ACA RefleXions

American Crystallographic Association
Structure Matters

Number 4

Winter, 2014

In 1981, 25 meters deep in the crust, miners at the Blocker-Lead Mine #4, Hot Springs, AR were amazed to see a gigantic cleft open up in a 3 meter thick quartz band, revealing the largest and most beautiful clear quartz ever found in this area. The cleft was almost vertical, so sophisticated scaffolding and machinery were required to extricate it without breakage. That same year a German admirer brought the giant quartz cluster to Germany to be the core of the crystal castle museum Riedenburg im Altmuehltal. Part of the museum's plaque is reproduced at left.

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President's Column - An Emphasis on Education and Outreach: Looking over this International Year of Crystallography (IYCr) as ACA President, I ponder ACA's mission and am left with two questions. How can our meetings better serve our members and attract new members? How can we excite and train the next generation of crystallographers?

Our strategic plan addresses these issues. We recently welcomed your comments on our mission, vision and objectives. Based on comments received so far, we are making education a stronger component of the 2015 Philadelphia meeting. We also plan to meet with ACA Past Presidents and Fellows to get more feedback.

The Philadelphia meeting will start Saturday with four excellent workshops on *High Pressure Single Crystal Diffraction, Serial Crystallography with XFELS*, *Rietveld Analysis* and *Small Angle Scattering*. We've introduced additional educational sessions during the meeting, providing training opportunities for more people than our traditional workshops have, both for new and experienced crystallographers.

The *Undergraduate and Graduate Student Reception* at noon on Sunday will showcase research posters by undergraduates as well as an educational talk. You can learn about strategies for *Engaging Undergraduates with Crystallographic Research* on Sunday afternoon. The Monday evening sessions will be *Professional Development: Communicating Your Science* and *Would You Publish This?*. The first is new and much needed for our young, early and mid-career scientists. The second, at which brief talks about structures with "issues" are presented by those with various levels of experience, is back by popular demand. An animated discussion about the merits of publishing the work follows each talk. An all-day session on Tuesday, *Standard Practices in Crystallography I: Data Collection Strategies* is the first in a series of best practices sessions organized by the Continuing Education and the Data, Standards & Computing Standing Committees as well as the General Interest, Service Crystallography, Small Molecule and BioMac SIGs. Finally, onTuesday evening there will be a session on *Diversity*. You can learn more about all these sessions at ***www.amercrystalassn.org/2015-scientific-program***.

These educational opportunities can help us fulfill our strategic plan objectives. They help us "serve as a leading professional society for scientific training for scientists engaged in the study of the structure of matter." For the 2016 ACA meeting in Denver, we will encourage the SIGs to plan more "how to" sessions for non-experts in the field and to explore ACA's many faces. These sessions enable us to communicate outside our main discipline, spawn dialog between structurally cutting edge research areas, and offer wider opportunities for training next generation scientists.

There are positive signs that fellow scientists are increasingly recognizing the value of crystallography and its equipment. Recent articles by thirteen emerging international investigators were featured in the online journal *ACS Virtual Select - Issues in Solid-State Chemistry* (***pubs.acs.org/JACSbeta/jvi/issue30.htl***). Each of the thirteen scientists were asked to name their favorite instrument. Of the eleven that responded, most selected the *single crystal diffractometer*. Two named other instruments and one nominated the espresso machine! Solid-state scientists and their journals certainly recognize the key role of crystallography and the diffractometer in solid-state material science. Our own ACA journal, *Structural Dynamics (**sd.aip.org**)* co-published with AIP Publishing, features cutting edge research using both conventional and new sources, instruments and methods.

And finally, I come back to IYCr 2014. Our first US and Canadian crystal growing contests have just ended. Our US/Canada Facebook Video Contest will have concluded at the end of 2014 (***www.iycr2014.org/aca/contests***). These activities generated a lot of excitement in local schools. In fact, I just got an enthusiastic email from the IYCr New York representative Miriam Rossi. High school science teacher Terri Campbell was given a small ACA grant to help run a crystal growing contest in the Valley Central High School in Montgomery, New York this fall. Each student got a pin with the IYCr symbol, grew alum crystals, made posters and proudly presented their results to teachers and fellow students. Forty-five high school students talked enthusiastically about their crystals**. "Fabulous!"** said Miriam. They'll be sending their best crystals to the US National Crystal Growth Contest at the University of Buffalo and putting the rest in their IYCr display case in their high school. There is indeed pride in growing your own crystals.

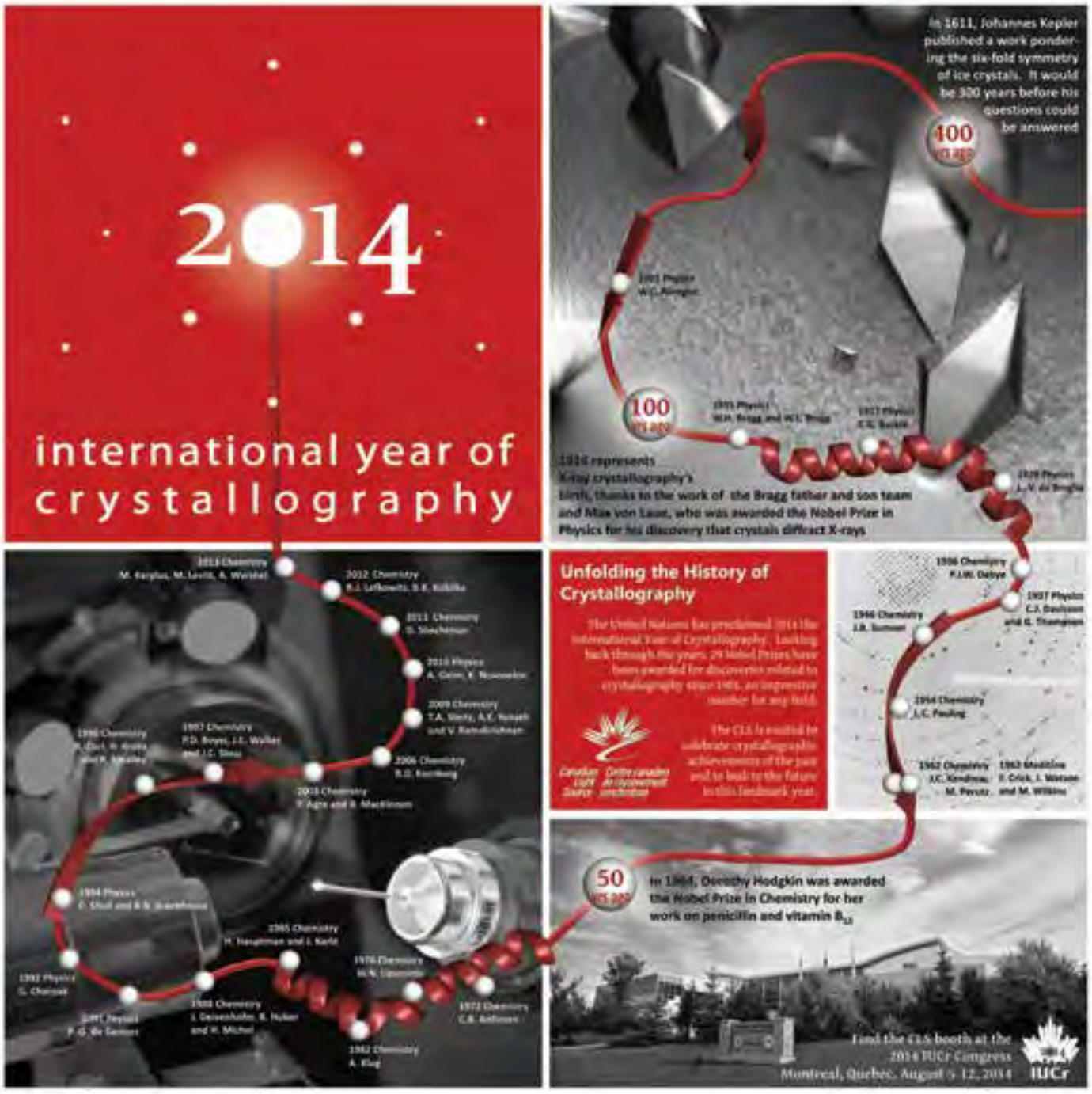
Melanie Washington, Robert Ulan-Gonzalez, Jon Brooks (a guest), Caitlin Thorn, and Emily Melville of Valley Centryal High School showcase their crystal. Photos by Terri Campbell.

As IYCr and my presidency wind down, I see us building up. We are building the structures through our strategic plan to keep our IYCr outreach momentum going, to enhance our image at home and in Washington, to better serve the current and future generations of structural scientists.

Martha Teeter

Reflexions from Canada

In addition to the hectic month of August, what with hosting the IUCr 23rd Congress and General Assembly in Montreal, Canadian Crystallographers held three other local meetings, all of which were well attended. The second annual Protein Structure, Function and Malfunction (PSFaM) Symposium was held June 13-15, 2014, at the University of Saskatchewan in Saskatoon. This year the meeting was ably organized and chaired by David Sanders and associates (Departments of Chemistry and Biochemistry at the U. of Sask). The meeting was a great success having 103 registrants, 30 poster presenters and 14 oral presentations chosen from the submitted abstracts. There were four invited keynote speakers: Andrew Emili and Trevor Moraes (University of Toronto), Kirk McManus (University of Manitoba) and William Montfort (University of Arizona). Following the ~1 ½ days of the symposium there was an award ceremony. Highlights from that ceremony included Michelle Kam who won the Louis Delbaere Prize for research carried out at the Canadian Macromolecular Crystallographic Facility (CMCF) beamlines at the Canadian Light Source in Saskatoon, Sask. Other equally deserving awardees were: Odette Allonby, Theerarat Praesertanan and Jeremy Marshall for the Poster Prizes and Andrei Grishin and Alla Gagarinova for their oral presentations. Clearly the success of the second annual PSFaM bodes very well for the continuation of this regional meeting in Saskatoon.



The second Canadian Regional meeting on which I would like to report is the 23rd annual meeting of the Buffalo-Hamilton-Toronto (BHT) Symposium held this year at McMaster University on Nov. 7, 2014. According to the report prepared by David Rose (University of Waterloo, Ontario), from which I am drawing my information, this meeting was attended by ~100 registrants - an attendance similar to that for the PSFaM meeting in Saskatchewan. The keynote speaker at the 23rd annual meeting of BHT was So Iwata (Imperial College, London) who spoke on two very hot topics: membrane protein crystallization and FEL/time-resolved data collection. In addition to dazzling the audience with his library of beautiful structures, So introduced several techniques and considerations regarding the special handling of membrane proteins. The afternoon saw presentations from seven trainees, including Monica Pillon (Guarne lab, McMaster), Ned van Eps (Ernst lab, Toronto), Sara Chavoshi (Saridakis lab, York), Kevin Leung (Shilton lab, Western), James Peek (Christendat lab, Toronto), Alan Ji (Prive lab, Toronto), and Natalie Bamford (Howell lab, Toronto). BHT also welcomed three new PIs to the region and heard about their research: JP Julien (Sick Kids, Toronto), Mike Suits (Wilfrid Laurier) and Vito Mennella (Sick Kids). As usual, loyal sponsors made the whole thing possible - Art Robbins, BioRad, Bruker, Rigaku, Formulatrix, ForteBio, MiteGen, Molecular Dimensions, ttplabtech, and Wyatt. They were also delighted to have a table from the ACA manned by Bill Duax. Rigaku and Art Robbins sponsored their usual wine and cheese social to end off the day. This meeting also marked the end of an era, as, after 23 years of leadership, Lynne Howell handed off the organization of the meeting to Jeff Lee and JP Julien. Thanks, Lynne - BHT would not have lasted 23 years without your dedicated contributions!

The Annual General Meeting (AGM) of the Canadian Institute for Neutron Scattering (CINS) was held at the University of Toronto, Nov. 14-15, 2014. I am very thankful to Thad Harroun (Brock University, Ontario) for sending me a summary of the results coming from that meeting. After having served as President of the CINS for many years, Dominic Ryan (Physics Department, McGill University)will turn over the presidency to Chris Wiebe (Department of Chemistry at the University of Winnipeg). The neutron scattering community of Canada wishes to thank Dominic for his many years of dedicated service as the President of CINS. Other changes within the administration of the CINS that took place at the Toronto AGM were: Thad Harroun will move from the Science Council of the CINS to the Board of Directors, and Thad's place on the Science Council will be taken by Jamie Noel (Western University). The Canadian Neutron Beam Centre (CNBC) at Chalk River, Ontario, operates six beam lines dedicated to research in materials science and engineering and to quantum materials. In the past year the CNBC counted 150 visitors using the beam lines at the Centre. In light of funding difficulties faced by the CNBC the operations are facing major problems in staffing of the beam lines. The Federal Government of Canada is working on a new nuclear agenda. Until this appears, the Canadian Nuclear Laboratories (CNL), a new name for the business end of the Atomic Energy Canada Limited (AECL), will continue to support the operations of CNBC. The CINS is independently updating a long-range plan for a new Canadian Neutron Centre that comprises a new reactor and a new neutron guide hall for materials research. The AGM endorsed the updates for the scientific program and have agreed to push forward with its publication regardless of the tardy release of the government's new nuclear agenda.

Finally, I would like to report on Canadian events celebrating IYCr. Louise Dawe (Wilfrid Laurier University, Ontario) has been the principal organizer of Canadian IYCr activities. Very recently she, along with Amy Sargeant, Christine Beavers and Jason Mercer, has put out a call for a North American IYCr Video Contest. It will be exciting to see what develops there. In March, the people at the Canadian Light Source produced a marvellous poster in honour of IYCr. The poster, seen on the previous page, can be downloaded at ***cmcf.lightsource.ca/research-highlights/#iycr2014***. Louise also organized a peer-shared poster conference at Wilfrid Laurier University in which her third-year students in crystallography prepared posters on various crystallographic themes and presented them to her first-year general chemistry students. What a great way to inspire young people into the wonderful world of crystallography!

There was a great deal of outreach for IYCr at the IUCr Congress in Montreal. I would like to highlight the film *Hidden Glory* based on a play by Georgina Ferry based on the life of Dorothy Hodgkin as taken mainly from letters that Dorothy wrote over her years in Oxford. Several of Dorothy's former students and colleagues in the audience were moved to give impromptu reminiscences of their time in her laboratory.

Despite poor or only local advertising of the events, there have been some regional celebrations of the IYCr. Marie Fraser and Masood Parvez (University of Calgary), sponsored by Sigma Xi, presented a special seminar and encompassing events on Sept. 18, 2014. The title of Marie's seminar was "*100 Years of Crystallography: Celebrating the IYCr*". Further north in Edmonton, Michael James and Mark Glover, with a host of keen post-doctoral fellows and graduate students, celebrated IYCr in a 4-day presentation from October 18-21, 2014. They had demonstrations of *Crystals, Symmetry, DNA Structure*, and *Single Crystal Diffraction*, as exemplified by optical diffraction and a host of protein structures that had been determined locally by x-ray crystallography. This celebration was presented at the Telus World of Science Museum in Edmonton. Both of these events in Alberta were well attended and enjoyed by students in elementary, junior and senior high school and by the general public. Who knows, perhaps we have nucleated the seeds of enjoyment gained by a lifetime of science in crystallography!

Michael James

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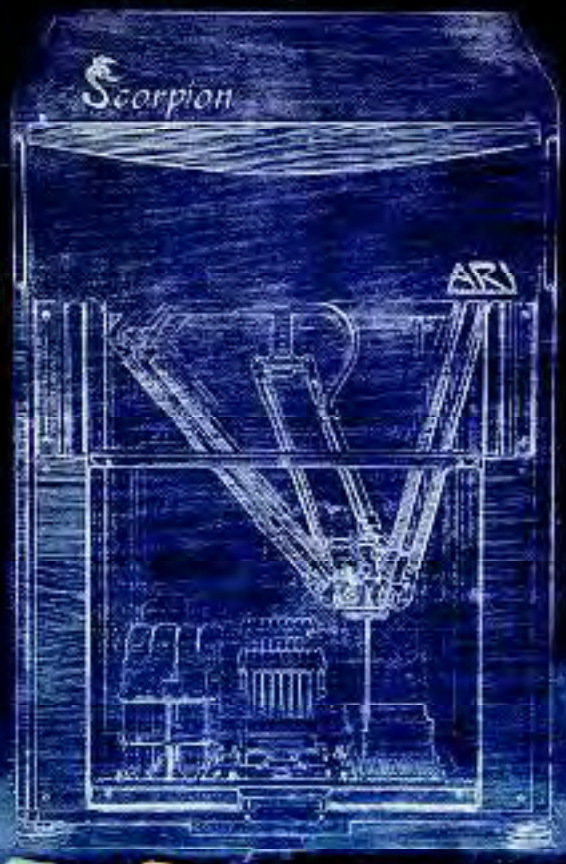
- ✓ Aspirate and dispense 1 ul to 1 ml
- ✓ Build multi-dimensional grids, pH, concentrations & titrate additives
- ✓ Set up 24-well plates, protein + screen
- ✓ Anything you can do with a handheld pipettor



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John R. Helliwell, Emeritus Professor, University of Manchester, was the ACA Patterson Awardee in 2014. In this Living History he summarizes his personal and professional life. Helliwell is known for his work as a pioneer in using synchrotron radiation, and his book* Macromolecular Crystallography with Synchrotron Radiation *is an essential reference work for researchers. He was Editor-in-Chief of* Acta Crystallographica *1996-2005 and President of the European Crystallographic Association 2006-2009. The video of his Patterson Lecture "Synchrotron radiation macromolecular crystallography: instrumentation, methods and applications" is available from the ACA History web page and from YouTube.

Patterson and Pattersons: Fifty Years of the Patterson Function, edited by Jenny P. Glusker, Betty K. Patterson and Miriam Rossi is my source book on A. L. Patterson, one of the greatest of crystallographers. In trying to find something to say about Patterson that was not already widely known, I turned to this book and found a story from Dorothy Hodgkin linked to Patterson's move from Canada to post-doctoral research with William Henry Bragg in London in the mid 1920s. When Patterson obtained a fellowship to do this his supervisor at McGill said that he should alter his ways and work hard to represent Canada well. When he arrived W. H. Bragg said, "Be sure that you have a good time and enjoy yourself."

