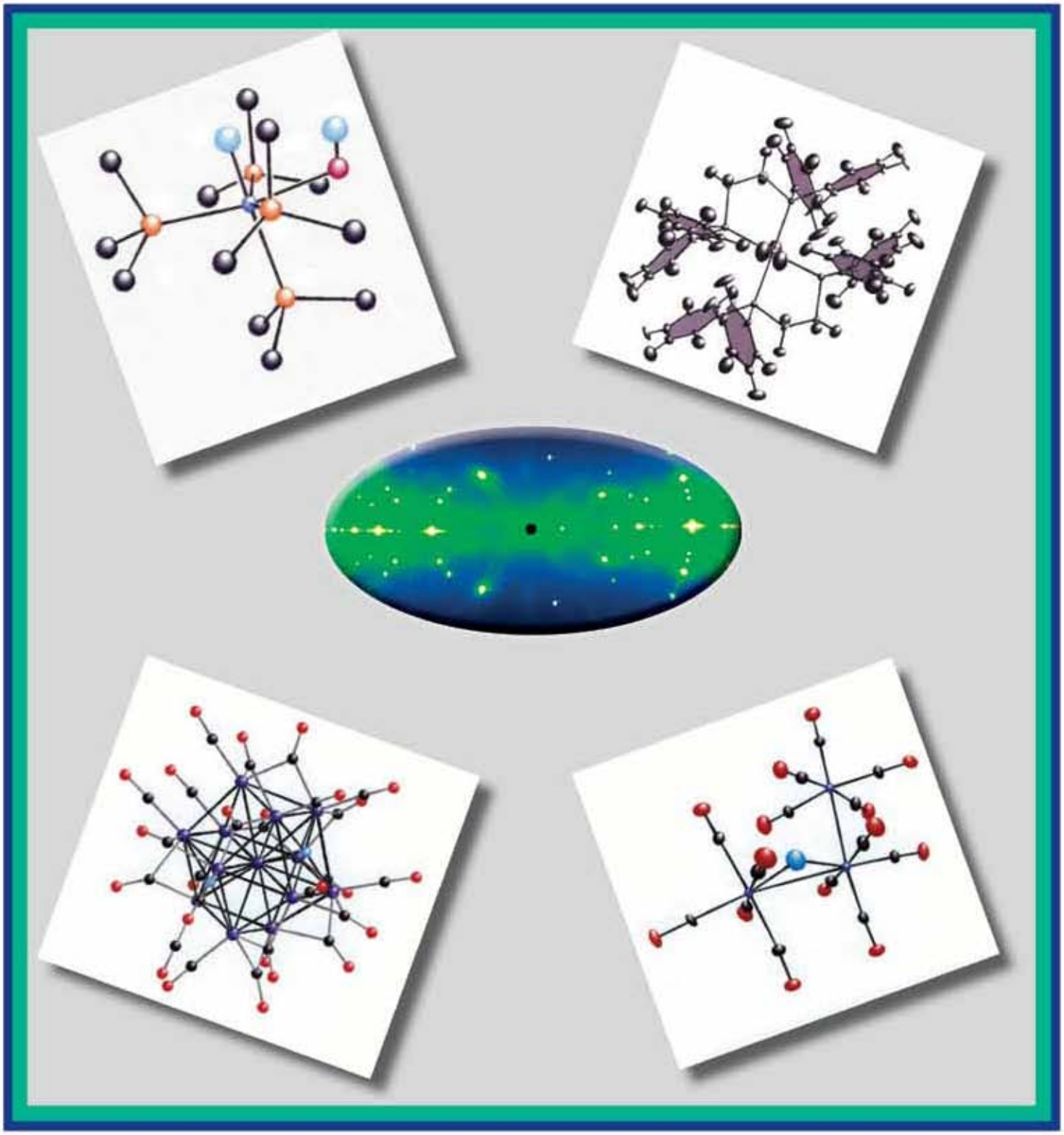
ACA RefleXions

American Crystallographic Association

Number 4

Winter, 2012



ACA - Bau Neutron Diffraction Award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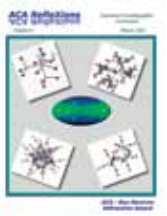

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ACA 2013 Award Winners

Election Results

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

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President's Column

Time flies. This is my fourth and final letter to you as President. By the time you read this, Cheryl Stevens will have taken the reigns. You will be glad to know that our election for 2013 is now complete--no recounts, hanging chads or other shenanigans. Martha Teeter has been elected Vice-President and will become President in 2014. James Kaduk was elected Treasurer, Graciela Delgado was elected to the Communications Committee, Kraig Wheeler to the Continuing Education Committee, and Tom Terwilliger to the Data, Standards and Computing Committee. Thanks to these fine folks for their willingness to serve, and for the other fine candidates who were willing to stand for election.

As for the general state-of-the-association comments, I am pleased to report that the Boston meeting was outstanding both scientifically and logistically and, thanks to a greater than expected on site registration, we even made a bit of money. As you know by now, the next meeting will be in Honolulu, July 20-24, 2013 (see pages 44-46 for more information). The hotel is very reasonably priced, and we expect that this meeting could be less expensive overall than Boston, so get your talks, posters, notebooks, and surfboard wax ready! The site for the 2014 meeting has been set for Albuquerque, New Mexico. We are hoping for a good turnout from south of the border, as we expand our efforts to include more Latin American scientists in ACA activities. Having Graciela Delgado on board the Communications Committee also gives us a chance to develop new scientific relationships with our neighbors to the south.

At the business meeting in Boston and in my column in the fall issue of *RefleXions*, I mentioned that the ACA was considering a new on-line journal. The American Institute of Physics, of which we are a part, has made us a generous and attractive offer to help get it going. Being us, we have yet to make a final decision but will have done so before the spring issue of *RefleXions* is published.

We are also moving ahead with our strategic planning process. Currently, the committee members for that important task are Cheryl Stevens, chair, Bill Duax, Judy Flippen- Anderson, S. N. Rao, Martha Teeter, Marcia Colquhoun and myself. Fred Dylla at the AIP is acting as our guide through the process. We will share the process as we go forward and would appreciate feedback. If you have any ideas you would like to share about how the ACA should move forward please send them to Cheryl (***cheryl.stevens@wku.edu***).

Our ACA Fellows program is now well established with the inauguration of our first two classes of Fellows in 2011 and 2012. However there are many more ACA members that should be accorded this honor and we welcome nominations. To remind everyone of how the process works, the procedure for nominating fellows follows my report.

Those are the important points for this report. Don't forget that there are some folks who have spent a good part of their lives supporting the ACA in various capacities, and I want to acknowledge them one last time while I have a chance. Judy Flippen-Anderson and Connie Rajnak as editors of *Reflexions*, Marcia Colquhoun, who does all the heavy lifting day in and day out, ably assisted by Crystal Towns, S. N. Rao and Bill Duax.

I will still have a year to go on council as Past-President and I am committed to the strategic planning committee and the ACA itself for the long term. I look forward to our continued interactions.

George Phillips

Nomination Procedure for ACA Fellows

1. A call for nominations for ACA Fellows will be published in the winter edition of *RefleXions* and on the ACA website. Nominations are solicited from any member (including retired members) of the ACA.

2. Nominations can be submitted at any time to the Buffalo office. The closing date for any given year is February 28th.

3. After February 28th, current Fellows will be polled for their evaluations of all nominations submitted since March 1st of the preceding year. The new class of Fellows will be appointed by Council based on the compiled results.

4. Self-nominations will not be accepted.

5. Nominations must include the following information about the nominee:

   a. Name, contact information (address, telephone number, email address), and professional affiliation.
   b. Nominees are expected to be members of ACA in good standing. Under exceptional circumstances Council may waive this requirement.
   c. Brief educational background.
   d. Professional history (positions, appointments, awards, honors).
   e. Membership in other scientific organizations.
   f. Service to the ACA and crystallography.

6. Nominations must include the following information about the sponsor:

   a. Name, contact information (address, telephone number, email address), and professional affiliation.
   b. Must be a current ACA member in good standing. The ACA office will confirm the sponsor's membership status.

7. In addition to that of the sponsor, two further letters of support must be included. The letters must clearly state how the nominee's research over a sustained period of time has had a significant impact on his/her field and detail how the nominee has contributed to the ACA.

News from Canada

The irony is striking. The week of October 24-26 was Gairdner week in Canada. The Canada Gairdner International Awards are given every year in recognition of major advances in medical research, often foreshadowing the Nobel Prize by 5-10 years. As part of the award process, awardees visit campuses across the country and give talks to high school students and university audiences. The culmination is a black-tie banquet in Toronto. The one theme that pervaded every one of the awardees' comments at the banquet was the central, critical role that curiosity-driven basic research played in their discoveries. Over and over, we heard how they never foresaw (and in some cases still do not foresee) practical applications of their advances, which spanned how cells and organisms are regulated by their circadian clocks, to the identification of the Fc receptors that mediate the action of antibodies.

Meanwhile, Liberal Member of Parliament Ted Hsu, from Kingston, Ontario, has continued his "Death of Evidence" tour. Ted, who is trained and has worked as a physicist, is one of the few voices being raised against the present trends in government science policy that de-emphasize curiosity-driven, investigator-initiated research in favor of matching funding schemes and partnerships with industry. Coupled with this philosophy is the closure of research facilities that threaten to generate evidence that disagrees with the government's ideology, such as the world-unique Experimental Lakes ecology research facility in western Ontario, the arctic research station, and investigations into environmental effects of oil sands development. This policy goes hand-in-hand with the gutting of much of the government's own internal research infrastructure, including the National Research Council, Fisheries and Oceans, Environment Canada, and others, hence the label "Death of Evidence".

It was striking that none of the discoveries celebrated by the Gairdners, nor those featured by the Nobel Prizes announced two weeks before, could have been accomplished under the current science policy and funding systems that are built on pre-defined applications and timelines, such as the short-term, fickle interests of industry. Unless Ted Hsu and his colleagues can mobilize the academic community and public opinion, it appears that Canada will be uncompetitive in major scientific advances (and international prizes) for generations to come.

In other news… The 21st annual regional Buffalo-Hamilton-Toronto (BHT) crystallography meeting was held at McMaster University on November 2nd. Our distinguished visitor this year was Todd Yeates (UCLA), who gave a fascinating account of his group's work analyzing protein symmetry, in particular why $P2_12_12_1$ is such a common space group for proteins. He left us with the tantalizing suggestion that his results might lead not only to improved approaches to protein crystallization, but also to designing protein 'cages' and other nano-materials. Todd was followed by a short update from Jim Britten of his talk at an early BHT (1992?) and a report from the Canadian National Committee. The afternoon session featured talks from new faculty (Todd Holyoak, Waterloo, and Joel Weadge, Wilfrid Laurier), and trainees from Queen's, Toronto, McMaster, Waterloo, and Western and Sick Kids. Pawel Grochulski came all the way from Saskatoon to give us an update on the status of the Canadian Light Source. As usual, the organization was led by Lynne Howell with loyal support from Rigaku, Art Robbins, Bruker, FortéBio, Formulatrix, Hampton Research, Molecular Dimensions, Norton and the CLS. Next year's meeting will be on November 8, 2013.

David Rose

From the Editors Desk:

Erratum: The Editors regret an unfortunate choice of words in the Fall 2012 *RefleXions* report on session 13.04 by Volker Urban and Lin Yang (page 40). This session was dedicated to the memory of Hiro Tsuruta, and the phrase used was: . . (Hiro Tsuruta) "who unexpectedly passed away in 2011". While unanticipated by Volker, Lin, and other colleagues in the small-angle scattering community, it was definitely NOT unexpected to either Hiro or his long time companion, Christine Trame, since Hiro died after a long and courageous fight with cancer.

Announcement: Surajit Banerjee (***sbanerjee@anl.gov***) has volunteered to fill the position of News and Awards Editor for *RefleXions*. We heartily welcome Surajit to the *RefleXions* staff and hope that you will make his job easier by sending him any information you come across about awards to ACA members including yourselves.

Nominations for 2014

ACA Awards: Nominations for the ***Patterson, Wood Science Writing***, and ***Etter Early Career*** awards are due by May 1, 2013. Nominations for ***ACA Fellows*** are due February 28, 2013.

ACA Offices and Committees: In the fall of 2013 we will elect a new Vice-President and one person to each of the ACA Standing Committees (Continuing Education, Communications, and Data, Standards and Computing). Suggestions are due to by February 15, 2013. Members of the nominating committee are Saeed Khan (Chair), Carrie Wilmot and Tom Koetzle. Full details describing the criteria for all ACA awards and offices can be found on the website.

2013 Dues are Due: Please renew promptly and remember to support your favorite ACA Award Funds. NOTE: It is now possible to renew online.

ACA website: www.AmerCrystalAssn.org.

Send all nominations to: Marcia@hwi.buffalo.edu

2012 Chemistry Nobel to Lefkowitz and Kobilka

Robert Lefkowitz (above left) and Brian Kobilka (above right) shared the 2012 Nobel Prize in Chemistry for groundbreaking discoveries that revealed the inner workings of an important family of such receptors: G-protein–coupled receptors (GPCRs). For a long time, it remained a mystery how cells could sense their environment. It was known that hormones such as adrenalin have powerful effects, e.g. increasing blood pressure and making the heart beat faster. Scientists suspected that cell surfaces contain some kind of recipient for hormones. But what these receptors actually consisted of and how they worked remained obscured for most of the 20th Century.

Robert Lefkowitz started to use radioactivity in 1968 in order to trace cells' receptors. He attached an iodine isotope to various hormones, and thanks to the radiation, he managed to detect several receptors; one of them, the β-adrenergic receptor was a receptor for adrenalin. His team of researchers extracted the receptor from its hiding place in the cell wall and gained an initial understanding of how it works.

In the 1980s, Brian Kobilka joined the team and was charged with isolating the gene that codes for the β-adrenergic receptor from the human genome. He managed to achieve this goal and the team realized that this receptor looked very similar to the rhodopsin receptor in the eye. They realized that there is a whole family of receptors that look alike and function in the same manner. This family is now known as GPCRs. About a thousand genes code for such receptors, for example, for light, flavor, odor, adrenalin, histamine, dopamine and serotonin. The studies by Lefkowitz and Kobilka are crucial for understanding how GPCRs function because about half of all medications achieve their effect through GPCRs. Furthermore, in 2011, Kobilka achieved another break-through; he and his research team captured an image of the β-adrenergic receptor at the exact moment that it is activated by a hormone and sends a signal into the cell. This image is a molecular masterpiece – the result of decades of research.

Crystal structure of activated beta-2 adrenergic receptor β2AR (red) in complex with G-proteins (green, cyan and yellow). Credit: S.G.F. Rasmussen et al., Nature 477, 549–555 (2011).

2013 Gregori Aminoff Prize to Gatti and Spackman

The Royal Swedish Academy of Sciences (RSAS) has awarded the 2013 Gregori Aminoff Prize in Crystallography to Carlo Gatti, (Italian National Research Council - above left) and Mark Spackman (University of Western Australia - above right) for developing experimental and theoretical methods to study electron density in crystals, and using them to determine molecular and crystalline properties. They have independently developed concepts for interpreting electron density distributions related to quantum chemistry theory, using multipole analysis of high-quality x-ray diffraction data. This approach has, in particular, significantly demonstrated and quantified the role of hydrogen bonding in molecular systems. 'Charge density topology' is important for classification of the type and strength of chemical bonding in solid compounds and molecules.

Carlo Gatti has developed the concept of Source Function that permits visualization of chemical bonds and other fundamental chemical properties using only information from observed electron density and its derivatives. In x-ray crystallography and materials sciences, the Source Function tool has been extensively applied to interpret a wide range of different bonding modes. Mark Spackman devised and implemented a new scheme for partitioning crystal space into molecular and atomic volumes limited by Hirshfeld surfaces, which reflect the nature and strength of interatomic and intermolecular interactions in quantitative terms.

Index of Advertisers

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First X-ray View of Martian Soil

NASA's rover ***Curiosity*** has completed its first x-ray diffraction experiment on Mars. It shows that the mineralogy of the Martian soil is similar to weathered basaltic soils in Hawaii. The rover located a deposit of soil and dust, scooped the dirt and delivered it to the CheMin x-ray diffractometer. The dust was sieved to grain size less than 150 μm, and delivered into a vibrating sample cell that was bathed in cobalt radiation. The diffraction signal was recorded on a CCD and sent by satellite from Mars to NASA's JPL labs, where it is being analyzed by the CheMin research team led by Principal Investigator, Dave Blake of NASA Ames Research Center. The identification of minerals in rocks and soils is crucial to the mission's goal of assessing past environmental conditions because each mineral records the conditions under which it formed. It is remarkable that the first robotic diffraction experiment on another planet took place on the 100th anniversary of the first x-ray diffraction experiment on Earth.

The x-ray diffractometer is called CheMin, short for "Chemistry and Mineralogy," and is one of 10 instruments on board. Aside from the science it returns, it is also a marvel for its instrument design. First conceived about 22 years ago, co-PI's Dave Vaniman and Dave Bish met Dave Blake (the 3 Daves) in a poster session where they were each proposing x-ray diffractometers for future space missions. Rather than competing, they decided to join forces and together formed a team that led the way towards building a light-weight, small, robust diffractometer that could travel through space at 14,000 mi/hour, land safely on a planetary surface and collect great data.

The instrument design was taken over by materials scientist, Philippe Sarrazin, who was able to create a design so small and compact that the final flight model weighs only 10 kg and is the size of a large shoe box. Through SBIR funding, a commercial instrument has been packaged in a briefcase and is now sold by Olympus for portable, *in situ* diffraction experiments in the field. The design won the Gold Medal at PITCONN in 2008 as the best new instrument of that year. The novel vibration mechansim employed to shake the samples, allowing poorly ground or "as-received" samples to be analyzed, won NASA's ***Commercial Invention of the Year*** award in 2010.

Powder is delivered to the instrument after passing through a sieve to eliminate grains that are too large for the sample chamber. The x-ray source is a small cobalt tube that required a new design for its high-voltage supply, since NASA had never flown a miniature high-voltage supply in space before.

In typical powder diffractometers, samples are carefully prepared and placed on sample slides that are aligned with rotating arms for the detector and x-ray source. This setup is too complicated and delicate for planetary exploration. Instead the sample is funneled into the arms of a tuning fork with thin kapton or mylar windows. The tuning fork vibrates the powder and provides grain motion that re-orientates the grains on a continuous basis, permitting the collection of a powder pattern on a CCD. The image from the CCD is returned to Earth.

