could not find it to bomb it." This research, he admits, is of little value now because "the smog is already there."

Upon completion of his PhD in 1946 he was offered an assistant professorship at the Univ. of Minnesota. He taught there for the next 13 years before moving to Harvard where he would become Professor of Chemistry from 1959-1971 and Abbott and James Lawrence Professor of Chemistry from 1971 until his retirement to *Emeritus* in 1990. During all this time, he continued the work on boron hydrides that he had started with Pauling at Caltech. (His musical education did not go to waste as he was a reputed classical clarinetist and performed in chamber music groups. He was the principal clarinetist with both the Pasadena Civic Orchestra and the Minneapolis Civic Orchestra.)

He pioneered the use of x-ray crystallography to study the structures of boranes at low temperatures and finally determined the unusual way that boron formed chemical bonds. He was able to elucidate the chemistry and structure of boron compounds, predict how they would react chemically, and provide groundwork for the synthesis of more complex boron-containing compounds. This was not a trivial task due to the highly unstable and explosive tendency of boron preparations.

Over the years his research interests evolved and his group solved the structures of many proteins. His structures of carboxypeptidase A and aspartate carbamoyltransferase were both the largest determined at the time. However, boron chemistry remained a passion for the rest of his career. Even when following other research pursuits, he would return to it "almost subconsciously within half a year. His dedication paid off and in 1976 he was awarded the Nobel Prize in Chemistry for his "*studies on the structure of boranes illuminating problems of chemical bonding*."

ACA Philadelphia 1988 - Top: Bill Lipscomb explains crystallography to Ben Franklin. Bottom: He shares his exploits with Judy Flippen-Anderson, Penny Codding and Caroline Duax.

While reading about his life, the accounts of his research successes were impressive but pale in comparison to the personal accounts of his character. Affectionately called The Colonel due to his Kentucky roots (he would later be made an official member of the Honorable Order of Kentucky Colonels), he was truly an inspiration. Those who studied under him describe him as a great mentor and admired teacher. He was encouraging, imaginative, and always accessible. Two of his doctoral students, Roald Hoffmann and Thomas A. Steitz went on to win Nobel Prizes themselves. All who knew him never fail to mention his sense of humour. A practical joker and a wise guy in life, he also brought comedy into science. In *Humor in Science*, he collected quotes from his papers. In one paper he wrote, "We admittedly made this observation with the benefit of hindsight. This science is known as retrospectroscopy." In another he included the footnote, "M. V. King and W. N. Lipscomb, to be unpublished." My personal favorite in the list was the time he observed, "Xue and Lipscomb, personal communication... A communication with myself!" He often quoted Sherlock Holmes in his papers, using that detective as a model for his own investigations. He was also a regular participant in the Ig Nobel Prize Award ceremony sponsored by Annals of Improbable Research. The Ig Nobel Prize is awarded to scientists whose research achievements "first make people laugh, and then make them think." His active participation in the Ig Nobels was not surprising as he was a man who made people both laugh and think at the same time.

*Abstracted by Bomina Yu from material collected by his son, James S. Lipscomb (**wlipscomb.tripod.com**)*

2012 M. J. Buerger Award to John Spence

John is a Regents' Professor at Arizona State Univ, Tempe where his research group studies condensed matter, biophysics and diffraction physics based on the use of electron and x-ray beams for imaging, spectroscopy and diffraction. State-of-the art equipment is used to do lithography at the angstrom level. The optical and superconducting properties of the resulting pattterned arrays of "Nano-rings" are being investigated. The group's quantitative convergent beam (QCBED) research allows for direct imaging of the chemical bonds in solids. Theoretical work continues on the inversion problem of multiple scattering, and experimental research is supported on the use of coherent sub-nanometer electron probes for the study of dislocation core structures and on electron channeling effects on x-ray production (ALCHEMI). His latest research is devoted to biological applications of femtosecond x-ray diffraction at Flash (in Hamburg) and at the Linac Coherent Light Source at Stanford where they use x-ray pulses so brief that they terminate before atoms move (in order to avoid damage), to determine the structure of membrane proteins and viruses which are difficult to crystallize.

2012 Charles Supper Instrumentation Award to Ron Hamlin

It is clearly recognized that progress in macromolecular crystallography has been crucially dependent upon advances in the availability of area x-ray detectors. Each new technology has gone through two essential stages: first, it is developed and demonstrated to work and second, it is refined and produced commercially.

