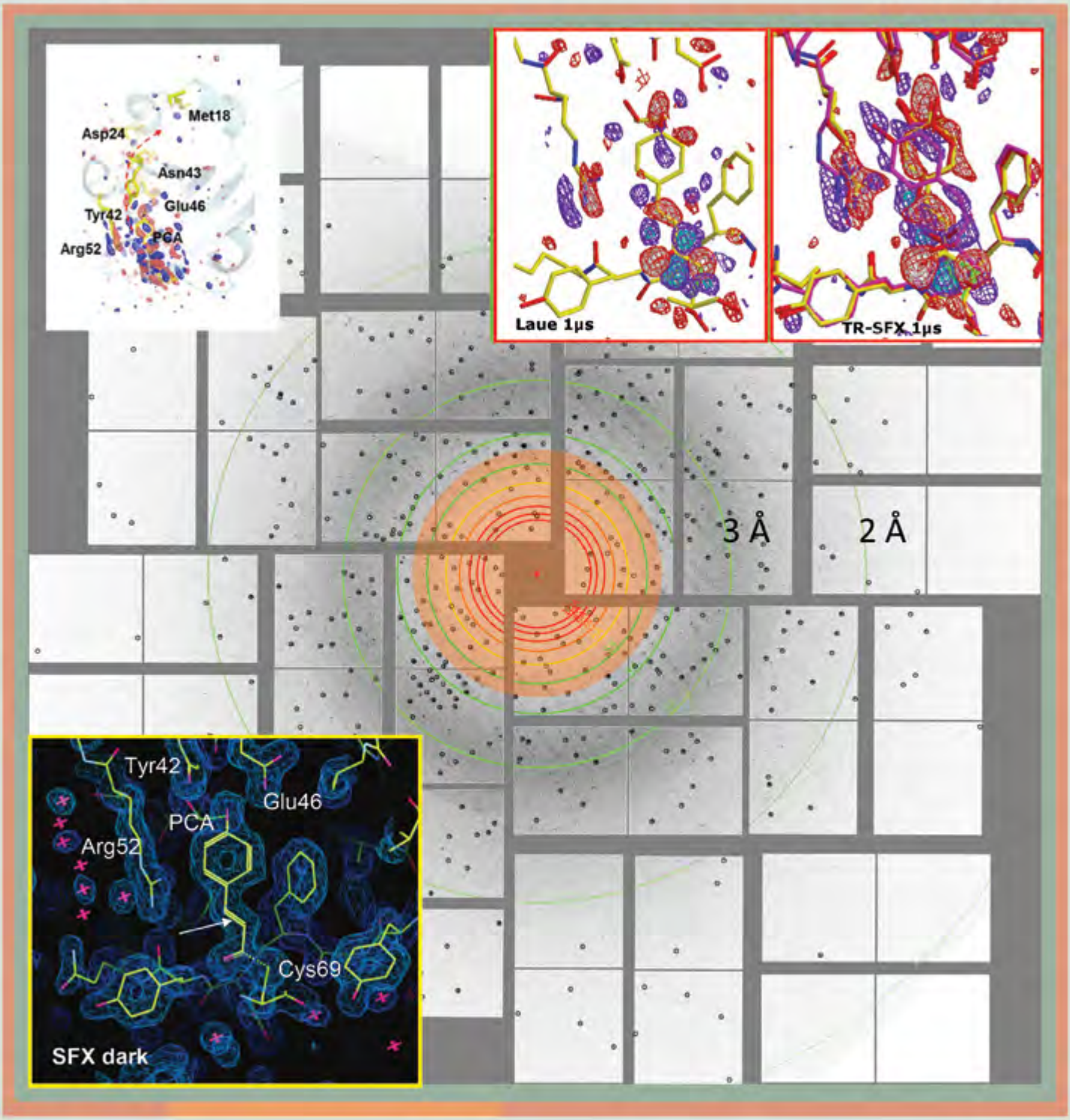
ACA RefleXions

American Crystallographic Association
Structure Matters

Number 4

Winter, 2015



Time-Resolved Serial Femtosecond Crystallography at Philadelphia ACA Meeting

ACA RefleXions

ACA - Structure Matters
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Contributions to ***ACA RefleXions*** may be sent to either of the *Editors*:

Judith L. Flippen-Anderson ..... **acareflexions@gmail.com**

Thomas F. Koetzle ..... **tkoetzle@aol.com**

Cover:	Connie Rajnak	Book Reviews:	Joe Ferrara
Historian:	Virginia Pett	Net RefleXions:	Anastasiya Vinokur
Photographer:	Peter Müller	News & Awards:	Chiara Pastore
Copy Editing:	Jane Griffin	Puzzle Corner:	Frank Fronczek

Spotlight on Stamps Daniel Rabinovich

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

Marcia J. Colquhoun, Director of Administrative Services
American Crystallographic Association
P.O. Box 96, Ellicott Station
Buffalo, NY 14205
tel: 716-898-8692; fax: 716-898-8695
marcia@hwi.buffalo.edu

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

ACA RefleXions (ISSN 1058-9945) Number 4, 2015. Published four times per year in the spring, summer, fall, and winter for the membership of the American Crystallographic Association, P.O. Box 96, Ellicott Station, Buffalo, NY 14205-0096. Membership in the ACA includes a non-deductible charge of $1.75 from membership dues to be applied to a subscription to *ACA RefleXions*. Periodicals postage paid at Buffalo, New York. POSTMASTER: Send address changes to ACA, P.O.Box 96, Ellicott Station, Buffalo, NY 14205-0096.

President's Column

It is with a heavy heart, yet one brimming with pride that I pen my final column as ACA President. The last year has been an amazing experience for me, as having the honor and responsibility of leading this august society has been truly gratifying, enlightening and in many ways, transformative. Perhaps my biggest take-away from the past year, however, has been recognizing the passion, commitment and pride ACA members have in our organization – 'member driven' puts it mildly!

I will take a final opportunity to thank our CEO Bill Duax; CFO S. N. Rao, Director of Administrative Serves and Meetings Manager, Marcia Colquhoun and our Membership Secretary, Kristina Vitale for their tireless efforts that keep the ACA running on our behalf. We are also lucky to have countless members who volunteer their time to make this organization what it is today. I would like to thank all of the Council members with whom I have served and acknowledge their efforts as well. The ACA is fortunate that Mike James will continue to represent our Canadian members and that Diana Tomchick will continue as ACA secretary. Personally, I am grateful to outgoing Past President Martha Teeter for her leadership and mentoring, as well as outgoing Treasurer Jim Kaduk for his breadth of experience and attention to detail. In 2016 Martin Donakowski will be the YSSIG Representative to Council and Hanna Dabkowska will continue to bring the IUCr perspective to our Council meetings. Moreover, the entire ACA is indebted to Tom Koetzle for his herculean efforts producing the fall issue of *RefleXions* with all the reviews from the Philadelphia meeting, and to Judy Flippen-Anderson for her work on *RefleXions* and for her tireless advocacy of our journal, *Structural Dynamics*. We are of course happy to welcome two new members to Council – Sue Byram as Treasurer and Amy Sarjeant as Vice-President. I think you will agree that we have a great line-up going forward, especially with Tom Terwilliger taking the reins as President.