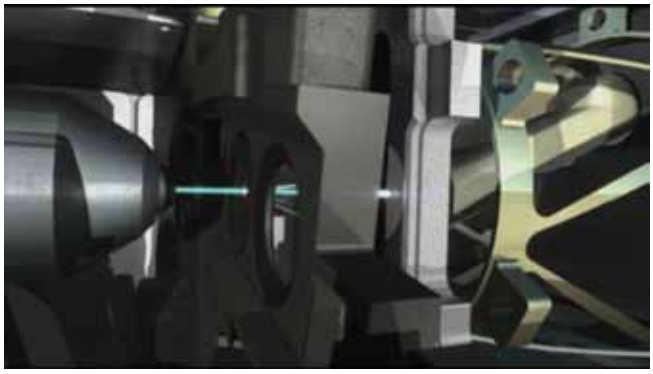
See page 38 for a listing of all participants on the CheMin team.

On the left is a typical powder diffractometer. The upper right is an image of the rover while it is being assembled, indicating the CheMin instrument in its place. The lower right shows Dave Blake using the briefcase sized version of the instrument.

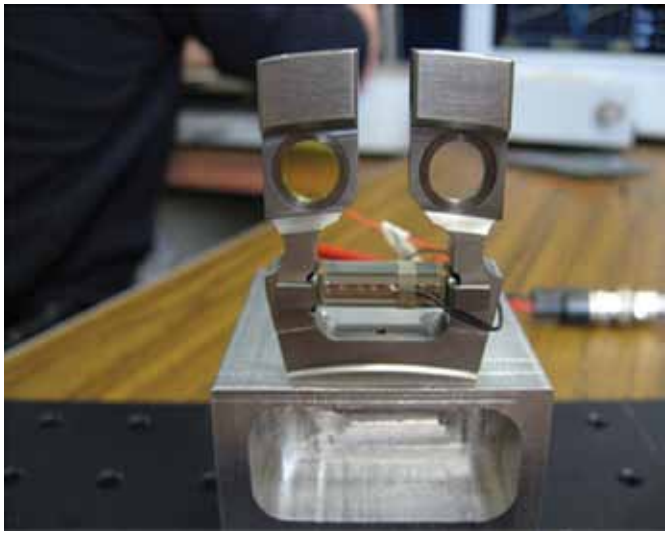
Self portrait of ***Curiosity*** at the Rocknest site, courtesy of Malin Space Science Systems.

NASA's Mars rover ***Curiosity*** used a mechanism on its robotic arm to dig up five scoopfuls of material from a patch of dusty sand called "Rocknest," producing the five bite-mark pits visible in this image from the rover's left navigation camera (Navcam). Each of the pits is about 2 inches (5 centimeters) wide.

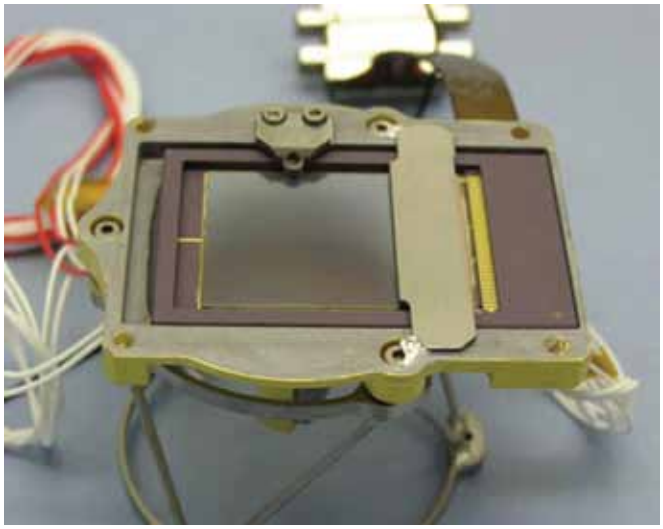
The fifth scoopful at Rocknest -- leaving the upper middle bite mark -- was collected during the mission's 93rd Martian day, or sol (Nov. 9, 2012). This image was taken later that same sol. A sample from that fifth scoop was analyzed by CheMin.



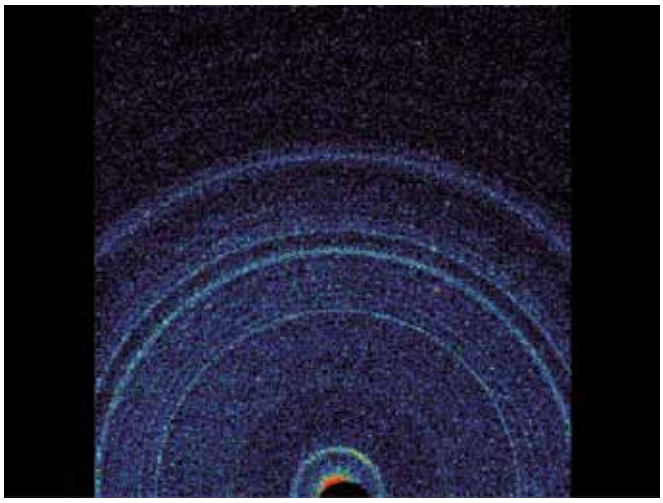
CADview image of the inner workings of the CheMin diffractometer. The x-ray source is on the left with a beam of x-rays intersecting the mineral grains in the sample chamber and the diffracted beams going to the detector on the right.



This image shows the cells that hold the soil samples that are vibrated by the Chemistry and Mineralogy (CheMin) instrument on NASA's ***Curiosity*** rover. When the rover delivers samples to CheMin, they are funneled into one of the windowed areas in the cell assemblies. These cell pairs are vibrated 2,000 times per second, like a tuning fork, by a piezoelectric device placed between the two arms of the fork. When vibrated, the particles flow like liquid. This movement enables the instrument's x-ray beams to hit all of the grains in random orientations over time. This innovative technology has been spun off for commercial use in miniaturized portable x-ray diffraction instruments. The powder vibration system enables poorly prepared or as-received samples to be analyzed without further sample preparation. This is useful in cases where extensive sample preparation is either not possible (e.g., on Mars) or when delicate materials (such as pharmaceutical products) would be destroyed or altered by extensive grinding. Implementation of the powder vibration system was a crucial step in enabling small portable x-ray diffraction instruments because many of the moving parts in conventional x-ray diffraction instruments could be eliminated. ***Image credit: NASA/JPL-Caltech/Ames***



This charged coupled device (CCD) is part of the CheMin instrument on NASA's ***Curiosity*** rover. When CheMin directs x-rays at a sample, this imager, the size of a postage stamp, detects both the position and energy of each x-ray photon. The technology in this CCD was originally developed by NASA and has become widely used in commercial digital cameras and other imaging devices. ***Image credit: NASA/JPL-Caltech/Ames***.



First x-ray diffraction pattern of Martian soil. This graphic shows results of the first analysis of Martian soil by the CheMin experiment on NASA's ***Curiosity*** rover. The image reveals the presence of crystalline feldspar, pyroxenes and olivine mixed with some amorphous (non-crystalline) material. The soil sample, taken from a wind-blown deposit, known as Rocknest, within Gale Crater, where the rover landed, is similar to volcanic soils in Hawaii. By directing an x-ray beam at a sample and recording how x-rays are scattered by the sample at an atomic level, the instrument can definitively identify and quantify minerals on Mars for the first time. Each mineral has a unique pattern of rings, or "fingerprint," revealing its presence.

The colors in the graphic represent the intensity of the x-rays, with red being the most intense. ***Image credit: NASA/JPL-Caltech/Ames***

Professor Dame Louise Napier Johnson (1940-2012)

Louise Johnson, biophysicist and structural biologist, died after a 13-month illness which she bore with quiet fortitude and grace. Her life and work impacted very many people worldwide, due both to her scientific activities in protein crystallography and enzymology, and her tireless interest and effort in supporting and encouraging scientists in developing countries to establish effective research laboratories as far apart as South America, the Middle East and Pakistan.

I am one of those whose life course was changed by a chance conversation with Louise, who I first met in 1987 when I was tutoring physics at Somerville College where Louise was then a Fellow. Over lunch she asked me what I was going to do when my fixed term contract at Somerville expired and since there was still a whole year to go, I threw away the comment 'Oh, I don't know, I will probably have to change fields since nuclear physics (my then research area) is no longer being funded in Oxford.' She visibly brightened and said 'We are looking for someone with just your skills at the moment to look after our new cutting edge x-ray equipment for protein crystallography which is about to arrive.' As a result of my rash statement and Louise's quiet persuasiveness, I visited her the very next day at the Laboratory of Molecular Biophysics (LMB) where she and her research group were then working on the mechanism of action of glycogen phosphorylase, a large protein (842 amino acids) present in muscle which turns inert glycogen into the sugar needed to power physical activity. They had succeeded in obtaining a structure (Johnson LN, March 1992. *FASEB Journal* **6** (6): 2274–8, Johnson LN, Barford, D, February 1990. *J. Biol. Chem.* **265** (5): 2409–2412) and showed how the enzyme was regulated by reversible phosphorylation and allosteric effects. In the early 1980s her group at Daresbury Laboratory near Runcorn was in the vanguard of those using synchrotron radiation for macromolecular crystallography (J Hajdu, K R Acharya, D I Stuart, P J McLaughlin, D Barford, N G Oikonomakos, H Klein, and L N Johnson, February, 1987. *EMBO J.* **6**(2): 539–546). Louise's lifelong interest in applying new techniques to structural biology questions came to the fore much later when she became Life Sciences Director of Diamond Light Source in 2003. There she oversaw the building and development of this highly effective national facility which is now bearing great fruit for the UK physical and biological sciences research community.

As a result of my visit to LMB that day I went to work there a few months later, and when Louise was appointed to the David Phillips Chair in Molecular Biophysics in 1990, worked under her until her retirement in 2007. Her management style was 'hands off' but 'attention on' in that she was always there if advice or guidance was needed, but did not offer it unless it was requested. She encouraged a highly cooperative working environment among the different groups and PIs in LMB which was extremely productive. Since synchrotron data collection time was allocated in aliquots of 24 or 48 hours and was much more efficient as a team effort, we regularly had the opportunity to work together closely with colleagues, thus developing a highly effective research effort. Although Louise did not normally accompany us on these trips to the synchrotron, during one of her sabbatical terms, she asked to be brought up to speed in using the current x-ray equipment and software for crystallography. She determinedly and methodically worked her way through our usual training program for new researchers, asking penetrating and pertinent questions at every stage. This was a great example to us of how a senior scientist should keep in touch with what daily research really involved, so that challenges faced by students and postdocs could then be better appreciated and overcome.

Her book written with Tom Blundell and published in 1976 (Blundell, TL, Johnson, LN (1976), *Protein Crystallography,* Academic Press, ISBN 0121083500), although now a collector's item judging by the price of a second hand copy on Amazon, is a classic text in the field worthy of attention today: I still regularly consult my well thumbed copy. Louise, with Wolfgang Baumeister, Alasdair C. Steven and Richard Perham, had just completed work on a book entitled *Molecular Biology of Machines and Assemblies* before she became ill, and it will be published in 2013.

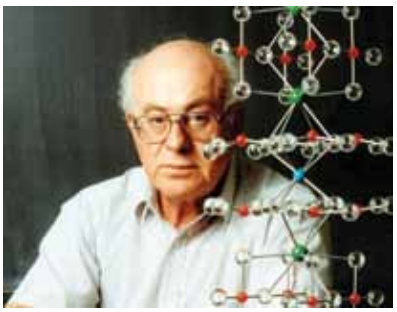
Louise was very modest and unassuming about her many achievements and honors, and this quality was brought home to me forcefully on one occasion in June 2010 when she very kindly offered to substitute in giving a conference lecture for me. At the time my husband was critically ill and I was unable to go and deliver it. We were trying to work out over the phone if she could give it on a Tuesday afternoon, and she mentioned she had to go to Cambridge on Sunday evening and for the whole of Monday and then to London on Tuesday morning, but that she might be free later in the afternoon. I assumed that the Cambridge trip was to visit her twin granddaughters, and asked after them, upon which she hesitantly told me that actually she was going to collect an honorary ScD degree from Cambridge. After some more convoluted discussion, it gradually transpired that the London engagement was at Buckingham Palace at a garden party given by the Queen, and that getting to Cardiff in time to give the conference lecture was unfortunately just not going to be possible. I was left wondering what her Wednesday commitments might be! Her schedules were punishing, and her energy amazing.

When Louise's death was announced, I received many e-mails from ex-LMB members expressing their appreciation for Louise's role in their lives, and retrospective realization of the positive atmosphere she nurtured: e.g. 'After working in other places, only now do I realize what a special place it was under her leadership', ' a great lady', and 'Such a big presence within the field'.

Thus because of Louise I am a protein crystallographer and no longer a nuclear physicist. She had an enormous and lasting influence on my life, as she also had on the lives of many others. Along with her numerous colleagues throughout the world, I will miss her inspiration both scientifically and personally. I feel privileged indeed to have both known and worked with her.

Elspeth Garman

Hugo Steinfink 1924 - 2012



Hugo Steinfink, past president of ACA and Professor Emeritus in chemical engineering at University of Texas at Austin, passed away at the age of 88, on August 25th, 2012, following complications from a cardiac procedure.

Born in Vienna, Austria on May 22, 1924, Hugo arrived in New York City in 1939 at the age of 15 with his brother and sister. Fortunately their parents were able to join them later. In 1941, he entered City College of NY, but his studies were interrupted by World War II when he served as an Army medic in the Pacific theatre in the Philippines. After an honorable discharge, he returned home and received a BS in chemistry in 1947, followed by a master's degree in 1948 from Columbia University.

After obtaining his master's, Hugo was employed by Shell Development Company, working in its Exploration and Production Research Department. Hugo once related to me how he became acquainted with the field of x-ray crystallography. When he arrived at Shell, Hugo's supervisor looked over his resume and upon seeing his experience as a medic and his chemistry background, declared that since the position had recently become vacant, Hugo would be handling the x-ray diffraction work at Shell. I'm fairly sure that Hugo was being modest when he said that he learned the craft slowly and felt that he needed to know more, but nonetheless he soon talked his boss into letting him attend one of Isidor Fankuchen's "Two Week Wonders" short courses.

This experience piqued Hugo's love of crystallography and in 1952, he returned to New York and Fan's lab, where he earned his PhD in x-ray crystallography at Brooklyn Polytechnic Institute in 1954. During his time there and with the help of Fan, the senior lab supervisor, Ben Post and a student, Josh Ladell, Hugo developed a low temperature Weissenberg camera *(Rev. Sci. Instr.* **24**, 882-3, 1953) and used it to determine the crystal structure of octamethyl cyclotetrasiloxane (*Acta Cryst.* **8**, 420, 1955) which is an important monomer in the production of silicone polymers and is now generically known as D4.

Ben Post, Berton Greenberg, Hugo Steinfink and Joshua Ladell at McMaster in 1986.

After obtaining his PhD, he returned to Shell Development Company in Houston as a research scientist. He specialized in silicate mineral and organo-silicon crystal structures and was recognized for his studies by election as a Fellow of the Mineralogical Society of America in 1956. He was also listed in *American Men and Women of Science, Who's Who, Who's Who in Technology,* and in *Who's Who in the South and Southwest*.

In 1960 Hugo left Shell Development for an academic career at The University of Texas at Austin, which was looking to bolster its "ceramics" programs. A January 12, 1962 *Time* article tells it this way: "The second-drawer engineering school at the University of Texas swelled with pride when it acquired a top-drawer man: the University of Illinois' chemist William Bradley, a leading authority on the molecular structure of materials. Masking its joy, as is proper in academic circles, Texas sent out a routine press release announcing Bradley's appointment—and thereby left untold a typical tale of the great game of faculty raiding."

"The plot to kidnap Bradley began three years ago, when Texas heard on the academic grapevine that middle-aged chemist Bradley wanted the help of a bright young scientist to complement his own work. Texas began to look. It soon learned that Bradley admired Hugo Steinfink, a young specialist in crystallography, then working for an oil company in Houston. Steinfink was lured to the Texas campus in 1960 with the promise of unlimited freedom and such research tools as a $30,000 refracterometer. The presence of Steinfink hooked Bradley, and the deal was clinched with a new, $4,000,000, eight-story laboratory."

Hugo was promoted to full professor in 1963 and appointed the Jewel McAlister Smith Prof. in Engineering in 1981. Later he was named the T. Brockett Hudson Prof. of Chemical Eng.. He was a core co-initiator of the Materials Science and Engineering Graduate Program of UT and guided the program through administrative channels to become a full-fledged MS and PhD degree granting program. He was honored by the University of Texas with many teaching excellence awards.

Hugo loved teaching and especially loved teaching x-ray crystallography. Every fall term he taught a theory class that was one of the few on campus that introduced students to symmetry concepts and a complete discussion of diffraction theory. Each spring he taught a diffraction lab class covering powder and single crystal methods as well as Laue photography. In the 1970s and 1980s he resurrected Fan's Two Week Wonders by teaching a one week complete course in powder diffraction as an engineering continuing education class.

Hugo authored and co-authored over 150 technical publications. His research over the years could be generally classified as structure-property relationships in solid state materials. Materials systems included silicates, zeolites, rare-earth and transition metal chalcogenides, and high temperature superconductors. I recall several sleepless nights as we tried to isolate the phase responsible for superconductivity after we heard about Chu's

work on Y-Ba-Cu-O mixtures in Houston. Indeed we determined the basic structure just as the spring 1987 ACA meeting started in Austin. A special evening session was added to the agenda for Monday, March 16 and several groups presented the same or similar results, two days before the "Woodstock of Physics" session at the APS meeting in New York on March 18.

Hugo always loved a good structure problem and even in his last months was working again on a novel cubo-siloxane structure with colleagues in the chemistry department.

Jack Dunitz, Herb and Edie Hauptman, Ellie Adman, Lisolette and David Templeton and Hugo Steinfink at ACA Atlanta, 1994.

Hugo was an active member of several professional societies. He was Chairman of the American Chemical Society, Central Texas Section in 1966 and was a member of the American Institute of Chemical Engineers, Phi Beta Kappa and Phi Lambda Upsilon, and Sigma Xi. He served on the US National Committee for Crystallography; was President of the ACA in 1995; was a co-editor of *Acta Crystallographica* from 1984 to 1993, and an Associate Editor of *American Mineralogist* from 1970 to 1972. He was also a board member of the American Institute of Physics from 1989 to 1995. In 1995, Hugo was a visiting professor at the University of Lille, France.