In approaching how to write this article, I decided it should not be a transcript of my talk. So, I have adopted an autobiographical style and also tried to give an insight into my work on diffraction methods and the associated instrument developments as well as their applications. Suffice to say that I have relied firmly upon the Patterson function in these developments, and I gave crucial examples of its use in my talk. It is a great honor for me to be selected for this Award from the ACA.

I was the first in my family to be interested in science and the second to go to university. My father was first to interest me in America, when he reminisced about his time in the Royal Navy. He would say how Americans would refer to the USA as "God's own country". I was mildly puzzled by this, as we knew that Yorkshire was God's own country, but it gave me an immediately positive view of the USA and I have now visited on many occasions. At school in West Yorkshire my best subjects were history, geography and mathematics, but at age 15 in the UK I had to choose between humanities or science. I chose to specialize in chemistry, mathematics, and physics, having given up biology, as I was too squeamish to even dissect a worm. My father was a policeman and he was moved around rather a lot; I had four schools between the age of 11 and 18 years. I had to develop a self-reliance both catching up on school course notes and always making new friends. My mother was a nurse. I was an only child. I played for my school at rugby and we travelled most Saturdays in the winter to different schools in West Yorkshire. I went to York University to read for a physics degree. It was a small class size (32 students) and this was important, as I was always able to do the physics undergraduate laboratory practicals on my own, which I especially enjoyed.

My DPhil (1974-1977) supervisor in Oxford University was Margaret Adams, and I was her first DPhil student. Charlie Bugg was a Visiting Scientist with Margaret through my first year and he was my proposer for my membership of the ACA. My interest in synchrotron radiation arose early on during my DPhil as I thought that the various experimental challenges for macromolecular crystallography could be handled better. In my DPhil project our crystals were quite typical and showed weak diffraction and long exposure times on our rotating anode x-ray source; solving the crystallographic phase problem seemed to me haphazard. As a graduate member of the UK Institute of Physics I heard that the Nobel Prize winning physicist Rudolph Mössbauer was to give a lecture at the Rutherford Appleton Laboratory, nearby Oxford, and during his talk he suggested the use of nuclear anomalous dispersion to solve the crystallographic phase problem. Also, again while I was a DPhil student, the IUCr conference book *Anomalous scattering* was published (edited by S. Ramaseshan and S. C. Abrahams, 1975). So these examples confirmed my view that it was a fertile time for a physicist like me entering protein crystallography — although at my interview one person said "don't bother, all the methods are fine as they are, there is no place for a physicist!"

Dorothy Hodgkin also informed me that she had received news (from Prof Sir Ron Mason) about some developments involving the first protein crystallography experiments ongoing at the Stanford SSRL in the mid 1970s, led by Keith Hodgson. I had the very good fortune to work closely with Keith some 10 years later along with Britt Hedman. Dorothy asked my opinion of the SSRL work and I reported back to her that I found the preprint that she had passed on to me very exciting! The opening sentence of Keith Hodgson's *PNAS* article was, "The use of synchrotron radiation as a source for single crystal x-ray diffraction studies has recently been the subject of considerable discussion and controversy." The first reference in this paper was to the pioneering work at DESY in Hamburg on synchrotron radiation (SR) biological diffraction of (predominantly) muscle fibers by Ken Holmes, Gerd Rosenbaum and Jean Witz This also I found an exciting paper.

So, as a DPhil student I thought a lot about "How to solve the phase problem?" A way to get the phase of a reflection was using resonant x-ray scattering: two wavelengths and an anomalous difference were needed. My DPhil was entitled "X-ray studies concerning the structure of 6-phosphogluconate dehydrogenase." In my thesis I included an Appendix on my efforts at the NINA synchrotron (Daresbury) in 1976 to optimize the platinum f''(anomalous scattering factor) at the L_{III} absorption edge of the $Pt(CN)_4$ derivative of my enzyme that I had prepared in my first year of research. I also had tried to measure diffraction data at NINA on small crystals of the protein despentapeptide insulin, with Guy Dodson's help. Incidentally Guy was quite merciless in making fun of my Yorkshire accent, which was very strong at that time. My local contact at NINA was Dr. Joan Bordas, who much later (in ~2010), when he was Director of the Spanish synchrotron radiation source ALBA, invited me to chair their Science Advisory Committee and be president of their Beamtime Panels.

Member of the UK SR Delegation to the USSR 1981 (shown here in Moscow outside the Institute of Physical Problems, USSR Academy of Sciences).

It was during my DPhil that I met my wife to be, Madeleine, in Holywell Manor, the joint Balliol and St Anne's Colleges Graduate Centre, where we were both resident. Madeleine was doing her DPhil with Professor Malcolm Green in synthetic inorganic chemistry. We married in 1978. She had several postdoctoral posts (with Gordon Stone, who later moved to Texas, Jim Howell and Dave Garner). Later, after a career break having our three children, she retrained and became a chemical crystallographer firstly at York University, at the initiative of Guy Dodson, and then for many years in Manchester University. Madeleine and I have published about ten papers together, one of which I highlighted in my Lecture; she has about 400 publications altogether mostly in her married name but also in her maiden name (Berry).

After I completed my DPhil, I embarked on postdoctoral research with Margaret in Oxford, funded by the Medical Research Council. I also won a Junior Research Fellowship at Linacre College. But within a few months I was offered a joint appointment at Keele University and at the Synchrotron Radiation Source (SRS) at the Daresbury Laboratory, which seemed to me to be an exciting opportunity. Although the protein crystallography community seemed skeptical about the future role of synchrotron radiation, I was able to obtain the UK community support in order to establish the first instrument for protein crystallography at the SRS, which was on bending magnet 7, SRS 7.2. There was serious rivalry between the different research communities to obtain a station on this first x-ray beamline. Although the initial SRS was not ideally suited to crystallography, especially with its horizontal source size of 14 mm, I could immediately realize 20 times our home lab rotating anode x-ray intensity, as an added benefit to the full tunability. The addition of a vertically focusing mirror brought us up to 100 times gain over our home lab intensity. Our first SRS protein crystallography (PX) users, UK and international, immediately started obtaining exciting results. The first users of SRS 7.2 of course included all the UK research laboratories undertaking protein crystallography of the time. Dr. Trevor Greenhough joined me at Keele and was very interested in the processing of oscillation camera data from SRS 7.2, vital to ensure quality data. I coordinated a "round robin study" of oscillation camera data processing and presented the results in a talk at the Ottawa IUCr Congress in 1981, along with a poster on SRS 7.2.

Being at Daresbury had major perks. I was a member of the UK Delegation on Synchrotron Radiation to the USSR led by the Daresbury Laboratory Director, the nuclear physicist Alick Ashmore. Before the trip I was telephoned by Maurice Wilkins, who wished me well, and by Max Perutz wanting me to undertake a protest on his behalf of a USSR dissident he was trying to help. I thanked both for their phone calls, but I was rather overwhelmed by both. Our delegation was treated exceedingly well in Moscow and in Novosibirsk. I realized that learning to give an after-dinner speech was going to be important, something I only made headway with when I became president of the local bowls, tennis and squash club in Stockport, near Manchester, much later. Daresbury was part of the Civil Service and my trip to the USSR also led to a briefing document being sent to me, which included "how to avoid compromising situations".

We were also getting noticed internationally; Howard Einspahr (pea lectin) and Steve Ealick (purine nucleoside phosphorylase, PNP) arrived early on from Birmingham Alabama, where they were based with Charlie Bugg. The PNP work, including an honorable mention of the role of SRS 7.2, was written up by Charlie in an article in *Scientific American* on structure-based drug design. Seeing my name quoted in *Scientific American* was something that my mother and father as well as my aunts and uncles took serious note of! Michael Rossmann also arrived promptly from Purdue University with his human rhinovirus crystals. His work at SRS 7.2, as well as his work at EMBL Hamburg, led to a protocol for virus crystal data collection, which was called "the American Method: shoot first and ask questions later". Michael and his coworker John Erickson wrote a paper about this R&D, which appeared in *J. Appl. Cryst.*; I am proud of the acknowledgement to me in that paper.

With SRS 7.2 up and running and UK with international (especially from USA and Sweden) users, a new opportunity arose to expand the technical specification with the advent of the SRS superconducting (5T) wiggler, built by the Rutherford Appleton Laboratory. This wiggler had a critical wavelength of emission of 0.9 Å, and adding this portion of the x-ray range for use would greatly extend the SRS 7.2 capabilities. In addition it had a higher intensity even at the SRS 7.2 favored wavelength range of 1.3-2 Å, due to the simple fall-off of the SRS spectral curve for a bending magnet field of 1.2 T, with its critical wavelength of 4 Å. Since this wiggler magnet could provide 60 mrad in total of beam radiation, rather than the 28 mrad of the bending magnet, we could also have a "straight through beam" setting for the 2θ arm. This would allow a white beam of X rays to pass through to the sample. At this time, 1984, the Cornell CHESS group of Keith Moffat published their seminal paper in *Science* advocating Laue diffraction for rapid data collection in protein crystallography for time-resolved structural studies in the crystal. The SRS 9.6, commissioning team included Andrew Thompson and also Miroslav Papiz, who joined me as a postdoctoral research assistant to commission and implement the FAST TV diffractometer, recently purchased from Enraf-Nonius based on the Medical Research Council Cambridge prototype of Uli Arndt. This commenced in 1984. It was a very busy time. I joined Daresbury as a full time employee, my first permanent job in science, in mid 1983. I was in charge of the SRS 7.2 user program, the development of a new instrument, SRS 9.6 and then its users. By mid-1985 I was suffering from severe exhaustion from long hours working, often missing a night's sleep and still trying to conduct a day job. I was also trying to undertake methods development research as well as user program local contact

support. When the opportunity arose, I moved back into a joint appointment with Daresbury, this time based at York University.

At SRS Daresbury ~1982. Left to right: Neville Greaves, Greg Diakun, J.R.H. and Paul Quinn

The research I did at Daresbury and from York at Daresbury on SRS 9.6, and the expanding user program, broke new ground in various research areas of macromolecular crystallography. We optimized anomalous scattering at the L absorption elements such as the common heavy atom derivatizing elements, Pt, Au and Hg. With Keith Hodgson and Britt Hedman in the (NATO funded) collaboration, we assessed how small the protein crystals could be, and tested crystals as small as 20 microns. Again with Britt and Keith, we showed that protein disulfides did split upon x-ray irradiation of a specific absorbed dose. I recorded broad bandpass Laue diffraction from a pea lectin crystal (these crystals were a gift from Howard Einspahr from the SRS 7.2 collaboration I referred to earlier), which led to a whole new software package for evaluating Laue diffraction patterns, in a collaboration with Daresbury colleagues Pella Machin, Mike Elder and John Campbell. (Mike and Pella were tragically killed in a climbing accident in Scotland in March, 1987.) There was also a spin-off into the initial SR small molecule microcrystals research program led by Marjorie Harding, then at Liverpool University, using the SRS 9.6 TV diffractometer. Most famous of all was the Foot and Mouth disease virus work of David Stuart, which even made it onto the BBC 9 o'clock evening news! The repertoire of SRS protein crystallography instruments improved further with the build of the rapidly tunable SRS 9.5. The Swedish Research Council provided the vital 50% of the funding for SRS 9.5. This allowed us to undertake two-wavelength phasing; specifically the work on a brominated oligonucleotide crystal was undertaken with my Manchester PhD student, Mark Peterson (see below).

Protein crystal perfection and the nature of radiation damage started to become a major research theme for me in the 1980s. The context was that I had ensured that the silicon and germanium monochromator crystals on SRS 7.2 and 9.6 were up to specification; I had travelled up to Durham University with them on the train to work with Brian Tanner's group to properly characterize them on their Bede double crystal rocking curve x-ray apparatus. The relevance of this to "How perfect were protein crystals?" I found fascinating. By this time the British Crystallographic Association had been launched and I was meeting not only biological but also physical, chemical and industrial crystallographers. I was learning about x-ray topography, powder diffraction linewidths, etc.

One day around 1986 or so, I was in my new office in the York Physics Department when Charlie Bugg rang me up and asked if I knew about microgravity protein crystal growth? More to the point how would I set about characterizing and comparing the perfection of protein crystals grown on earth as "ground controls" and the space-grown ones? I mentioned my monochromators and their being, well, simply perfect. There were fundamental physical and chemical questions: How perfect could protein crystals be? What happened to their mosaicity upon x-ray irradiation? At the SRS, a high brightness lattice had been introduced involving an improved, i.e., lower source emittance. So, what was the sample acceptance? At the ADONE synchrotron in Frascati, with Marcello Colapietro, I measured protein crystal monochromatic rocking widths on his four-circle diffractometer and with a very small angular x-ray divergence. At SRS 9.5, by using a long distance from the protein crystal sample (2.4 m) we, with PhD students Susanne Weisgerber and Eddie Snell, recorded USA space shuttle grown and control earth grown diffraction spot sizes; the space ones showed a significantly smaller spot size. Later, with Naomi Chayen and Eddie we expanded on this research considerably and published a book together, *Macromolecular Crystallization and Crystal Perfection* (OUP and IUCr). The arrival of microgravity research brought, I think, an increased rigor on these topics to our field. In reviewing Andre Authier's book *Early Days of X-ray Crystallography* I was fascinated to learn of Patterson's publication on particle size broadening, work he had started in a research period in Germany after he completed his work with W. H. Bragg in London. This was a connection to Patterson I had not expected!

The work we (Cruickshank, Helliwell and Moffat) undertook on the multiplicity and angular distribution of reflections in Laue diffraction, published in *Acta Cryst. A*, overturned some misconceptions in the field; that a Laue diffraction spot should always contain multiple Bragg reflections and that quantitative crystal structure analysis was not possible with Laue intensities. In our first theory paper (1987) prime number theory refuted the first misconception. A paper I wrote with colleagues published in *J. Appl. Cryst.*, with several follow up crystal structure analysis case studies, refuted the second misconception. Our 1987 theory paper abstract had concluded by mentioning its relevance beyond synchrotron Laue diffraction and on to neutron Laue diffraction.

In the early 1990s I was contacted by Clive Wilkinson and Mogens Lehmann about the possibility of the Institut Laue Langevin (ILL) introducing the neutron Laue method for biological and chemical crystallography with neutrons. In neutron biological crystallography, protonation states (as deuterium) of ionizable amino acids such as histidine, aspartic acid and glutamic acid, as well as more detailed information on the orientation of water (D_2O) molecules, could be determined at diffraction resolutions around 2 Å. The idea was that neutron fluxes were low compared with x-ray fluxes and harnessing a wide spectrum of emitted neutron wavelengths would open up a range of new and more challenging projects for crystal structure analysis of higher molecular weight proteins and/or smaller crystals of proteins, which had been previously out of reach of monochromatic neutron beams. At the same time I noticed that concanavalin A crystallizations that my PhD student Susanne Weisgerber had set

up had grown very large, to several mm^3. In 1997 we published our first neutron protein crystal structure using the neutron Laue data measured at the ILL on the EMBL LAue Diffractometer (LADI), processed with the Daresbury Laue software.

I was asked to lead the MX Working Group for the planned ESRF, the first 3rd generation SR source. This was finally approved in the late 1980s after many workshops and meetings, initially within the ESRP (European SR Project, based at CERN in Geneva). It was as part of the ESRP work that I visited Roger Fourme, leader of the Paris LURE SR Source protein crystallography instrument; Roger and I worked on aspects of beam heating and x-ray irradiation damage with the incredibly intense x-ray undulator source beams that the ESRP would introduce to users for the first time in the world. We produced a report (Helliwell and Fourme 1983 "The ESRF as a facility for protein crystallography: A report and design study" (ESRP Report IRI-4/83(1983), pp. 1-36). I later became a consultant for ESRF and EMBL Grenoble. Through the 1990s and into 2000 I served successively on the ESRF Scientific Advisory Committee (SAC) as vice-chair and as chair, on the ESRF Machine Advisory Committee representing the SAC and the ESRF Council as a member of the UK Delegation.

With Alfons Haedener, Basel, 1998.

By 1989 I had moved to the University of Manchester as Professor of Structural Chemistry, as I mentioned briefly above, again jointly with Daresbury, and was able to combine my interest in methods developments at the synchrotron for crystallography with my own steadily increasing structural studies research program. In Manchester I had been joined by Bill Hunter from Olga Kennard's Lab in Cambridge and in turn he recruited Gordon Leonard. There was a lot of knowledge around me in oligonucleotide and protein structures! I learned a great deal from Bill and Gordon and was very sorry to see them leave Manchester, Bill to introduce protein crystallography in Dundee and Gordon to ESRF. Bill had introduced me to Alfons Haedener; Alfons and I entered a very productive collaboration (MAD and Laue) on the enzyme hydroxymethylbilane synthase (HMBS, described further below). With Joe Gilboa and Joe Yariv at The Weizmann Institute, Israel we made extensive studies of the lectin concanavalin A including eventually a chemical crystallography style "bond distance analysis". The hydroxymethylbilane synthase project made good use of the x-ray sensitive ESRF (Jean Pierre Moy) electronic detector, and we could measure a large number of Laue patterns from a crystal, allowing high-quality electron density maps to be determined. We used a Hal Wycoff design flow cell, the device first shown to me by David Phillips at my DPhil interview in Oxford in 1974! We also undertook Se-methionine MAD phasing, inspired by Wayne Hendrickson, of the active form crystals of HMBS at SRS 9.5 and ESRF BM14; the respective seleno anomalous difference Patterson maps facilitated the development of these first instruments for MAD on SRS and ESRF.