While we are on the subject of changes, and I hope you are sitting down, some significant changes are afoot in Buffalo. Both Bill and Marcia have announced their pending retirements. Yes – you read that correctly. They have given us three years notice (which is more than anyone could hope for!), and we have our work cut out for us to keep the momentum of their 25+ years of effort and contributions going strong. Please take a moment to thank them both but don't panic, we've still got a few years to get oriented for the future.

Speaking of the future, these announcements prompt an array of questions. Most notably, what will the ACA look like in three, five or ten years and beyond? In many respects the timing of these developments is coincident with a number of other, very real challenges. Previous President's columns have reflected on challenges facing many societies: declining membership, the role or value of societies like the ACA in today's climate of social media, open access publishing, etc. As such, I feel that we have an opportunity here to look deeply and thoughtfully at how we structure the ACA to not only meet, but get out in front of a number of these issues. Major personnel changes also present an opportunity to reflect on the overall organizational chart. I think the ACA should do just that and consider a range of models going forward.

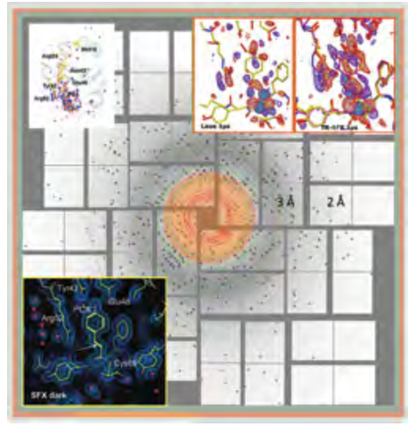
Financial challenges, including the ACA's dependence on our annual meeting for revenue and the issues confronting many societies regarding relevance, are not trivial. We should acknowledge and embrace these challenges and look ahead to leveraging our resources using best practices delineated in the broader scientific community. ACA's participation in the Council of Scientific Society Presidents (CSSP) has helped foster an awareness of challenges/opportunities in this arena, as has my engagement with AIP's Board of Directors. The latter has led me to believe we can make even more use of our parent organization.

What does this mean in the near term and how do we develop a succession plan? Immediate steps include the formation of a succession committee. Council (at the Fall meeting) voted to create such an entity and I have been charged with populating it. We will happily entertain volunteers or suggestions and I intend to have the committee established in advance of the spring Council meeting. An official charge is still in the works, yet one may obviously infer from this column what needs to be accomplished: figure out what to do next, who will do it, where will it be and how much it will cost … all the while maintaining the identity of the ACA, promoting its mission and tackling any and all challenges head on. No sweat …. Deep breath! I look forward to working with all of you on this and I will make these activities the priority of my term as Past President.

My summer President's column alerted you to some personal professional developments wherein I was selected as an AIP State Department Science Fellow. As such, I have begun a sabbatical this past August in the Bureau of International Security and Nonproliferation, Office of Weapons of Mass Destruction and Terrorism (ISN/WMDT). I look forward to the next issue of *RefleXions* where I can provide a few more details as to this experience. Security clearance comes with a few challenges, and clearing one's report for print is one of them. That said, I am on the Nuclear Forensics team and am hard at work on strengthening the core capacities of other countries to prevent and investigate illegal uses of radioactive materials. Engaging with the broader international community is indeed intriguing and I am becoming keenly aware of different perspectives and approaches to problem-solving around the world. I have had some unique travel expriences thus far and, despite my interest in nuclear science, I seem to impress more folks when I engage on crystallography! Stay tuned for a more detailed AAR (or 'After Action Report,' as they say in the biz!).

Thank you again for the honor and privilege of serving as ACA President. I hope I did not do too much damage and I look forward to the future of our science and of our society.

Chris Cahill



What's on the Cover

Marius Schmidt, an invited speaker in session 2.1.5: Structural Dynamics, chaired by Keith Moffat and George Phillips, kindly supplied all the figures shown on the cover. The background is a diffraction pattern from photoactive yellow protein (PYP) microcrystals; the data was collected on the CSPAD, (Cornell-SLAC-Pixel-Area Detector). The central orange mask denotes electronic attenuation to boost the dynamic range.

At upper left: a strong **D**ifference **E**lectron **D**ensity (DED) map from TR-SFX x-ray data. Some dark state residues are shown in yellow; the dark state structure is displayed by the light blue ribbon. Negative difference electron density is in red, positive in blue. Large features up to -22σ / +18σ are present.

The images at upper right zoom into the chromophore pocket of PYP; the image in the upper right corner is a 1 µs pump-probe delay from time-resolved serial femtosecond crystallography (TR-SFX), the yellow color denotes dark state; magenta and red, pR1 and pR2, respectively. For comparison, the image immediately to the left is the corresponding 1 µs Laue map. The photocycle examined by time-resolved crystallography contains six intermediates: IT, ICT, pR1, pR2, pB1 and pB2. Difference electron density is in red/white (negative) an blue/cyan (positive).

At lower left: dark PYP structure in yellow and electron density from x-ray FEL (Free Electron Laser) data collected at the LCLS (Linear Coherent Light Source). All images on the cover are from a paper: *Time-Resolved Serial Crystallography Captures High-Resolution Intermediates of Photoactive Yellow Protein,* ***Science***, 5th December 2014, pp 1242-1246. [DOI:10.1126/science.1259357], corresponding author: Marius Schmidt.

Haas, Abad-Zapatero and Petsko Highlight Technological Developments

In this issue of *RefleXions* David Haas and Cele Abad-Zapatero recount their Living History autobiographies. Both Cele and David worked with Michael Rossmann at one point in their career, David in 1962-1965 and Cele in the late 1970s and early 1980s. Both memoirs emphasize the important technological advances that enabled data collection and refinement of larger structures such as viruses and protein complexes.

David describes his experiments in the Rossmann lab, freezing lactate dehydrogenase crystals with sucrose cryoprotectant to extend crystal lifetime in the x-ray beam (1970). At the time, it seemed to him that there was very little interest in data collection at low temperature. In 1975 Greg Petsko extended these experiments to many other proteins by replacing the crystallization solution with high concentrations of organic solvents such as methylepentanediol or ethylene glycol. Nevertheless, in the early 1980s while he was in the Rossmann group Cele didn't use the freezing method; he ascribes the long delay in adopting this technique to the lack of devices to maintain frozen crystals reliably. It was not until the late 1980s that Håkon Hope successfully promoted this method, which is now routine. From the point of view of the history of science, the substantial gap between initial discovery and widespread application of low-temperature data collection illustrates our reliance on the instrument-makers.