A true scholar and scientist, Hugo was most proud of his family – his adoring wife, Cele of 64 years; his children Dan Steinfink (Beverly) and Susan Steinfink Soussan (Henri); grandchildren David Steinfink (Ashely), Adam Steinfink, Sarah Steinfink Cogliandro (Michael)and Nicole S. Soussan. He was blessed with a great-grandchild, Samuel Steinfink. He is also survived by his brother, Emil. Hugo took great pride in his children and grandchildren, sharing their successes in life with all who would listen. He was a patient and giving man who was there 100% for anyone in the family at all times. Hugo combined his brilliance, sense of fairness and curiosity with a dry wit for which he was so loved and will be forever in the hearts of his family and friends. He shared his life experiences from his childhood in Nazi Vienna to the latest books he thought worthwhile for all to read. He truly had a love of learning and instilled his thirst for knowledge in his children and grandchildren.

Hugo was an avid tennis and squash player most of his life. He traveled the world including a safari in Africa for his 80th birthday and later to the Galapagos. He was not only fiercely loved by his family and many friends, but also respected by his colleagues and students.

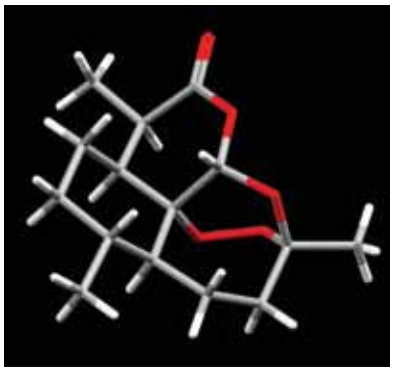
Steve Swinnea

CCDC Takes Crystallography into the Garden!

Although plants produce a vast array of chemical compounds, many of which have been found to be of use to humans, the natural world and the chemical world often seem distinct. However, the usefulness of many plant-derived compounds in medicine, flavorings, textiles, and dyes etc. has encouraged chemists to study these compounds, often using x-ray crystallography.

Working with the Cambridge University Botanic Garden, the Cambridge Crystallographic Data Centre (CCDC) has recently launched the "Chemicals from Plants Trail" around the Garden. Twenty-two plants are highlighted with descriptions of the interesting chemical compounds they contain. Crystal structures for all of these compounds are included in the Cambridge Structural Database (CSD).

Included on the trail is Artemisia annua (sweet wormwood), the source of artemisinin. Also known as Qinghaosu, it has been used in traditional Chinese medicine since around 200 BC. Artemisinin is active against Plasmodium malaria. As the plant grows quickly to harvestable age, it provides a cheap source of the drug. However, the World Health Organization does not recommend its use as a monotherapy as there is some evidence to suggest that some malarial parasites are already developing resistance.



Artemisinin: JN Lisgarten, BS Potter, C Bantuzeko, RA Palmer; J.Chem. Cryst. (1998), 28, 539, (CSD refcode QNGHSU03)

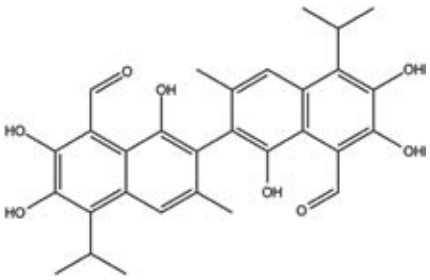
The structure shown at left is unusual in that it contains a peroxide bridge- one of very few instances of this in nature.. The O-O bond is broken when the molecule comes into contact with the Fe(ii) in heme, which is produced in the infected blood cells. Free radicals are produced which destroy the parasite. One problem with using artemisinin, however, is its poor solubility in water which chemists have tried to improve synthetically.

As well as medicinal plants, the trail also includes plants used as foodstuffs, such as Capsicum annuum. The compound capsaicin (Chili Pepper) accounts for the heat of chili peppers. However, the hot sensation is caused by chemically stimulating heat sensors in the body and does not actually raise body temperature. Similarly, menthol (from mints, also on the trail), stimulates the cold receptors, without actually decreasing body temperature.

GM Battle, GO Kyd, CR Groom, FH Allen, J Day, T Upson, J. Chem. Ed. (2012) 89, 1390-1394.

The heat of chili peppers is measured using the Scoville scale, named after Wilbur Scoville. As originally devised, the test involved diluting a solution of the pepper abstract in sugar water, until a team of tasters could no longer detect the heat. The degree of dilution gives its measure on the Scoville scale. Today, the concentration of capsaicin is measured by HPLC.

Capsaicin is the princi-pal ingredient in the pepper spray used for riot control and personal protection. The pain pathway activated by capsaicin is the same one activated by tarantula venom!



Gossypol (as dipropyl ether clathrate) M Gdaniec; Acta Cryst. C: Cryst.Struct. Commun. (1991), 47, 1296, (CSD refcode KIVCAT).

When applied topically, capsaicin can be used in small quantities to treat pain. As nerves are overwhelmed by the burning sensation, they lose their ability to report pain.

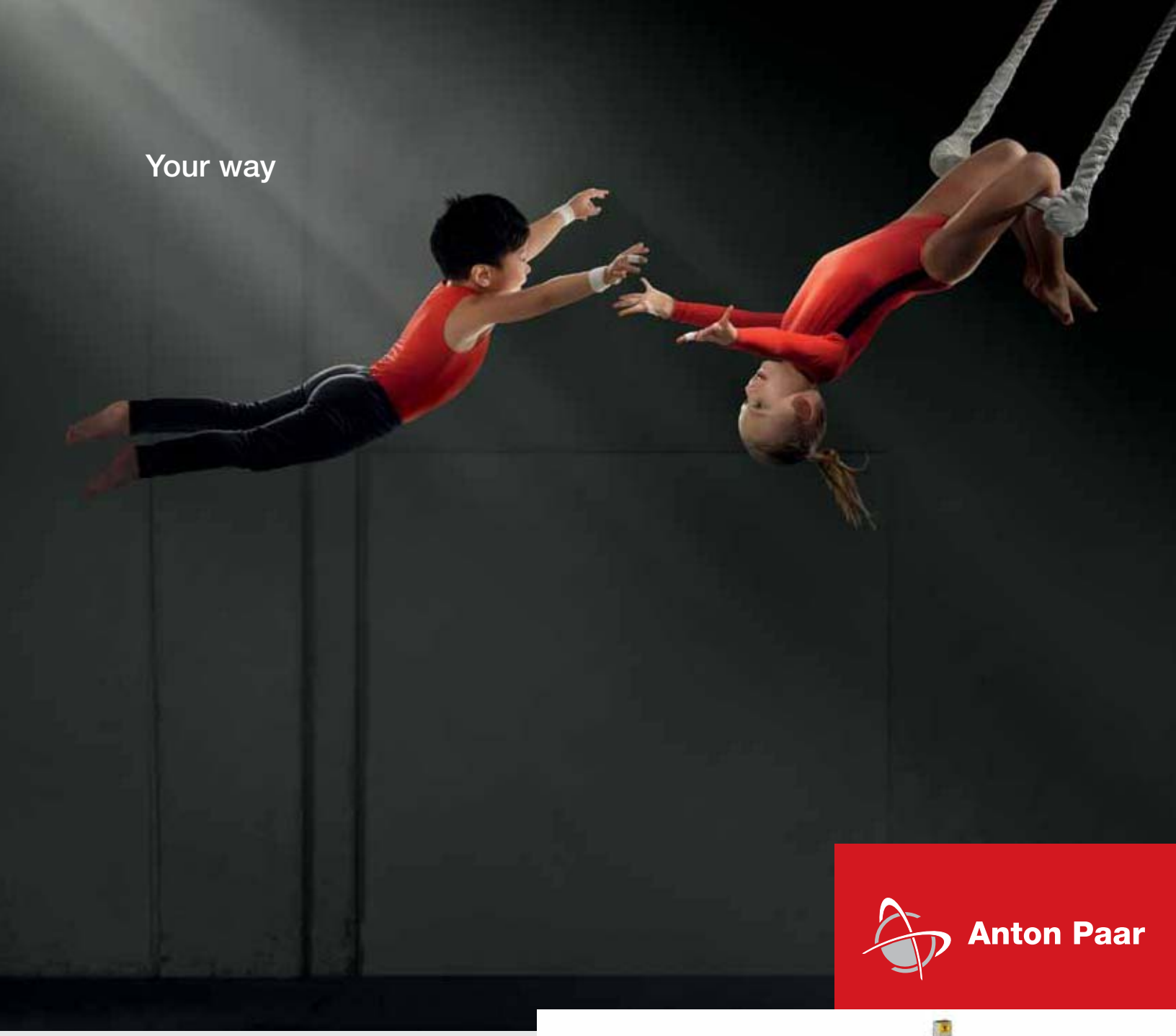
Cotton seeds (from Gossypium) provide a rich potential food source. However, the presence in the plant of the poisonous compound gossypol, has limited their use in this way. Attempts are being made to genetically modify some cotton plants to reduce the quantity of gossypol in the seeds to make them safe to eat, while preserving the quantity in the stems and leaves as needed to protect the plant from herbivores.

Gossypol has been tested in China as a male contraceptive, but trials were halted when it was discovered that its use led to permanent infertility.

Each plant on the trail has an information board and QR code which links to the online version of the trail. This contains more information on the plant and the compound(s) of interest and their uses, a 2D diagram and a representation of the 3D structure. You can also link to the full x-ray structural data in WebCSD. Even if you can't visit Cambridge in person, the virtual Trail can be followed at ***www.bit.ly/CCDCTrail***.

The Trail is designed to appeal to people of all ages and all levels of chemical knowledge and hopefully will demonstrate how x-ray crystallography can help us understand some of the chemistry going on all around us.

Gwynda Kyd



Anton Paar

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What does the U.S. National Committee for Crystallography do?

The USNCCr (sometimes referred to as USNC/Cr) has as its mission to represent the interests of the US crystallographic community to the International Union of Crystallography (IUCr) and to advocate in other forums, as you may have read in the Spring 2012 *RefleXions* article. It should be noted that this community includes all crystallographers employed in the US, regardless of citizenship. Here, I would like to talk about what the USNCCr does.

Individual crystallographers do not join the IUCr, rather countries do, by becoming adhering bodies to the IUCr. In the case of the US, the National Academy of Sciences (NAS) is the adhering body and the parent organization of the USNCCr. Within the Academy, the Board on International Scientific Organizations (BISO) hosts the national committees, including the USNCCr. Every three years there is an IUCr Congress, which includes a General Assembly. It is at this Assembly that elections are held and other business is discussed and voted on. The US delegation to the Assembly has five members, each of whom has one vote. The US delegation is nominated by the USNCCr and approved by the NAS president. In addition to this function, the USNCCr participates in a number of other activities.

The USNCCr has four subcommittees, including one on crystallographic databases, and one on crystallographic research resources. The latter focuses primarily on neutron- and synchrotron-based diffraction user facilities since they have become increasing central for almost all types of crystallography, with the possible exception of small-molecule single-crystal studies. In fact, one area for future consideration will be how to encourage growth of synchrotron and neutron diffraction in this arena. The USNCCr is also interested in enabling US crystallographers to join together to articulate their needs within the user facility community. In the area of databases, we have invited speakers to our meetings to discuss topics of current interest, such as "what is an appropriate delay for release of an electron density map from TEM-based crystallographic publications?"

US Delegates to the IUCr Congress in Madrid (August 2011). From left to right: Victor Young, Chris Cahill, Katherine Kantardjieff, Brian Toby, Joseph Ng

The committee is made up of twelve individual members plus a chair, vice-chair and secretary/treasurer. Committee members are elected to a three year term so four new members are elected each year. Unless elected as an officer, members can only serve two consecutive three-year terms and are limited to a maximum of twelve years on the committee. It is important that the committee be truly representative of the diversity within the crystallographic community and this is taken into account when selecting candidates to run for election to the committee.

Historically, the committee has expended considerable effort in two areas: helping foster crystallography in Latin America and improving crystallographic education. Both efforts have resulted in reports prepared in cooperation with the ACA that can be downloaded from the USNCCr web site (***sites.nationalacademies.org/PGA/biso/IUCr/PGA_071551***). In addition, thanks to NSF support, the committee has provided travel fellowships to facilitate the attendance of young scientists to the triennial IUCr congresses. The committee publicizes this program, selects the recipients and then organizes activities for them at the congress. Most recently the travel program has been transformed into a young observer program with participants invited to attend the assembly and other events. The committee has also participated in mentoring programs for younger scientists at both ACA and IUCr meetings.

The USNCCr also has an interest in crystallography beyond the US and is looking at ways to increase interactions between crystallographers in all the Americas. At recent IUCr congresses, we have arranged mixers to bring together the IUCr leadership, our committee members, and crystallographers from Canada and Latin America. The USNCCr has provided funds to subsidize students to attend the ACA crystallographic summer school.

In the future there are plans to do more in both Latin American outreach and in education, but another major undertaking for the committee will be to bring attention to the International Year of Crystallography (IYC 2014). For this to be effective, outreach to other organizations and communities is essential. Individuals who are interested in working on activities to publicize crystallography to the general public or the greater professional community should .contact ***brian.toby@anl.gov.***

The 2014 IUCr Congress, hosted by the Canadian National Committee, will be held in Montréal and the 2017 Congress will be in Hyderabad, India, but it is not too early to think about a bid in the Americas for 2020 or 2023. Toward that end the committee would like to encourage people to think about hosting a future congress in the US and to contact ***brian.toby@anl.gov***, if you are willing to work on preparing a bid.

Brian H. Toby

Advanced structural refinements with OLEX2

The first official US OLEX2 workshop on advanced crystal structure refinement techniques took place during the 2012 ACA meeting in Boston. Forty one enthusiastic participants from six countries came together for a full-day hands-on session on the opening day of the conference. The workshop was organized by Oleg Dolomanov and Horst Puschmann (OLEXSYS), and Ilia Guzei (University of Wisconsin-Madison), and cosponsored by the ACA, General Interest and Small Molecule SIGS, and OLEXSYS. The instructors began by demonstrating the OLEX2 GUI to introduce the participants to the multifunctional and thoughtfully laid out menus, submenus, and basic program features. Several practical examples of advanced structure handling were shown on the big screen and all participants were given ample time to repeat the steps on their laptops. Real time help from the instructors ensured that each person fully benefited from the exercises. Three instructors per 40 participants was the right ratio because unexpected issues surfaced with both Windows and MacOS, but the OLEX2 creators were able to expeditiously quench the fires. Most experienced crystallographers in the audience knew what was needed for each non-routine example structure, and the workshop showed them HOW to accomplish that with OLEX2. The highlights of the well-paced session were disorder modeling with (a) group or atom splitting algorithms built in the Refine menu and (b) idealized geometries, a procedure made exceptionally convenient within OLEX2 based on Ilia's library of idealized geometries (***xray.chem.wisc.edu/Resources.html***). The workshop closed with a demonstration of facile crystal structure report generation within the *Work->Report menu*; the full HTML report with tables is followed by a summary. All examples were meticulously described in easy-to-follow workshop notes that were distributed prior to the meeting. If you are interested in the workshop notes please contact the workshop organizers (***iguzei@chem.wisc.edu; horst@olexsys.org***). The frequently updated "Ilia's notes on OLEX2" are available at ***xray.chem.wisc.edu/Resources/Manuals/Ilia_Guzei_notes_on_OLEX2.pdf.*** OLEX2 is a large and powerful program that is conveniently interfaced with other popular programs such as SHELXL and SIR. OLEX2 is being actively developed with program updates and customer support second to none. OLEX2 may be downloaded free from ***www.olex2.org/.*** The Boston OLEX2 workshop received a lot of praise from the participants and there are plans to conduct another OLEX2 workshop at the 2014 IUCr Congress in Montreal.

Left to right: Horst Puschmann, Oleg Dolomanov, Ilia Guzei. (Photo by Peter Mueller)

Ilia Guzei

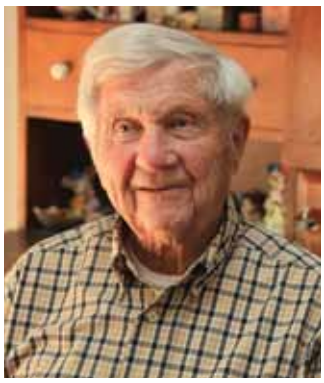
B.C. Wang on Dick Marsh: As a new PhD, I was very impressed by Dick's knowledge of crystallography and calculations. Two cases come to mind that I will never forget. When I showed him a Weissenberg photograph from the first cobalt complex I obtained in his lab, he looked at it and immediately gave me an estimate of the crystal's cell constants. Impressively, his estimate was within 5% of the calculated values. I later learned how to do this trick *after* he shared his secret. However, I never mastered the second one. Dick had memorized the logarithmic table. He could multiply two or three numbers in his head simply by adding their corresponding logarithmic values, and then convert the sum back to get the result. He could get the answer as quickly, or more quickly than I could with my slide rule!

Working in Dick's lab was a very valuable and pleasant experience. For example, every day around 10:30 am he would stop by the offices of students, postdocs and visiting scientists in our building and say "coffee time". Crystallographers from all over campus would then converge in the cafeteria for a short gathering. Those were memorable moments for me to meet many crystallographers and visiting scientists at Caltech at the time.

Some 30 years later Bob Sparks and I invited Dick to lecture at the ACA Summer School in Crystallography, which was held at the Univ. of Georgia from 1997-2001. Dick was very enthusiastic about the School. However, in 1997, we were uncertain if he would be able to lecture, but he did come. We found out upon his arrival at UGA that he and Helen were actually celebrating their 50th wedding anniversary that week and he detoured to UGA to give the lectures. We were all very appreciative and happy to celebrate this special occasion with him.

John Rose on Dick Marsh: Dick is probably best known by the community for his untiring work in checking for, and correcting, bad crystallography — such as missed space group symmetry in published structures or presentations. Crystallographers were wary of "being Marshed". To quote Peter Müller "Together with Richard Harlow's 'ORTEP of the Year' award, Marsh's work has encouraged careful work and crystallographic craftsmanship for decades." According to one Marshee (who wishes to remain anonymous), being Marshed was not a pleasant experience since colleagues ribbed you about missing obvious clues (e.g., funny or inconsistent bond lengths) and overall your reputation as a crystallographer was tarnished. Dick's analysis of the Cambridge Structural Database over the past 30 years has identified and corrected hundreds of structures and his work in structure validation has spawned several tools (e.g., PLATON/ADDSYM) to help validate crystal structures. In 2003, Dick was honored by the ACA as the inaugural recipient of the Kenneth N. Trueblood Award for outstanding achievement in chemical and computational crystallography. To quote Jenny Glusker (Chair, Trueblood Selection Committee), "Dick Marsh is a rare individual among crystallographers, an outstanding teacher and researcher who has greatly influenced so many students and faculty, as did Ken Trueblood during his 50 year career."