A big structural research theme developed with the lobster coloration protein crustacyanin; this was work carried out in collaboration with Naomi Chayen at Imperial College and Peter Zagalsky at Royal Holloway College. I also had a new PhD student with me in Manchester, Michele Cianci from Padova University, Italy and also an EU funded research visitor from Poland, Andrzej Olczak. Along with Pierre Rizkallah at Daresbury we solved the crystal structure of apocrustacyanin A1 utilizing softer X rays (λ = 2.0 Å), at SRS PX7.2 (which Pierre had "un moth-balled"), SRS PX9.6 and SRSPX9.5. With the apocrustacyanin A1 crystal structure we solved the beta-crustacyanin crystal structure using data recorded at SRS MPW 14 (this latter beamline development was led by Colin Nave). Our lobster crustacyanin research, published in PNAS in 2002, hit the media! Articles appeared in *The Times*, *The Guardian*, *The Independent* and it was featured also on radio and TV. Later science writers gave their descriptions, e.g., in *Physics Today* (written by Charles Day), which I especially liked. Madeleine set about crystallizing numerous carotenoids and considerably expanded the available carotenoid x-ray crystal structures and their associated colors. This combination of chemical crystallography along with the biological crystallography proved to be a strength of our lab. Through the 2000s we both presented these results at a variety of conferences having by now been able to travel together, as our children had grown up and "flown the nest".

The x-ray laser arrival was clearly very exciting, I thought, from the outset. In 2002 I was Director of SR Science based full time at Daresbury. I firmly encouraged UK participation. In 2004 I published some ideas of how one might optimize its use in protein crystallography in a conference proceedings paper (the International Symposium on Diffraction Structural Biology, ISDSB, held in 2003 in Japan) in the *Journal of Synchrotron Radiation*. My paper describes finding "marker" seleno atoms in Se-met amino acid residues from two wavelength dispersive differences and secondly use of longer wavelengths along with back scattering to still realize at least 2.5 Å diffraction resolution. In general, though, the biological crystallography community reaction to the x-ray laser was as controversial as the earlier reaction on whether synchrotron radiation would be useful in protein crystallography! In Manchester, with my final year undergraduate project and master students, we started investigating electron-rich heavy-atom clusters binding to lysozyme as a test protein; tantalum bromide (Ta_6Br_{12}) and the platinum hexahalides, especially platinum hexaiodide, were interesting. My idea was that with protein samples as small as a single molecule in the x-ray laser beam their diffraction patterns would be exceedingly weak and so we would need both

recognizable markers, like the Se-met above, and the nicely shaped octahedral platinum hexahalides. These would also provide an increase in the x-ray scattering efficiency of a protein sample. I spoke on these ideas and results at the ECM28 in 2013 held in UK. At the x-ray laser session in Albuquerque I made the additional suggestion that fully loaded ferritin, with its protein shell enclosing some 2000 iron atoms, would make a splendid test "nanocluster" to spray past the Linac Coherent Light Source LCLS Stanford x-ray laser beam. John Spence, who sat nearby, looked at me and said "ferritin is planned".

I heartily thank all my PhD students and post docs over the last 35 years for the research and development work we have undertaken, as well as the people I mentioned above. I would like to mention that I collaborated for many years with George Habash, Durward Cruickshank and Jim Raftery. I am very grateful to CCP4 whose software I have extensively relied upon, as well as my students and I learning a great deal at their Study Weekends, as well as SHELX software (for full matrix inversions) and Xplor/Phenix software (for neutron macromolecular crystallography). I also heartily thank Daresbury Laboratory and the universities of York, Oxford, Keele and Manchester; and all the SR and neutron facilities for their collaboration since 1976. I especially thank my wife Madeleine.

J.R.H. taking a stroll between APS SAC meeting sessions, pointing to the Tesla sign. (Tesla makes SR source magnets; Tesla is also the unit of magnetic field named after Nikola Tesla.)

When I received the email from the ACA President Cheryl Stevens that I had been selected to receive the 2014 ACA Patterson Award, I immediately told Madeleine that I could not have achieved it without her. The ACA conference in Albuquerque was, of course, a wonderful experience. As well as the Patterson Award Lecture I gave two other lectures, on the use of high-photon energies in macromolecular crystallography and on involving undergraduates in protein crystallography research. My past PhDs (Dora Gomez, Michele Cianci, and Eddie Snell) and collaborators (Zygmunt and Ulla Derewenda, Howard Einspahr and Keith Moffat) hosted a marvelous dinner for Madeleine and me near the Albquerque Convention Center.. I was proud also to enter the ACA 2014 Conference Banquet alongside the ACA President Prof Martha Teeter. As with all the ACA meetings I have attended over the years, I greatly enjoyed all of this ACA meeting. Thank you to the ACA!

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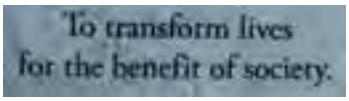
Notes of a Protein Crystallographer:



I was a totally disoriented foreign student when I arrived at the University of Texas (UT) at Austin in the Fall of 1972. I had been admitted to UT thanks to the Institute of Internal Education (IIE) and supported by a Fulbright scholarship with intentions of pursuing a graduate degree in biophysics. I had a general idea of what that was, but I did not know that I was going to focus on the emergent (and by then mature) field of protein crystallography. It all happened because, in the lab of my advisor (Larry Fox), there was a beautiful blue protein purified from a blue-green algae (*A. quadruplicatum*) that I was lucky enough to crystallize on my first try. That event changed my life. Approximately forty years later, on July 12, 2014, my colleagues from those years and other successive generations of students, postdocs, colleagues and friends of Marvin L. Hackert and Jon D. Robertus met on the UT campus to honor the two faculty members who have devoted their professional lives to training and educating generations of protein crystallographers and structural biologists. Notable absences were Hugo Steinfink and Ray Davis, distinguished crystallographers of the UT campus (both past presidents of the ACA) who passed away earlier. It was a 'close family' symposium under the title of *Celebration of 40 Years of Protein Crystallography at UT-Austin* organized by my colleague from those youthful years - Art Monzingo.

From the evening reception and get-together the night before, to the banquet at the end of the academic sessions, and the 'ritual' inner tubing excursion on Sunday down the chute on the Comal River in New Braunfels (which I unfortunately did not attend), it was a memorable weekend. There was time to catch up with close colleagues (John Priestle, Robyn Stanfield), friends and families, and also a substantial amount of getting to know the later generations that came through the UT labs after I left in 1979.

It is not the purpose of these notes to make a technical and scientific review of the meeting. Suffice it to say that the presentations by the alumni, friends and colleagues of the two honorees were excellent. I just wish to convey the spirit of friendship, camaraderie and sheer delight at spending a couple of days together sharing the science and honoring Marv and Jon. The morning of Saturday, July 12, slipped away with talks about drug discovery, nitric oxide signaling, intrinsic disorder of proteins, rare and exotic antibodies (BEVO-bodies), integrins, immune therapy, intron debranching enzymes and Amyotrophic Lateral Sclerosis. After a busy lunch, the exciting science continued in the afternoon with talks on: proteome evolution, nuclease in cell death and inflammation, design of drugs against *Schistomosomiasis*, DNA damage regulation, rhodopsin and GPCR activation, non-canonical base pairing, filamin domains and structural studies on the thiamine transporter of *Listeria*. All in all, it was an exhilarating and full program.

Sculpture of Barbara Jordan - the quotation leading off the article is taken from one of red granite engraved panels around the memorial.

After a brief break to stroll around campus, there was a banquet that evening. Several speakers, among them Art Monzingo, Ernest Villafranca and myself, as the most senior members of the group, gave emotional accounts of their years at the incipient laboratories of protein crystallography that Marv and Jon developed into an inspiring environment for the many generations that passed through their labs. The transforming effect of those years in the minds and hearts of many of the attendees was made patently clear by the anecdotes and conversations of many of the participants. Time passed too quickly and it was soon time to return to our current lives with many of the participants still doing research. Among the beautiful Battle Oaks at the entrance to the UT campus on 24th Street, one can find a secluded corner with a larger-than-life sculpture of Barbara Jordan, a remarkable woman who authored the following quotation: *I've always felt that as long as you are alive, you should be doing something that makes a difference…. You don't have to do big, gigantic things. Just do things incrementally that make a difference*. Indeed, this is what Marv Hackert and Jon Robertus have done during their tenures as protein crystallographers on the UT Austin campus for over forty years; and many of us, myself included, were transformed by their efforts.

Cele Abad-Zapatero

Attendees to the symposium honoring Marv Hackert and Jon Robertus (first row, fourth and fifth from the left, respectively).

Molecular Beauty

I am soliciting nominations for "beautiful molecules", together with a .jpg image and short note describing why a molecule or molecular complex is beautiful to you. If many come to mind, please distill the list to the top 2 or 3 'beauties'. I will review the nominations and submit a summary to a forthcoming edition of *RefleXions*.

In perspective, when we speak of beauty in nature (e.g., a flower, a cloud formation...) what characteristic is immediately shared in our conversation? One aspect of molecular beauty is architectural form, illustrated here by two examples, Hans Deisenhofer's co-chaperonin structure (top) and Tim Richmond's nucleosome structure (bottom - both with artistic enhancements for my 3D printer). Surely others come to mind: symmetry, shape, contrasting patterns, etc.

Benjamin Franklin, in Poor Richard's Almanack, 1741, wrote:
Beauty, like supreme dominion Is but supported by opinion

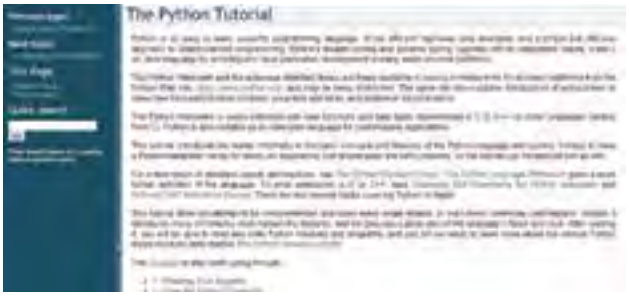
Ed Meyer
molecular-sculpture.com

NetfleXions

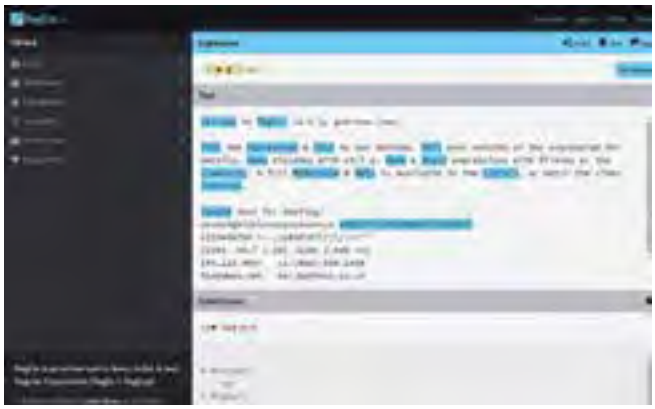
There was a time when working in a scientific field brought with it a certain familiarity with computers. If you were born before 1980, chances are you know what a DOS prompt is, and more importantly, what to do with it. Do you find yourself searching for ways to use the keyboard when facing a fancy new point-and-click GUI? Can you remember the days of the VAX, before the internet, when line printers or punch cards ruled the earth. OK, admittedly some of those things predate this fearless scribe, but I do find myself yearning for those times now and again. When I teach crystallography to new students, I occasionally have to stop and explain when I tell them to insert an ACTA "card" in their "ins" files. Some habits die hard. But maybe they shouldn't die at all.

I'm not saying we all need to go back to the halcyon days of science when in order to process data, first you had to write the program to do it. There is, however, a certain joy in being able to make a computer bend to your will, to have your CPU do all the dirty work for you. In the current age of sentient diffractometers that can solve a structure and generate glossy automated reports it's easy to become complacent, to sit back and let the software take you where it will. But what if you don't like where it's going? Or what if you need more than what your software is giving? Then it's time to think about writing some automation scripts, designing your own programs, or writing plugins to your favorite software packages. Perhaps over time, your little script will go on to change the face of crystallography.

Like most things in life, if you're interested in learning, there's help for you online. For the novice scripter or experienced programmer alike, there are several great websites out there that can help you on your way. If you're considering plunging into Python or you simply want to remember the correct way to define a dictionary, the Python website (***www.python.org***) has you covered. If you know nothing of scripting and need something to guide you through, the tutorial at ***docs.python.org/2/tutorial/index.html*** is just the thing. You'll go from writing "Hello world!" to automated file maneuvering in no time flat.



While you're worrying away at your scripts, you might find yourself in need of a fancy regular expression to search for just the right string of text. If you're like me and can never quite remember the syntax, then head on over to ***www.regexr.com.*** This tidy website has all the information you need to craft the perfect regex, and has functionality to test it out on your own files. Simply paste in some sample text, start writing out your regular expression and watch in real-time to see if it matches what you hope it does.



For more serious programmers out there, you may already be familiar with Numerical Recipes. This book contains information and lines of C++ code for myriad mathematical problems facing scientific programmers. Luckily for you, the book is available on-line at ***www.nr.com***. Non-subscribers can access a limited number of pages of the current edition per month. However, for a small subscription fee, full users can have complete access to the text, as well as online repositories of code. Older versions of the text are available with no restrictions. Numerical Recipes can help you tackle Fast Fourier Transforms and Linear Least Squares with ease. And, if you are so inclined, you can call NR code directly from your Python script. If FFTs are really your thing, you can find all the code you need for C and Fortran and a host of other languages as well at ***fftw.org*** .

If you're the sort of person who finds joy in writing the most efficient "if…then" statement, then hopefully you'll find some help in the sites above. If you've always shied away from lines of code, maybe this article has inspired you to try your hand at scripting away some of crystallography's more mundane, rote tasks. If you read this piece and had a list a mile long of even more helpful sites, do send them along, and perhaps *Netflexions* will feature them in another issue. But if you do read anything from these words, let it be that computers are not immutable black boxes. They can be coaxed into doing all sorts of amazing things for you and, by extension, for the entire crystallographic community. All you need is a little imagination; the help is available on-line.

Amy Sarjeant

Reciprocal Space Visualization - MAX3D

The MAX3D workshop was offered to introduce attendees to the routine examination of 3-dimensional diffraction data. Area detector scans for single crystal or texture analyses provide us with examples for 3D reciprocal space visualization. Attendees installed the MAX3D software on their laptops in advance of the workshop and came prepared to explore.

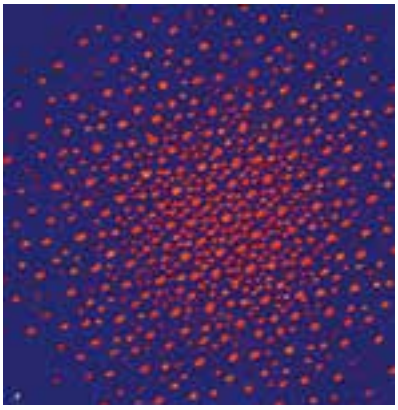


Figure 1. $Al_{70}Pd_{22}Mn_9$ Quasicrystal (Geetha Blakrishman, Warwick)

The workshop opened with a survey of various examples of reciprocal space objects, including quasicrystal diffraction, solid-state incommensurate and diffuse scattering, fibre diffraction, protein diffraction, texture analyses, thin film analyses, etc. Use of various MAX3D tools for studying interesting diffraction features was demonstrated.

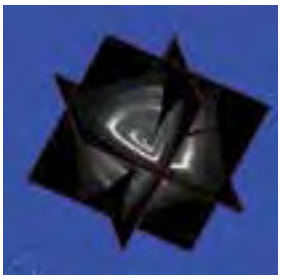


Figure 2. Slices through fibre diffraction pattern on squid pen (Malkel Rheinstudter, McMaster)

In the second part of the workshop the participants worked through a sample dataset, learning how to load raw diffraction frames into MAX3D and create a 3D reciprocal space object. They adjusted the opacity of various intensity ranges of the object to focus on interesting features of the diffraction pattern. They practiced 3D cropping and reloading subsets of the pattern at higher voxel resolution. They experimented with switching between 3D, slice and 2θ sphere viewing modes.

In the final part of the workshop we examined data provided by the participants. Figure 3 shows a partial scan of a protein (*PDBID 3K9I*). By zooming in on a region of the pattern and rotating the 3D object, we could clearly see that there were 2D sheets of diffuse scattering associated with the diffraction pattern. This system was discussed in detail in Poster S-11 by James Clarage, Anam Ahmed, Mary Faltaous and Lukas Cara at the 2014 ACA Albuquerque meeting.

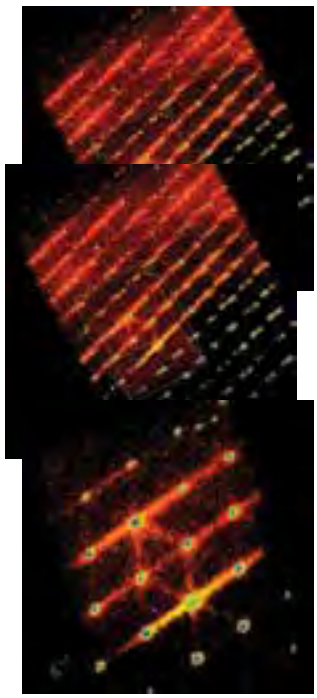


Figure 3. Diffraction from a protein (PDBID 3K9I), zooming in to see the sheets of diffuse scattering (James Clarage, St. Thomas).

The workshop participants seemed to be quite enthusiastic and excited about their new-found ability to become intimately acquainted with their experimental data. The audience included professors, students and professional crystallographers. Comments were made regarding a new understanding of diffraction and reciprocal space. The potential of creating and using these images for teaching was also discussed. Participants included Lawrence Andrews, Bhandari Yuba, Eileen Brady, James Clarage, Robert Evans, Lokesh Gakhar, James Holton, Matthew Jensen, Chao Li, Tracy Nixon, and Dale 'Mystery Man' Swenson. The workshop was organized and presented by Jim Britten. MAX3D is authored by Jim Britten (***britten@mcmaster.ca)*** and Weiguang Guan of McMaster University.