In the early 1970s another instrumental development, the commercial oscillation camera with software to process the data, was a game-changing advance that Cele used both in graduate work with Marv Hackert and later in the Rossmann lab. Then during the 1970s synchrotron sources of x rays began to come online. The structure solution of rhinovirus by the Rossmann group (1985) was possible because of the rapid data collection and high resolution available at synchrotron sources. Cele also notes the advances in structure solution and refinement during the 1970s and early 1980s: non-crystallographic symmetry algorithms to solve virus structures and constrained-restrained refinement techniques by Joel Sussman (CORELS) and by Konnert and Hendrickson (PROLSQ) to refine proteins. Finally, Cele describes his pioneering application of computer graphics software FRODO (T. A. Jones) to refine the structure of lactate dehydrogenase.

Recent research, however, causes reevaluation of formerly groundbreaking technology. Although Greg Petsko was one of the early champions of low-temperature data collection, in his 2015 Buerger lecture ("Forty Years of Crystallographic Studies of Protein Structure, Function and Dynamics or Some Like It cold – But Should They?") he notes that temperatures below about 200-220 K result in significant changes in protein structure and dynamics. He calls this the "skeleton in the closet of structural biology" and he argues that by collecting data at low temperature we discard information we really want – flexibility of side chains, vibrational motion, protonation state, metal ion spin – the intricate variations in structure at room temperature that are responsible for binding, catalysis and product release. He suggests that the latest technological development, the x-ray free-electron laser, will provide the means to obtain room temperature structures for every unique protein in the PDB. If you missed his lecture in Philadelphia, you can view it online on YouTube from the ACA History website.

Virginia Pett

Memoirs: David J. Haas

David J. Haas's memoir gives a perspective on how scientific discoveries are made and recognized. He set out to test whether crosslinking a protein might stabilize the crystal and ended up discovering that freezing crystals vastly extends their lifetime in the x-ray beam. The value of this observation was not appreciated until much later, when freezing crystals at synchrotron sources became necessary.

I was born in Buffalo NY, but after WWII my family moved to south Texas, where I was raised in a farming community near the Mexican border. After attending several local colleges in Texas, I decided to transfer to the University of Buffalo where I still had relatives living in the Buffalo area. I graduated from the University of Buffalo (now SUNY at Buffalo) in 1962 with a physics degree, and then entered the Department of Biophysics in the Medical School. The department was closely associated with Roswell Park Memorial Cancer Institute where the Crystallographic Center had been established in 1960. This new center was created to house "The Protein Structure Project". David Harker was provided with a million dollars in 1949 for "The Protein Structure Project" by Irving Langmuir. Isidor Fankuchen apparently had sufficient interest, space and facilities for such an organization and invited David Harker to establish it there. The plan was to remain for about ten years and arrangements were made in 1960 to move the entire group to Buffalo. For the first few years in Buffalo, the crystallography group was situated in the basement of Roswell Park Research Building, and then in 1968 the Crystallographic Center was constructed on the Roswell Park Campus.

David collecting diffraction data with the original Harker-Furnas Goniostat at Roswell Park Memorial Institute, 1964.

With David Harker (photo credit: AIP Emilio Segre Visual Archives, Physics Today Collection) as my advisor I specialized in x-ray crystallography at the Crystallographic Center, where I used the original goniostat units (Eulerian cradle) for collecting diffraction data and superficially participated in the ribonuclease protein work. My thesis project was to solve the crystal structures for six organic molecules which were known protein denaturants. Performing x-ray data collection on the GE goniostats required manual data collection. I spent hours isolated in the x-ray room dialing numbers into these units. All the data were punched into Hollerith cards, and I used one of two IBM 1620 computers which were at the Roswell Park Computer Center and the UB Engineering Department. There were boxes and boxes of punched cards to transport for the structure determination. All the software programs were supplied by Dr. Ahmed in Ottawa, Canada, which proved to be essential to my success. After solving the structures of the six organic molecules in a matter of months and providing some assistance to the ribonuclease group, each of the crystal structures was published as a paper in *Acta Crystallographica*, which presented me with much needed exercises in scientific writing and drawing electron density maps/structures by hand. I can say that Harker was surprised at how fast I determined these structures, and he instructed me to write my thesis, including all the data that I had sent for publication. I graduated in February 1965.

Harker was a marvelous instructor, and he was intimately involved with the various departments at the University of Buffalo. Besides the daily lunchtime discussions between the staff members (Doretta Norton, G. Kartha, Lena & Jake Bello and staff), the laboratory was frequently full of visitors including Max Perutz.

During this time I met my wife, and we married on June 10, 1962. Sandra and I have been partners ever since! She had unforeseen skills and talents which were demonstrated beyond her raising our three sons. Besides having her name on many patents, Sandra was Vice-President of Temtec, Inc. – the business that we operated for 21 years (1981-2002). She excelled as the HR and customer service manager.

Meanwhile, Harker had contacted several British protein crystallographers to locate a postdoctoral position for me. This was already five years after the structures of myoglobin and hemoglobin had been determined, and David C. Philips had just finished with the structure of lysozyme (March 1965). We knew it was an exciting time in Britain for protein crystallographers. Phillips responded that he would have a postdoc position available for me after September 1965. I immediately accepted. Harker suggested that in the intervening months I should learn as much as I could about the new direct methods that were just being perfected by the Karles in Washington, DC. Jerry Karle invited me to his lab for several months. Isabella and Jerry Karle were really wonderful, and I attempted to learn as much as I could about direct methods during this stay. I worked with a research assistant S.A. Brenner on collecting data on dimethylmalonic acid, and we published a paper using Symbolic Addition Methods to determine the structure. Isabella and Jerry were always available for discussions so my time with them was quite beneficial. Also, during the summer they frequently had barbeques for the laboratory staff and their spouses at their home in Falls Church. Great comraderie!

Sandra and I arrived in London September 1965. We spent a few days at David Phillip's home, getting oriented and learning the language! I spoke at length with my officemate – Charles Bunn who was a well-known industrial crystallographer. The real excitement at the Royal Institution had been the March Friday Evening Lecture by David Phillips on the structure and function of lysozyme, the first enzyme structure to be determined. (He was now working on the *Scientific American* article.)