Dick Marsh on Dick Marsh: My crystallographic history began in September, 1945, the day after I was discharged from the Navy in New Orleans (chosen because it was the home of my fiancée, Helen Laterriere). I walked into the registrar's office of Tulane University with my G.I. bill in hand and asked if I could get into graduate school. They accepted me, with the warning that most classes were already filled. One that they found for me was held in the neighboring Sophie Newcomb College, the female counterpart of Tulane. The course was called something like "X-ray Crystallography", which I had never heard of, and was taught by R. C. L. Mooney, who warrants a digression.



Mooney had, a few years earlier, been accepted into graduate school at Caltech (my undergraduate school). But when Mooney arrived at Caltech, both sides were surprised: Caltech, because Mooney was a female (the "R" turned out to be "Rose"); and Mooney, because she did not know that Caltech, at that time, did not accept female students. What to do? My understanding is that Linus Pauling gave her a temporary appointment as research associate and helped arrange for her to transfer to the University of Chicago as a student of Will Zachariasen. She received her PhD there. After teaching at Newcomb she moved to MIT, where she later married the noted physicist John Slater.

Rose Mooney's office-laboratory-classroom contained a single x-ray tube and a Laue film holder — period. But she was a fine teacher, and I greatly enjoyed her crystallography class. As I recall, at that time Tulane did not offer a PhD program in chemistry, and after one year I was accepted at UCLA. Helen and I were married on August 11, 1947; as a wedding present I took her on a honeymoon trip of two thousand miles to the west coast, permanently displacing her from her family, all her friends, and the only city she had ever lived in. She seems to have forgiven me.

After my first year at UCLA I chose as my advisor Jim McCullough, who worked with organic selenium compounds. (He liked to tell stories about his evening trips home from his lab, and how all the other passengers moved to the far end of the streetcar when he climbed aboard.) I stayed far away from synthesis, but eagerly helped with McCullough's crystallographic research. One of his recent graduate students had been Gabrielle Hamburger (later, Donnay), and it was somehow comforting to have Gabrielle Hamburger, Martin Buerger, and C. W. Bunn so active in crystallography at that time.

At first our Fourier and structure calculations were carried out with pencil and paper, and with slide rules and logarithms. But soon we obtained a set of Patterson-Tunnell strips, which were similar to the world-renowned Beevers-Lipson strips, for carrying out Fourier summations. Mechanical calculators were also becoming available. Some would even do division, which caused large clanks as the carriage bumped up and down in moving from column to column. Servicemen from Friden, Marchant, or

Monroe suppliers were in frequent demand. I received my PhD at UCLA in 1950. (My thesis was described as "sophomoric" by one of the committee members.) I then accepted a post-doctoral research appointment at Caltech, and held such an un-tenured position until I became emeritus in 1990.

The post-war years were tremendously exciting for diffraction crystallographers. The influx of students under the GI bill and the availability of funding from such agencies as the Office of Naval Research and the National Foundation for Infantile Paralysis led to rapid advances in diffraction equipment, structure determination and refinement methods, and particularly in computing capabilities. As early as 1947 Ray Pepinsky, Penn State, developed XRAC — a two-dimensional array of sine-wave generators where the amplitudes and phases could be adjusted and combined to present, on an oscilloscope, a two-dimensional Fourier map. It was in constant demand from crystallographers everywhere. In 1950 SWAC was installed and maintained by Ken Trueblood and Bob Sparks at UCLA. It contained over 2000 vacuum tubes, and was programmed for least-squares refinement. As I recall, it would play "The Star-Spangled Banner" correctly when all the tubes were working. The age of computers had begun.

Crystallography was particularly exciting at Caltech, because of Linus Pauling. *The Nature of the Chemical Bond* had been published in 1948, and he and Bob Corey were preparing to publish their descriptions of the α–helix and the β-sheet. Many graduate students, postdoctoral fellows, and visitors from other institutions all over the world were at Caltech, working on structural problems of all sorts. (In 1956 Jack Dunitz, Leslie Orgel and Alex Rich published a joint paper from Caltech on the structure of the new aromatic compound ferrocene.) A special occasion, in 1953, was a conference in Pasadena on protein structures with attendees from around the world. I shall not forget one occasion. A young scientist, whose name I don't recall, gave a dry and, perhaps, confusing presentation on methods of estimating the scaling factor for diffraction intensities from globular proteins. At one point he showed a slide of the relationship between $I(q)$ — the measured intensity — and the diffraction spacing q. There was a question from the audience. It was W. L. Bragg: "Doctor, just what is your $I(q)$?" There was a long silence.

Dick Marsh and Linus Pauling at Pauling's 85th birthday celebration (CalTech, 1986).

My first paper from Caltech was with Pauling, on the structure of chlorine hydrate — one member of a number of crystalline gas hydrates stable somewhat above 0°C. Pauling, through his studies on intermetallic compounds, had developed a truly amazing insight into symmetric polyhedra, and he found that a polyhedron with twelve pentagonal faces and two hexagonal faces — a tetrakaidecahedron — and with equal edges of about 2.7 Å (a typical O–H···O bond) would fit into a cubic lattice so as to create a cage of water molecules able to accommodate the Cl_2 molecule. This cage approximated an oblate spheroid with a diameter at the equator large enough to hold a Cl_2 molecule but with a polar diameter slightly too small. In order to approximate the disordered arrangement of Cl atoms — bonded together and with populations decreasing with latitude — we resorted to Bessel functions to calculate the diffraction intensities. The R for comparing calculated and observed intensities was 0.32. While this value seems high, it was based on intensity estimates from several 30° oscillation photographs (prepared in a cold room at 4° C) which consisted of powder lines superimposed with many single-crystal reflections; estimating intensities was difficult and imprecise. Other models devised by us and other workers gave notably worse agreements.

As I think back to the time that I spent in that cold room with frozen, fumbling fingers I remember Lindo Patterson, then at McGill University in Montreal, boasting of the low-temperature experiments he carried out during the winter using diffraction equipment mounted immediately outside his office window.

At that time I also worked on the structures of a number of intermetallic compounds, mostly with David Shoemaker (before he moved to MIT and married Clara Brink). They included NaPb, with its fascinating Pb_4 tetrahedra; MgB_2; Ag_5Zn_8; and $NaZn_{13}$. The stoichiometry of such compounds interested quite a number of workers in the field who thought that the Fibonacci series might somehow be involved.

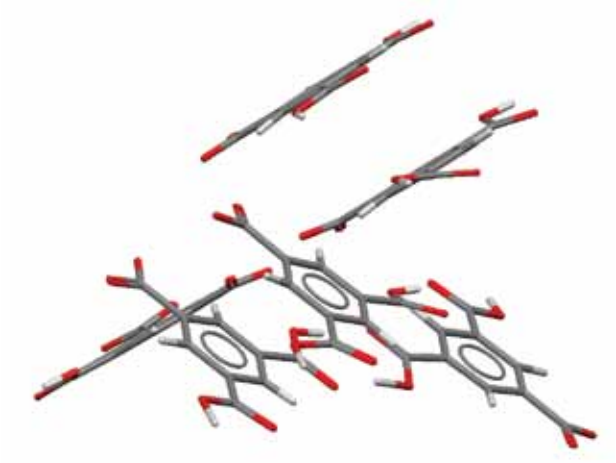
In 1952 Pauling saw a paper reporting the structure of the β (monoclinic) form of selenium, Se_8. He immediately knew it must be wrong. Rather than being an 8-membered ring as in the α (also monoclinic) form, one atom was displaced by about 1.1 Å so as to form a broken chain. It turned out that the problem could be corrected if the **y** coordinate of that atom were changed from **y** to **0.5 - y**. Since the structure determination was based on zero-level Weissenberg photographs (as was usual at that time), the only data that would be affected were the *hk0* reflections with *h* odd. The original author had reported problems in interpreting the *hk0* data, and the $R(F)$ for them was 0.31. Measured intensity values for these reflections were not included in the paper, but a reproduction of the *hk0* Weissenberg photograph was; we were able to estimate intensities directly from it and obtained an R of 0.18 for our revised structure. This experience no doubt influenced my later interests in incorrect structures.

A year or so later I became involved in a structural study on silk fibroin. This was a particularly interesting fibrous protein, since the worm's gland could be both stretched and rolled so as to achieve two-dimensional order, as expected for a β-sheet structure. Weissenberg photographs indicated not only the repeat distance along the polypeptide chain but the spacings between the sheets. There were two such spacings — a small one to accommodate the glycyl and alanyl residues and a larger one to accommodate the remaining residues. I believe this model has survived the test of 60 years. A vivid remembrance of that study is the daily

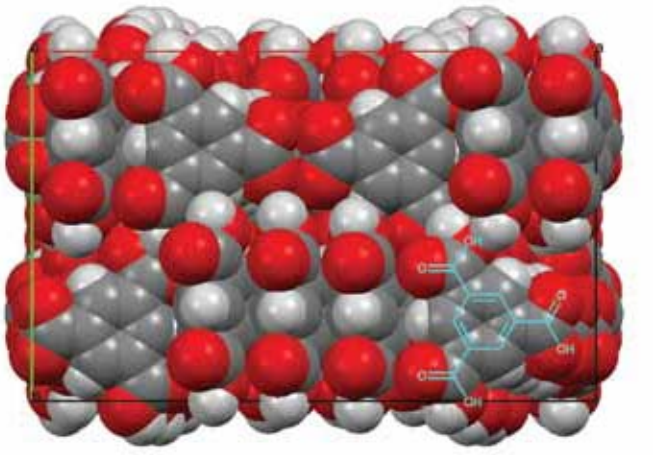
sessions of about one hour in Robert Corey's office, editing the one or two paragraphs of text that I had prepared the previous evening. Corey was a wise and gentle man, and he never once used the term "sophomoric".

At about the same time Joe Kraut, then a graduate student at Caltech, was spending happy hours at the local beaches collecting sea-gull feathers for his structural studies on feather-rachis keratin. As far as I know that rich, interesting diffraction pattern has not yet been satisfactorily explained.

I should like to mention one other structure determination, from 15 years later; it was part of Dave Duchamp's PhD thesis. The compound was trimesic acid — the symmetric tri-carboxylic acid derivative of benzene. Crystals were monoclinic, space group *C2/c*, with 48 molecules per cell (6 per asymmetric unit). This was a big computer chore for those times, but the structure was going to be interesting since an initial rotation photograph



Structure of trimesic acid, drawn from CSD entry BTCOAC by Jeff Deschamps (D. J. Duchamp & R. E. Marsh (1969). Acta Cryst. B25, 5).



clearly showed the Fourier transform of a six-membered ring and *h0l* Weissenberg photographs showed nearly exact **mm** symmetry. Complete data were collected, and the intensities of 11,563 independent reflections were estimated visually. As an aid to figuring out the structure, the Fourier transform of the molecule was generated from a cardboard mask placed in the path of a parallel light beam obtained from a pair of 12-inch lenses; comparing this optical transform with precession photographs suggested the orientations of the molecules in the **a, c** plane. The final least-squares refinement included 979 parameters and required about two hours on an IBM-7094 computer. All of this was carried out while Dave was developing the CRYM computing system of Fortran-based crystallographic programs. The resulting structure was based on six-membered rings of molecules hydrogen-bonded together to form pleated "chicken-wire" arrays; layers of three such arrays interpenetrated one another in a truly fantastic way. Maybe one can imagine Father Nature asking his wife, "How did you come up with that one, dear?"

For the past many years I have been concerned with the problem of incorrect structure determinations — almost invariably a mis-assignment of space group — appearing in the crystallographic literature. Small-molecule crystallography is, perhaps, unique in the amount of over-determination (in the ratio of observations to parameters) that it affords; there should be very little room for error. I somehow take such errors personally: they should not happen in MY field of study. Fortunately, in the past few years they have decreased in number, thanks to computer programs such as Checkcif and to slowly-successful pleas to journal editors to insure that authors make use of these programs. My recent surveys have suggested that the "wrong structure" disease may be getting close to extinction.

A couple of other highlights of my career: In 1993 I served as president of the ACA. Fortunately, Bill Duax was the Chief Executive Officer, S. N. Rao the Treasurer, Marcia Colquhoun the Director of Administrative Services, and Judith Flippen-Anderson and Connie Rajnak the *Newsletter* Editors. The ACA is extremely fortunate to have them still in place.

For a few years I participated in the ACA summer course in crystallography, first at Pittsburgh with Bryan Craven and then at Athens, Georgia, with B. C. Wang. These courses seemed to me to be very valuable, for both the students and the instructors, and I am sure they remain very valuable today. A vivid memory from the 1998 session was watching Herb Hauptman, also an instructor in the course, in the middle of downtown Athens leading a group of about 50 local residents singing (in French) the Marseillaise on the day that France won the World Cup.

My 67-year tour through crystallography has been delightful and fulfilling beyond description. With very few exceptions, the people I have been associated with (far, far too numerous to mention) have been stimulating and delightful. I have truly been blessed. Thank you, R. C. L. Mooney.

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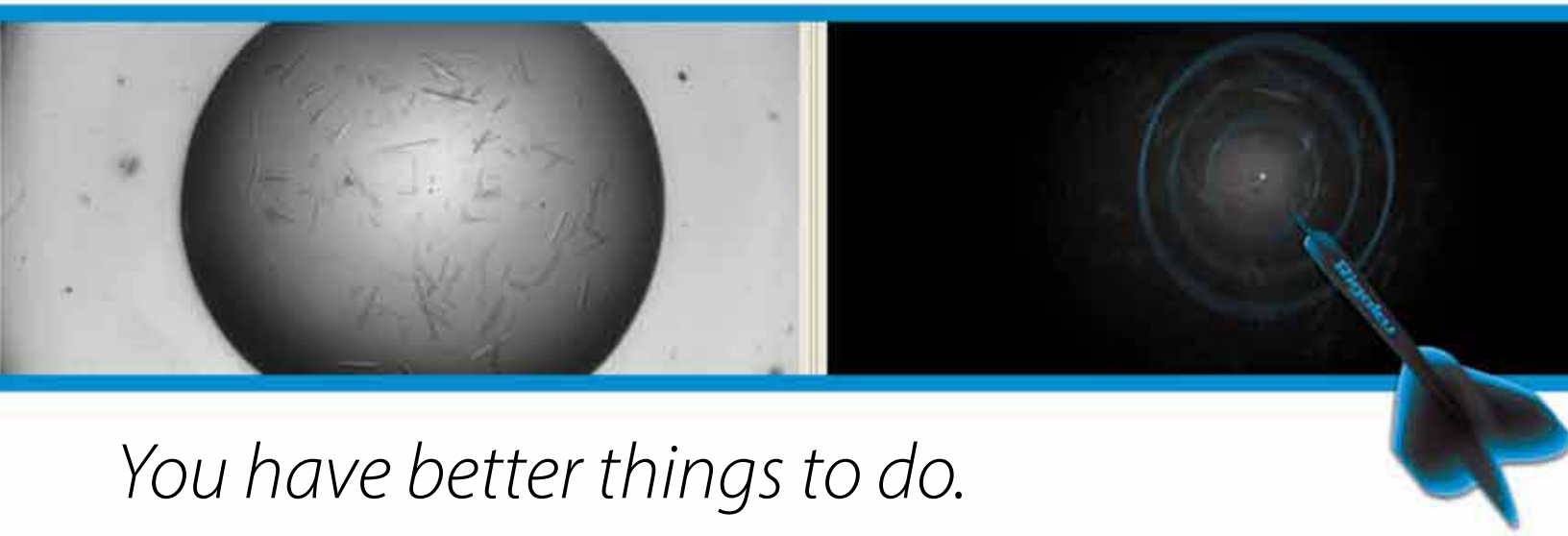

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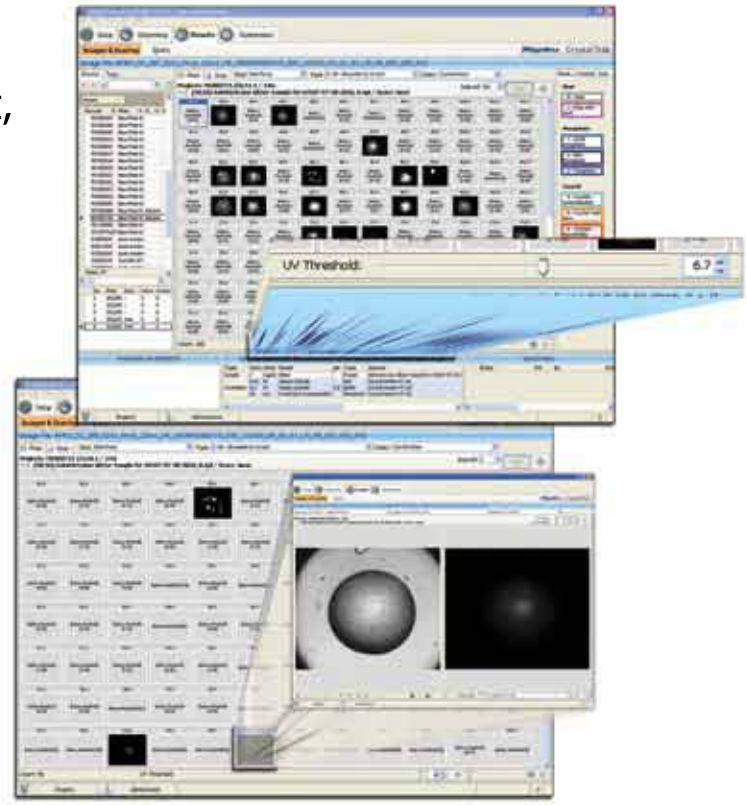

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After her graduate work at the University of Pittsburgh, Helen M. Berman moved to the Institute for Cancer Research in Philadelphia, where she began her studies of nucleic acid complexes with carcinogens and drugs. She continued her research in nucleic acid interactions at Rutgers University, where her interests in computing and databases led to her work as Director of the Nucleic Acid Database and as Director of the RCSB Protein Data Bank. Under her leadership the scientific and educational mission of the PDB has greatly expanded; there are now many convenient ways to search, display, and compare the information contained in the over 85,000 structures in the PDB. Helen has been recognized with many awards, notably the 2006 Buerger Award from the ACA and the 2012 Carl Brändén Award from the Protein Society.