Ron has been a leader in both stages of all the modern generations of major area x-ray deterectors. He earned his PhD in physics from UC San Diego where his early work with Nguyen-Huu Xuong (2004 Supper Award winner) led to the development of a highy successful multiwire area detector. Then in 1983 Hamlin (together with Xuong and Chris Neilson) formed Area Detector Systems Corporation (ADSC) to sell the detector. When image plates were developed, ADSC teamed with MAR to make them readily available in the US. When Sol Gruner's group (CHESS) demonstrated the potential of the phosphor-coupled CCD detectors (1991-1993) Ron immediately recognized their potential. He worked closely with Gruner's group along with Walter Phillips' group at Brandeis to develop a highly successful line of CCD detectors which can now be found at synchrotron sites all over the world.

Like Charles Supper, Ron has provided the crystallographic community with innovative commercial products for decades, and guided each step in the design, fabrication, and use of his products.

ACA 2012 Warren Award to Paul Fenter

Paul Fenter is a pioneer of x-ray methodology for understanding the structure of interfaces, particularly those involving liquids or soft matter. His relentless and creative pursuit of the mechanisms underlying otherwise routine scattering methods has led to substantial breakthroughs.

His primary contribution has been in developing the method of x-ray reflectivity for studying surface structure. On the experimental side, he has pioneered the use of area detectors, like CCD's, which allow significant enhancements in data collection efficiency and accuracy. He has pushed the use of resonance methods to obtain chemical sensitivity to the point of being able to obtain element-specific density maps of interfaces with very few prior assumptions.

More recently, the reflectivity work has been extended to crystal truncation rods (CTR) which involve the crystal lattice as well as the interface under study.

Another recent breakthrough is his invention of the XRIM method of imaging structure at a buried interface such as mineral water. This uses the reflectivity or CTR information to produce real-space images by applying a Fresnel Zone Plate as a lens to magnify the sample. While several crystallographers were busy attempting to interpret the coherent diffraction from interfaces, Paul Fenter was the sole originator of the idea to combine the diffracted beams together again to form an image.

-

Sol Gruner elected to American Academy of Arts and Sciences

The American Academy of Arts and Sciences has recently announced their class of 2011. Among the 212 new elected Fellows is ACA member ***Sol Gruner,*** Professor of Physics at Cornell University where he studies biological physics, polymer and other soft condensed matter physics, x-ray and synchrotron radiation science and scientific instrumentation. By using small angle x-ray scattering, protein crystallography, and computational quantum chemistry, he probes how pressure impacts protein structure and function. His group also works on the development of x-ray detectors and nanocomposite self-assembling materials, such as polymers and inorganics. He is also director of the Cornell High Energy Synchrotron Source (CHESS).

Keith Hodgson and Louise Johnson elected into the National Academy of Sciences

The National Academy of Sciences recently announced the election of 72 new members and 18 foreign associates from 15 countries in recognition of their distinguished and continuing achievements in original research. Among the new members is ACA member ***Keith Hodgson*** from Stanford University. Hodgson is David Mulvane Ersham and Edward Curtis Franklin Professor of Chemistry, and Associate Director for Photo Science at SLAC National Accelerator Laboratory. His lab studies bioinorganic and biophysical chemistry. By using novel x-ray absorption spectroscopy methods, his research group has characterized the polynuclear molybdenum-iron-sulfur cluster in the active site of the enzyme nitrogenase. Other studies include dioxygen activation and oxidation by iron, the copper function in electron transport, and electronic structures of iron-sulfur clusters.

Louise Johnson, David Phillips Professor in Molecular Biophyhsics, Laboratory of Molecular Biophysics, Oxford Univerisy was named as a Foreign Associate. Louise retired from the university in 2007 but has retained an interest in protein kinases and their regulation in health and disease with special focus on the kinases involved in the regulation of the cell cycle. She has also been associated with the Diamond Light Source where she studies coherent diffraction imaging of cells and macromolecular assemblies and where she also explores ways in which free electron laser x-ray sources may be exploited.

Kavli Prize Winners at the White House

On June 6, 2011, President Barack Obama met in the Oval Office with the seven U.S. recipients of the 2010 Kavli Prizes to recognize and honor their seminal contributions to the three fields for which the Prizes are awarded -- astrophysics, nanoscience and neuroscience.