It was suggested that I might investigate the effects and possible uses of crosslinking protein crystals, to increase mechanical stability and reduce radiation damage. No other experiments on reducing radiation damage had been successful. With an ample supply of surplus lysozyme crystals from Philips, I first tested crosslinking to different degrees, and lysozyme was an excellent test model as the crystals were very stable and rugged. Brief exposure to a dilute solution of glutaraldehyde produces only a "surface crosslinking". I found that the "surface-crosslinked" crystal would remain unchanged and basically normal. A measure of the degree of crosslinking was to denature the crystal and observe the volume of swelling. The less the crosslinking, the greater the swelling. The surface-crosslinked crystals, when denatured, swelled to enormous sizes, each crystal edge increasing more than three times. Most important, with denatured surface-crosslinked lysozyme crystals, slowly removing the denaturant and returning the crystal back to its original supernatant caused the crystal to shrink again and recover its x-ray diffraction pattern. This proved to be a remarkable renaturation property which shows that the protein molecules could actually recrystallize themselves. I presented several papers at European crystallographic meetings and published a short note in *Acta Crystallographica* in 1968.

One of my fondest memories about working at the Royal Institution was the daily 4 p.m. tea gathering. Most of the staff appeared for the daily discussions (Gareth Mair, Colin Blake, Louise Johnson, Tony North, Ragupathy Sarma) including Sir William Lawrence Bragg. I recently read in Georgina Ferry's

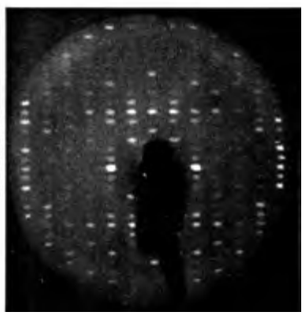
book on Max Perutz that these tea breaks were begun by Sir William Henry Bragg when he first took over management of the Royal Institution laboratory in 1923.

In the fall of 1966 David Philips informed me that he was moving the group to Oxford University and that I would need to find another laboratory to continue my NIH Fellowship. He

Sandra and I arrive in Israel from England at the Weizmann Institute of Science with our son Stuart.

suggested the Weizmann Institute in Israel and arranged for me to work in the Crystallography Group of the Chemistry Department with Wolfie Traub and Gerhard Schmidt. Until recently I had no idea why he made this suggestion, but it appears that he attended a meeting in Israel earlier in 1966 and was impressed with the quality of the people and work at the Weizmann Institute of Science. Wolfie Traub indicated that we should just take a ship to Haifa, and they would be ready for us at any time. As my NIH Fellowship was not transferable, Wolfie said the Weizmann Institute would also provide a Weizmann Fellowship which included housing and a stipend. (Thank you Mr. and Mrs. Van Leer for your Fellowship.) The Weizmann Institute proved to be a remarkable scientific institution, and what an experience for both Sandra and me.

Taking all my lysozyme materials and chemicals, I continued work on the effects of crosslinking protein crystals. I determined that crosslinking had little or no effect on reducing radiation damage by exposing various crystals for days in the full-power x-ray beam and then taking precession photographs of a standard pattern. This was quite disappointing! Fortunately, there was an unused crystal-freezing apparatus setup on one of the Philips x-ray generators. Considering whether crosslinked crystals would remain intact when frozen, I determined that crosslinked crystals fractured from ice crystals in exactly the same manner as native (uncrosslinked) crystals. Then I discovered that crosslinked crystals could be put into almost any solution of salts or organic solvents (cryoprotectant) because the crosslinking prevented the crystal from dissolving in the supernatant (as well as providing structural stability). With surface crosslinked lysozyme crystals in different concentrations of sucrose, frozen crystals gave excellent diffraction patterns above a certain sucrose concentration (sufficient to prevent ice formation). I confirmed that freezing in sucrose did not damage the crosslinked crystal by taking standard diffraction patterns repeatedly before and after diluting out the cryoprotectant.



Precession photograph of the first successful frozen protein crystal, crosslinked lysozyme at -50°C.

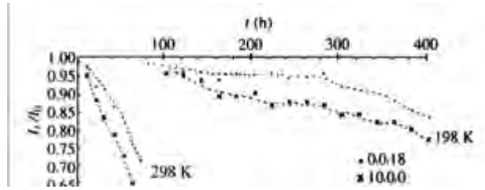
Then I discovered that lysozyme crystals could have their supernatant slowly changed to the appropriate compound concentration "without crosslinking" simply by selecting the appropriate compound (at room temperature and taking more precession x-ray patterns). These frozen *native crystals in sucrose cryoprotectant* gave excellent diffraction patterns, and I was quite impressed with their stability. (Note: The term cryoprotectant used here had not been created at this time.) Exposing several crystals to many days of x-rays at full power while taking repeat precession patterns demonstrated that the frozen lysozyme crystals showed substantially less radiation damage than native lysozyme crystals at room temperature. Hence, a solution to the radiation problem may be at hand! I was unable to continue this work at the Weizmann because the Six Day War began on June 5, 1967, and I had sent my wife and newborn son back to London for safety. I had already taken sufficient precession patterns for publication to demonstrate that radiation damage is absolutely reduced by freezing protein crystals! Fortunately, I had already arranged for a position with Michael Rossmann at Purdue when I returned to the United States.

The Rossmann laboratory was a beehive of activity with M. J. Adams, A. J. Wonacott and A. McPherson all working on the lactate dehydrogenase (LDH) project. Michael had the latest equipment and the group was always willing to help me learn the new methods. Within the first months, I wrote the short paper describing my findings of reduced radiation damage at low temperatures and presented my finding to the Rossmann crystallography group. They were skeptical that the benefits of extending the useful life of their crystals would be worth the "perceived" complexity and difficulty of building, installing and operating cooling apparatus. I believe that everyone expected the radiation damage reduction to be only a few hours, not the hundreds of hours that finally came to be with low-temperature x-ray data collection. And certainly, no one could even imagine the importance of freezing crystals with synchrotron radiation sources! Again, I would not have had a convincing argument for reduced radiation damage without the lysozyme precession photographs from the Weizmann Institute. The general notion at the time was that freezing protein crystals was no different from freezing food – I do not believe anyone in the laboratory knew the Birds Eye frozen food story, and it appeared that freezing anything, in general, was a bad idea!

After extended deliberations, Michael Rossmann agreed to loan me one of the Picker Automated diffractometers, and he would fund the purchase and construction of the most primitive freezing apparatus, as it probably would only be used once for my project. (Thank you Michael!) The glass laboratory fabricated a co-axial gas delivery jet for directing the nitrogen gas onto the

Freezing apparatus in the Rossmann lab for collecting the first data from frozen LDH crystals.

crystal with a dry air cylindrical barrier jet surrounding the nitrogen stream. The crystal would be mounted in a Lindemann glass vial in the conventional manner along with a small amount of mother liquor. The work would be performed on LDH as this was the protein being worked on by Michael Rossmann and sufficient crystals were available. The same sucrose cryoprotectant was successfully used as demonstrated previously.



Cryoprotected LDH crystals show less radiation damage at 198 K than unprotected crystals at 298 K.