I was born in Chicago and raised in Brooklyn, NY. My father was a physician, and my mother was a housewife who also acted as his office assistant for his medical practice. From as early as I can remember, I was strongly encouraged to pursue a medical career. Growing up, I attended New York City public schools and was always a very good student. After my junior year in high school, I was fortunate enough to be able to be in an NSF-sponsored program run by Moses Tendler at Yeshiva University. In that program, high school students took classes in the morning and were then assigned to research labs in New York City. I went to work in Ingrith Deyrup's laboratory at Barnard College. Ingrith, a biology professor, was studying active transport in kidneys. As part of my work in her lab, I had to learn how to work with animals from mice and rats to groundhogs. I coaxed the animals out of their cages that were on a roof of a college building on Broadway. After anesthetizing the animals, I removed their kidneys and performed further experiments under the direction of very kind and competent graduate students. It was quite an introduction to biology.

Helen and Barbara Low (Professor Emeritus of Biochemistry and Biophysics, Columbia University), who recently gave an invited lecture on penicillin to Helen's undergraduate honors class at Rutgers.

Largely at Ingrith's urging, I applied to Barnard College and was accepted. Barnard was a small women's college associated with Columbia University, and turned out to be the perfect school for me to attend. At Barnard I decided to major in chemistry. At the end of my second year, my physics professor Daniel Greenberg arranged for me to work in Barbara Low's (b. 1920) laboratory at Columbia College of Physicians and Surgeons. So in 1962 at the age of 19, I had my first experience working with crystals and I loved it. Every day I went into the cold room, selected a crystal that had been soaked in heavy atom solution, mounted it in a capillary, and took pictures on a precession camera. Barbara gave the undergraduates tutorials every week. Through these experiences, we learned about symmetry and diffraction and reciprocal space. By the end of the summer I knew that I wanted to be a crystallographer.

Helen and members of the Pittsburgh lab at a lab picnic in 1965 (David Zacharias, George Jeffrey and son, Ryonosuke Shiono and daughter).

When I graduated in 1964 I decided to pursue my graduate training at the University of Pittsburgh with George Allen "Jeff" Jeffrey. This meant of course that I had to leave my beloved New York to go to the Wild, Wild West (Yes, *The New Yorker* cover cartoon, in March 1976, by Daniel K. Wallingford is completely accurate). As per Jeff's advice, I took the minimum number of courses and began research very early on. Bryan Craven, Bob Rosenstein, Dick McMullan, Martin Sax and Ryonosuke Shiono trained the students in formal and informal settings. My research project involved determining the structures of carbohydrates, some of which were very challenging and provided a perfect test bed for the newly emerging direct methods. Many of the authors of these programs visited Pitt and I got a chance to use these programs and learn from the masters including Peter Main, Paul Beurskens and Syd Hall. I also became enamored of computing and how it was essential for our science. The students in my era also contributed to the Pitt experience. Sundaralingam directly preceded me, as did Sung-Hou Kim. Ned Seeman and George de Titta arrived just as I was finishing my degree. The experience at Pitt was intense and challenging. In addition to crystallography, Jeff was very interested in structure classification and comparison. It is clear to me now that this had a huge influence on my thinking.

In 1966 Sung Hou had moved on to Boston for his post doc at MIT, and through him I met the students of Cy Levinthal including Joel Sussman. I became fascinated by the world of protein folding. As part of my PhD qualifier, I had to create a hypothetical grant proposal. Strongly influenced by the work I had seen at MIT, I proposed to perform structure-based sequence comparisons of known proteins, make model peptides of conserved regions, and then determine the crystal structures to see if the fragments kept these structural features. Of course, this work would require access to protein structure coordinates—not something easily available at the time.

Once I completed my PhD and post doc at Pitt, I went to work in Jenny Glusker's laboratory at the Institute for Cancer

Research (ICR) in Philadelphia. During that period I worked with Joel Sussman, Sung-Hou Kim and Ned Seeman on the structure of a dinucleoside UpA. Since we worked in different cities and it was the 1970's, we referred to ourselves as the "East Coast Conspiracy".

Ned Seeman, Joel Sussman, Helen, and Sung-Hou Kim in front of MIT.

In that same time, I became very involved in trying to set up a repository for protein structures. Among the activists in this effort were Edgar Meyer and Gerson Cohen. We wrote letters to people and even had a petition sent to the ACA asking for support. In 1971, I went to the meeting on *Structure and Function of Proteins at the Three Dimensional Level* at Cold Spring Harbor Laboratory and further discussed the idea of a protein data resource. Protein crystallographers had already been talking about how to set up an archive and Walter Hamilton (Brookhaven National Laboratory) readily agreed to take on this project, especially since Edgar was working on a protein library at BNL. After forming an agreement with Olga Kennard at the Cambridge Crystallographic Data Centre, the Protein Data Bank was formally announced and after Walter's death, Tom Koetzle took over the leadership of that project. My involvement was advisory in nature; I was content that the PDB existed.

Walter Hamilton, Helen, and Tom Koetzle on the way to a meeting in Aarhus in 1972.

At ICR, I had a small research group who worked on drug nucleic acid fragments and the systematics of nucleic acid structure in collaboration with Stephen Neidle in London. I also became involved in setting up the research computing facilities for what was now the Fox Chase Cancer Center (FCCC). In 1979 my son Jason was born. Several of the female faculty began to discover the challenges of raising a family and maintaining a productive career, and we encouraged the establishment of a day care center at FCCC. All was wonderful and well until I was diagnosed with breast cancer in 1982 and again in 1986. In the midst of treatment I had to put together the abstract book for an ACA meeting, and thanks to Judy Flippen-Anderson we managed to meet all the deadlines. The experience of having cancer and working in a cancer center was very challenging and in 1988 I decided that I needed a new venue. In July 1989, I moved to Rutgers University as a Professor of Chemistry.

Stephen Neidle and Helen in his office at King's College London in the late 1970's.

Helen and her group at Rutgers in the early 1990s.

All my interests came together at Rutgers: crystallography, computers, nucleic acids, proteins, systematics. And I had the added bonus of being able to transfer knowledge to new generations of students. On the nucleic acid front, we continued to study structures of fragments and with Bohdan Schneider did a study of the hydration patterns around nucleic acids. We discovered that the patterns are local and predictable for the bases. With Wilma Olson, we established the Nucleic Acid Database as a repository for nucleic acids. The idea of that project was to create a home for nucleic acid structures of all sizes, which meant combining structures from the PDB and the CCDC. The NDB became a test bed for creating a searchable relational database. I became involved in creating the mmCIF dictionary working with Paula Fitzgerald, Phil Bourne and John Westbrook and used that formalism as the underlying structure of the NDB. By assuring me that collagen and nucleic acids had much in common, Barbara Brodsky, a professor at the medical school, convinced me to work on collagen. Together with Jordi Bella, we solved the structure of a model peptide of collagen and using the same methods Bohdan had developed for nucleic acid hydration, we

discovered predictable water patterns in collagen. One of the great pleasures of all this work was the participation of very bright undergraduate students. It was wonderful to work with them in the same way that my early mentors worked with me.

Meanwhile, the Protein Data Bank continued to grow at BNL. Joel Sussman became the lead in 1993 and for a time we worked together on the challenges involved in supporting the infrastructure required to manage these data. When the NSF issued a call for proposals in 1998, I decided that it was time to step forward and try to create a new generation PDB. I formed the RCSB consortium with Phil Bourne at the San Diego Supercomputer Center at the University of California San Diego and Gary Gilliland at the National Institute of Standards and Technology. We were funded to manage the PDB and its approximately 9000 structures.

mmCIF meeting in Brussels with John Westbrook, Phil Bourne, Paula Fitzgerald, Sydney Hall, and Shoshana Wodak.

Somehow, we got through the transition and were able to keep the resource going without any breaks in service. We learned to build the resource systematically and met the challenges of a production environment in which there is an expectation of 24/7 services. In 2003, we joined forces with PDBe headed by Kim Henrick and PDBj headed by Haruki Nakamura to form the Worldwide Protein Data Bank (wwPDB), thus ensuring that the PDB would remain a single, uniform and global service. And in 2011, with more than 80,000 structures in the archive, a symposium was held in Cold Spring Harbor commemorating the 40th anniversary of the PDB.

I feel very lucky that the dreams and aspirations I had as a young woman have come to fruition and that I have the privilege of continuing to do productive work. My son is now grown and a physicist. I discovered that I have the BRCA 1 mutation and yet have somehow survived. My dream is that in my lifetime we can understand biology and medicine at the molecular level so that it will be possible to circumvent the errors of our genes.

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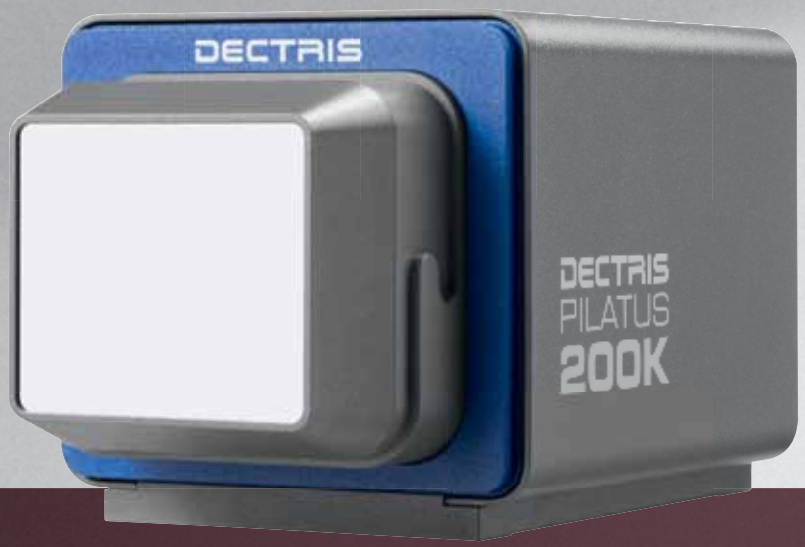

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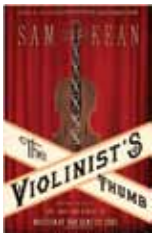


The Violinist's Thumb and Other Tales of Lost Love, War and Genius as Written by Our Genetic Code by Sam Kean, Little Brown Books, 2012, ISBN: 978-0-316-18231-7.

I heard about this book while listening to an interview with the author on *Science Friday*. I had read and thoroughly enjoyed Kean's earlier book, the *Disappearing Spoon*, and so bought a copy of TVT immediately. Many of the topics described are well known to this community but his treatment of the subject is refreshing. More importantly I learned some new and interesting tidbits about DNA.

The book is divided into four parts. The first part titled, *A, G, C, T and You* covers our understanding of what genes and DNA are and how we came to understand them. The work of Mendel (peas), Meischer (pus) and Morgan (fruitflies) gives us the basics we need to understand the genetic code. Of course, Watson, Crick and Franklin are mentioned here as well.

Next, *Our Animal Past*, covers the work of McClintock who elucidated the molecular basis of evolution. We also learn how the entire history of life on earth is encoded in our genes, how packed our genes are with foreign DNA, and when and how humans with 46 chromosomes diverged from other primates with 48 chromosomes. This latter story is underscored by the discovery of a healthy man in China with 44 chromosomes.

Part III, *Genes and Geniuses*, looks at how genetic records show we've gone through several evolutionary bottlenecks and how lucky we are to be here. The author looks at how genes and brain size relate as well as how we might use art in the mating process.

The last major section, the *Oracle of DNA*, looks at the forensic analysis of the DNA of famous people, for example Tutankhamen, who died at the age of 19 from what was probably too much inbreeding. A little bit of modern history comes out in the description of the battle between Venter and Watson and then Venter and Collins, with the result that neither group would have been successful in sequencing the human genome without the other. The author also reviews cloning and epigenetics.

In the epilogue the author describes his own experience with having his genome sequenced and the trepidation associated with finding out whether one has the genes for a specific familial disease.

The only flaw I could find was the lumping of the great apes and monkeys into a group called *monkeys*, as opposed to *primates*. It is not a big mistake, but means one has to be careful about other statements.

International Tables for Crystallography, Volume F, Crystallography of Biological Macromolecules, Editors Eddy Arnold, Daniel M. Himmel and Michael G. Rossmann, Second Edition, 2011.

I did not read this encyclopedia cover to cover. This is the first book I have reviewed for which I have not done this. Given its size and the fact that this is a second edition, I think you will forgive me. However, I did look carefully at sections that were new or had received major updates.

The book attempts to collate the sum total of all knowledge in macromolecular crystallography by soliciting experts on specific topics. It is very well indexed and referenced

If you place the first and second editions side by side, the first thing you will notice is that the second is a full centimeter thicker than the first. This is because many sections of the book have been updated. Others have received few or no update as they are historical and complete as originally written and some others should have received a refresher. Part 24, which covered software, has been dispersed into the sections for which the particular package is relevant.

When the first edition came out, I bought two copies, one for myself and one for my company. I reference mine frequently. The only books more worn on my shelf are my *IT Volume C*, and my *CRC Handbook of Chemistry and Physics* from graduate school.

Part 1 provides a historical perspective on crystallography from the editors and three contributors. For the most part it was not updated, but this is, along with Part 25, the story of the determination of the structure of lysozyme and is a must read for everyone. We often forget how easy crystallography is today and these parts remind us it wasn't so easy not so long ago. Part 1 did receive new sections by Himmel, Spence and Sun.

Part 2;2 (Einspahr and Weiss) covers the quality indicators for crystallography from diffraction data, various structure solution methods and refinement. The most commonly used indicators are tabulated at the end of the section.

Part 3;2 (Ernst, Yansura and Koth) describes membrane protein cloning, expression and purification.

Part 4 provides a current survey of crystallization methods (Sauter, *et al.*), modification of proteins to aid in crystallization (Derewenda) and high through put methods (Choi).

Part 8;1 (Helliwell) covers the current state of synchrotron radiation sources. Part 9 covers data collection. 9;1 is an updated version of the original (Dauter and Wilson) and covers the basics of monochromatic data collection. 9;2 (Earnest and Cork) reviews automatic sample changing and 9;3 (Shapiro) covers the new field of diffraction imaging.

Section 10;3 (Garman) describes radiation damage to crystals, an important topic not included in the first edition.

Section 11;7 (Yeates and Tsai) on detecting merohedry is completely new and is complemented by Section 18;12 which covers structure determination in the presence of twinning (Yeates and Sawaya).

Part 13;5 on the use of MOLREP (Vagin and Teplyakov) is also completely new.

Section 16;1, on *ab initio* phasing (Sheldrick, *et al.)* has received numerous updates in this edition and includes a discussion of the deceptively simple charge flipping method, while section 16;3, *ab initio* phasing or low resolution Fourier syntheses (Lunin, Urzhumtsev and Podjarny) is completely new.

Part 17;1, Macromolecular model building and validation with *Coot* (Emsley, Lohkamp and Cowtan) replaces the section on *O* from the first edition.

Part 18, Refinement, has a number of new additions. The sections on Atomic Resolution Refinement (Dauter *et al*.), ARP/wARP (Lamzin *et al*.), SHELX (Sheldrick), PrimeX (Bell *et al*.), are not new but have been updated while a section on PHENIX (Adams *et al*.) is completely new.

Part 19 covers other methods and includes several updated sections related to cryoEM and single particle reconstruction.

Part 21, Structure Validation, has new sections on KiNG (Chen *et al*.) and MolProbity (Chen *et al*.). Part 22 covers Molecular Geometry and Features. Section 22;3, Hydrogen Bonding in Biological Macromolecules, (Baker) has been updated.

Part 23, Structural Analysis and Classifications, has been refreshed with a new version of Protein-Fold Classification (Orenco and Thornton) as well as a new section on the interaction of halides with protein crystals (Vallelios *et al*.).

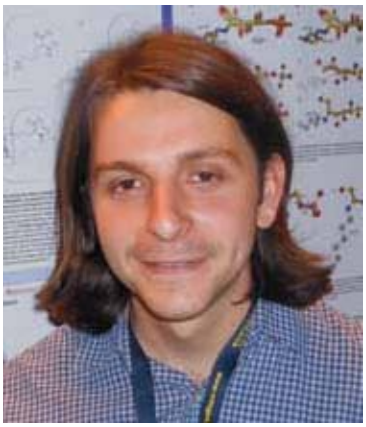
In Pursuit of the Unknown: 17 Equations That Changed the World, Ian Stewart, Basic Books, New York, 2012. (342 pp.). ISBN 978-0-465-02973-0.

Ian Stewart's latest book, *In Pursuit of the Unknown: 17 Equations That Changed the World*, offers a refreshing juxtaposition of theoretical and anecdotal material concerning, as the book's title implies, 17 equations that have fundamentally affected the various disciplines of math and science; these equations range from *Pythagoras' Theorem* (a sure throwback to any high school geometry class) to the *Black-Scholes Equation* (a financial market model that earned its namesakes the Nobel Prize in 1997) to *Maxwell's Equations* (another high school throwback- Advanced Placement (AP) Physics) and the *Navier-Stokes Equation* (derived from the application of Newton's Second Law to fluid motion). Stewart begins his discussion of each equation with some sort of anecdote, then progresses into the historical context of the equation, and concludes with insight into the theoretical nature of the equation and how the equation will continue to maintain its relevance in its respective field. Each discussion manages to maintain a balance between entertainment and enlightenment that can only be applauded in mathematic literature. The historical breadth and explanatory depth of Stewart's book is admirable. He transitions smoothly from his discussions of older mathematical concepts, such as the controversial development of calculus and *Newton's Law of Gravity*, to more recent ideas, including Einstein's *Theory of Relativity and Information Theory*. Additionally, Stewart dispels many modern misconceptions concerning the applications of these equations, and not only addresses appropriate situations for their use, but corrects inappropriate situations in which they can be mistakenly applied.

All in all, *In Pursuit of the Unknown* is an engaging and enjoyable read, appropriate not only for those interested in broadening their mathematical horizons, but really for anyone. It is humbling to realize just how essential mathematics is in the modern world.

Jeanette S. Ferrara, Princeton, Class of 2015

The following notes were written by recipients of travel grants to attend the ACA meeting in Boston (2012). They wre asked to comment on their personal exeriences at the meeting: the venue, the events for young scientists, the overall program and their own presentation. They all were very grateful for the awards and for many attendance would not have been possible without it. The 'kids' are the future of our science - please keep this in mind and contribute generously to the ACA student travel fund.