Jim Britten

Contributors to this Issue

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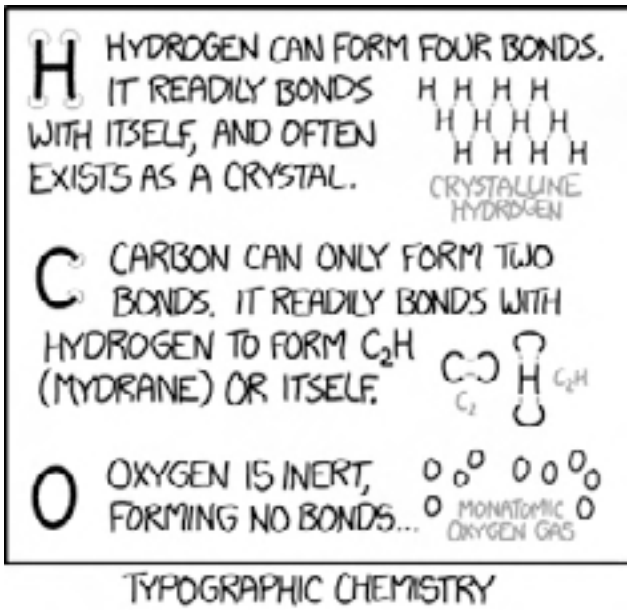
Cartoons: This page from XKCD.com and on Page 41 from Nearing Zero by Hank Kim at www.lab-intio.com



U.S. National Committee for Crystallography Report of the Twenty-Third Congress and General Assembly of the International Union of Crystallography

The National Academy of Sciences (NAS) is the adhering body to the International Union of Crystallography (IUCr), and the NAS manages the relationship with the Union through the US National Committee for Crystallography (USNC/Cr). While the American Crystallographic Association (ACA) also plays a major role in our profession, this professional society is only one of the several regional affiliates of the IUCr.

Every three years the Union hosts a Congress. This year it was held in Montreal, Quebec, Canada on August 5-12 and organized by the Canadian National Research Council in Montreal, the first time that it has been held in the Americas since the 1996 meeting in Seattle, WA.

An important part of the meeting is the General Assembly (GA), where the IUCr policy decisions are made, such as elections of the Executive Committee (EC), presentation and voting on resolutions, and update on Union initiatives. The US delegation (Brian Toby, Chair, Chris Cahill, Katherine Kantardjieff, Brian Matthews and Joe Ng) was absolutely delighted to have a former ACA President, Marvin Hackert, elected as the new IUCr President. One of the highlights of the General Assembly was the approval of a new Latin America Crystallographic Association (LACA) as the fourth regional associate of the IUCr (besides the ACA, the European, and the Asian societies). This shows the significant growth of crystallography and the long tradition of practice in many of the Latin American countries, which extends back more than half a century. While it is common to observe in every General Assembly one or two countries interested in joining the Union, this meeting was noteworthy since eleven countries (all from either Africa or Latin America) submitted their applications to join the IUCr. Algeria, Cameroon, Costa Rica, Morocco, Pakistan, Turkey, Uruguay and Venezuela are now members of the Union. The rest of the countries did not present enough evidence of meeting the criteria; therefore, they were asked to resubmit their application for the next General Assembly. Two bids were presented to host the IUCr Congress in 2020, for Paris and Prague, and the delegates selected thebid from the Czech Republic.

At this GA, we the lost two excellent women on the EC and did not add any new female members. It is important, valuable and simply right to strive for diversity on IUCr commissions and committees; this includes gender balance as well as geographic and area factors. To address this, the national committees need to put forward a set of highly qualified individuals to run for elections that address all these areas where diversity is needed. This process is best completed almost a year in advance of the next General Assembly, which will meet in Hyderabad in 2017.

This year, the USNC/Cr obtained a grant from the National Science Foundation that provided 19 travel grants to US early career scientists to attend the Congress as part of the USNC/Cr Young Observers program. This program encourages early career scientists to attend the IUCr General Assembly where they are exposed to the field of science policy. In addition, each awardee is paired with a senior crystallographer who acts as a mentor for the duration of the Congress. Also, the committee held a US reception, which was attended by 70 US and international crystallographers. This activity provides American crystallographers the opportunity to network with international peers.

In addition, the USNC/Cr staffed a booth for promoting US sites for the IUCr Congress in 2023. We held a contest where visitors indicated their favorite US city from among four options (Boston, Chicago, Honolulu and San Diego) to host the IUCr Congress in 2023. The USNC/Cr will be working in the next three years to complete a bid that will be presented at the next IUCr Congress, which will be held in Hyderabad, India on August 21-29, 2017. The committee will work with the ACA in the preparation of the bid, and a team of volunteers will be needed. If you are interested in helping with this, please contact Joseph Ng, USNC/Cr vice-chair (and chair-elect) at ***ngj@uah.edu***.

Of course, the meeting included far more than discussions on IUCr governance. The Congress offered an amazing array of speakers, and a typical day offered six keynote presentations in two time slots, one plenary presentation, eight morning micro-symposia, and another eight in the afternoon. I found myself absorbed in science talks from breakfast until the evening. The scientific highlight of the meeting for me was the plenary presentation given by Dan Shechtman from the Technion, who reviewed his discovery of an "impossible" 10-fold symmetry electron diffraction pattern, which we now know denotes quasi-crystalline ordering. This led directly to the understanding that not all materials with long-range order are periodic, which has changed how we define what a crystal is. The speaker explained why he was confident that his observation was indeed something novel and not something more conventional, such as a twin. The solo Nobel Prize awarded to Shechtman would be well deserved just for establishing a strong experimental case and then standing up unyieldingly to the scientific establishment until his results could be accepted, let alone for discovering a new form of matter. Another very memorable part of the meeting for me was a theater performance rather than a scientific talk. The biographer of Dorothy Hodgkin, Georgina Ferry, created a one-woman play, *Hidden Glory: Dorothy Hodgkin in Her Own Words*, using actual quotations from Hodgkin's letters and other writings. A video of this play was shown, and it was worth much more than missing a lunch to watch it. In fact, after watching the video, I went on to read the reissued biography (timed for the IYCr?) to learn more about this great scientist

Brian H. Toby Chair 2012-2014, USNC/Cr

The 2014 USNC/Cr Young Observers Program at the IUCr Montreal, Canada.

This past August, several thousand crystallographers descended on Montreal to attend the 23rd Congress and General Assembly of the IUCr. Much has already been written about the social and scientific aspects of the Congress, and results of the voting at the General Assembly have spread throughout the community. There was abundant fanfare over the International Year and its associated activities. But such a large convention space, teeming with the top names in our field, can prove a daunting experience to young members of our profession who may, perhaps, be attending their first scientific meeting ever.

Thanks to NSF funding (CHE 10001907), the U.S. National Committee for Crystallography (USNC/Cr) provided travel awards to nineteen young scientists to help them travel to the Congress and developed a social program give them support as they navigated this enormous event. This Young Observers program accepts applications from young crystallographers, either students still working towards their BS, MS or PhD or professionals already out in the workforce but within 5 years of their degree. The program is competitive, with roughly half of all applicants receiving an award. Once chosen, the applicants are invited to select a mentor from a pool of established crystallographers who are well known to the community. A special dinner is held during the Congress so the YOs can meet with their mentors and discuss any number of issues. In addition to the one-on-one mentoring experience, this year we had a panel discussion focusing on various career choices and pathways leading from grad school to successful – and fulfilling! – employment.

The YOs are invited to attend the General Assembly meetings, to get a sense of how the Union operates and how decisions are made and policies are crafted. Many members of the crystallographic community are largely unaware of the inner workings of the IUCr, so this experience helps shed a light on what can seem to be a very mysterious process. One particular YO, Bradley Hintze from Duke University, was able to participate in the Biological Macromolecules Commission and had a voice in discussions on data deposition. Anastasiya Vinokur from the University of Wisconsin, wrote extensively about her experiences as a Young Observer:

It is very scary to go to your first conference alone. You can liken that feeling to walking into a high school cafeteria on your first day as a new kid. There are a lot of people, a lot of languages, a lot of interesting and challenging talks, and not a whole lot of familiar faces. But when I thought I would have to eat lunch alone, muddle alone through the difficult terminology of the latest talk I heard, someone waved at me. It was my mentor, Christine, from the Young Observers program and all of the anxiety melted away. I was not alone. In fact, I already belonged to a small community by virtue of coming to the IUCr Congress through the Young Observers program.

I cannot adequately express my gratitude for the opportunities that this program gave me. As a graduate student of a young professor working on a project not yet funded, my chances of going to a big conference like the IUCr Congress were limited. But Young Observers changed that. They covered my travel expenses and most importantly gave me the confidence that my work was interesting not only to the solid state community, but to crystallographers as well.

Young Observers opened a window for me to a wider community. I sat one afternoon at the USNC/Cr booth and listened to an impromptu history of crystallography from people who witnessed it unfolding. I attended talks by crystallographers about whom I had only read in textbooks. I watched the union delegates waltz through the challenges of politics and science. This is a vibrant, ever-changing community and I felt excited to become part of it.

I am just at the beginning of my scientific career, but I see the path that I want to take; there is a place for me among the world's crystallographers. Attending the IUCr 2014 this summer widened my horizons, taught me new concepts, introduced me to new people, and made me, I hope, a better scientist. I look forward to attending the ACA meeting in Philadelphia next summer so as to learn more and to grow more.

As a mentor, the YO program is just as rewarding. Having the chance to meet the next generation of crystallographers provides the opportunity to see the Congress and our community from a fresh perspective. These young scientists are pursuing research that will continue to define what we consider crystallography in future years. To have the chance to listen to their triumphs and trials, and to offer advice and guidance as they plan their future is truly an invigorating experience.

We hope that this program will always be available to younger US scientists and though Hyderabad, 2017 seems far afield and a long time off, we will certainly need mentors and volunteers to help organize the program, review applications and advise a Young Observer. Look for more on this in 2016 or contact the chair-elect of the USNC/Cr, Joe Ng ***(ngj@uah.edu)*** in advance of the IUCr2017 Congress to express interest.

Amy Sarjeant and Anastasiya Vinokur

ACA Members Matthew McGrath and Caitlin Murphy Selected for AIP Science and Technology Fellowships: I am pleased to report that two ACA members have been selected as AIP S&T Fellows for 2014-2015: Matthew McGrath, who will be working in the Office of Conservation and Water at the Department of State, and Caitlin Murphy, working on Capitol Hill in the office of Senator Al Franken (D-MN). The AIP S&T Fellowships are available at the Department of State and in Congress. (For details on how to apply for both programs, see page 68 of the fall 2014 issue of *RefleXions*.)

In this issue we are introducing Matthew and Caitlin and have asked them to provide a short note on what drew them to apply for the fellowships. Going forward, Matthew and Caitlin both have agreed to provide updates on their experiences; these will appear in future issues.

Judy Flippen-Anderson

Matthew McGrath: Since defending his PhD in physical chemistry at the University of Minnesota in 2007 as a Department of Energy CSGF fellow, Matthew has worked in four different countries, including two years of Peace Corps service at a public university in central Africa and two years as an NSF international postdoctoral fellow. He is currently working just outside of Paris, France, on a large project to incorporate forest management at the European scale into climatic simulations. His fellowship will not begin until early next year (2015), as he needs to finish up his current project in Europe.

Matthew writes: In many ways, my career to this point has been preparing me for the AIP State Department Fellowship. The purpose of the fellowship is to give scientists experience in the creation of foreign policy. Since defending my thesis, my life has been focused outside the United States. I've had the opportunity to witness diverse cultures, speak varied languages, and integrate myself into communities partially and wholly unlike the Midwestern town in which I grew up. These experiences have led me to develop habits and ways of thinking that are culturally-sensitive and diplomatic; in short, exactly the type of personality required for success in the US Department of State. In addition, they've ingrained in me an international way of viewing solutions, which is, in essence, the goal of foreign policy.

Being trained as a scientist, I have a particular way to approach problems, which is not necessarily identical to standard government workers, many of whom come from backgrounds in law and the humanities. I have been looking at science diplomacy fellowships for several years, as I had strong interests in both science and international affairs. The opportunity to apply my scientific training to problems of international importance was enticing, even if the problems I'll be looking at are completely unrelated to what I've been trained in. One problem I've always had as a scientist is the feeling that my work wasn't relevant. Many of us spend a good part of our careers struggling to explain what we're working on to family and friends. At the Department of State, the work you have in a day can change with events that happened while you were sleeping. It's not difficult to explain to someone your work when they've already read about it in *The Washington Post*.

One final aspect of the fellowship that appealed to me is the work environment. In the laboratory, the goal is to answer a question with 100% accuracy; anything less won't (shouldn't?) make it past the referees. This often means taking weeks, months, and years to perform all the research and literature review required. At the Department of State, time is a driving factor. A principal is meeting with an ambassador tomorrow and issue X is certain to come up. What does the principal need to know about issue X? This sort of environment trains you to think on your feet and work well under pressure, reaching out to contacts that know the information you're looking for instead of spending time learning it yourself. A completely different experience than what most scientists are used to. I strongly believe that, after the fellowship, I will be a better thinker, communicator, and scientist, even if I don't run a single experiment during my time at the Department of State.

Caitlin Murphy: Caitlin received her PhD in geophysics from Caltech in 2012, where she used high-pressure experiments to improve the current understanding of Earth's metallic core and ran multiple geophysical field excursions to image seismic faults in Southern California. Before taking up her AIP Congressional Fellowship, Caitlin served for two years as a Carnegie Postdoctoral Fellow at the Geophysical Laboratory in Washington, DC, where her research explored earth and energy materials under high-pressure conditions including measurements at DOE-funded synchrotron and neutron facilities.

CaitIin writes: I chose to join the ACA because its mission perfectly reflects my research interests: understanding how the atomic-scale structure and interactions in a material dictate its macroscopic properties. For me, this fundamental question underlies all of the earth and materials science research in which I have been involved. For example, I have investigated how the vibrations of iron atoms at high-pressure conditions are correlated with the elastic and thermodynamic properties of Earth's core; probed the local bonding environment of hydrogen in select hydrogen-storage materials; and explored the defect mechanism that leads to the coloration of heat-treated orange sapphires.

While I truly enjoyed all of these projects—and the amazing scientists they introduced me to—I felt that the focus of my work was narrowing with time, and that it was becoming increasingly removed from societal benefits. Although I strongly believe that this type of research is important for the advancements of all scientific fields, it no longer felt like a good fit for me. Therefore, I decided to apply for the AIP Congressional Science Fellowship, which represented the perfect opportunity for me to perform a public service, while still drawing upon my science background.

I am still at the beginning of the 2014-2015 AAAS Science & Technology Policy Fellowship program, but I have immensely enjoyed my experience so far. The two-week orientation program that kicks off the fellowship program (for all S&T fellows) was incredibly stimulating, and a refreshing change of pace from my independent postdoctoral research. We had the privilege of hearing from very impressive speakers about the history of our government, and how data-based arguments influence/inform/interact with the federal policy-making process. In addition, we participated in hands-on exercises that demonstrated how complicated it can be to balance scientific and political factors, and exposed us to the complicated relationships among (and within) the three branches of government. I loved the breadth of topics that were covered during this two week period, and the connections that were drawn between scientific research and the policy decisions that impact our society.

I am also very much enjoying my current position as the Energy and Environment Fellow in Senator Al Franken's office. So far, I have worked on a wide range of topics, from Minnesota mining projects and rail transportation issues, to electrical grid resiliency and winter fuel supplies. It is a very fast-paced environment, and I have learned an incredible amount in just four weeks. I love the team effort that is required by the nature of the work, in addition to the opportunity for independent research and thinking.

Finally, I would highly recommend the fellowship program to early career scientists who find themselves wondering if a research position is right for them, and particularly those that wish science played a larger role in our political process. It is a great opportunity to plant the seeds of change, although one year is likely not long enough to see a new idea come to fruition; on the other hand, the short-duration of the program is ideal for those who may want to return to academia after trying out a different direction. As for me, I am open to many career paths following the fellowship program; one of the things I am really looking forward to this year is learning about the ways I can make a difference outside of academia, while continuing to apply the skills that I gained throughout my academic career. No matter what, I am confident I will leave this program with a new set of skills, an incredible amount of new knowledge, and a new list of career opportunities that I was not familiar with before this year.

John Cowley Medal: John Spence, the Regent's and Richard Snell Professor of Physics at Arizona State University, received the John Cowley Medal on September 12, 2014, during the 18th International Microscopy Congress in Prague.

The Medal awards lifetime achievement of an international leader in the field of diffraction physics or microscopy and honors the memory of John Cowley, who pioneered these techniques and established the electron microscopy facility at Arizona State University.

John Spence was the recipient of the 2012 Buerger Award, named an ACA Fellow in 2014, and has received many other honors. He graduated in physics from the University of Melbourne and moved to Oxford, UK, for his post-doctoral research. Currently he is the Director of Science for the National Science Foundation's BioXFEL Science and Technology Center, which supports the application of X-Ray Free-electron lasers (XFEL) to structural biology.

Spence's multifaceted cutting-edge research makes use of electrons and x-rays for imaging, spectroscopy and diffraction, spanning the fields of physics, material science and biophysics. He is author of some 450 papers, covering: electron and x-ray holography; optimization of cryomicroscopy imaging techniques; atomic scale imaging of materials defects; and predictions of materials properties by atomic quantum mechanics. Recently he has focused his attention on the application of femtoseconds long x-ray pulses to solve the crystallographic structure of difficult-to-crystallize membrane proteins and viruses, using the Linac Coherent Light Source at Stanford, the world's first hard x-ray laser.

Sigma Xi Proctor Prize: On November 7th ACA member Jenny Glusker received the 2014 Sigma Xi's William Procter Prize for Scientific Achievement. The prize is intended for a scientist who has made an outstanding contribution to scientific research and has demonstrated the ability to communicate the significance of his/her research to scientists from different disciplines. Her talk was titled "Crystals and their Amazing Internal Structures".

Jenny Gusker started her postgraduate career in the laboratory of Dorothy Hodgkin, in Oxford, working on the hexacarboxylic acid derivative of vitamin B12 and determining the structure of the corrin ring. She then moved to the USA to work in the laboratory of Robert Corey at Caltech where, in collaboration with the fresh Nobel Laureate Linus Pauling, she started to study the structure of peptides and proteins. When she moved to the Institute for Cancer Research in Philadelphia, now part of the Fox Chase Cancer Center, she joined Lindo Patterson's lab, and continued her interest in B12 structures. She then became principal investigator, focusing on: the structural study of small-molecules related to cancer; the structural aspects of the Krebs cycle and citrates; the coordination of metal-ions in proteins; the interaction of ligands with metal ions; and the enzymes aconitase and xylose isomerase. She is currently Professor Emeritus at the same institution, and she collaborates with researchers at Los Alamos and Oak Ridge National Laboratories on neutron diffraction projects.