I assembled all the equipment and fabricated simple control circuits, purchased a suitable air dryer and several bathroom scales for tracking the weight on the nitrogen-filled Dewars. After determining the pounds/hour usage of the liquid nitrogen, I would calculate when the "feed" Dewar had to be manually refilled from the storage Dewar. Of course, this was typically in the middle of the night! I scheduled regular monitoring of two reference reflections so as to measure the actual x-ray deterioration during the hundreds of hours of exposure. The results of this first x-ray data collection from a frozen crystal were published and I also presented a paper at the next ACA meeting in 1969. I can only say that there was basically "no interest" in this work whatsoever! Furthermore, I never heard a word about freezing protein crystal for the next 30 years until 1999 when I again revisited Michael Rossmann at Purdue. He said, "What a wonderful technique cryocrystallography had become". Actually, I could hardly remember the work, so Michael gave me a copy of our 1970 paper to read!

As a side note, during 1969, I developed an instrument for setting dihedral angles on metal atomic models that made it very easy to accurately fabricate the backbone for known protein structures. A manufacturer became interested in the "Dihedral Angle Dialer" and manufactured it for several years. What is interesting is that I sent a request to the Purdue University Intellectual Property Committee for permission to apply for a patent, but they just had no interest in scientific patents. And now I can note that if I had applied for a patent on the process for freezing protein crystals for radiation damage reduction, they surely would also have refused to consider it! Scientific patents were just for science, not commercialization! How the world has changed!

In 1970, I entered industry by joining Philips Electronic Instruments in Mt. Vernon NY as Principal X-ray Scientist and was immediately appointed Radiation Safety Officer. (I now know that being the RSO was considered by the managers as an awful waste of time!) The Mt. Vernon facility was the original Philips plant set up in the United States by N. V. Philips in 1935. The facility manufactured analytical x-ray equipment and sold industrial x-ray systems as well as other Philips instrumentation. I remained on the ANSI Committee for X-Ray Analytical Instruments for many years, but 1977 was the most valuable as we published the revised X-ray Safety Standard N43.2-1977.

My first project was to complete the software for the Automatic Powder Diffractometer System which I believe was the very first commercial computer-controlled x-ray diffractometer system. It used the Philips Digital Controller (4k with optional 4k for analytics) and would scan 35 consecutive powder samples without human intervention. The automatic sample changer and strip chart recorder/paper tape data output would keep an industrial laboratory fully operational on a continuous QC and analysis basis. After completing the software, I wrote the instruction manual and provided technical expertise for the salesmen and at trade shows. As a high-speed automated instrument, it was very advanced for the early 1970s and many were sold to industry worldwide.

About 1975, I participated in making the analytical x-ray safety film for the Bureau of Radiological Health ("The Double-Edged Sword"). The film provided safety advice and precautions for individuals who work with analytical and x-ray spectroscopic equipment. The film appears to have been successful, and I was told that it has continued to be shown into the 21st century. (I recently saw it on YouTube!)

In 1973, I was asked to assist in designing the first Philips "Dynafluor" Airport X-ray Security System because on January 5, 1973, the FAA had instituted mandatory passenger security screening: walk-through metal detectors for people and low-dose x-ray for baggage and hand-carried articles. (Several engineers at Philips Government Systems, Mahwah NJ, were the inventors of the original low-dose security system in 1970.) During 1973 and 1974, the Philips Industrial Group initially built a lead-lined moving-tunnel unit and then supplied a large conveyorized low-dose x-ray unit to several airlines (Dynafluor IV) that proved to be a "dinosaur". I initiated a stealth project to create a lightweight, mobile, low profile system that provided a successful second-generation system for many airlines (Dynafluor VI). In addition to selling hundreds of units worldwide, the Dynafluor VI provided a modern Electronic Security Screening System similar to the current airport units with low profile, short tunnels, high speed and easy-to-use. So during the 1970s, Philips became a major supplier for aviation security equipment. About a dozen patents were issued for the various Dynafluor Security Systems but Philips terminated the business before enforcing any of their patents.

Philips Electronic Instruments moved to Mahwah, NJ in 1976.

I remained with them until 1983 and was mostly involved in low-dose x-ray security matters. One surprising item was that until 1976 neither the FAA nor any airline had actually provided a visual training program (slides or movie) for security personnel (guards) who operated the metal detectors or low-dose x-ray systems at the airports. Philips decided that this was important (as well as an excellent marketing tool) so we arranged to rent a truck, place a low-dose x-ray unit with an electric generator inside so that we could photograph the actual x-ray images of guns, explosives and bombs. I did this on an Army firing range in Virginia with a substantial variety of explosives and weapons. These high-quality photographic images of actual explosives provided the FAA with an excellent slide-training program for aviation security personnel. The slide set was used for years by airlines security managers all around the world and probably saved many lives because it provided actual x-ray images of guns, bombs, and other hazardous items.

During the late 1970s, I developed an idea for a new type of security ID badge which would prevent the reuse of temporary badges and parking permits for visitors, contractors, etc. After several years of laboratory work at home, Sandra and I introduced the self-expiring Visitor Badge, which changed color a day after being issued to prevent reuse. Our first badge was a coated paper badge with a photochemical that turned blue when the individual left the facility and entered daylight. It was sensitive only to short UV light and was an effective daytime temporary ID. However, our second self-expiring badge changed color by dye migration and was a one-day Time Expiring Badge. Between 1981-2002, more than 20% of all visitor badges issued in the United States were TEMPbadge badges. The business was sold in 2002.

We have returned to the Weizmann Institute of Science several times and supported them with a graduate student fellowship, exactly the same kind that I received in 1966. We were very pleased when Ada Yonath received the Nobel Prize in 2009 for the ribosome structure, using cryocrystallographic techniques. As it turns out, she was a graduate student in the Weizmann Institute's Crystallography Department while I was there in 1966.

One of my desires was to become involved in historical artifacts before they reached the museums, so between 1995 and 2005, I volunteered for many archeological digs and research projects in Israel, Great Britain and Canada. These have provided an ongoing excitement for Sandra and me, particularly when we visit one of the dig sites, and I can show people the inch or so in the "square" that I dug through!

During 2006, I became involved in a short research project for the Smithsonian Institution on the official biography of James Smithson. The author, Heather Ewing, had begun researching this book in 2000 and because of a publication deadline of June 2007, was unable to research the archives of the Royal Institution of Great Britain on Albemarle Street (the Institution where the Braggs had been directors, the Institution in which James Smithson had been a founding member, and the Institution where I spent 18 months of postdoctoral work in 1966 with David Phillips). With a letter of introduction from the "Historian of the Smithsonian Institution", I spent three week in the Royal Institution's vault looking through all the original minutes and notes from 1799 to 1829, the year that James Smithson passed away. My notes and digital photos of the relevant pages were passed on to Heather Ewing who published the book in late 2007 (*The Lost World of James Smithson* by Heather Ewing, 2007).