Sam Light

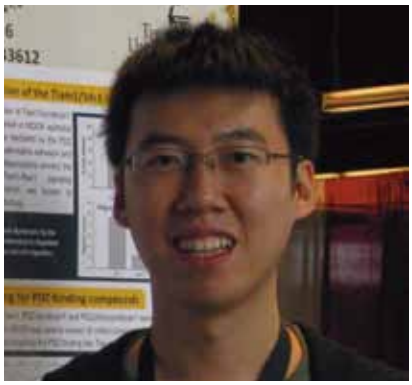
I found attendance at the meeting to be very rewarding. The broad scope of topics represented at the sessions helped me keep abreast of developing trends in structural biology and several talks unexpectedly bore direct relevance to my research – casting some of our data in a new light.

My poster presentation was also a decidedly positive experience. The research I presented focused on the connection between certain physical chemical principles and conformational changes that occur at an enzyme active site. Partly because the topic was more concept-based than most structural biology research, I was unsure how the poster would be received. Acceptance of the basic line of reasoning and apparent interest in the conclusions by many viewers provided encouragement and reaffirmed the work's importance in my mind. In addition, meeting and interacting with people at the poster session was rewarding in its own right.

Only in small part because of the tropical locale, I hope that I will be able to attend the conference next year.

Kathryn McCulloch

This meeting was a wonderful experience for me. It was my fourth meeting and I enjoyed becoming reacquainted with people I had met earlier. Everyone was welcoming and eager to share their science, which made the conference a lot of fun. Boston is a great city, with good food and a lot to do in the evenings. I returned from the meeting having heard many interesting presentations and aware of new techniques to try. It is always intriguing to learn about advances in technology, such as the new pixel array detectors and sample centering techniques like SONICC. I most enjoyed the events geared toward young scientists, such as the mixer and the Blackboard sessions on data collection. It was nice to meet others that are also in early stages of their careers and to hear about their experiences. The Blackboard sessions were informative because even when one is familiar with the programs being discussed, there are always new little tricks and tips to be learned. I am very much looking forward to attending next year.



Xu Liu

As a new member of ACA, this was my first meeting and the travel award allowed me to attend the entire conference. I found the meeting to be a comprehensive forum of crystallography, manifested by the breadth and depth of its scientific program. It was a great opportunity for me to network with a wide range of colleagues from fellow students to professors and beamline experts. I also attended the coot/refmac workshop on first day, which provided excellent systematic training on structure refinement. Not only did I boost my knowledge on general refinement procedures and low-resolution data processing tricks, but also I reduced the R- factor of my own structure by 4% during the practice session. I also liked having seminar and poster rooms in the same hotel, which was convenient and comfortable for all attendees. In addition, it was a pleasure to walk on the pier along the Atlantic ocean and on the campus of Harvard University after the sessions. Overall, I learned many valuable things including current advances and future directions, which will help me develop my career in protein crystallography. I am looking forward to more such interactions at next year's conference.

Adam Lietzan

The Boston meeting was a wonderful experience. The breadth of topics covered was, at times, overwhelming. There were so many interesting topics that it was often difficult to decide which session to attend. I particularly enjoyed the new format introduced this year in the *Data Collection with the Pros* session. Having the opportunity to see Zbigniew Dauter screen protein crystals, analyze diffraction data and troubleshoot problems that arise during data collection in real time

was truly informative. Exposing young crystallographers, such as myself, to proper data collection and analysis is an aspect of the conference I hope the ACA never abandons.

I also enjoyed the session entitled *Protein and Small Molecule Crystallography at Undergraduate Institutions: Research, Pedagogy and Professional Development*. It's comforting to see numerous researchers striving to increase the accessibility of x-ray crystallography to undergraduate students. Such initiatives serve to invite participation and broaden the excitement in crystallography for future generations.

Attending the ACA was an invigorating experience. I would like to thank all the individuals who organized this spectacular meeting and I look forward to attending many more in the future.

Li-Kai Liu

I enjoyed Boston and tried to take advantage of everything the meeting offered. The experience not only expanded my knowledge but helped guide me to the correct resources, people or information, that could shape my career path. Particularly, I was fortunate to be invited by Joseph Orgel to present preliminary results from my current thesis project and the positive interactions and feedback from the audience were very precious to me. Since a series of sessions ran in parallel, I was kept busy trying to attend as many talks of interest to me as possible. I also had the chance to talk to presenters at the poster sessions and to interact with representatives from the commercial sector. Overall I got to see not only how improvements in technology are advancing basic research in crystallography but to see how people make use of it to understand the composition of molecules or to come up with innovative applications. I feel lucky to work in this field and will certainly come back to another meeting.

Jonathan D. Cook

Not only was this my first ACA, it was my first time presenting my work at an international conference! I must say, I wasn't expecting the kind words and support that I received from all of the interested scientists that visited my poster. I truly felt that people cared about the science I was presenting!

The program was well rounded and I found that I learned something new in every session that I attended. I particularly enjoyed Andrea Thorn's talk on twinning during the Refmac workshop, and meeting with George Phillips during the Young Scientists Interest Group Mixer. We made some new friends from the University of Rochester and bumped into some old friends from across the US and Canada.

The Westin was a great place to spend a week, and Boston was beautiful. We managed to tour around Harvard and MIT during our stay, and even grabbed a pint of beer at the bar made famous in the television show "Cheers".

I am pleased to say that I am now a card-carrying member of the ACA, and I am looking forward to next year's event!

Ming Dong

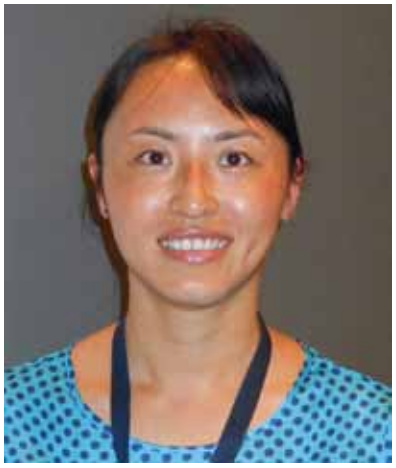
ACA 2012 was a great opportunity for me that could be very helpful for my future professional career. Being able to network with a large number of researchers having common scientific goals, challenges and interests expanded my horizons beyond my own research and experience and I was inspired by many of the talks.

I am an ACA member and this was my first meeting. Presenting at the poster session was a great opportunity to practice my presentation skills. I also got different perspectives and feedback that will be very helpful to my own research. It was especially good to meet other graduate students and learn about their research. Attending a workshop was great training that will broaden my crystallographic expertise.

I also made the most of the opportunity to talk to vendors and learn more about the latest equipment and techniques. The location of the hotel was good. It gave me a chance to visit one of the oldest cities in the states. Overall the program was great, not only covering my own interests, but offering opportunities to expand my knowledge beyond my own research. I would love to come back next year.

James Hall

This was my first time attending an ACA meeting and I have to say I was very surprised at the quality of both the program and the meeting location. I thought the hotel was a great venue and am especially grateful to the ACA for negotiating the reduced price for student rooms as this made it more affordable. The program was highly diverse with great coverage of my personal areas of interest as well as those that I would not normally be exposed to, such as the more technical aspects of detector design. In addition to this I found the exhibitors very approachable and more than willing to discuss their latest products with me which was really useful as it enabled me to find out about the latest developments in industry. I was also fortunate enough to be able to present a talk at the meeting which was well received. All in all this was both a productive and enjoyable meeting and I certainly look forward to attending ACA meetings in the future.



Wenhua Wang

The meeting was a great experience for me. It was my second ACA meeting but it was the first time I felt I had sufficient knowledge to fully appreciate the richness of the program.

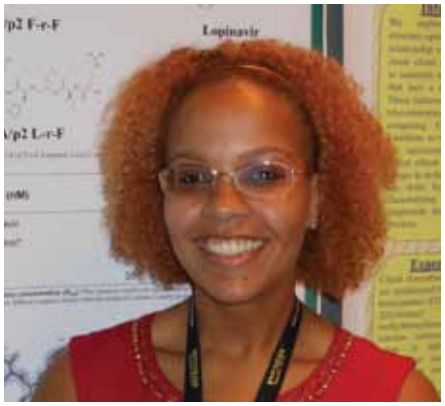
The sessions were well assembled with many informative talks. I especially loved the session *From Constructs to Crystals* in which many crystallographers' wisdom and tricks used to obtain crystals sparkled. The *Emerging Sources* sessions broadened my knowledge beyond that of classical crystallography. The *Membrane Protein and Structure-Guided Drug Discovery* sessions were still hot and eye-catching. I also enjoyed Donald Caspar's elaboration about *The History of Structural Biology*. It was a big plus of this meeting.

The social events and poster sessions were great venues to meet new people. Many fresh ideas came to me during the active discussions and I also learned how other mentors and labs function, which will definitely help me when I start to look for a post-doctoral position. One thing that was a little bit disappointing was that some people I wanted to talk to did not show up to their posters. I certainly appreciated all the good comments and feedback I received at my own poster.

Visiting the industrial booths and seeing some of the latest equipment and techniques was another fantastic part of the meeting. I really valued the opportunity to participate and I look forward to attending future ACA meetings.

Bhupinder Sandhu

This was my second experience at an ACA meeting. Once again the meeting hosted a large and diverse number of professionals and this time it was my privilege to present a talk on my research. It was an unforgettable experience. The remarks and comments following my talk will be helpful in my future research. In addition to hearing many excellent talks and viewing posters in so many different interesting research areas (it was often hard to choose which talk to attend at particular time) I was able to interact with many crystallographers to discuss my work as well as current topics in crystallography. It was nice to see again many familiar faces from the ACA summer school held in June this year where I shared many good experiences. I was able to see the beautiful sights in Boston and experience the city's rich history and culture. I am very grateful for having had the opportunity to attend meeting and I am looking forward to the ACA meeting in Hawaii next year.



Tamaria Dewdney

This was my first ACA meeting as well as my first visit to Boston and I thoroughly enjoyed my experience. Boston is a wonderful city with a rich historic culture and spectacular seafood. It was very welcoming to receive so many ribbons at registration; student, travel award winner, and first time attendee. I was very interested in the sessions on macromolecular crystallography and complimentary techniques where I learned a great deal about SAXS. The events for young scientist such as the mixer gave me an opportunity to network with my peers as well as with experienced scientists from both academia and industry. I gave a poster presentation this year that provided me the opportunity to discuss my work and receive important suggestions and advice regarding my project. My poster earned the Mattaiya Sundaralingam Pauling Poster Prize at the awards banquet. I am extremely grateful for this honor. The energy and

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excitement about crystallography was refreshing; encouraging me to return to the lab with renewed vigor to obtain new structures. Overall, I had a wonderful experience and hope to return to the ACA meeting in 2013.

Elena Aksel

This was my first time at ACA and it was an invaluable experience. During my PhD work I focused on the crystallographic structure of ceramics, so this conference introduced me to many new aspects of crystallography. I enjoyed the symposium on the *100 Years of Diffraction* and learned a great deal about the applications of crystallography for protein and pharmaceutical studies. However, I wish there were more sessions focused on materials.

I gave an invited talk in the *Total Scattering Analysis* session and received the 2012 Margaret C. Etter Student Lecturer Award from the Neutron Scattering SIG. This talk was a great opportunity for me and many intriguing discussions followed my presentation. I was able to follow up with several distinguished scientists in my field and get their feedback on my results. I also enjoyed the evening poster sessions where I was able to network with people from a wide range of fields. The conference as a whole was a wonderful experience for me.

Elena Forcén-Vázquez

The 2012 ACA meeting was my first experience outside Europe and it was great! Both the organization and the scientific program were excellent. There were lots of things to do and learn. At the Olex2 workshop I was able to improve my knowledge and learn about the new features of the program directly from the authors. Speakers in the scientific sessions included a large number of experts in fields that use crystallography. The *Transactions* Symposium in honor of Bruce M. Foxman was a delight; it was a pleasure for me to meet the people whose work over the years has been a reference for many others. I was given the opportunity to present a talk about my work in the *Cool Structures* session, thanks to which I could share and discuss many ideas with a good number of colleagues. Visiting the exhibits showed me that it was possible to discover new products and devices and talk about our necessities, wishes or doubts with the technical teams from the instrument companies. I also visited some nice posters and met face to face with their authors. In addition, the social program with the opening reception, the mixer and the banquet was a success; it was a good chance to meet people, especially the young participants. Thank you for the opportunity. I had a wonderful time in Boston, and I hope I can attend future ACA meetings.

Faye Clair Bowles

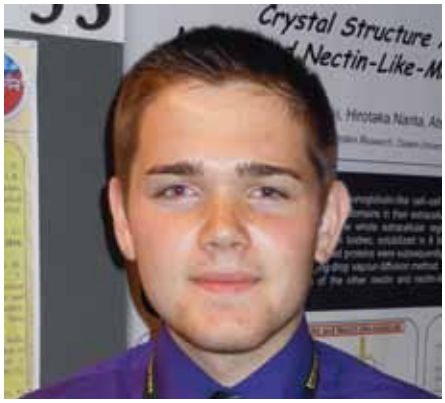
I just wanted to give a huge thank you to everyone who worked behind the scenes to make this year a success! This was my second ACA meeting and having it in Boston was remarkably historical. I learned more in one afternoon than my whole high school career! The young scientist session was fun! I cannot say much about my presentation, because I gave it! I loved giving it, no pressure and tons of fun! The receptions are always a great way to network and see everyone! I felt the program covered a wide range of topics, and it seemed to be scheduled in such a way that I could attend them all! I was in talks all week long, not saying it was a bad thing! My presentation on Tuesday went very well! It was my first presentation, and of course, I got the jitters! After my presentation, I had so many people come up to me ask me questions and I even networked some! My goals for the next meeting are to be a chair-elect for a SIG and to do another talk. I hope to stay actively involved in the ACA and look forward to seeing all my new friends in Hawaii!!

Marni Williams

ACA Boston was the first such meeting that I have attended that focused mainly on the field of crystallography. With a background in parasitology and using crystallography as a tool to understand mosquito immunity against malaria parasites, the meeting provided me with lots of new information. I thoroughly enjoyed the talks by the experts in the field as well as meeting fellow students. I also attended a workshop where I learned about new software tools for protein crystallography. The meeting was well organized and there was ample opportunity for interaction as well as for learning about new technologies from the exhibitors. The setting at the Westin hotel was convenient and receiving the travel award made it possible for me to stay at the conference venue. There were a large number of posters which meant that I did not receive as much attention as I would have liked, but I suppose that is normal at such a large meeting. I will definitely try to attend the next meeting in Hawaii if time and money permits, but for now I first need to solve a new protein structure!

Martin Donakowski

I really enjoyed the meeting in Boston and for reasons I had not anticipated. I came as an inorganic solid state crystallographer and knew the conference would consist largely of protein crystallography – but there were still great sessions related to my inorganic research. I thought that I would not enjoy the small molecule crystallography talks as my compounds do not contain any carbon; however, the principles of symmetry analyses and the capabilities organic chemists have in the design of crystals left me with many inspirations and techniques. It was these talks – not directly related to my work – from which I benefitted the most. This was my first oral presentation at a conference and I was happy to receive a thoughtful question afterwards. The talks were short in length which made it difficult to cover all of the background I wanted to in my talk, but ultimately it made for a good format to quickly learn about varied topics. The camaraderie was incredible: the Olympic games were playing so it made for the perfect atmosphere to meet people from different fields and different countries.

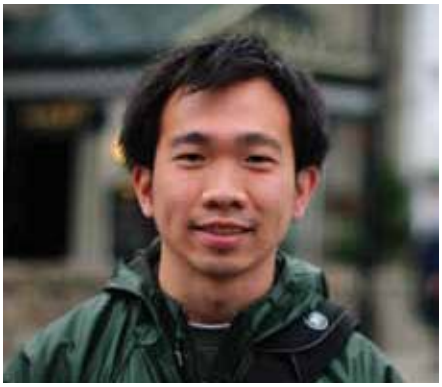


Max Kaganyuk

I'm a senior chemical engineering student at the University of Washington. My research professor urged me to apply for the 2012 ACA conference, which I am glad he did as I really enjoyed my experience. I attended to present my research on non-linear optical crystals that I worked on during a summer REU internship with Werner Kaminsky. I had a good experience presenting my research. The small size of the meeting allowed for an intimate setting for sharing your work with other researchers. The location was also ideal for touring the city of Boston. I got the chance to visit both MIT and Harvard. My trip was made possible by the travel grant and I urge, as my professor urged me, any students interested in presenting their research to consider applying for the 2013 ACA meeting.

Matthew J. Whitley

This was my first ACA meeting and I enjoyed my time at the conference very much. My research involves macromolecular crystallography, and I found plenty of interesting scientific content at the meeting to hold my attention. I was especially pleased by the breadth of content, which ranged from applications of crystallography in structural biology and enzymology to practical data collection strategies to technical crystallography topics such as advances in hardware and the latest capabilities of synchrotron beamlines. The wide variety of material presented allowed me to concentrate on the topics of greatest interest to me personally while still updating myself on developments in the wider world of crystallography. I also enjoyed the poster sessions, as they allowed plenty of time for conversing with the presenters in a relaxed atmosphere. I thought the Boston meeting was an overall success, and I look forward to attending additional ACA meetings in the future.



Allan Pang

I have been an active member of the British Crystallographic Association for over two years, but it was only this year that I decided to join the ACA and attend my first international conference. I was very fortunate that, even as a first timer, my abstract was chosen for an oral presentation. I am grateful that it was well received (although, I wish I had more time to explain and expound some more about my project).

What surprises me about the ACA Meeting is the number of attendees. I felt

at a bit of a loss as to who to talk to since there were so many people from other countries there. It was a bit disappointing that I did not have much time to talk to everyone. On the other hand, it was a great experience to get some tips from experts, and as a final year PhD student, I was also able to provide some helpful comments to a number of younger students. The conference provided a good venue for me to network with crystallographers of varied expertise.

I have to congratulate and applaud the people behind the program. I really enjoyed the variation of the talks. Sadly, I could not attend all of them as some of the good sessions (and interesting for me) were happening at the same time. I also enjoyed the exhibit show. They also gave some new ideas how to deal with difficulties I have encountered with my project. Overall, it was a pleasant experience and I will not think twice about attending the next one!

Pranoti Navare

This was my second ACA meeting and I was very pleased to have been selected to give an oral presentation in one of the General Interest sessions. For me, the best part of the meeting was the two sessions honoring Bruce Foxman and I found all the talks to be very interesting. It is worth mentioning that the talks on topotactic transformations, materials for sustainable future, and small molecule structures for important scientific advances were thought provoking. I also got the opportunity to interact with various exhibitors, and learn more about the current developments in x-ray instrumentation that enable the collection of high quality diffraction data. It was great to meet with other post-docs, graduate students, and researchers from the pharmaceutical community as well as to exchange interesting ideas with scientists whose text books/papers I have read. I am definitely looking forward to attending the 2013 ACA meeting in Hawaii.