The 2010 Kavli Prize in Nanoscience was awarded to ***Donald M. Eigler*** and ACA member ***Nadrian (Ned) C. Seeman*** for their development of unprecedented methods to control matter on the nanoscale. Eigler demonstrated it was possible to pick up and precisely place individual atoms at will, creating a whole field of quantum engineering. Seeman conceived the idea of using DNA as a building material for nanoscale engineering. Inventing DNA nanotechnology, he pioneered the use of DNA as a non-biological programmable material for a countless number of devices that self-assemble, walk, compute and catalyze. These discoveries promise breakthroughs in future applications in fields ranging from electronics to biology.

The Kavli Prizes (awarded biennially) are a partnership between The Kavli Foundation (U.S.), the Norwegian Academy of Science and Letters and the Norwegian Ministry of Education and Research. The 2010 Kavli Prize Laureates were announced last year and received their awards in a ceremony held in Oslo, Norway. The call for nominations for the 2012 Kavli Prizes occurs this fall.

President Obama greets Kavli Prize Laureates-Nadrian (Ned) Seeman (New York University) is 4th to the left of President Obama. Credit for photo: White House.

E. Dodson, C. Giacovazzo and G.M. Sheldrick Awarded the Ninth IUCr Ewald Prize

The ninth IUCr Ewald Prize has been awarded to ***Elinor Dodson*** (Top - Department of Chemistry, University of York, UK), ***Carlo Giacovazzo*** (Middle - Institute of Crystallography-CNR, Bari, Italy) and ***George.M. Sheldrick*** (Bottom - Lehrstuhl für Strukturchemie, Göttingen, Germany) for the enormous impact they have made on structural crystallography by designing new methods and providing them to the crystallographic community in algorithms that are constantly maintained, renewed and extended. Their invaluable contributions to the computational side of the field have led to leadership with the program suites CCP4, SIR and SHELX, respectively. Daily, all over the world, thousands of crystallographers are profiting from their excellent achievements. The presentation of the Ewald Prize will be made during the Opening Ceremony of the IUCr Congress in Madrid in August 2011.

2011 Travel Award Winners

Argentina
Ana Bianchi
Unive Nac de La Plata
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McGill
Ireland
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Singapore
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Thailand
Orrasa In-Noi
Suranaree U of Tech
United Kingdom
Phoebe Allan
Univ of St. Andrew
Briony Yorke
Univ of Leeds
United States
Mayank Aggarwal
Univ. of Florida
Debasis Banerjee
Stony Brook Univ
Christopher Davies
Purdue
Jeremiah Gassensmith
Northwestern
Thomas Grant
Hauptman-Woodward
Benjamin Greve
Georgia Inst. of Tech
Shimelis Hailu
Howard University
Mark Hunter
Arizona State
Christopher Kane
Georgetown
Melanie Kirkham
Oak Ridge Natl Lab.
Vishal Koparde
VA Commenwealth
Anna Kowalska
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Eric Reinheimer
Cal. State Poly - Pmona
John Roudebush
UC - Davis
Clare Rowland
Northwestern
John Sander
University of Iowa
Nathan Schley
Yale
Ian Stokes-Rees
Harvard Medical
Elzbieta Trzop
SUNY - Buffa
Tara Michels-Clark
Tennesee
Cortnie Vogelsberg
UCL
Hsiu-Wen Wang
Indiana
Weina Wang
Duke
Christopher Williams
Duke
Erik Yuki
Univ of Minnesota

2011 Margaret Etter Awards

Etter Early Career Award
Yurij Mozharivskyj
Michigan

Etter Student Lecturers
Bio-Mac SIG
Rebekah Nash
UNC Chapel Hill
Materials Science SIG
Phoebe Allan
Univ.of St. Andrew
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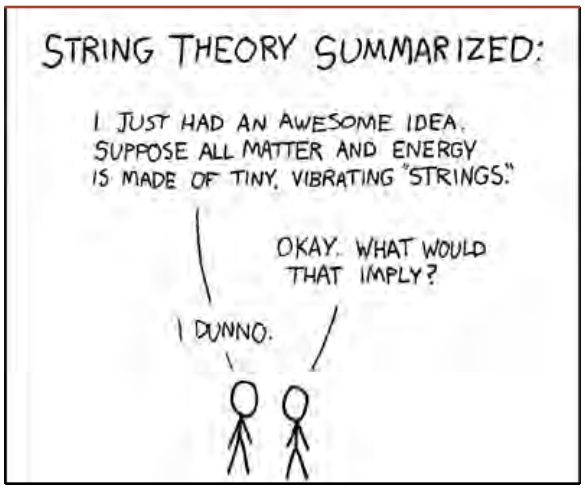