Beginning in late 2005 with a book project, I spent three years of archival research to determine the people instrumental in developing secure identification credentials and, in particular, who invented the original photo ID badge. During 2007 another project of interest was the invention of the first low-dose security x-ray system, and how the United States Government (and the public) were convinced to pass laws requiring 100% mandatory physical screening of aviation passengers. The first low-dose x-ray system was developed by an engineering group at Philips Government Systems in Mahwah NJ in 1970 by George W. Shepherd Jr. (deceased) and Neal Diepeveen. The Philips group worked "as an unauthorized project" for three years and demonstrated their system to government and airline officials on Sept 25, 1970 in a hanger at Washington National Airport. This was sufficiently convincing for the airlines and the US Government

The original "Saferay", the first low-dose x-ray system developed at Philips 1968-1970.

to institute and pass laws for mandatory security screening of aviation passengers. With 100% mandatory physical screening begun on January 5,1973, the passenger aviation industry was basically saved from worldwide terrorism and criminals. And two new industries were created: metal and explosives detectors for people and low-dose x-ray for baggage and hand-carried articles. Shepherd and Diepeveen were nominated in 2015 for the National Medal of Technology and Innovation.

In 1999, after becoming aware of the success of biological crystal structure determination, I have once again begun reading, watching and attending crystallographic lectures as well as ACA meetings. The entire field of cryocrystallography is new to me, but Elspeth Garman provided me with a number of technical articles on the subject. WOW! In 2006, I attended the cryocrystallography session held at the ACA meeting in Chicago and have been watching many historical lectures on the internet (like the ACA historical videos). I am amazed by the enormous technical growth in biological structures determination in the past 40 years. Crystallography has really become an extraordinary research and industry tool for society!

Notes of a Protein Crystallographer: From Altar Boy to Sorcerer's Apprentice

Cele Abad-Zapatero was educated in Spain; he came to the USA on a Fulbright at the University of Texas at Austin. Michael Rossmann presented him with the drawing at left (by Kathy Schuster) when he left Purdue for Abbott Laboratories. In this memoir Cele describes his crystallographic research as well as his lifelong interest in the intersection of science and art. He ends with a prediction for future directions in biological research, as well as some reflections on the impact of structure-based drug design. Cele's complete memoir with references will appear online at the ACA History website. Some of his experiences, thoughts and reflections have been published in the book Crystals and Life: A Personal Journey (IUL, 2002).

Contingency of life. I owe my existence to a tragic event during the Spanish Civil War (1936-1939). My paternal grandparents had seven children and made a living by working the dry and poor soil of the Castilian plateau. Thus, my father was sent away at a very young age to a seminary in Catalonia, near the city of Barcelona. During his time at the seminary he showed great aptitude for music; he played the organ regularly and on weekends he was asked to play at social events such as weddings.

One weekend, during my father's absence from the community, a group of anticlerical demonstrators entered the seminary. The novices were either shot or disbanded from the community. Thus, my father returned to an empty seminary house. He left the priesthood and returned to his birthplace. In the larger nearby town of Aranda de Duero (province of Burgos) he met my mother. She was the daughter of a very lively and intelligent man, part mason, part architect and draftsman and indeed part musician also; I was named after him.

I should have been a Dominican monk. Initially, I went to the parochial school where my father was a teacher and I was part of the choir of altar boys that sang at the services of the parish. As my father discovered my interest and aptitude for study, he dreamed of his second son being a Dominican scholar. However, at the age of 14 I had to choose between two alternative and exclusive paths: the 'sciences' or the 'humanities'. I vividly remember sleepless nights and anguished ruminating on this issue. In the end I chose the science course, much to the chagrin of my father.

Students of the parochial school of Santa María (Aranda de Duero, Burgos, Spain) circa 1956. Author is in the center of the first row of three.

Finding a profession. I have very fond memories of the two years of 'superior bachalaureat' (ages 15-16). I studied very hard and I was rewarded by what I felt to be an extraordinary expansion of my interests and my perception of the power of the natural sciences to explain the world. There was no regret in the fact that I had chosen sciences as my future path.

A very important part of the geology curriculum was an introduction to crystallography so that the different crystal forms of the various minerals could be studied in the appropriate context. At the time, I was not particularly interested in this part of the material but I understood very well the symmetry groups and crystal forms; it all seemed so well organized.

The subconscious avocation about crystals and crystallography appeared again in my first year at the University of Valladolid (Spain). As part of the classwork in geology we had to assemble cardboard models of the different forms of crystals in the various minerals. Building the models, and preparing for the exam required an enormous amount of time that I happily spent in my father's library room, as opposed to going out with friends.

After five years of college, having a university degree (*Licenciado*) in physics would allow me to teach at the high school level in some remote places in Spain. However, through the years of study at the university I had experienced a pulling force towards biological subjects. By accident, I found a short typed note at the bulletin board of the University of Valladolid announcing Fulbright Scholarships to pursue graduate studies in the USA. Late in June 1972, my dream was realized. I received a telegram from the Fulbright Office in Madrid saying that I had been offered a scholarship to do graduate work at the University of Texas at Austin. My dearest young wife Victoria and I traveled to the USA in the fall of 1972. I started my graduate studies under the mentorship of J. Lawrence Fox and Marvin L. Hackert working on the structure of two beautifully colored proteins (C-Phycocyanin and B-Phycoerythrin) extracted from algae.

Structure of the first viruses. The years that I spent at Purdue University as a postdoc were extraordinary. The international nature of the crystallography group lead by Michael Rossmann was multifaceted and stimulating. In the late 1970's, the frontier of macromolecular crystallography was to obtain the first atomic structure of viruses, and in particular the class of viruses described as spherical or isometric.

In addition to the large amount of data that needed to be collected to solve these structures, plus the difficulties of obtaining heavy-atom isomorphous derivatives, the major issue was the design and development of algorithms to average over the NCS of the crystals. The electron density maps without the averaging were too noisy and uninterpretable. Michael's vision of the power of NCS averaging was critical for the solution. Tomato Bushy Stunt Virus was solved first (S. Harrison at Harvard), followed by Southern Bean Mosaic Virus (SBMV, Purdue), trailed by Satellite Tobacco Necrosis Virus (Bror Strandberg, Uppsala). The most striking result of these studies was that the capsid proteins that enclosed the RNA of these viruses all had the same 'jelly-roll' fold. The structural and evolutionary implications were enormous

Somehow, the achievement of this group of devoted postdocs

and colleagues inspired me to write the lyrics of a ballad. The 'Ballad of the 2.8 Å Structure of SBMV' was sung at a party organized by Michael and Aud Rossmann at their home on Nov. 4, 1979. The full text of the ballad was also published in the 2013 issue of the bulletin of the Spanish Society of Virology.