Rama Sashank Madhurapantula

I joined the ACA earlier this year just as abstracts were invited for the conference. Little did I know that I would be giving a 10 minute talk on what I have been working on in the last year since the start of my doctoral work at Illinois Inst. of Technology Chicago in Joseph Orgel's Laboratory.

This was my first international conference ever and I was delighted when the abstract I submitted was accepted for a talk in the *Flesh and Blood: Intact & in situ Connective Tissue Diffraction Studies of Animals Plants & Insect Bodies* session. My research involves fiber diffraction on glycated rat tail tendons. We want to help understand the process of non enzymatic glycation of type I collagen in diabetic conditions.

I was even more elated when I was awarded with a travel grant that motivated me to make the best presentation I could. It was an awesome opportunity to present in the presence of the biggest names in fiber diffraction like Barbara Brodsky and Gerald Stubbs in a session chaired by Joseph Orgel and Olga Antipova.

The location was wonderful except for the fact that it was expensive even after I got the travel award. The arrangements were great and I got a chance to meet people whose research is parallel to ours and very interesting to me as I could closely relate what they were doing to what I see myself doing in the foreseeable future.

At the end of the meeting, I was nominated for the position of the secretary of the Fiber Diffraction SIG. This will greatly motivate me to work harder and better on my project in the coming years. I seriously couldn't have asked for better than this at this point in my career. I look forward to attending the next ACA meeting.

Sergai Kalynych

I thoroughly enjoyed the conference and have undoubtedly grown scientifically from my attendance. Many of the talks provided me with the ideas which will be useful for advancing my own research. The conference was organized exceptionally well and facilitated scientific exchange among students, postdocs and senior researchers on many levels. For me personally, it was also quite exciting to see the faces behind the names I've previously only seen on the author list of the top scientific journals. I also found the equipment exhibits particularly useful as they provided direct interactions with the manufacturers. I was impressed by the latest tools and technologies that are becoming available to the scientific community involved in macromolecular crystallography. Lastly, I would like to mention that I really enjoyed participating in an event for young scientists. It was a pleasure to get to know the graduate students from academic institutions across the globe. I don't think the meeting location could been chosen any more appropriately. The hotel was only steps away from beautiful Boston harbor with many excellent restaurants in the immediate vicinity. I hope that the next year is fruitful in terms of the scientific findings so that I could present my research developments at ACA Hawaii.

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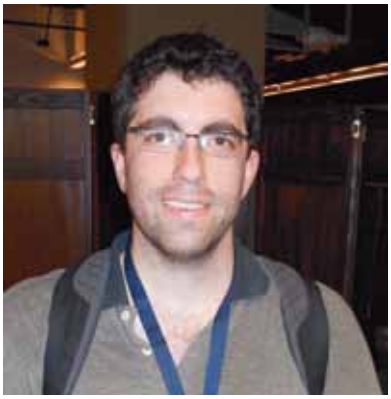


Christian Huck-Iriart

Boston mixes the beauty of a modern city with a little bit of Harry Potter. This was my first ACA meeting and I was very glad to be part of this wonderful reunion that honored the city where it was located. I applaud the effort of the organizers and senior members to include young people as part of the community. I am working with complex soft matter systems using scattering techniques. At the meeting I found lots of interesting topics that gave me several nice ideas for my work. In my opinion, the scattering section might be improved by the incorporation of a workshop focused on Small Angle Scattering. In general it was a very good conference attended by plenty of good people.

Shraddha Thakkar

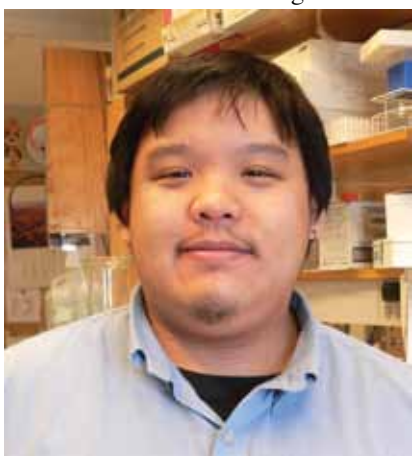
I am a graduate student at University of Arkansas for Medical Sciences. This was my second ACA meeting and once again it was a great and memorable experience for me. It was very beneficial to my career and it gave me many new perspectives about crystallography. I was honored to have been selected to speak in the *Structure-Guided Drug Discovery* session as the winner of the industrial-SIG Etter Student Lecturer Award. It was exciting to present my research along with leaders in the field and I was able to meet many well-known crystallographers. A number of parallel sessions were equally interesting and it very hard to decide which session to attend.

In addition to the talks, the poster sessions also covered diverse research from many different areas of crystallography and they were very well attended. The meeting had the right blend of people, from very well known academic and industrial researchers to enthusiastic students. The exhibits showcased the latest instruments and technologies, and choosing Boston as the venue for the meeting was excellent. I look forward to attending future meetings.

Sozanne Solmaz

After my non-voluntary abstinence from crystallography meetings for multiple years I was able to attend this year in Boston. The meeting offered me an excellent opportunity to get updated in the latest advances in x-ray crystallography, ranging from tips for the refinement of low resolution structures, to data collection cues from the pros and the use of long-wavelength x-rays for phasing. Other highlights for me were the lectures on the advancement of x-ray lasers.

I was selected for an oral presentation on our model of the transport channel of the nuclear pore complex, which is based on the structures of the interacting domains of the three proteins that line the channel. Its hallmark is a flexible mid-plane ring composed of Nup54 and Nup58, which can undergo large-scale conformational changes, leading to fluctuations of the channel diameter from ~20 to 45 nm. Several participants were intrigued by this feature, leading to some good discussions afterwards during the coffee-breaks and poster sessions. Overall, it was a very successful meeting and I would like to return next year. The only thing that could be improved is to have more common meals to facilitate better networking.



William Wan

The meeting was a good opportunity for me to present my own research and to learn about the new and exciting research of others. I gave a talk in the *Fibril-Forming Pathological Peptides* section, which allowed me to discuss my work and exchange ideas with other researchers in my field. In addition to this, the overall program of the meeting was diverse enough for me to explore different topics outside my own research area. I enjoyed being able to sit in one session on the latest synchrotron technologies and then move on to another about structural biology. As a student, I had ample opportunity to meet other students from around the world as well as to talk to professors and scientists outside my own university. In particular, I enjoyed Don Caspar's presentation on the history of structural biology. His talk gave us a great view of how past scientists gained their particular insights, and was useful in getting us to think about how to tackle the problems we work on now.

Yen-Tin Lai

This was my first ACA meeting and I loved it! Being a structural biologist, I was impressed by the wide range of topics that were covered. The latest developments about using crystallography to study biology were discussed by researchers from all over the country. Among all the wonderful talks, I enjoyed the award sessions and the lectures about the historical context of crystallography the most. It was inspiring to learn from established and famous researchers. Besides listening to talks, I also presented my research results as a poster. It was very helpful to exchange opinions and receive advice from other crystallographers. The evening activities were very relaxing, especially after spending all-day in the lectures. In the young-researcher-mixer, I not only met other students but also researchers at more advanced career stages. It was very exciting to discuss what might be a better career path with young PIs who have just started their own labs. It decreased the anxiety deep in my heart about the uncertainty of my academic career. This wonderful trip was capped by the recognition of my research with a Pauling poster award. I definitely will attend next yesr

Vijay Kumar

This was my first ACA meeting and I found it a very good learning experience. I met people from several backgrounds and made good scientific connections. The program was nicely arranged and. the events for young scientists were useful and it was good to get to know other new young researchers and hear about their exciting research. My presentation was very well received. However, in the future: 1) please include more variety of vegan/ vegetarian food during the YSSIG mixer, and 2) it would be great if the speakers presentations could be available after the meeting. I am much eager to attend next year.

D. Sean Froese

The meeting was a great experience. The location was excellent. The conference hotel was also a fine choice and a student-postdoc discount made it a viable place to stay. I really enjoyed the meeting format, with so many different talks going on at once, there was always a topic of interest being covered, even for someone without a crystallographic background like me. The drawback is that sometimes too many interesting lectures were occurring simultaneously; but I think the organizers struck a nice balance of concurrent subjects so that was not a large problem. As an invited speaker, I really appreciated the warmth and interest from my section chair, Zachary Wood, as well as from those in the audience. Waiting for my turn to speak, I was struck with the experience and presentation skills of those who went before me, but this did not diminish the respect I was shown. Finally, I really appreciated the poster sessions. .

Timothy Munsie

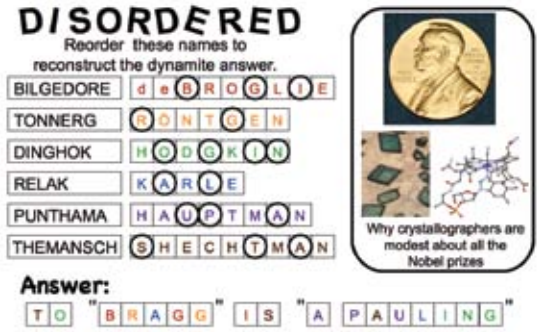
The most valuable part of the conference for me was meeting people and becoming part of the community. The depth of knowledge of the attendees made me realize how much more there is to learn and how rich the subject is. This was my first academic talk and just giving its was a great experience. I spoke on crystal growth methodology and how I'm using diffraction techniques to better understand and characterize the optical floating zone. The reception of the talk seemed to be quite positive based on the quality of questions and the discussions that resulted.

These will significantly help me to decide the next steps to take in my research and reinforced the value that crystallography has had and will continue to play. Even more importantly, the contacts and friends that I've now made give me the confidence to reach out to the rest of the community when I need help understanding or extending my research, which I've come to realize is an invaluable thing to someone who spends a significant part of their time trying to make new and novel materials. The conference was an interesting experience and I can only hope that I can come back in the future.

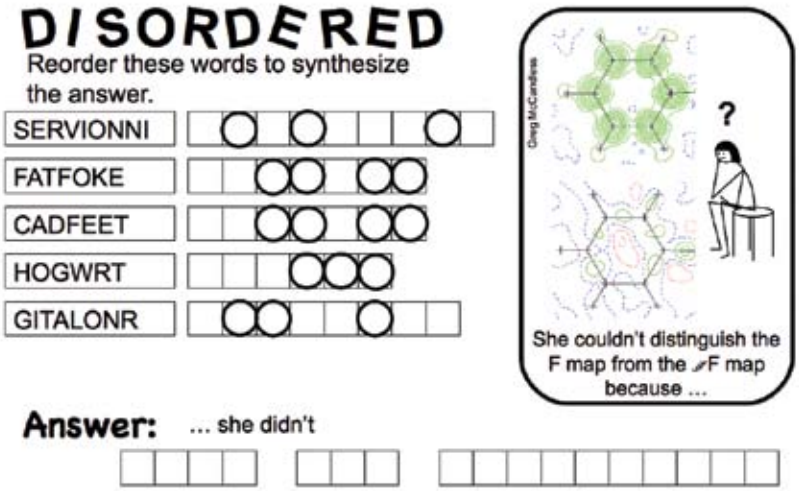
Sanaz Khorasani

This was not only my first international conference but my first time in the USA as well. The ACA meeting was very enjoyable, well organized and provided me a great opportunity to meet many foreign scientists. The poster sessions were interesting and encouraged interaction which allowed me to learn a lot from established researchers and other students. I was fortunate to attract a lot of interest to my poster, and to talk to many excellent crystallographers who have previously published papers related to my project. The compliments and advice were greatly appreciated and very encouraging. The young scientist mixer was awesome; it gave me an opportunity to speak with other students from all over the world and to become acquainted with their current studies and future career prospects.

Solution to the fall puzzle



New puzzle for winter 2012



Most of the speakers and attendees at the Women's Symposium, ACA McMaster University, 1986 were identified - can anyone provide names for the five still eluding us ?. In front, Judy Flippen-Anderson; first row, left to right: Helen Berman, Connie Chidester, Norma Duke, Gabrielle Donnay, Suzanne Fortier, Carol Brock, Jane Griffin, Kay Onan; Second row: Jenny Glusker, Ann Glusker, ?, Martha Teeter, ? in back, and ? in front, Miriam Rossi, ? behind Miriam, Penny Codding, Virginia Pett, Kim Watson, Marie Fraser, ?

Crystallography History Puzzle:

What are "wheaks" and "relps"?

What is "the Bucessera"?

What does "Vernished" mean?

Who was "A. L. Pon"?

What do the following words have in common?

BASSET, BULGAR, CARBON, CARNAL, CARPET, CITRUS, DOGSEX, FARMER, MUPPET, POSSUM, SURFER, WASHED

(puzzle adapted from *BCA News*)

quality

expertise | development | range | quality | support

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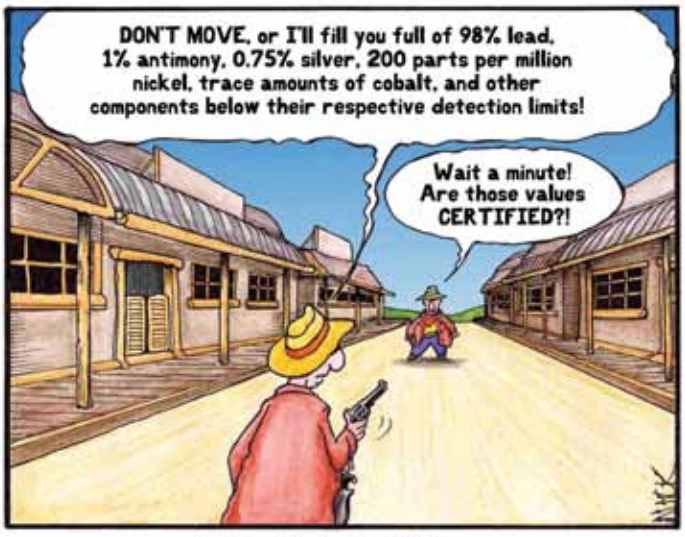
What's on the Cover

Single-crystal neutron structures from Brookhaven and Argonne National Laboratories. ***Upper Left:*** $[Rh_{13}H_2(CO)_{24}]^{3-}$: The First Accurate Characterization of Five-Coordinate Hydrogen Atoms. Bau, R. *et al*. *Science* (1997), **275**, 1099-1102. ***Upper Right:*** [*cis*-IrH(OH)$(PMe_3)_4]^+$. Milstein, D. *et al*. (1990) *J. Chem. Soc., Dalton Trans*., 1429-1432. ***Lower Left:*** $HReMn_2(CO)_{14}$. Bullock, R.M. *et al*. *J. Am. Chem. Soc*. (1992), **114**, 5125-5130. ***Lower Right***: $RuH(H_2)(PPh_2CH_2CH_2PPh_2)_2]^+$. Albinati, A. *et al*. (1997) *Inorg. Chim. Acta* **259**, 351-357. ***Central image:*** A neutron Laue pattern of a Nickel-Aluminum alloy crystal produced by the KOALA Laue Diffractometer at the Bragg Institute, ANSTO at Lucas Heights, Syndey. ***Credit for the molecular images:*** Tom Koetzle and Judith Otto.

Contributors to this Issue

Elena Aksel, Surajit Banerjee, Helen Berman, Faye Clair Bowler, Jonathan Cook, Graciela Delgado, Tamaria Dewdney, Martin Donakowski, Ming Dong, Joe Ferrara, Jeanette Ferrara, Elena Forcen-Vazquez, Frank Fronczek, Elspeth Garman, Ilia Guzei, James Hall, Christian Huck-Irart, Jim Kaduk, Max Kaganyuk, Sergai Kalynch, Sanaz Khorasani, Vijay Kumar, Gwynda Kyd, Yen-Tin Lai, Adam Lietzan, Sam Light, Xu Liu, Li-Kai Liu, Rame Sashank Madhurapantula, Dick Marsh, Kathryn McCulloch, Timothy Munsie, Pranoti Navare, Allen Oliver, Judith Otto, Allen Pang, Virginia Pett, George Phillips, David Rose, Bhupinder Sandhu, Amy Sarjeant, Sozanne Solmaz, Charlotte Stern, Steve Swinnea, Martha Teeter, Tom Terwilliger, Shraddha Thakkar, Brian Toby, William Wan, Wenhua Wang, Kraig Wheeler, Matthew Whitley, Marni Williams.

The CheMin team: Steve Chipera, Cherie N Achilles, Albert Yen, Allan Treiman, Joy A Crisp, David F Blake, Jack Farmer, Douglas W Ming, Philippe Sarrazin, Elizabeth B Rampe, Shaunna Morrison, Thomas F Bristow, Robert T Downs, Richard V Morris, David L Bish, David Vaniman.



Analytical Chemists in the Wild West

Cartoon from Nearing Zero (***www.lab-initio.com/***)

Emilio Segrè Visual Archives 2013 Calendar

Niels Bohr's atomic model has had an immense impact on the history of physics and is an icon of the scientific revolutions of the 20th century. Even today, high school students are presented with the model as an introduction to "the new physics." Bohr's achievements include the establishment and leadership of one of the most successful research institutions in the world, an interpretation of quantum mechanics with far-reaching philosophical implications, the explanation of nuclear fission, and a personal political mission for an "open world" in the face of the nuclear bomb. The History Programs of the American Institute of Physics and the Niels Bohr Archive, Denmark, celebrate the model's 100th anniversary with this calendar of select historical photos from his career. ***Order it online: http://photos.aip.org/calendar/***

FYI: The AIP Bulletin of Science Policy News

FYI summarizes science policy and budget developments in Washington affecting the physical science community. Summaries are issued two or more times every week. *FYI This Month* is distributed on a monthly basis, briefly summarizing major developments that were covered in more depth in *FYI*. Electronic subscriptions to *FYI* and *FYI This Month* are free; they are provided by AIP as a service to the science community. Subscribe at ***www.aip.org.***

Some of the latest *FYIs* included:

* - STEM Visa Bill Passes House; Stopped in Senate.
* - New Chairman for House Science, Space, and Technology Committee.
* - Update: U.S. Helium Program and U.S. Production of Molybdenum-99 .
* - Update on Actions Affecting Spending for Science Conferences.