Jenny is the recipient of many awards, notably the Fankuchen Award of the ACA and the Garvan Medal of the American Chemical Society. She served as President of the ACA in 1979 and as editor of *Acta Crystallographica D* (macromolecules). One of Glusker's major interests is crystallography education; the 3rd edition of the popular textbook *Crystal Structure Analysis: A Primer* by Glusker & Trueblood appeared in 2010. She is the co-author or co-editor of a number of books on crystallography and the history of crystallography.

The ACA History Portal hosts Jenny's memoir, which describes her wonderful journey through crystallography (***www.amercrystalassn.org/jp_glusker***). The article above was adapted from Virginia Pett's introduction to the memoir.

Earle K Plyler Prize: ACA member Majed Chergui, from the École Polytechnique Fédérale de Lausanne, is the recipient of the 2015 Earle K. Plyler Prize for Molecular Spectroscopy & Dynamics of the American Physical Society. The Society honored him "for developing new methods and redefining the boundaries of molecular spectroscopy through extending the temporal and spectral range, and for his pioneering work in ultrafast X-Ray spectroscopy for studies in solution and the solid state."

Majed is the current editor-in-chief of *Structural Dynamics* co-published by the ACA and AIP Publishing. He studied and worked in the United Kingdom, France and Germany, before becoming Professor of Experimental Condensed Matter Physics at the University of Lausanne in 1993 and Professor of Physics and Chemistry at the Federal Institute of Technology, Lausanne in 2003.

His research aims at capturing the real-time conformational changes in condensed phases (proteins, liquids or solids) as well as in metallic and semiconductor nanostructured materials. To do so, he has pioneered ultra-fast x-ray absorption spectroscopy and ultrafast 2-dimensional spectroscopy in the ultraviolet spectral range. He has also developed novel optical laser pump-x-ray probe techniques using picosecond and femtosecond hard x-ray pulses from a synchrotron.

Some selected topics that Majed is currently investigating in his lab are: determining the role that solvation dynamics plays in

chemical and biochemical reactions; understanding the ultrafast charge transfers occurring between metal ions and ligands in transition-metal complexes (including metalloproteins) and the conformational changes that they generate; investigating the dynamics of biosystems using time-resolved non-linear spectroscopy in the UV (using aromatic amino acids as naturally occurring probes); and developing computational methods to calculate x-ray scattering patterns at the femtosecond time-scale. These type sof ultrafast time-resolved diffraction experiments offer access to vibrational and rotational dynamics and are now possible using Free Electron Lasers.

Biophysical Society Fellow: ACA member George Phillips has been appointed a Fellow of the Biophysical Society for his efforts to elucidate the structural and dynamical properties of biological macromolecules using x-ray crystallography, and for his commitment to biophysical training both at graduate and at post-graduate levels. He will receive the honor on February 8, 2015, during the annual meeting of the Society in Baltimore.

George is a past-president of the ACA, ACA fellow and a co-editor of *Structural Dynamics*. After spending 12 years at the University of Wisconsin-Madison as a professor, he is now the Ralph and Dorothy Looney Professor of Biochemistry and Cell Biology at Rice University, his alma mater.

His profound interest in structural biology has led him to broadly diversify his research. His team studies how heme-binding proteins coordinate oxygen, investigates new methods to capture the dynamic properties of macromolecules and characterizes proteins from hyperthermophilic bacteria to engineer thermostable proteins with possible commercial application. He and his research group are also involved in structural genomics and computational biology projects. Finally they collaborate with the Great Lakes Bioenergy Research Center to develop cellulosic ethanol, a biofuel produced from wood, grass and inedible parts of plants and derived from lignocellulose.

Gregori Aminoff Prize: On March 31, 2015, during the annual meeting of the Royal Swedish Academy of Sciences, Ian Robinson, Chair of Physics at the London Center for Nanotechnology (LCN) at University College London, will receive the 2015 Gregori Aminoff prize for "his development of diffraction methods for studying surfaces and nanomaterials."

Ian Robinson obtained his Master's degree from Cambridge University, UK, and his PhD from Harvard. He worked at Bell Laboratories (formerly known as AT&T Bell Labs) until 1992, when he became Professor at the University of Illinois at Urbana-Champaign. In 2006 he moved back across the pond to take up the professorship at the LCN. In 2000 he received the ACA Warren Award.

He was one of the first scientists to implement the use of x-ray radiation for the study of material surfaces in the 1980s, introducing a paradigmatic shift in material science. Until then, materials were mainly studied using less sensitive electron diffraction techniques that did not allow high-resolution atomic structural analyses. Nowadays one of his main research interests is to develop 3D coherent diffraction imaging methods that can provide high-resolution maps of single nanoparticles. At the Research Complex at Harwell, where he holds a part-time appointment, he has recently applied these 3D imaging techniques to study the structure of human chromosomes.

ICDD Awards: The International Center for Diffraction Data (ICDD) awarded the 2014 McMurdie Award and the 2014 Distinguished Fellow Award to Evgeny Antipov, from Moscow State University. The award recognizes "distinguished work that improves the Powder Diffraction File™ database in its purpose of identifying and characterizing materials". Antipov contributed extensively to improve, extend and promote the database and served as ICDD Ambassador to the Eastern European Community.

The ICDD also named two ACA members as new Fellows. Graciela Diaz de Delgado is a chemistry professor from the University of the Andes in Merida, Venezuela and has chaired the Grant-in-Aid Committee in 2012-2014; she applies diffraction methods to study organic molecules, such as carboxylic acids, metal carboxylates, natural products and synthetic intermediates of drugs. Robert Papoular is senior physicist at the Saclay Institute for Matter and Radiation, operated by the French Atomic Energy Commission, and has chaired the X-ray Diffraction Methods Subcommittee 2012-2014. His main research interests involve solving crystal structures from powder diffraction data.

ACA History Website Adds "ACA Beginnings": ACA Historian Virginia Pett and Webmaster Patti Potter have inaugurated a new section to the ACA History website. "ACA Beginnings" will contain articles and photographs documenting the history of the organization and the people who have made it a vital forum for scientists interested in structure and the significance of structure for understanding mechanism and function. See ***www.amercrystalassn.org/history_beginnings***.

The first item in this new section is the text of a 1974 talk by Martin Buerger relating how the ACA was formed at mid-century. Buerger was the inventor of the precession camera and the author of many books describing fundamentals of crystallography and how to obtain undistorted photographs of the reciprocal lattice. He was president of both the American Society for X-ray and Electron Diffraction (ASXRED) and the Crystallographic Society of America (CSA), the two precursor organizations that united to form the ACA in 1950.

Do you have photos to contribute to this new section of the website? Send high-resolution scans (with names, place and year) to Virginia Pett (***pett@wooster.edu***). If you would like to write a paragraph or two about your recollections of significant moments in the history of our society, please send them. The stories could be humorous, too, since ACA members have always been fun and interesting people. And if you have suggestions for other items to include, send them also.

Virginia Pett

Editors note: Every time I click on the ACA History site I am excited to see how much has been added, and it just keeps getting better. The lion's share of the credit for this site goes to Virginia Pett who has become one of the ACA's most dedicated volunteers and is totally committed to seeing this site live up to her vision of what it should be. Virginia is the chair of the Ad-Hoc ACA History Committee, and she would welcome help from any member interested in helping curate materials that could be uploaded to the site. Ilia Guzei has already joined this Committee and is responsible for resurrecting and producing the video from the symposium featuring Nobel Laureates at the 1988 ACA meeting in Philadelphia. Unfortunately, volunteers, no matter how dedicated, are not enough to keep the site growing and improving – that costs money. So remember to support the History Site when you make your yearly contributions along with renewing your membership (which is due now). You can also make a donation using the 'Donate Now' button on the ACA home page. We hope that you will visit the History Site often and check out its exciting new offerings.

Judy Flippen-Anderson

Frank Allen FRSC 1944-2014 : It is with great regret we announce that Frank Allen died, November 10, 2014, aged 70. Frank joined the Chemical Crystallography Group at the University of Cambridge in 1970 and played a pivotal role in the establishment of the Cambridge Structural Database. He went on to become the Scientific Director and then the Executive Director of the Cambridge Crystallographic Data Centre. Following his retirement in 2008, Frank remained with the CCDC as an Emeritus Research Fellow, enabling him to continue to indulge his passion for structural chemistry. Frank's research involved collaboration with many scientists around the world, resulting in over 200 papers. He was also a wonderful teacher, supervising more than 20 doctoral students and introducing many more to structural chemistry through workshops over many years. His contributions to other influential organizations, his vigorous editorship of *Acta Crystallographica Section B*, the numerous conferences he organized and presentations he made meant Frank was known to and respected by crystallographers the world over. Frank has long been a leading figure in international crystallography, and was a wonderful colleague, becoming a friend to all those who worked with him. He will be sadly missed.

(This information was taken from the CCDC website (***ccdc.cam.ac.uk***). A full obituary will be published by the IUCr (R. Taylor, *Acta Cryst. (2014). B70*, 1035–1036)).

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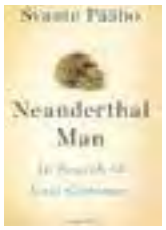
Neanderthal Man: In Search of Lost Genomes: Svante Pääbo, Basic Books, New York, 2014, 275 pp., ISBN 978-0-465-02083-6.



Neanderthal Man recounts Svante Pääbo's scientific and personal journeys studying the genetic makeup of ancient and extinct animals and humans, which culminated in 2010 with the publication of the full genomic sequence of a Neanderthal. Dr. Pääbo is the Director of Genetics at the Max Planck Institute for Evolutionary Anthropology in Leipzig, Germany. One of the remarkable outcomes of the work described in the book was the discovery that modern humans and Neanderthals must have interbred while they both inhabited our planet.

Neanderthal Man tells the story of the author's long and painstaking development of methods required in preparation for sequencing the ancient Neanderthal genome. It took years to develop techniques for extracting ancient DNA from tiny samples of bone or other tissues of animal or Neanderthal remains. The detection and prevention of contamination from modern DNA entails a significant part of Pääbo's body of work, and there are some technical descriptions in the book that may not appeal to non-molecular biologists. Technological and instrumental breakthroughs in DNA sequencing that arose out of the human genome projects were critical to the final result. Once the Neanderthal genome was sequenced, as described by Pääbo, a major analysis and statistical undertaking was required to interpret what the sequence actually told him about our relationship to Neanderthal man. Besides the interpretation that humans probably interbred with Neanderthals, there are implications about how and when human and other hominids originated and dispersed across the continents. That is a very fascinating aspect, especially when one thinks about the enormous time scales over which this all occurred compared to a single human lifetime.

In his book Dr. Pääbo describes the triumphs but also the heartbreaks of a hard driving and extremely ambitious career as a successful researcher. Pääbo attempts to share his decision-making processes, his quests for funding, his need for collaborations, his management style, and the importance of attending scientific conferences to hear about other people's work and how it stimulated creative thinking about his own work. Most of us do not make the magnitude of discovery that this book describes, but we all share the happiness of seeing a scientific result before anyone else in the world until it is published. Also, Dr. Pääbo is very matter-of-fact about aspects of his personal life.

Laurie Betts

The Science of Shakespeare: A New Look at the Playwright's Universe by Dan Falk, Thomas Dunne Books, New York, 384 pp, ISBN: 978-1250008770

Dan Falk's latest work is an exciting exploration of the relationship between one of literature's greatest playwrights and the scientific world of his time. Even though each chapter title is a quoted line from one of the Bard's plays, Falk begins them by establishing the historical context of relevant scientific inventions and discoveries, and works his way towards connecting Shakespeare to these developments. He then returns to these specific lines in the plays that allude to either a crucial moment in scientific history or its repercussions in shaping a newfound scientific social consciousness. What drives the book is Falk's tangible passion not only for the historical scientific context in which Shakespeare's plays were written, but for the plays themselves.

In Chapter 9, titled "'Does the world go round?': Shakespeare and Galileo," Falk explores the relationship between the work of the playwright and that of the astronomer. Interestingly, although Shakespeare's birthplace in Stratford-upon-Avon is now a bustling tourist attraction, Galileo's birthplace in Pisa is a private residence, marked by a small plaque and the Italian flag. The latter hardly seems fitting given Galileo's myriad contributions to the fields of astronomy, physics, mathematics, engineering and philosophy.

Galileo is perhaps best remembered for developing an improved telescope and for the astronomical advancements he was subsequently able to make in support of Copernicus' heliocentric theory. With his improved telescope, Galileo made a name for himself as the first person to identify three of Jupiter's moons. This discovery revolutionized the field of astronomy, because it had previously been believed under the Aristotelian theory of cosmology that all celestial bodies orbited the Earth.

How does this relate to Shakespeare, you may wonder? One of Shakespeare's later plays, Cymbeline, features Jupiter (the Roman god) descending from the heavens. Even though he is certainly apostrophized in many of Shakespeare's other works, this is the only moment in which he makes a physical appearance onstage, which is certainly noteworthy since Cymbeline was written after the publication of Galileo's discovery. Falk concedes that it cannot conclusively be proven that Shakespeare read Galileo's research but, given Galileo's notoriety as a challenger of Catholic doctrine, it seems unlikely that Shakespeare would not have heard of his work. Even if it is merely a coincidence, it is a fascinating one.

I found Falk's book to be a quick and stimulating read, fast-paced and delightfully written.

Jeanette S. Ferrara

Stuff Matters: Exploring the Marvelous Materials that Shape our Man-Made World by Mark Miodownik, Houghton Mifflin Harcourt Publishing, New York, 272 pp, ISBN: 978-0544236042.

Stuff Matters, is a delightful approach to the history and the science of modern materials by a materials scientist. His structure and approach for the book is unique, unlike anything I've encountered yet in popular science nonfiction.

Miodownik starts with a black-and-white photograph of himself sitting at a table on the roof of his flat. Each chapter begins with a reproduction of that photograph, but with an arrow pointing to a different object and a label describing the

object's composition. He offers a brief history of each material, laced with a personal anecdote or two, and often accompanied by a hand-drawn illustration of its molecular composition.

Perhaps the most entertaining chapter is that on chocolate. A self-professed "chocaholic," Miodownik's passion for the popular food is evident. Given the fame of Swiss chocolate, I had always thought that the solid bar form was invented in Switzerland, but it was, in fact, an English firm called Fry and Sons that first produced "eating chocolate." However, this chocolate, which had thirty percent sugar added, was too bitter. The Swiss were the first to use milk to combat this bitterness, essentially inventing what we now know as milk chocolate. They used the powdered milk recently introduced by Nestlé, a company that was attempting to give a localized commodity with virtually no shelf-life a transportable quality and a longer shelf-life.

It was quite fortunate for the Swiss that Nestlé was pioneering powdered milk at the same time that Fry's introduced their too-bitter eating chocolate. Adding regular non-powdered milk to the chocolate would have been disastrous. Chocolate powder is hydrophilic, and will absorb water; however, because fat and water do not dissolve in each other (fat is hydrophobic), the chocolate powder would eject its fat coating, making the resulting liquid lumpy and generally regarded as unappetizing. One can only imagine the differences in our modern world if powdered milk had never been developed.

Miodownik's passion for the subject (of) matter as a materials scientist is evident in his prose, and makes the book a quick and easy read. There is very little technical jargon that might impede the enjoyment of the book by someone not trained in materials science, or even the sciences in general. Miodownik is a man who loves what he does, and sees his work in the world around him. This book is a testament to his desire to inspire excitement for materials science in those around him as well.

Jeanette S. Ferrara

Proof: The Science of Booze: Adam Rogers, Houghton Mifflin Harcourt Publishing, New York, 2014, 272 pp., ISBN 978-0-547-89796-7.

This book is exactly as its subject matter would suggest: fun. Rogers' own passion for a good brew comes through quite vividly, and motivates the text quite nicely.

Rogers attempts to trace the 'life' of alcohol, from its 'conception' via fermentation to its 'haunting' of the human body via the infamous hangover. He also touches on the history of alcohol as a beverage fit for human consumption.

Rogers' claim that there is no substantial scientific explanation for the hangover (and likewise, there is no 'cure-all') intrigues me. As I have been required to read The Odyssey multiple times for academic purposes (as well as having read it once as a child for pleasure), I found it particularly entertaining – and perhaps a bit disconcerting – that a hangover severe enough to result in psychiatric dissociation is called Elpenor syndrome. Its namesake was one of Odysseus' sailor companions in Homer's epic, who got drunk and fell asleep on the roof of Circe's castle only to fall off and die when he woke.

I had always been told, and believed, that hangovers were caused by dehydration, and that the best prevention and cure was simple hydration. Rogers does not deny that drinking alcohol dehydrates you, but he claims that this dehydration does not solely account for the painful reality of the morning after.

Rogers also debunks the myth that vodka does not cause hangovers, as well as the myth that more drinking (i.e., Bloody Marys) is an effective cure. Studies have shown that people who drink enough vodka to raise their blood alcohol content (BAC) to between 0.1 and 0.15 % get hangovers, as do people who drink enough of almost any other kind of alcohol. Morning cocktails may temporarily delay the crippling effects of a hangover, but the hangover is inevitable.

Rogers quite entertainingly details the results of his own self-proclaimed hangover experiment, where he and two of his friends decided to get very drunk (BAC over 0.1) and test the effectiveness of various hangover 'cures'. However, their breathalyzer was broken, so in order to ensure that they would have a hangover, they overcompensated and drank quite a bit. Rogers believes that they went so over the limit of 0.1 that anything they tried the next morning proved ineffective. Although Rogers admits the 'experiment' was hardly scientific, it is a nice anecdote upon which to end his book. All in all, Rogers' Proof is a fun read, light enough for summer but also substantial enough to make it worthwhile.