AUGUST 2011

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

SEPTEMBER 2011

19-22 **40th Congress of the Italian Crystallography Assn.** Siena Italy. ***www.unisi.it/eventi/aic2011/index.htm***

OCTOBER 2011

4-7 **Trends and Perspectives in Neutron Instrumentation: From Continuous to Spallation Sources.** Tutzing Germany. ***www.jcns.info/Workshop_2011***

28-30 **Symposium Celebrating the 40th Anniversay of the PDB,** Cold Spring Harbor, NY. ***meetings.cshl.edu/meetings/pdb40.shtml.***

NOVEMBER 2011

20-24 **1st Asia-Oceania Conference on Neutron Scattering.** Tsukuba Japan. ***j-parc.jp/MatLife/en/AONSA/index.html***

MAY - JUNE 2012

8-12 **14th Int'l Conf. on the Crystallization of Biological Macromolecules (ICCBM 14).** Huntsville, AL. ***iccbm14.org***

31-10 **Present and Future Methods for Biomolecular Crystallography.** The 45th crystallographic course at Ettore Majorana Centre, Erice, Italy. ***www.crystalerice.org/Erice2012/2012.htm***

JULY 2012

28-1 **ACA2012, Westin Boston Waterfront Hotel, Boston, MA.** ***Program Chairs: Bruce Foxman (foxman1@brandies.edu) and Bruce Noll (bruce.noll@bruker-axs.com); Local Chair: Peter Mueller***

Bruce Foxman

Bruce Noll

Peter Mueller

NOTE: New meeting for mat - Workshops still on Saturday but then 4 days instead of 5 - beginning on Sunday, July 29 and concluding on Wednesday, August 1st.

AUGUST 2012

7-11 **ECM-27**, Bergen, Norway. ***www.ecanews.org/meetings.php***

SEPTEMBER 2012

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

DECEMBER 2012

20-24 **AsCA'12.** Adelaide, Australia. ***www.asiancrysassn.org***

AUGUST 2014

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

The IUCr photograph archive (www.iucr.org/gallery)

The IUCr web site now hosts an archive of photographs that provides general access to a large and growing collection of images of crystallographers.

The photographs in these collections represent, for the most part, candid snapshots of crystallographers at work, at national and international meetings, and occasionally at play. Although they include some official photographs from major events, primarily they document the lives of crystallographers as seen spontaneously by their colleagues and friends.

Contributing to the archive*:** The IUCr is happy to host collections from individual crystallographers, who should contact the IUCr Webmaster (scripts.iucr.org/cgi-bin/contactus***) for assistance. The main purpose of the archive is to make publicly available an extensive photographic record of the crystallographic community. Contributors are requested to consider posting their images under a Creative Commons Attribution License (see next section).

Images from the collection used in this issue of *RefleXions* were contributed to the IUCr by Bill Duax and Syd Hall.

Contributors to this issue: Sidney Abrahams, Bill Busing, Ed Collins, Angela Criswell, Bill Duax, Jack Dunitz, Joe Ferrara, Greg Good, Syd Hall, Ashfia Huq, Menahem Kaftory, Cheryl Klein Stevens, Tom Koetzle, Patrick Loll, Krystle McLaughlin, Edgar Meyer, Connie Rajnak, SN Rao, Howard Robinson, David Rose, Amy Sarjeant, Ned Seeman, Jim Silverton, Eddie Snell, Shankar Subramaniam, John Tanner, Crystal Towns, John Westbrook, Bomina Yu, Christine Zardecki. Photo of Keith Hodgson provided by Diana Rogers.

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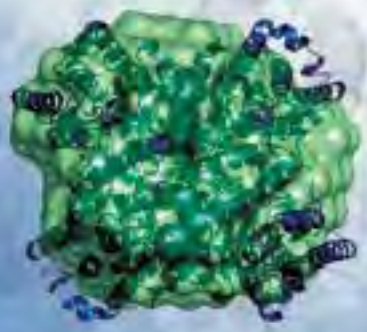

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