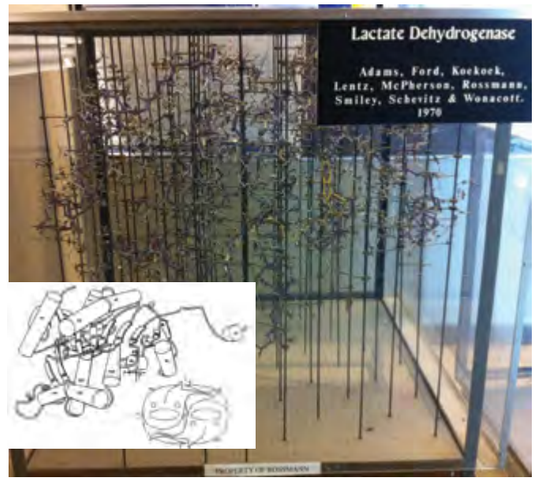
Wire model of the protein capsid of SBMV built at Purdue around 1980 by the author.

Refining the Classics. After the work on virus structures, I stayed for a few more years at Michael's lab taking the challenge of refining one of largest protein structures that had been solved in the 'golden age' of protein crystallography, Lactic Dehydrogenase (LDH, which also contained the iconic 'Rossmann fold').

Even in the early 1980s, structures were built using mechanical Kendrew parts and refining a medium-large protein structure was a challenging feat manually as well as computationally. A collaboration of Michael Rossmann with Joel Sussman (Weizmann Institute) and T.A. Jones (University of Uppsala, Sweden) explored new computational methods and pioneering computer graphics to do the work; for me the attraction was irresistible. Sussman had developed the refinement program CORELS (Constraint-Restraint Least Squares) and Jones had created the remarkable computer graphics program FRODO specially designed to build and refine protein structures in the computer, superseding the mechanical models. I spent a significant amount of time in each laboratory and within a few months of work I managed to decrease the R-factor of the early LDH wire model from 0.45 to 0.24 with a dramatic improvement on the stereochemical parameters of the model. Similarly dramatic results were obtained soon thereafter with the refinement of Beef Liver Catalase at Purdue (by I. Fita, A. Silva), using FRODO and the restrained-refinement program PROLSQ developed by Hendrickson and Konnert. The refinement of protein structures, even the larger ones, was a laborious but feasible endeavor after those years. In addition to the professional excitement, our two dearest children (Inés and Pablo) were born while at Purdue. Adventures in structure-based drug design.

Although I was an academic at heart, visa issues, family responsibilities and the inability of finding an academic position in Spain made me look for opportunities in the pharmaceutical industry. Luckily, I managed to find a promising position at Abbott Laboratories in the northern suburbs of Chicago. Victoria and our two young children moved in the spring of 1985.

The early projects. There was an immense sense of optimism in those years among all of us protein crystallographers in the



LDH Kendrew model built at Purdue University in the late 1960s contrasted with FRODO display of the same structure.

pharma industry. The notion was that our results would feed into the molecular modeling being done by the computational chemists and feed back into the medicinal chemists, allowing the design of 'intelligent' compounds faster. At the beginning though, the structure solution of novel target proteins by MIR methods or even the refinement of existing structures for relevant biological targets of interest was very time consuming. The Protein Data Bank had not reached a significant coverage of folds or structures of many proteins of biomedical interest (particularly from humans or from important pathogens). Crystals diffracting at high resolution were difficult to obtain. The ingenuity of chemists and the expediency of the molecular modelers beat our results, often by months. We recognized that the results from our 'structure-based' methods had a rather limited impact on the outcome of successful projects at the clinic.

However, there was one program where the SBDD technology had an important effect: a critical enzyme in the reproductive cycle of the HIV virus was a small aspartic protease, about half the size of pepsin. This family of enzymes had a long tradition in crystallography starting from the early work of J.D. Bernal on pepsin; it was also an important target for the design of anti-hypertension agents interacting with renin – a structural relative of pepsin. There was a long history of active compounds against this class of enzymes at Abbott labs and by an uneven mixture of SBDD (J. Erickson, C. Park, V. Stoll) and chemical ingenuity within the team of medicinal chemists, Abbott Laboratories managed to market important potent compounds against the AIDS virus: Norvir, Ritonavir and later Lopinavir.

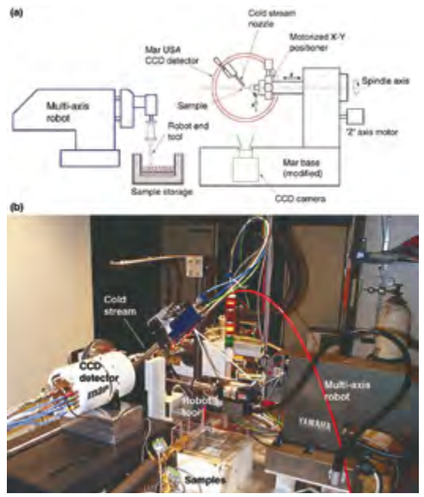
Access to synchrotrons. The pharmaceutical industry members came to the conclusion that they needed independent, routine access to synchrotron radiation sources to expedite the application of SBDD to drug discovery projects. These projects could not compete for synchrotron time with the high profile, cutting-edge, academic structures. A consortium of several pharmaceutical companies proposed to design, build and equip

beamline stations at the APS for drug discovery projects named Industrial Macromolecular Crystallography Association (IMCA), under contract with the Illinois Institute of Technology (IIT). The managements and legal departments of the pharmaceutical giants struggled with the unprecedented notion of sharing a resource with their competitors. However, the respective teams of protein crystallographers argued that it was imperative to proceed if the new methodology was to be used effectively. The names of Noel Jones, Joel Oliver, Keith Watenpaugh, Bill Stallings, Tim Morrison, John Chrzas and others should be included here. I feel proud that I was part of changing the *modus operandi* of SBDD in the pharmaceutical industry.

With the possibility of obtaining high quality data rapidly, and the parallel developments of high performance computer graphics, reliable refinement algorithms and superior software tools, as well as the expansion of the available structures in the PDB, protein crystallographers could provide *rapid* structural responses to drug discovery projects. Quite often, it was now possible to beat the computer modelers to address medicinal chemistry questions based on 'experimental results', not hypothetical models. It was also possible to tackle the structure determination of more challenging targets, and with the help of new members of the laboratory, S. Muchmore, D. Bussiere and C. Dealwis we solved the structure of Erm C′, an important structure in the mechanism of erythromycin resistance in bacteria using the NSLS and the Se-Met method pioneered by Wayne Hendrickson and coworkers.