Jeanette Ferrara

Structural Dynamics

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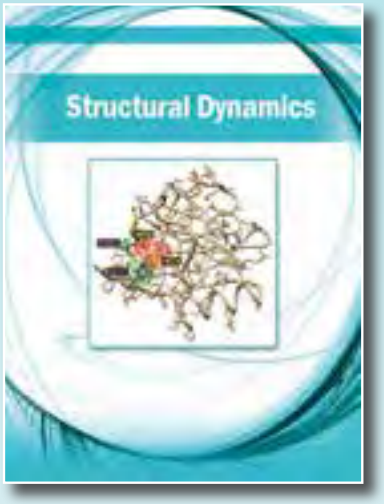

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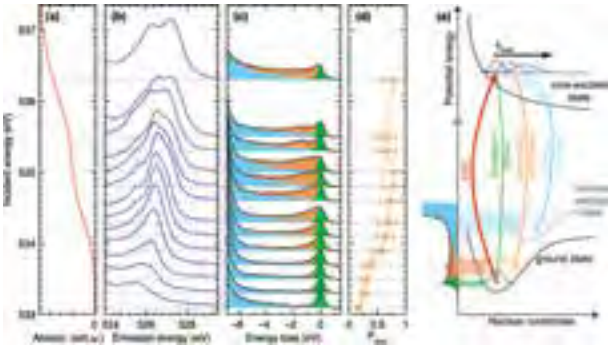
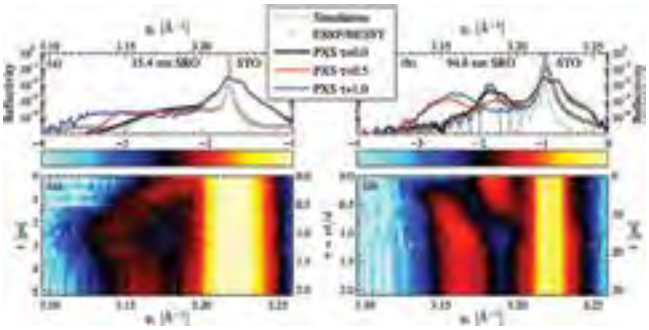
Liquids and Solutions: Dynamics of the OH group and the electronic structure of liquid alcohols: Simon Schreck, Annette Pietzsch, Kristjan Kunnus, Brian Kennedy, Wilson Quevedo, Piter S. Miedema, Philippe Wernet and Alexander Föhlisch - Struct. Dyn. 1, 054901 (2014); doi:10.1063/1.4897981



Abstract: In resonant inelastic soft x-ray scattering (RIXS) from molecular and liquid systems, the interplay of ground state structural and core-excited state dynamical contributions leads to complex spectral shapes that partially allow for ambiguous interpretations. In this work, we dissect these contributions in oxygen K-edge RIXS from liquid alcohols. We use the scattering into the electronic ground state as an accurate measure of nuclear dynamics in the intermediate core-excited state of the RIXS process. We determine the characteristic time in the core-excited state until nuclear dynamics give a measurable contribution to the RIXS spectral profiles to $\tau_{dyn} = 1.2 \pm 0.8$ fs. By detuning the excitation energy below the absorption resonance we reduce the effective scattering time below τ_{dyn}, and hence suppress these dynamical contributions to a minimum. From the corresponding RIXS spectra of liquid methanol, we retrieve the "dynamic-free"density of states and find that it is described solely by the electronic states of the free methanol molecule. From this and from the comparison of normal and deuterated methanol, we conclude that the split peak structure found in the lone-pair emission region at non-resonant excitation originates from dynamics in the O–H bond in the core-excited state. We find no evidence that this split peak feature is a signature of distinct ground state structural complexes in liquid methanol. However, we demonstrate how changes in the hydrogen bond coordination within the series of linear alcohols from methanol to hexanol affect the split peak structure in the liquid alcohols.

Materials: Ultrafast lattice response of photoexcited thin films studied by X-ray diffraction: Daniel Schick, Marc Herzog, André Bojahr, Wolfram Leitenberger, Andreas Hertwig, Roman Shayduk and Matias Bargheer - Struct. Dyn. 1, 064501 (2014); http://dx.doi.org/10.1063/1.4901228



Abstract: Using ultrafast X-ray diffraction, we study the coherent picosecond lattice dynamics of photoexcited thin films in the two limiting cases, where the photoinduced stress profile decays on a length scale larger and smaller than the film thickness. We solve a unifying analytical model of the strain propagation for acoustic impedance-matched opaque films on a semi-infinite transparent substrate, showing that the lattice dynamics essentially depend on two parameters: One for the spatial profile and one for the amplitude of the strain. We illustrate the results by comparison with high-quality ultrafast X-ray diffraction data of $SrRuO_3$ films on $SrTiO_3$ substrates

Articles coming soon

A split-beam probe-pump-probe scheme for femtosecond time resolved protein X-ray crystallography, by Jasper J. van Thor and Anders Madsen

Molecular alignment dependent electron interference in attosecond UV photoionization, by Kai-Jun Yuan and André D Bandrauk

More upcoming special topic issues:

Soft X-ray in Energy and Time (SXET) – This issue will have reports on the current status and new developments in soft x-ray absorption and emission spectroscopy as well as its resonant processes towards the Heisenberg limit (time versus energy limit). It will feature technical and methodological developments

for high energy resolution or ultrafast time-resolved approaches addressing new scientific questions for solid, liquids, gases and interfaces. Guest Editor: Emad Flear Aziz

Ultrafast Structural Dynamics – A collection of papers discussing the latest developments aimed at understanding real-time structural changes in materials science, chemistry, and biology using a variety of techniques including: Ultrafast electron diffraction, scattering and microscopy; Ultrafast x-ray diffraction, scattering and spectroscopy; and Ultrafast multidimensional vibrational and electronic spectroscopies. Guest Editor: Steve Johnson.

Why publish in Structural Dynamics?

Metrics: An average time from submission to publication of ~77 days is highly competitive with many of the journals produced by the industry leaders, and an average download per article in 2014 of more than 600 is a clear indication of both the high quality of the papers and the wide exposure they have had even in the inaugural year of the journal.

Structural Dynamics is a gold open access publication - all articles published in the journal will be freely available to all readers giving authors the broadest possible distribution of their research and statisying all open access mandates being handed down by various governmental funding agencies.

Publication Charges & Open Access Fees : Open access is also an "author pays" model. The submission charge was waived for first 50 papers published in *Structural Dynamics*. Starting in 2015 authors will be assessed an Article Processing Charge of ***USD2200,*** which covers the cost of publication and allows the author to retain copyright through a Creative Commons Attribution 3.0 Unported license.

ACA members can take advantage of a special discounted article processing charge of USD1500 when publishing in Structural Dynamics. The corresponding author must be the ACA member (***membership.amercrystalassn.org/***).

Waivers may be available for certain authors. The ability to pay does not influence whether or not a manuscript is accepted for publication. Please check the journal website for more details: ***scitation.aip.org/content/aca/journal/sdy/info/about***

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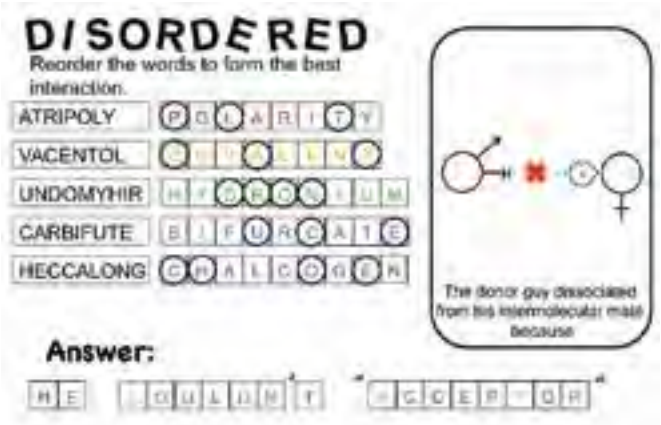
Puzzle Corner

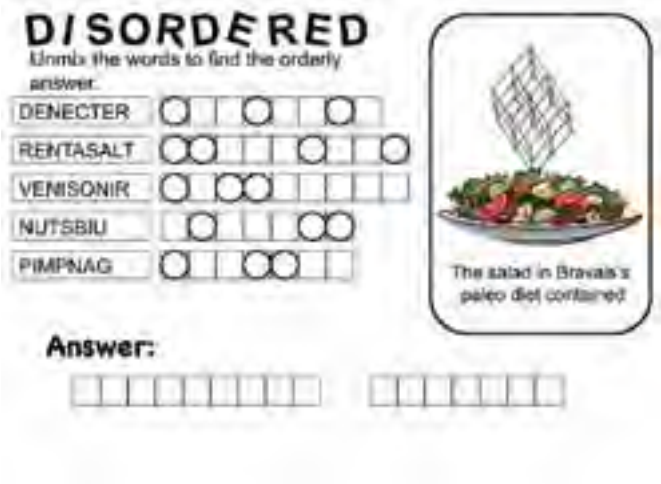
In this issue, we have the solution to the last ***DISORDERED*** puzzle, a new one, and the solution to the Fall issue's Crystal Connections Puzzle. We asked what the answers to these six clues have in common:

Number of US constitutional amendment ratified in 1868
"____ can be as bad as one" according to Three Dog Night
Most stable F isotope
The Ides of March
53Mod7
2001 Roger Maris movie

The answers are 14, 2, 19, 15, 4, and 61, which are, in order, the space group numbers for the six most populous space groups in the Cambridge Structural Database, $P2_1/c$, P-1, C2/c, $P2_12_12_1$, $P2_1$, Pbca. The answer was provided by Greg McCandless (Dept. of Chemistry, University of Texas at Dallas). Greg points out that, in this context, Three Dog Night's assertion that "One is the loneliest number" is incorrect. Space group P1 is the 10th most popular space group in the CSD (~0.9% of entries). The loneliest number is 99, space group P4mm, with only one entry.

Frank Fronczek





ACA Election Results

Council Officers

Vice President
Tom Terwilliger
Secretary
Diana Tomchick

Standing Committees

Communications
Katrina Forest

Continuing Education
Andy Howard

Data and Standards
Stephen Burley

SIGS
Biological Macromolecules
Chair-elect: Barry Finzel
General Interest
Chair-elect: Graciela Diaz de Delgado
Secretary: Jason Mercer
Industrial
Chair-elect: Eugene Cheung
Light Sources
Chair-elect: Allen Orville
Materials Science
Chair-elect: James Neilson
Neutron Scattering
Chair-elect: William Ratcliff
Powder Diffraction
Chair-elect: Tiffany Kinnibrugh
Service Crystallography
Chair-elect: Vic Young
Small Angle Scattering
Chair-elect: Alex Hexemer
SAS Amendment - Passed
Small Molecules
Chair-elect: Stacey Smith
Young Scientist
Chair-elect: Martin Donakowski
Secretary: Kimberly Stanek

Canadian Division
Secretary: Brian Patrick

Vice-President -Tom Terwilliger

Laboratory Fellow, Los Alamos National Laboratory, Los Alamos, NM

Statement: The ACA plays a crucial role in the promotion and development of the field of crystallography along with its sister organizations around the world and with the IUCr. As one of the leaders of the ACA I will endeavor to maintain the current vitality of the ACA and also to help the ACA develop and promote a vision for the future of crystallography. Our annual meetings are major events that provide a forum for a wide range of science benefitting from crystallography. The meetings also have a strong emphasis on methods and the nuts and bolts of structure determination and analysis that I feel is essential to the strength of the field. Continuing these strong traditions will be a top priority of mine. The standing committees and SIGs play an important role in communicating the ACA vision, assisting members with continuing education, setting standards for data and reporting, and helping young scientists, all while helping maintain continuity within the organization. Continuing the roles of these standing committees and interest groups and helping to invigorate them will be another important priority. It will also be important to continue the development of a vision of where crystallography should go. There are many new developments both in crystallography and in other structural fields that affect the work and future of crystallographers. In macromolecular crystallography the change from crystallography as a profession to structural biology as a profession has changed the training of students and the research focus of nearly all in the field. It will be important to ensure that there is sufficient training in crystallography available, and that there are sufficient researchers who continue to develop the field, as the methods that exist today are far from optimal. Also in macromolecular crystallography it will be important to recognize the developments in all technologies for structural biology and to bring together complementary methods.We have had a long and productive history and we can look forward to a long and productive future as well. I am looking forward to helping the ACA continue to lead in developing this future.

Secretary - Diana Tomchick

Professor, Departments of Biophysics & Biochemistry, University of Texas Southwestern Medical Center, Dallas, TX

Statement: I have belonged to the ACA for almost 30 years, and I gladly support its activities and am proud of its role in the crystallographic community. I welcome the opportunity to actively assist the ACA as Secretary, and as a member of Council. My crystallographic experience began with small molecules as an inorganic chemist, and I was a recipient of a student travel award to the 14th IUCr Congress in 1987 in Australia, as well as a recipient of a Pauling Prize in 1990. My training eventually led me to my current position as Director of a campus-wide core facility that provides expertise in macromolecular structure. This position requires significant organizational skills as well as scientific expertise, and for many campus research groups I am the professional "face" of crystallography. Perhaps my most important role is as an educator, as I provide expertise in current crystallographic methods to members of the campus community through the classroom and individual consultation on structural projects. The ACA provides a critical resource for crystallographers to network and keep abreast of scientific and technical advancements, and to educate the next generation of scientists as well as the general public. As Secretary I will work diligently to support the efforts of the organization as well as the other officers and various committee chairs in furthering these goals.

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Communications Committee - Katrina T. Forest

Professor Bacteriology Depart, University of Wisconsin-Madison

Statement: Student membership in the ACA was fundamental to my training as a crystallographer and to my sense of belonging in this community. During my academic career, I have been the lone structural biologist in a microbiology department; connecting with colleagues at other universities and staying current on crystallographic methodologies have been important benefits of ACA membership. I look at serving on the Communications Committee as a way of giving something back to the ACA.

While we may live for those fleeting moments in which we realize we have discovered something about the natural world that no one else is yet aware of, our findings are only fully realized when they are explained to others. Our responsibilities as scientists include communicating our results with colleagues, funding agencies, students, and the general public. I have enjoyed opportunities during my career to discuss our research with local newspapers and television stations, to present it to interested citizens at public outreach events, and to share our science during campus workshops for middle school students. My lab has also expanded our definition of science communication by hosting Artists in Residence whose own artistic output, influenced by the experimental goings on in the lab, serves as a novel way for us to communicate the beauty in science to the general public.

As a member of the Communications Committee I will work with my colleagues to maximize exposure of our annual ACA meetings, work with the ACA Historian to coordinate videotaping of and special volumes dedicated to plenary lectures, solicit contributions for *RefleXions*, serve as an ambassador for the value of crystallography to funding agencies, and seek additional opportunities to communicate the importance of crystallography to the general public.

Data, Standards & Computing - Stephen K. Burley

Distinguished Professor, Rutgers University; Director, RCSB Protein Data Bank; Director, Center for Integrative Proteomics Research, Rutgers University; Member, Rutgers Cancer Insttute of NJ; Adjunct Professor, UC San Diego

Statement: At Rutgers University (***proteomics.rutgers.edu***) I am currently leading efforts to create new outreach and instructional vehicles describing the best practices for using data resources and tools in structural biology to broader audiences in biology, life sciences and physical sciences. I see great potential for the Data Standards and Computing Committee (DSCC) and the ACA working to identify exemplar curricula and materials to support such instructional programs for both scientific and general audiences.

For many years, I have been actively involved in the PDB efforts developing community-based standards for deposition, publication, and archiving of macromolecular structural models and underlying experimental data. I believe the DSCC and ACA can play an important role in promoting and strengthening the progress from these efforts, and in meeting the continuing challenges of developing standards for new diffraction, hybrid experimental, and integrative methodologies.

The crystallographic community benefits from the availability of structure data hosted in a variety of data repositories. An important role of the DSCC and ACA is to increase community awareness of the sustainability challenges faced by these repositories, and to promote successful models of sustainability that ensure their continued availability and high levels of service. There are also opportunities to extend successful models of sustainability to other communities developing repositories for experimental data complementary to crystallographic data.

Continuing Education - Andy Howard

Associate Professor, Biological & Chemical Sciences Dept., College of Science, Illinois Institute of Technology, Chicago, IL

Statement: Small-molecule and macromolecular crystallography have become increasingly de-professionalized over the last three decades in the sense that non-specialists can participate in and use crystallographic structure determinations. This is a good thing in that it increases the size of the community that can capitalize on the utility of crystallographic techniques, but it comes at a price: many of the practitioners of these techniques have only a meager understanding of the underlying physics and chemistry. The result is that if our hardware and software do not yield answers on the first try, these users have no way of diagnosing problems and working around them, and they frequently have an inadequate understanding of what parts of our analyses are reliable and what parts are not. The task of crystallographic educators should be to provide this community of users with enough knowledge and wisdom about the fundamentals of the subject, and the ways that the field is advancing, that these non-specialist users can solve their own problems and have a deeper appreciation for its principles. Educators should also help practitioners to recognize the strengths and weaknesses of crystallographic analyses, and in particular to know what the confidence limits are for the conclusions that they derive from their data. The ACA Continuing Education Committee should involve itself in in-reach to specialists so that they can keep up with the latest theoretical and experimental approaches. But its charge should, increasingly, involve outreach to the wider scientific community so that those non-specialists will know how to overcome roadblocks and understand the advantages and limits of crystallographic methods. I am looking forward to working with other members of the Committee to explore ways to accomplish both these in-reach and outreach goals.

Cover Design by Connie Rajnak

Cora Lind-Kovacs showed this image of the world's largest quartz cluster at her talk in the *Transactions Symposium:* **100 Years of Crystallography** the first day of the Albuquerque ACA meeting. She talked about *Fun with Crystals, Light and Symmetry--IYCr Outreach Activities*, describing how she got to visit the Crystal Museum Riedenburg in the Altmuehl Valley in Germany in 2007 while visiting a friend. This museum was established to provide a home to the magnificent quartz cluster. The plaque displayed at the site describes the discovery and extraction of the crystal group.

Translated into English the plaque says: 25 meters deep in the crust, a gigantic cleft opened up in front of the eyes of the surprised miners who were working inside an approximately 3 meter thick quartz band, more than 25 meters below the surface in dense sandstone rock. It contained the largest and most beautiful clear quartz ever found in this area.