ACA Election Results

Council Officers

Vice President
Martha Teeter
Treasurer
Jim Kaduk

Standing Committees

Communications
Graciela Delgado
Continuing Education
Kraig Wheeler
Data and Standards
Tom Terwilliger

SIGS

Biological Macromolecules
Chair-elect: Eddie Snell
Fiber
Chair-elect: Joseph Orgel
Secretary: Rama S. Madhurapantula
General Interest
Chair-elect: Peter Mueller
Secretary: Amy Sarjeant
Industrial
Chair-elect: Richard Staples
Materials Science
Chair-elect: Tyrel McQueen
Neutron Scattering
Chair-elect: Katherine Page
Powder Diffraction
Chair-elect: Michael Lufaso
Service Crystallography
Chair-elect: Peter Mueller
Small Angle Scattering
Chair-elect: Zhang Jiang
Small Molecules
Chair-elect: Amy Sarjeant
Synchrotron Radiation
Chair-elect: Corie Ralston
Young Scientist
Chair-elect: Yulia Sevryugina
Secretary: Jarrod French

Canadian Division

Secretary: Brian Patrick

Vice-President - Martha Teeter

Statement: 2014 has been proclaimed the International Year of Crystallography (IYCr). We should use this opportunity to increase public awareness of crystallography; to increase the awareness of the way crystallography underpins most of the technological developments in our modern society; to illustrate the universality of science; to increase the awareness of the way crystallography underpins investigations of cultural heritage artifacts; to promote education in crystallography and also to promote its links to other sciences.

As a crystallographer and science educator, I am keenly aware of an anti-science attitude among certain political candidates, corporations and their think tanks, and anti-science educators. I think crystallography provides wonderful opportunities to develop an awe of the natural world and the scientific method for children and adults. I am an advocate for multi-disciplinary approaches to teaching science as well as for scientific research. I would advocate for the many disciplines of crystallography represented in the ACA.

This juxtaposition of IYCr with anti-science trends presents tremendous opportunities to use crystallography to increase public and political awareness of science and its benefits. I plan to make this a major emphasis in my term on council. I envision enabling creation of a series of both short and longer videos and visual aids to bring crystallography before the world and document the accomplishments of diffraction, curriculum units for science teachers to professors, and creation of material to help politicians understand science and its contributions. I hope to elicit the creativity of old and young crystallographers in bringing this message to the world.

Funding for crystallographic research, which is very often interdisciplinary, is another priority for me. I will listen and learn from current and past councilors as to other issues facing the ACA at this juncture.

I appreciate this great honor and the chance for me to give back to a society that has provided much for me. I am thrilled to have the opportunity to represent a discipline of creative, honest individuals who are curious about the science, and many of whom have invented new crystallographic and computational tools to solve problems. This is a great time to share crystallography with the world.

Treasurer -James A. Kaduk

Statement: The duties of the ACA Treasurer consist of acting essentially as an internal auditor, representing the ACA on the AIP Committee of Society Treasurers and the USNCCr. As a member of the ACA Council, the Treasurer helps to set policy and strategy for the organization. I hope to continue to bridge the gaps between the powder/single crystal communities, as well as the materials/biological communities. The ACA is well run, and an obvious job of the council is to ensure that it stays that way, and has sufficient reserves to endure any rough patches. I believe in complete transparency, and hope to publish an annual report to summarize the financial and scientific accomplishments of the ACA to the wider world.

Continuing Education - Kraig Wheeler

Statement: Continuing Education within the context of the ACA describes a wide range of educational initiatives. The CEC serves as one of the critical service arms of the organization. It is distinguished as the only committee responsible for providing readily accessible professional development and thus its success (or demise) has far reaching implications.

My past service to the ACA has been enriching and I am excited by the opportunity and new challenge of serving on the CEC. For the last 18 years, my experience as a faculty member at a predominantly undergraduate institution has provided many opportunities to explore and support the education of x-ray crystallographers. Inspiring students through purposed instructional activities and research programs still holds much interest to me. This passion coupled with outreach activities (collaborations, organizing workshops and sessions) plus managing a small-molecule single-crystal x-ray facility has given me a unique perspective that should be of benefit to the ACA community.

Given the changing climate of the crystallographic community (instrumentation, software, and users), it is imperative that the committee develop accessible high-impact programs that reach a broad demographic of users such as:

Workshops and summer schools: The current offerings of ACA sponsored workshops and summer schools provide significant opportunities to train novice to seasoned users on the various aspects of crystallography. Because such activities are basic to the mission of the committee, evaluating existing practices and extending current directions to other projects would provide excellent opportunities to foster innovative instruction.

Next generation users: The success of tomorrow's crystallographers and users will require formal instruction and hands-on experiences with crystallographic theory, data, and instrumentation. Though this group most often includes post docs and graduate students, it is now increasingly apparent that there is considerable value in capturing an even younger crowd such as undergraduates and high school students. Academic and industrial institutions often serve as the initial point of exposure to our field; however, the ACA (the leading voice of crystallography in North America) should also play a pivotal role in the development of the next generation of x-ray users.

As with any organization, developing excellent training programs requires effective planning, promotion, oversight, and execution. The CEC is vitally important to the progress of our organization and profession and as such I am commited to support and strengthen existing initiatives and will help identify strategies to initiate new programs and resources.

Communications Committee Graciela Delgada

Statement: The ACA continues to incorporate new and better ways of communication. ACA publications have increased awarness of the association in the scientific community and should continue to grow in quality and scope. In today's world, any ideas and proposals coming from people of different latitudes should be welcome to better disseminate the important role that crystallography has played for decades in improving our quality of life. As a South American member of the ACA since 1987, I would like to contribute, through the Communications Committee, in the important task of making more people aware of the impact that crystallography has had and will continue to have in our lives. As a member of the steering committee established to organize the Latin American Union of Crystallography I will actively participate in the activities to be organized for the International Year of Crystallography (IYCr). I will also take this opportunity to strengthen the relationship between the ACA and the Latin American crystallographic community.

Data, Standards, and Computing Committee - Thomas C. Terwilliger

Statement: I am pleased to have been elected to help represent the ACA in the current international discussions of two major ideas for crystallographic data deposition and data interpretation. The first discussion is on the issue of deposition of diffraction images as a standard part of a PDB deposition. My personal view is that this is highly desirable if it can be accomplished with relatively low cost and relatively low burden to the investigators (see ***forums.iucr.org/viewtopic.php?f=21&t=79***). I will continue to listen to the views of ACA members as the discussion continues. The second discussion, related to the first but separate, is on continuous improvement of macromolecular crystal structures. The idea is that methods continually improve, so applying today's methods can improve yesterday's structures, and applying tomorrow's methods will improve today's structures. The question is whether it would be useful to change our paradigm of having a fixed interpretation of a crystallographic dataset into one where both the original and improved models might co-exist.

We gratefully acknowledge the continued support of our CORPORATE MEMBERS and welcome new members

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Etter Early Career
Eric Ortlund

Bau
Tom Koetzle

Fankuchen
Richard Dickerson

Trueblood
Tom Terwilliger

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Hawaii 2013
American Crystallographic Association

July 20 - July 24, 2013
Sheraton Waikiki
Student rooms: Princess Kaiulani
Deadlines:
Abstracts: March 31, 2013
Travel Grant Applications: March 31, 2013
Advance Registration: May 31, 2013
Hotel Reservations: June 18, 2013
Abstracts accepted online only
40% of all talks will be from contributed abstracts

Submit abstracts - Register - Full call for papers
Sponsorship Opportunities
Information for Exhibitors

www.amercrystalassn.org

Workshops

Biological SAXS - Theory and Practice
Organizers: Richard Gillilan & Eddie Snell

Introduction to GSAS-II Crystallographic Analysis System
Organizers: Robert von Dreele & Brian Toby

Get the Most out of the Cambridge Structural Database
Organizer: Pete Wood

Award Symposia

Bau Award in honor of Tom Koetzle
Trueblood Award in honor of Tom Terwilliger
Fankuchen Award in honor of Richard Dickerson
Margaret C. Etter Early Career Award in honor of Eric Ortlund

Transactions Symposium

Neutron & Synchrotron Sources: Role in Crystallography
Session I - Small Angle Scattering
Session II - Supramolecular Assemblies
Session III - Emerging Characterization Facilities and Tools
Session IV - Chemical Crystallography

Organizers: Richard Gillilan, Greg Hura, Christine Dunham, Eric Montemayor, Antonio dos Santos, Jonathon Hanson, Christine Beavers, Simon Teat

Evening Session
Enabling Partnerships for Broader Crystallographic Data Accessibility – Chairs: Joe Reibenspies, John Rose & John Westbrook

Microsymposia

SAS

Dynamic & Flexible Structures in Biomolecules (I) – Chairs: Michal Hammel & Yun-Xing Wang
Nanostructured Thin Films - Frontiers of Grazing Incidence Scattering– Chair: Detlef Smilgies
Membrane Protein Scattering – Chair: Shuo Qian

BioMac

Structural Enzymology (I) – Chairs: Gerald Audette & Rebecca Page
Structural Enzymology (II) Neucleotide Metabolism Modification & Interactions – Chairs: Zachary Wood & Hideki Ahara
Host Pathogen Interactions – Chairs: Erica Saphire & Graeme Conn

BioMac and YSSIG

Structure Validation – Chairs: Ed Collins & Andrew Torelli
Structural Biology for the Home Laboratory – Membranes – Chairs: George Lountos & Ward Smith
Exciting Structures – Chair: Angeline Lyon

BioMac and Synchrotron

Complementary Methods in Crystals and in Solution (I) – Chairs: Mike Becker & Eddie Snell
Complementary Methods in Crystals and in Solution (II) – Chair: Eric Ortlund

SAS and Neutron

Applications of SAS and Reflectometry in Energy-Related Materials – Chairs: Lilin He & Alex Hexemer

YSSSIG

Etter Early Career Award Symposium – Chair: Albert Reger
Career Odyssey Panel – Chairs: Katherine Hicks & Megan Sikowitz

Small Molecule, Service and Canadian Division

Cool Structures – Chairs: Richard Staples & Yulia Servyugina

Industrial

From Knowledge to Design: Data Mining in Materials Chemistry – Chairs: S. Ruetzel Edens & Peter Wood

Synchrotron

Multi-crystal and Micro-crystal Data Collection – Chairs: John Rose & Marian Szebenyi
Femtosecond X-ray Pulses: Tools for Crystallography – Chair: Michael Bogan
Femtosecond X-ray Pulses: Biological Applications – Eaton Lattman
Specialized MX Experiments – Chairs: Stephan Ginell & Gerd Rosenbaum

GIG

General Interest – Chairs: Xiaoping Wang, Jeanette Krause & Allen Oliver

Materials, Neutron, Powder, Service and Small Molecule

Materials for a Sustainable Future & Structure/Function of Metal-Org. Frameworks – Chairs: O. Borkiewicz, P. Khalifah & X. Wang

Materials, Neutron, and Powder

Nanomaterial Structure from Diffraction Data (I) Theory & Modeling – Chair: Thomas Proffen
Nanomaterial Structure from Diffraction Data (II) Experimental Advances – Chair: Katherine Page
Materials Discovery – Chairs: Fernando Uribe-Romo & Daniel Shoemaker
Better Ways of Finding Atoms (MEM & Other Techniques) – Chair: Saul Lapidus
Nanodomains and Beyond – Chair: Craig Bridges

Powder and Small Molecule

Contemporary Crystal Engineering – Chairs: Tomislav Friscic & Travis Holman

Powder, YSSIG, Service and GIG

Reviewer Practices – Engaging New Crystallographic Reviewers – Chair: Peter Mueller

Small Molecule, BioMac, Continuing Ed, GIG, and Canadian Division

Building Protein and Small Molecule Research Capacity at an Undergrad Inst. – Chairs Roger Rowlett & Kraig Wheeler

BioMac and Canadian Division

Structural Enzymology (I) – Chairs: Gerald Audette & Rebecca Page

Service and Canadian Division

Improving Structural Models Through Conformational Tips & Tricks – Chairs: Louise Dawe & Jason Mercer

SAS, Materials and Powder

Microstructural Evolution (Mesoscale)/Geologic Catalytic and Engineering – Chair: Ken Littrell

ACA Hawaii - July 20 - July 24, 2012

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 Waikiki Hotel.

New Schedule: The 2013 Meeting will have a 4-day, 5 concurrent session pattern such that there will still be as many talks as during a 5 day meeting. The meeting will start with workshops on Saturday, July 20, and scientific sessions on Sunday, July 21 and will end on Wednesday, July 24, after the Awards Banquet.

YSSIG Social Events: **Due to the new shorter meeting format the *Mentor/Mentee dinner* and the *YSSIG Mixer* will be combined into a single 'not to miss' event - stay tuned for further details that will be posted on the meeting website.**

Obtaining a VISA: Advanced 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 distributed only on CDs with a hardcopy Program Schedule.. We are not planning on having a meeting bag so if you would like one you should remember to bring your favorite from an earlier meeting.

Hotel Info: FREE WI-FI is included 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 which helps keep registration fees affordable.

All of our contracts include a number of lower cost rooms available to students. Room sharing can make them even more reasonable - use the ***Room Sharing*** feature under accommodations on the meeting web site.

As further incentive to stay in the conference hotel, a number of lucky attendees will be selected at random to receive one night's accommodation free!

Financial support: Young scientists will be available to apply for travel support through the ACA and the IUCr. Applications should be made by the abstract deadline on the meeting web site.

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.

Registration fees

Category	Early (before May31)	Late (after May 31)
Regular Member	$500	$700
Retired Member	$195	$295
Post doc Member	$250	$350
Student Member	$195	$295
Nonmember*	$700	$950
Post doc Nonmember*	$350	$450
Student Nonmember*	$285	$385
Guest**	$ 65	$ 65

WK.01 Biological SAXS - Theory and Practice	Student/Post-doc	$100
	Academic	$150
	Corporate	$250

	Students / Others
WK.02 Introduction to GSAS -II Crystallographic Analysis System	$75 / 100
WK.03 Getting the Most out of the Cambridge Structural Database	$130 / 170

Workshop fees will increase after May 31, 2013

Social events

Opening Mixer	included in reg. fee
Banquet	$70 ($35 students)
YSSIG Event	TBD

* The nonmember registration fee includes a complimentary one year ACA membership.
Those registering as nonmember post docs or nonmember students must include documentation of this status with the registration form.
**Guest registration includes Opening Reception and Exhibit Show.
Register on-line or download forms to register by fax or mail.

www.amercrystalassn.org/content/pages/2013-homepage
Questions: aca@hwi.buffalo.edu

JANUARY 2013

18-20 **CUWiP Conference for Undergraduate Women in Physics,** Colorado School of Mines & Denver West Marriott. Contact Ariel Bridgeman at ***abridgem@mines.edu.***

MAY 2013

26-29 **4th International Symposium on Diffraction Structural Biology.** Nagoya, Japan ***sbsp.jp/ISDSB2013/homepage/index.html***

JUNE 2013

16-20 **Workshop on Dynamic Structural Photocrystallography in Chemistry and Material Science.** Univ. of NY at Buffalo, SUNY. . Organizer: Phillip Coppens ***chem9988@buffalo.edu.***

JULY 2013

20-24 **ACA 2013 will be back in Hawaii at the SheratonWaikiki.** Program Chairs Allen Oliver ***aoliver2@nd.edu*** and Jeannette Krause ***jeanette.krause@uc.edu***

AUGUST 2013

4 - 9 **ICCOSS-XXI** International Conference on the Chemistry of the Organic Solid State, Oxford, UK. ***iccoss2013.org***

11-16 **ICCGE-17, 17th Int'l Conf. on Crystal Growth and Epitaxy.** University of Warsaw, Warsaw Poland. ***science24.com/event/iccge17/.***

25-29 **ECM28.** University of Warwick, UK. Contact: Sandy Blake, Chair of ECM28 at ***a.j.blake@nottingham.ac.uk. ecm28.org/.***

MAY 2014

20-24 **ACA 2014 Annual Meeting,** Albuquerque, NM, Albuquerque Convention Center & Hyatt Regency Hotel. Program Chairs: Christine Beavers, & Petrus Zwart. Local Chairs: Zoe Fisher & Kate Page.

AUGUST 2014

5-12 **XXIII Congress and General Assembly of the IUCr,** Montreal, Quebec, Canada. **www.iucr2014.org/.**

ACA Small Molecule Course 2013

The 10-day course will be offered from June 23 through July 3rd, 2013 at Northwestern University, in Evanston IL. This intensive course will emphasize both the theoretical and practical aspects of chemical crystallography. Diffraction theory, symmetry operations, structure solution and refinement, powder diffraction techniques and high energy sources are some of the topics that will be discussed. No prior knowledge of crystallography is expected from attendees. However, a good understanding of undergraduate level chemistry, physics and mathematics is desirable. Attendees are advised to read either: *Crystal Structure Analysis: A Primer*, 3rd Ed. by Jenny P. Glusker and Kenneth N. Trueblood (Oxford Univ. Press, 2010) or *Crystal Structure Determination*, 2nd Ed. by Werner Massa (Springer, 2004) as preparation for the course. While the course is geared toward the graduate level, applications from strong undergraduates will be considered. The course is limited to a total of 25 attendees. In previous years there has been a broad demographic of participants from both the US and abroad with affiliations in academia, government and industry. The faculty comprises experienced crystallographers with varied research backgrounds from national labs, industry and academia.

Instruction is divided into three sections: Theory lectures are given during the morning sessions; workshops and data collections will occur in the afternoon and evening sessions. Participants will receive hands-on experience preparing crystalline samples for single-crystal and powder diffraction experiments; setting up and running data collections; processing data; and solving and refining structures. Several single-crystal and powder instruments will be available for the duration of the course, and attendees are encouraged to bring their own samples for data analysis. Commonly used software packages and crystallographic databases will be made available on university computers. Attendees are not required to bring their own computers.

Application information and registration fees can be found on the course website at ***www.acasummercourse.net***. Housing is available on-campus at Northwestern for approximately $500 for the duration of the 10-day course. A limited number of partial scholarships are available for student-level attendees based on scientific ability, and expected benefits from participating in the course. Some meals will be provided, and there are many dining options both on and off campus.

Northwestern University is located on the shores of Lake Michigan, just north of Chicago, in Evanston IL. The campus is linked by public transportation to O'Hare and Midway International Airports and Union Station (Amtrak).

For further information, please see our website at ***www.acasummercourse.net*** or e-mail us at ***info@acasummercourse.net***. Applications will be considered on a rolling basis, with a deadline of April 1st. We encourage international participants who require visas for travel to the US to begin the application process early.

Amy Sarjeant, Allen Oliver & Charlotte Stern

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