As seen in the reconstruction sketch, the cleft was almost vertical, with an inclination of 80º. This required the design of sophisticated scaffolding and machinery to prevent breakage of this magnificent quartz formation. Thankfully, the cleft was filled with fine clay, which protected the sensitive crystals from damage during extrication.

At right: the reconstruction sketch, also shown on the plaque at the site.

Cora Lind-Kovacs

The following notes were written by the 2014 recipients of travel grants and/or the young researchers selected for the SIG Etter Award Lectures. They were asked to comment on their personal experiences at the meeting: the venue, the events for young scientists, the overall program and their own presentations, and whether they are (and plan to continue to be) ACA members. Many would not have been able to come to the meeting without the financial support provided by ACA members that generously contribute to the travel award funds.

Yusong Guo – BioMac Etter Student Lecturer: It was such a great experience for me to attend the ACA meeting in Albuquerque, especially as a Student Lecturer Award recipient. During the talk, I received many interesting questions that will help us further explore our research. The overall atmosphere of the meeting was very warm and kind. Another fantastic thing was that I won the hot air balloon ride raffle sponsored by Rayonix -- Another once-in-a-lifetime experience!

If I could suggest one change to improve the meeting, perhaps there could be more panel discussions between senior and younger scientists. The career development panel went very well, but the only problem was that there seemed to be not enough time. I'm currently an ACA student member, and I'll definitely continue my membership.

Jordan Cox – Small Molecule Etter Award Lecturer: By far my favorite thing about this year's ACA meeting was the *Career Odyssey Panel* on Sunday night. Most people have heard career advice from others before, and generally I find it vague, sometimes frustratingly so. However, at this session we heard from professionals in crystallography-related fields who had much more to say than the inspirational, if not particularly helpful "follow your passion." Not only was "getting a job" discussed, but we were given many interesting and instructive insights into how to succeed in that job. What skills, both scientific and managerial, are important and how we could cultivate those skills. As a young scientist, these were messages that I enjoyed hearing. It was a good reminder that, while my goal is to get a job, that isn't the endgame. Once I've worked so hard to get a job I want, I'll also want to excel at that job and prove to those I work for that they have found the right person for the job.

The range of careers on the panel was just as exciting. Hearing from people with such a wide array of backgrounds, career tracks, and current jobs, it was very interesting to see what the possibilities are from where I currently am in my career. What future career I think I'll want to have often depends on the day of the week. Some days it's a professorship and other days it's as a national lab researcher. Of particular interest to me were the contributions from Margaret Gordon and Joseph Orgel, as well as the similarities and differences in their respective careers. While the panel may have simply intensified my indecision, I certainly left with a greater understanding of what life in a scientific career can be like, and how I can make the most of my career now and into the future.

This meeting was the first conference I had ever attended, so with nothing to compare it with, it was difficult to think of anything I would like to see changed. I am currently a member of both the American Chemical Society and the ACA and I plan to maintain my membership in the ACA in the future.

Jacob Trotta – Industrial Etter Lecture Award: I recently graduated from Villanova University with a BS in chemistry. I will be attending Cornell University in the fall to pursue a PhD also in chemistry. I am a member of both the ACS and the ACA, and will likely continue my membership in the ACA if the graduate research I pursue involves crystallography. As an undergraduate, the large majority of my research experience was completed while interning at Alkermes, Inc., where I started working in the summer of 2011. I was invited to the ACA meeting by Peter Wood to give a lecture at a session co-sponsored by the Industrial and Young Scientist SIGs.

This was my first time attending any kind of professional meeting, and I had a great experience. One thing that really struck with me was David Sargent's talk on *Automated Crystal Harvesting with the RodBot*. The presentation demonstrated the amazing ability of an *in situ* robot to collect single crystals from crystallization systems through human control or software automation. This is done in either case without damage to the single crystals due to the unique physics of the RodBot's propulsion, making it viable to automate single crystal harvesting in the crystal screening process. I also enjoyed the exhibit show, and in particular relished the opportunity to talk with members of the Cambridge Crystallographic Data Centre (CCDC). The opportunity the Cambridge Structural Database (CSD) presents for insight into otherwise inaccessible crystallographic information constantly amazes me. Crystallography aside, I am also happy to say that I took an excursion to the Sandia Peak Ski & Tramway on the outskirts of Albuquerque, enjoying a spectacular view of the New Mexico landscape with a coworker and friend from Alkermes, as well as newly made friends from the meeting.

Though overall I thought the ACA meeting was great, I did find that the crystallography of small organic molecules was underrepresented, especially in oral presentations. I would hope that future meetings strive to find a better balance of biomolecule and small molecule crystallography.

Finally, I am above all indebted to Alkermes for both their financial support in attending the meeting and their constant, unwavering encouragement.

Rama Sashank Madhurapantula – Fiber Diffraction Etter Lecture Award: So there I was reading the PhD comics page when I got an email from my advisor that I should submit an abstract for the ACA meeting at Albuquerque. I always wanted to see that city, not at all because of all the frenzy created by "Breaking Bad" (oh wait!!). So I wrote and submitted my abstract for the session titled *Flesh & Blood: Intact and in-situ Connective Tissue Diffraction Studies of Animals Plants and Insect Bodies*. I was excited to be selected for a 15 minute talk on my work as a doctoral student on the effects of non-enzymatic glycosylation, or as we call it *glycation*, on the structure of type I collagen in rat tail tendons and the biochemical implications of these changes in terms of vulnerability to matrix metalloproteinases. This was my second ACA meeting, and I was nominated and elected the secretary of the Fiber Diffraction SIG for 2013-14. So this was


Krystle McLaughlin


Margit Fabian


Patricia Langan


Kimberly Maize


Donghyuk Shin


Alisa Glukhova


Mohammed Tata


Brian Dolinar


Rama Madhurapantula


Kimberly Lincoln


Patrice Kenfack Tsobnang


Jaime Jensen

the first time I was attending the conference as a SIG officer.

Things got even better when I was informed by the chair of the Fiber Diffraction SIG, Olga Antipova, and chair-elect, Joseph Orgel, that my presentation had been chosen for the Margaret C. Etter Student lecturer award for the SIG. This is a huge honor for a student who has so far spent only 3 years trying to understand the field and knows what you would call a tiny droplet in the ocean that is fiber diffraction, and the financial support that came with the honor was much appreciated. My presentation went great and I was pleased to be able to answer the questions from the audience from my current understanding of the field.

I attended the YSSIG mixer for the first time this year and I met students and post docs from labs from all over the world, which was great fun. I had a chance to walk around a bit of the city of Albuquerque and hang out with some new friends that I made during my visit. I also attended the *Career Odyssey Panel*, which was very informative for students who want to get into research and academia.

All in all, it was an interesting and exciting visit to the conference this year. I was nominated to stand for re-election as the secretary of the Fiber Diffraction SIG. I am thankful to the SIG for having selected me for the talk, the award and the nomination. I am deeply honored to be in the company of some great scientists at a stage of my career where contacts and connections mean a lot in terms of rounding me as a better scientist and extending my knowledge of the field.

Patricia Langan – Neutron Scattering Etter Lecture Award: The most helpful thing for me was having a large neutron crystallography session in which to participate. Because of the number of talks and the ease of attending them all in one or two sessions, rather than having to jump around from room to room, it was very easy for me to access the people who could speak to issues that I may have also experienced in my experiments. I would like to see more sessions on neutron crystallography at future meetings. The ACA is currently the only professional society of which I am a member and I plan on continuing that association.

Vicky Doan-Nguyen – Powder Diffraction Ettter Lecture Award: I appreciated the opportunity to meet other crystallographers in general but also specifically in the fields of total x-ray scattering and GISAXS. I also enjoyed meeting other students and the opportunity to present my work as a lecture. I thoroughly enjoyed the riveting scientific discussions with experts in my area of GISAXS.

I would suggest providing access to coffee on-site. This is a minor issue, but travel time to an off-site Starbucks is huge if it's not during a designated coffee or lunch break.

I am currently a member of the ACA, the American Physical Society, and the Materials Research Society and plan to continue as an ACA member.

Patrice Kenfack Tsobnang: I am PhD student in the University of Yaoundé I (Cameroon) and Université de Lorraine interested in small molecule crystallography and powder diffraction. As with many Cameroonian and African people working in the field of crystallography, one of my aims is to promote this science in Africa in general and particularly in my country.

This was my first international conference with such a large number of participants so I was very interested to learn that ACA members are organized into scientific interest groups (SIGs) that allow them to get to know one other and interact easily. I was particularly pleased to find the Young Scientist SIG that encourages students and early career scientists to participate in the activities of the ACA. They have used the SIG to build a strong network with professors and experimental researchers, which is both beneficial for the young scientists and important for the Association. I was particularly impressed to see undergraduate students participating in this SIG and attending the meeting.

I was fascinated by the plenary lectures and especially the presentation on the investigations of Dorothy Hodgkin. I was very impressed with all the talks and posters that I attended. I learned much about the modern methods used to teach crystallography. I enjoyed the session on *Engaging Undergraduate students with X-Ray crystallography* and the *Transactions Symposium: 100 Years of Crystallography*. I also learned much about the activities that happened around the world during IYCr. I was happy to see the wide breath of crystallography and to appreciate how much this science is helpful for diverse research activities and technology.

The discussion following my talk in the session *Producing and Transporting Energy: Thermoelectrics, Superconductors, Photovoltaics, and Magnets* was very helpful as were the discussions in *General Interest I and II*, *Innovative Ways of Finding Atoms from Powder Diffraction Data*, *Cool Structures*, *Advances in X-ray and Neutron Scattering Techniques under Non-ambient Conditions*, and *Structural Studies of Radioelements*. I learned a lot and found answers to some questions that I had during my own experiments. These talks have also inspired me to continue our research project.

I want to thank the organizing committee for trying to organize linked sessions to avoid overlap, although I did have to choose between *General Interest II* and *Advances in X-ray and Neutron Scattering Techniques under Non-ambient Conditions*. Maybe increasing the number of days of the conference would make it easier to avoid this overlap as well as more time for poster sessions.

Kimberly Lincoln: I had a great time at the meeting, met some really cool people, and learned a lot of new stuff pertaining to x-ray crystallography.

I really liked the friendly atmosphere that I felt from others at the meeting and that there was a diverse group of scientists coming from a broad range of fields such as physics, chemistry, biology, engineering, etc. It was really cool to learn how diverse x-ray crystallography is.

The one thing I would change about the meeting is how the talks were organized with respect to the program. X-ray crystallography is an extremely versatile tool that is used in so many fields of science, so the program could have been better tailored with respect to a particular field of interest. For example, I saw talks pertaining to organic catalysis, inorganic catalysis, protein crystallography, powder diffraction, and small molecules. Being an inorganic chemist who has a strong interest in metal-


Christopher Durr


Jie Qiu


Paulina Dziubanska


Yusong Guo and Gerald Audette


Yi Tian-Teng


Kevin Knox, Pavel Juhas, Vicky Doan-Nguyen, Simon Billinge

Jesse Hopkins

based redox chemistry it was difficult for me to see all the talks that I wanted to because a lot of them overlapped. Thus, I would advise that the talks be listed under the respective fields, such as organic, inorganic, protein crystallography, small molecules, and redox chemistry. In this way a person like me who is interested in seeing talks related to metal-based redox processes could find them all in one session. I hope that helps. I have a few other ideas as well, and if you are interested in hearing them then please contact me further.

I am a member of the American Chemical Society as well, and do plan on keeping my ACA membership. I would like to be more involved with the conference in general, and have volunteered to participate in organizing next year's conference. Overall I had a great time at the meeting, enjoyed meeting people from all over the world and established some contacts that will be useful for my future career as a scientist, and I am even in the process of setting up a collaboration with someone I met there.

Krystle J. McLaughlin: The 2014 ACA meeting was a wonderful experience for me as I was honored to not only present my research in a poster session, but to help organize the student-centered lunch reception. As always, I enjoyed the breadth of crystallography topics and the ability to talk with many researchers. One of my favorite talks was the Wood Writing Award presentation and lecture by Daniel Rabinovich, as he made description of the intersection of crystallography and stamps very engaging. I also really enjoyed the YSSIG mixer as it was fun and a great time to meet other young scientists as well as some established ones who were in attendance. I joined the ACA in 2007 as a graduate student and plan to continue my membership as I transition into my first faculty job. I think that if ACA could offer more professional development resources at meetings it would be beneficial to all early career members including students and postdocs. I look forward to attending more ACA meetings in the future, and I thank the ACA for supporting my attendance both as a student and postdoc.

Peter Randolph: This was my first ACA Meeting. Overall it was an amazing experience and, I hope, the first of many. The highpoint for me was presenting my research as an oral presentation in the *Exciting Structures* session. Not only was I able to showcase my current research, but I also received advice from a variety of sources, which I am now integrating into my research.

In addition to presenting my research, there were a number of other highlights. I attended a meeting of the Young Scientists SIG, another first. During this meeting, I discovered a variety of ways to get more involved in the ACA and volunteered to co-chair a session next year. There were many enriching talks this year, including the *Blackboard Sessions* (which were extremely useful for me), *Supermolecular Assemblies*, and the *Chemistry and Biology with Novel Scattering Techniques*. The poster sessions offered a great forum to see and discuss others projects. Finally, Alburquerque was a lovely city that I had never had the opportunity to visit before and am now looking forward to visiting again.

Jaime Jensen: Not only was this my first ACA meeting, it was also my first international conference and I was very excited to have my abstract selected for a talk during the *Etter Early Career Award Symposium*. I presented my recent structural work toward elucidation of the signaling activation mechanism through the receptor for advanced glycation endproducts (RAGE). The session attendees were very welcoming and encouraging, and a couple of individuals provided valuable feedback for my future research directions.

The program was highly diverse, and I was able to attend many lectures both within and outside of my areas of research and interest. I especially enjoyed the *100 Years of Crystallography* series and the *Career Odyssey Panel*, which was a great resource for this crystallographer-in-training. The relaxed atmosphere of the poster sessions was great; I certainly benefitted from the one-on-one Q&A with presenters whose work caught my attention. The exhibit show was also very useful; I was able to troubleshoot some equipment problems with the experts and gather practical information on crystallization screens I had not previously used. One of the greatest aspects of the ACA meeting was the multiple opportunities to network with established scientists and meet with my peers in the Young Scientists SIG. I connected with many delightful individuals with whom I hope to remain in contact. I was continually impressed with the support extended to trainees within the field. Overall, my experience at the ACA meeting was superb. I plan to continue my membership with the ACA, and I sincerely hope that my research in the next year is fruitful so that I can attend ACA 2015 in Philadelphia!

Yi Tian-Ting: To celebrate the 100th year of x-ray crystallography, the ACA conference at Albuquerque provided the opportunity to consider, discuss and review the status of education and research in the broadly defined discipline of crystallography. I found all the sessions, ranging from instrumentation and methods development, to application and structural studies, very useful and informative. I benefited greatly from all the interactive seminars and mixing with other meeting attendees. I was also inspired by the plenary talks regarding women in crystallography by Martha Teeter and Jenny Glusker with special focus on Dorothy Hodgkin. Dorothy Hodgkin was a great example of good character and great science. I wish I were born 20 years earlier! Another presentation worth mentioning is the *The World of Crystallography on Postage Stamps* by Daniel Rabinovich. What a refreshing talk where *Einstein meets Magaritte*. Overall, it was a wonderful experience for me as a first time attendee. I would like to thank all of the friendly members in the YSIG, who made my integration into the ACA community easy. Last but not least, thanks to all the fellow researchers I met for all the great ideas and laughter. I look forward to seeing you all again next year in Philadelphia.

Chris Durr: I very much enjoyed my first ACA meeting. My favorite part of the meeting was having the opportunity to meet leaders in the field of crystallography. What amazed me was how helpful and welcoming everyone was to younger scientists. The connections I made in Albquerque led to my attending the ACA summer school which taught me a great deal more about crystallography.,

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If I could suggest one change it would be to include more small molecule crystallography. In particular I'd be interested in how small molecule crystallography was used to solve chemical problems or explain a chemical process.

I am currently a member of the ACS and the ACA. I intend to remain a member of both.

Jie Qiu: The best thing for me is the existence of the Young Scientists SIG, which gave graduate students and postdocs the opportunity to be involved in the organization of the conference.

I attended the session on *Structural Studies of Radioelements* and found that only a few people working in this area attended the conference. Is it possible to invite or encourage more people in this area to attend so that we could have more chances to communicate with one another. I am a member of the American Chemical Society and ACA and plan to continue both.

Margit Fabian: I was impressed by the variety of fields and countries represented by the meeting attendees. I liked the way the sessions were organized and thought the networking opportunities were outstanding. I found Jenny Glusker's talk on women in crystallography with a focus on Doroty Hodgkin to be quite impressive. The plenary lectures provided me with new information on specialized fields using crystallography.

It was a great experience to take part in the SIG Meetings: Materials, the Neutron & Powder joint meeting, Fiber Diffraction and Young Scientists. From these communities I learned how an effective scientific community can function and how I can become part of the overall scientific network

It was my second conference in this area and I learned much in field of biomaterials, nanoparticles, magnetic materials and new methods for structure analysis. For me it was very useful to listen to presentations about instrument development. I enjoyed all the presentations and particularly the following: *Scattering and Energy Storage Materials*, *Discovering Emergent Phenomena and Magnetism With Neutron and X-Ray Powder Diffraction* and *Earth/Environmental Sciences*.

The magical city of Albuquerque was a worthy choice for a conference like ACA 2014. I'm member of ACA, and it would be a great pleasure to continue my membership.

Paulina Dziubanska: I am really delighted that I had an opportunity to meet some of the world's most famous crystallographers as well as many talented young scientists from all over the world. I would suggest making the space around each poster a little bit bigger. Unfortunately many people gave up attending the poster session due to the crowds in this area. I am a student member of ACA and I am currently considering renewing my membership.

White House Report Recommends Nanotechnology Grand Challenges

A new report issued by the President's Council of Advisors on Science and Technology (PCAST) urges coordinated federal action to support the development of commercial products based on discoveries from nanotechnology research. Among the report's recommendations is the establishment of a series of Grand Challenges to focus future nanotechnology R&D.

The *Report to the President and Congress on the Fifth Assessment of the National Nanotechnology Initiative* was approved by PCAST and was released to the public in October.

Early in the report it states: *The primary conclusion of our 2014 PCAST review is that the United States will only be able to claim the rewards that come from investing in nanotechnology research and sustaining an overarching Federal initiative if the Federal interagency process, the Office of Science and Technology Policy (OSTP), and the agencies themselves transition their nanotechnology programmatic efforts beyond supporting and reporting on basic and applied research and toward building program, coordination, and leadership frameworks for translating the technologies into commercial products.*

The report focused on how future nanotechnology R&D funding should be spent. Twelve overall recommendations were made. The three most important recommendations were:

The primary active program-management structure should be driven by the Federal and OSTP commitment to the concept of nanotechnology Grand Challenges.

We reiterate the need for an ongoing, separate standing committee of cross-sector nanotechnology experts that advises, but does not evaluate, the nanotechnology activities of the U.S. Government. We also iterate the need for a functional interagency process via the National Science and Technology Council, the Committee on Technology, and the Nanoscale Science, Engineering, and Technology (NSET) Subcommittee that is able to make cross-agency funding priorities when needed to address nanotechnology Grand Challenges.

We reiterate the need to assess Federal nanotechnology research and commercialization funding through a more formal system of metrics.

The report defines a Grand Challenge: *A large, outward-facing effort with a specific, measurable goal. A Grand Challenge has a well-defined technical goal with a story-telling case that inspires different sectors to invest in achieving the goal. Most Grand Challenges address an issue of significant societal impact.* The report continues: *A nanotechnology Grand Challenge should be audacious but achievable and stimulate the network of activities that will drive scientific ideas to commercial nanotechnology and catalyze new discovery for technologies of the future.* Examples of Grand Challenges include: *Nano-enabled desalination of seawater, nano-enabled solid-state refrigeration*, *nano 3D printing for manufacturing*, and *a nanoscale therapeutic for a major cancer type.*

Extracted from AIP FYI #154 by Richard M. Jones (November 7, 2014)

Editors note: In earlier issues of *RefleXions* we tracked the progress of creationist activities in a number of states and countries. After the verdict in the Kitzmiller v. Dover Area School District was handed down in 2005 one might have expected the issue to be settled but such is not the case. Indeed, the owner of Hobby Lobby is in the process of building an eight-story Bible museum in downtown Washington, DC. The National Center for Science Education (NCSE) continues to concentrate its activities on keeping both evolution and climate science taught as part of public school science curricula. The following news items have been taken from the NCSE website (***ncse.com***).

Evolution in a new PRRI survey: Attitudes toward evolution and the compatibility of science and religion were addressed in a new survey from the Public Religion Research Institute (which, as NCSE previously reported, was mainly focused on climate change). Presented with "Evolution is the best explanation for the origins of human life on earth," 24% of respondents completely agreed, 29% mostly agreed, 14% mostly disagreed, and 27% completely disagreed, with 5% of respondents saying that they didn't know or refusing to answer. (November 24, 2014)

Corrected textbooks adopted in Texas: The Texas state board of education voted to adopt a slate of social studies textbooks for use in the state on November 21, 2014. Among the books approved were several textbooks that, after criticism from NCSE and its allies in the scientific, educational, and civil liberties communities, were revised by their publishers (including Pearson and McGraw-Hill) to eliminate misrepresentations of climate science. (November 21, 2014)

Creationist legislation in Brazil: A bill introduced in the Brazilian Chamber of Deputies would, if enacted, require creationism to be taught in the country's public and private schools. (November 21, 2014)

Opposition to new science standards in South Dakota? : A South Dakota state senator dislikes a proposed new set of state science standards, according to the *Sioux Falls Argus Leader* (November 18, 2014). At a November 17, 2014, public hearing — the second of four — on the standards, Phil Jensen (R-District 33) expressed concern about the treatment of evolution and climate change. (November 18, 2014)

Update from Scotland: The Public Petitions Committee of the Scottish Parliament heard testimony supporting the proposed ban on teaching creationism as scientifically credible in Scotland's public schools on November 11, 2014, according to the Press Association (November 11, 2014). The committee agreed to write to the Scottish government, the Educational Institute of Scotland, the Scottish Secondary Teachers' Association and the Association of Headteachers and Deputies in Scotland to receive their views on the matter.

Ohio's antiscience bill progresses: Ohio's House Bill 597 — which if enacted would require students in the state's public schools to "review, in an objective manner, the scientific strengths and weaknesses of existing scientific theories in the [state science] standards" — was passed on a 7-2 vote by the House Rules and Reference committee according to the *Cleveland Plain Dealer* (November 5, 2014).

Over at last for Freshwater: On October 6, 2014, the Supreme Court of the United States declined, without comment, to hear John Freshwater's appeal of the Ohio Supreme Court's decision to uphold his termination as a middle school teacher. The decision brings the long and complicated controversy over Freshwater's inappropriate religious behavior in the classroom — including teaching creationism and misrepresenting evolution as scientifically controversial — to a final conclusion.

Santer in "97 Hours of Consensus" : Ben Santer, a member of NCSE's board of directors, is among the ninety-seven climate scientists featured in Skeptical Science's *97 Hours of Consensus campaign* (***skepticalscience.com/nsh/#***). Launched on September 7, 2014, the campaign features hourly statements on climate change from a group of 97 leading climate scientists along with their playful caricatures.

ASIH calls for repeal of Tennessee's antiscience law: At its 2014 meeting held in Chattanooga, Tennessee, the American Society of Ichthyologists and Herpetologists adopted a resolution encouraging the state of Tennessee to repeal the antiscience law — nicknamed the "monkey bill" — adopted there in 2012. (August 22, 2014)

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SAS with Membranes and Membrane Proteins – Chairs: Fred Heberle & Shuo Qian
Structural Modeling for SAS – Chairs: Tomas Weiss & Xiaolin Cheng
Evolving Techniques for SAS – Chairs: Cheng Wang & Michal Sabat
SAS, BioMac, YSSIG
Application of SANS/SAXS to Structural Biology – Chairs: Kushol Gupta & Alvin Acerbo
YSSIG
Career Odyssey – Chair: Smita Kakar
Professional Development: Communicating your Science – Chairs: Jarrod French & Andy Torelli
Etter Early Career Symposium – Chairs: George Lountos & Andrey Yakovenko
YSSIG, BioMac
Solutions to Crystallization: Protein Crystallization for Crystal Growth – Chairs: J. Luft & J. Newman
Hot Structures I - Intracellular Protein Regulons – Chairs: Hyun-Joo Nam & Yi Tian Ting
Hot Structures from Membrane Systems – Chairs: Anna Baker & David Lodowski
Evening Session on Diversity – Chairs: Krystle McLaughlin & Eileen Brady
Structured Nucleic Acids – Chairs: Eric Montemayor & Manual Swairjo
Play it Cool? Ambient and Cryogenic Approaches – Chairs: Doug Juers & James Fraser
BioMac, YSSIG, Canada
Molecular Machines – Chairs: Gerald Audette & Tim Maier
Mechanistic & Spectroscopic Structural Enzymology – Chairs: Chris Bianchetti & Mohammad Taha
BioMac, Canada
Structural Glycobiology – Chairs: David Rose & Michael James
Light Source, BioMac, SAS
Structural Dynamics- Chairs: Keith Moffat & George Phillips
BioMac Light Source, MNP
Combined Methods in Data Analysis – Chair: Peter Chupas
Light Source
Advances in Multi-crystal Approaches and Serial Crystallography – Chairs: Nadia Zatsepin & Cornelius Gati
Imaging with X-rays: Hard and Soft Electrons and Light – Chairs: Vivian Stojanoff & Gerd Rosenbaum
Industrial, BioMac
Structural Informatics for Drug Design and Development – Chair: Mark Oliveira
Ind., Powder Service
From Fingerprinting to Full ID: PXRD – Chairs: Richard Staples & Curt Haltiwanger
Industrial, NMP
Powder Pair Distribution Function and Pharmaceuticals – Chairs: Simon Billinge & Peter Stephens
Ind., Small Mol
Crystal Engineering Form & Function – Chairs: Peter Wood & Tomislav Fiscic
YSSIG, Small Mol
Important Science from Small Molecules Structures – Chairs: L. Falvello, P. Gonzalez & A. Albinati
Cool Structures – Chairs: Allen Oliver & Chris Durr
Small Mol
How I Spent my Summer Vacation at Small Molecule Summer Schools – Chairs: A. Sarjeant & J. Lee
General, CEC
Engaging Undergraduates with Crystallographic Research – Chairs: Roger Rowlett & Joe Tanski
General Interest – Chairs: Stacey Smith and Peter Müller
Service, Canada, Small Mol, GIG
Would You Publish This? – Chairs: Louise Dawe & Brian Dolinar
Service, YSSIG
Publication Practices – Chairs: Kimberly Lincoln & Larry Falvello
Service, General, BioMac, CEC, Data Standards Committee
Standard Practices in Crystallography I: Data Collection Strategies – Chair: Peter Müller
Service, Light Sources, BioMac, Ind
Experiences and Opportunities with Central Facility Services – Chairs: C. Beavers and B. Sankaran

ACA Philadelphia - July 25-29, 2015

Who Needs to Register: Everyone must submit a registration form (including invited speakers) with the appropriate fee. Registered participants will receive conference materials and a name badge securing admission to the Opening Reception, the Exhibit Show and Scientific Sessions, at the ACA Registration Desk within the Sheraton Hotel.

Obtaining a VISA: Advance planning by foreign travelers is critical. We recommend all foreign travelers consider the following when making plans to travel to the US:

Identify whether a VISA is needed.

VISA applications should be made 90 days in advance of the travel date. For further information contact: the US Department of State (travel.state.gov/visa/visa_1750.html).

Staying Green: The full set of abstracts will be availabe through the ACA website. Program information will also be available through your smartphones and tablets.

Young Scientists:

Travel Support: is available from both theACA and the IUCr. Applications should be made by the abstract deadline on the meeting web site.

Session Room Monitors: We are pleased to offer registered Students & Post-docs attending the 2015 Meeting the opportunity to defray meeting expenses by participating as Session Room Monitors.Session Room Monitors operate audiovisual equipment, and room lighting, photograph the speakers (cameras provided), track and record attendance, and perform other tasks requested by the session chairs. Monitors will be compensated at a rate of $10 per hour. You must commit to at least one, full-day (8:00a.m.-5:00p.m. or when the session ends). Positions are assigned on a first-come, first-served basis. If you would like to participate, please contact: aca@hwi.buffalo.edu.

Meeting Orientation: Our focus is to orient new 'young scientists' and first time attendees to the structure of the ACA Meeting and how to make the most of their experience. The orientation is scheduled for Saturday, July 25 at 5:30pm and will last about an hour.

Bruker - Young Scientists Mixer: High energy fun, great food and some of the most exciting venues make the Young Scientists Mixer a great place to connect with scientists ranging in experience and disciplines. Sponsored in part by Bruker AXS, the Young Scientist Mixer is one of the meeting's most popular events and is FREE to registered Students & Post-docs (ticket required). The mixer will be held on Sunday, July 26.

Accommodations: A limited number of rooms for students and postdoctoral associates are available at a reduced rate at the Sheraton. You must be a registered Student or Post-doc to be eligible for this rate (First-come first-served). ***Room sharing*** is an another option for those looking to save money on their hotel accommodations.

Registration Fees

Category	Early (before May 31)	Late (after May31)
Regular Member	$505	$705
Retired Member	$200	$300
Post doc Member	$255	$355
Student Member	$200	$300
Nonmember*	$705	$955
Post doc Nonmember*	$355	$455
Student Nonmember*	$290	$390
Guest	$ 65	$ 65
Banquet	$70 ($35 students)	

Workshop I: Intro to Modeling High-Pressure Single-Crystal Diffraction Data
Students & Postdocs $120; others $160

Workshop II: Serial Crystallographic Data Analysis with Cheetah & CrystFEL
Students & Postdocs $100; Academic $150; Corp. $250

Workshop III: Reitveld Refinement Analysis
Students & Postdocs $125; others $165

Workshop IV: SAS: Structural Biology & Soft Matter
Students, Postdocs & Academics $130; others $250

* The nonmember registration fee includes a one-year ACA membership.

Those registering as students or postdocs or must include documentation of this status with the registration form.

The opening reception is included in the registration fee. Guests are also welcome to visit the exhibit show.

Register on-line or download forms to register by fax or mail.

www.amercrystalassn.org/2015-mtg-homepage
Questions: aca@hwi.buffalo.edu

Hotel Info

WI-FI will be complimentary in the sleeping rooms, so bring your laptops and stay connected to home and office. The room rates at the Sheraton are competetive with other properties in the vicinity. We are able to offer these rates by committing to fill a certain number of rooms. By staying in the conference hotel you will help us meet our room block commitment, which also brings with it the free meeting space that helps keep registration fees affordable.

The Organizing Committee will observe the basic policy of non-discrimination and affirms the right and freedom of scientists to associate in international scientific activity without regard to factors such as ethnic origin, religion, citizenship, language, political stance, gender, or age, in accordance with the statutes of the International Union.

ACA Summer Course in Chemical Crystallography

June 20th – July 1st, 2015
Northwestern University

Applications will be accepted starting January, 2015
www.acasummercourse.net

Sponsored by:
The American Crystallographic Association
The US National Committee for Crystallography
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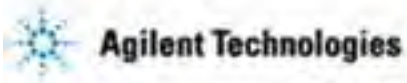

NORTHWESTERN
UNIVERSITY

JANUARY 2015

14-16 **BioXFEL STC Annual Conference.** Ponce, Puerto Rico. *www.bioxfel.org/events/details/6*

MARCH 2015

8-12 **Ultrafast Dynamic Imaging of Matter.** Grindelwald, Switzerland. *www.udim2015.ethz.ch*

MARCH - APRIL 2015

30-2 **BCA Spring Meeting.** University of York, UK. *www.crystallography.org.uk*

JUNE 2015

7-11 **International Conference on Structural Genomics 2015: Deep Sequencing Meets Structural Biology**. Rehovot, Israel. *www.weizmann.ac.il/conferences/ICSG2015*

JULY 2015

25-29 **ACA 2015 Annual Meeting.** Philadelphia, PA, Sheraton Philadelphia Downtown. ***Program Chairs: Kraig Wheeler & Louise Dawe. www.AmerCrystalAssn.org***

AUGUST 2015

23-28 **ECM 29,** Rovinj, Croatia. ***Program Chair: Nenad Ban. ecm29.ecanews.org***

DECEMBER 2015

5-8 **AsCA2015 Science City.** Kolkata, India. *asca.iucr.org/meetings*

JULY 2016

22-26 **ACA 2016 Annual Meeting**. Denver, CO, Sheraton Downtown Denver. ***Program Chairs: Amy Sargent & Edward Snell. www.AmerCrystalAssn.org***

NOTE: New schedule for ACA 2016: The meeting will begin on ***Friday, July 22***. The ***workshops*** will be scheduled for all-day on Friday with the ***opening reception*** on Friday evening. The ***exhibit show*** will open Friday night and end after the Monday poster session. ***Poster sessions*** will run Saturday - Monday and the ***microsymposia*** will run Saturday - Tuesday. The ***awards banquet*** will take place Tuesday evening and ***session planning for 2017*** will be on Wednesday morning.

2015 Dues are Due: Please renew promptly and remember to support your favorite ACA Award Funds. ***NOTE: It is now possible to renew online***

membership.amercrystalassn.org

Call for Nominations - 2015 - 2016 Awards

2016 Bau Neutron Diffraction Award: Established in 2010, this award recognizes exceptional research achievement in neutron diffraction. The Award consists of a $1,500 honorarium and reimbursement of up to $1,500 for travel expenses to accept the award and to deliver the award lecture at the ACA annual meeting (Selection committee: A. Wilkinson, T. Koetzle, A. Huq).

2016 I Fankuchen Award: To recognize contributions to crystallographic research by one who is known to be an effective teacher of crystallography. There are no geographic or age restrictions. The honoree delivers a lecture at the ACA annual meeting and at the recipient's home institution or at another institution of the recipient's choice. The Award consists of a $2,500 honorarium and up to $2,500 in travel expenses. (Selection committee: D. Rose, W. Furey, C. Lind-Kovacs).

2016 TrueblоodAward: To recognize exceptional achievement in computational or chemical crystallography. The Award consists of a $1,500 honorarium and reimbursement of up to $1,500 for travel expenses to accept the award and to deliver the award lecture at the ACA annual meeting. (Selection committee: T. Terwilliger, P. Adams, W. Hendrickson).

2016 Margaret C. Etter Early Career Award: To recognize outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career. The Award consists of a $1,000 honorarium and a plaque. The winner is also expected to present a lecture at the ACA annual meeting.

The deadline for nominations for the 2016 ACA Awards is April 1, 2015. The Charles E. Supper Instrumentation Award and the E. A. Wood Science Writing Award are given on an irregular basis and nominations may be submitted at any time.

2015 ACA Fellows: Serves to recognize a high level of excellence in scientific research, teaching, and professional duties, but also service, leadership, and personal engagement in the ACA and the broader world of crystallography and science. Our Fellows program celebrates the excellence of our own members from within the ACA, and promotes their recognition worldwide to constituencies outside of the ACA, such as their employers, other scientific societies, and the government. See ***www.amercrystalassn.org/aca-fellows*** for information on the nomination procedure. ***Nominations for 2015 ACA Fellows are due by February 28, 2015.***

2016 ACA Offices and Committees: In the fall of 2015 we will elect a new Vice-President, Treasurer, and one person to each of the ACA Standing Committees (Continuing Education, Communications, and Data, Standards and Computing). Suggestions are due by February 15, 2015. Members of the nominating committee are Ward Smith, Martha Teeter and Louise Dawe.

More information for all ACA Awards is available on the ACA website: www.AmerCrystalAssn.org.

Send all nomination suggestions to: Marcia@hwi.buffalo.edu

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