Crystallographic screening and ACTOR. From the very beginning of SBDD it was clear that protein crystallography could be of great value in the optimization process. However, there were internal and external pressures to expand its role. Another new member of the laboratory, V. Nienaber, played a critical role in expanding the role of crystallography to the screening of limited mixtures of small compounds (typically 8-10) using pre-grown crystals of the target. Unknown to us, a similar approach had already been explored by Wim Hol, Christophe Verlinde and coworkers. However, the idea of screening compounds using crystals presented the challenge of how to develop methods for higher throughput crystallography using in-house x-ray sources. With the guidance of Steve Muchmore, this problem was taken as a major engineering challenge by the automation department at Abbott Labs and with the total involvement of Jeff Olson, Ron Jones, Jeff Pan, Michael Blum and others, they addressed the problem of automatically mounting, centering and exposing the frozen target crystals. This was the origin of the ACTOR (Automatic Crystal Transport Orientation and Retrieval) robot tested and developed at Abbott Laboratories in the late 1990s. Protein Tyrosine Phosphatase 1B (PTP1B), a target for diabetes, was used for the first ligand screen runs. The commercial implementation of ACTOR received an R&D 100 Award for 2002. After this proof of concept, many similar devices became common particularly in beamlines and synchrotron stations, where minimizing unproductive beamtime is high priority and automatic data collection is now routine.

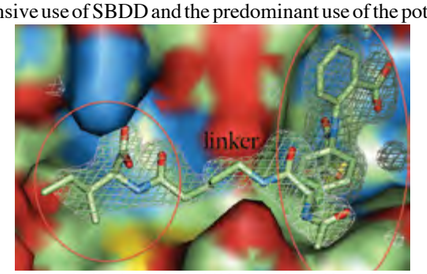
Fragment-based drug design. Our relationship with the NMR group at Abbott was cordial but also competitive. The NMR group proposed using smaller molecules (or 'fragments': SAR



ACTOR prototype robot at Abbott Laboratories protein crystallography lab.

by NMR) as a promising way to solve the problems derived from attempting to optimize hits with difficult synthetic pathways or poor pharmacokinetic properties. PTP1B, a protein target for which we had excellent crystals diffracting at high resolution in our in-house lab provided an excellent ground for a productive collaboration. Small inhibitor fragments were identified by NMR techniques and soaked in PTP1B crystals to establish their mode of binding in the active site, and later linked with other small compounds binding to an adjacent site. Further work was needed to achieve enough specificity compared to the T-cell PTP1B and to improve pharmaco-kinetic properties.

Atlas of Chemico-Biological Space (AtlasCBS). The praises and achievements of SBDD during the approximately thirty years (1985-2015) that it has been in the spotlight cannot be denied: its accomplishments are superior to its limitations. However, the extensive use of SBDD and the predominant use of the potency of



An early PTP1B dual-site inhibitor designed in collaboration with the NMR group at Abbott Laboratories.

the compounds as a guide often resulted in compounds that were potent but did not have favorable pharmaco-kinetic properties; typically they were very large and very polar.

In the late 1990s, the guidelines suggested by Lipinski and known as the 'rule of five' (Ro5) provided an easy rule-of-thumb to address some of these issues. On the tenth anniversary of the

publication of Lipinski's paper, I wrote a brief essay arguing that we should look for other 'variables' to guide drug discovery. Earlier, Jim Metz and I had extended the notion of 'Ligand Efficiency' that had been originally proposed by Hopkins and colleagues (2004). We suggested that a combination of efficiency variables (size efficiency and polar surface efficiency) should be used to guide drug discovery in a more effective way. After my retirement from Abbott, I have been expanding these ideas to map chemico-biological space (AtlasCBS) and also to use them by applying rigorous methods of Multiple Parameter Optimization. I do hope to be able to stay scientifically active to see what happens at least for the next decade.

Science and the Arts. As I matured scientifically, I began to see science and art as the two most unique activities of the human mind. I began writing a play about the historical encounter of John D. Bernal and Pablo Ruiz Picasso, probably the most influential artist of the 20th century. They were both known for their left-wing politics. They met at Bernal's flat in November 1950, and Picasso left a mural drawing at the apartment. A dramatic rendering of this encounter was presented as the play 'Bernal's Picasso' written in collaboration with Jill Campbell that was stage-read at the 2008 APS User's meeting.

In investigating the source of inspiration of the cubist painters, I encountered the scholarly work of the art historian Linda D. Henderson. This was a revelation! The dramatic photographs published by Roentgen in his scientific communications opened the eye of scientists, artists and laypersons alike to an unseen

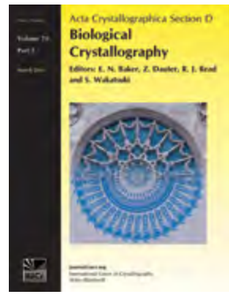
The play Bernal's Picasso at Argone National Laboratory, May 2008. (Left to right, front: Picasso, J.B.J. Fourier, Rosalind Franklin, W.L. Bragg; back: Art; Science.)

reality that was beyond the perception of the naked eye. As thoroughly documented by the work of Prof. Henderson, this notion appeared in the press, popular publications, and hobbyist magazines and made it to 'artistic manifestos' of the upcoming artistic movements. I was absorbed by the *direct* influence of the discovery of x-rays and the search for 'other views' of reality by the painters, particularly the cubists, in the early 1900s. I am now certain this is not the only time that science has expanded the vision of the arts (*i.e.*, Renaissance and the use of perspective).

Notes of a Protein Crystallographer. I found the scientific and intellectual atmosphere of Spain under Franco (1939-1975) particularly oppressive, with the power of the Catholic Church dominating many aspects of the educational system in Spain. In addition, the majority of the professors provided a very narrow view of their fields without inspiring in the students any sense of what the scientific endeavor was all about. The teachings were typically a repetition of well-established patterns and scientific facts. The inter-relation among the different sciences was never discussed. Certainly, there was not the remotest notion of any connection between the sciences and the arts.

During my years at Abbott Laboratories, daily immersed in the practical applications of macromolecular crystallography, I wanted to present a wider perspective on the scientific findings. I wrote brief essays in *Structure* and *Acta Crystallographica* highlighting some historical, human or artistic connections between crystallography and other branches of science and art. These ruminations made my intellectual life far richer. Shorter versions of those essays and others that were not suitable for publication in scientific journals have appeared in *ACA RefleXions*. Altogether, I probably have published over twenty essays. I do hope that they have also enriched the lives of the readers. I mention one in particular that relates the beautiful rose windows of the gothic cathedrals (Fig. 7) to their mathematical symmetry and to a recent oligomeric structure.

Crystal Ball. What would I do if I were a student again? On the biology side I would focus on the vast field of neurobiology; on the structural side I would explore the formation and evolution of dissipative structures and their role in mental processes.



Acta Cryst. D cover relating the symmetry of the rose windows in gothic cathedrals to the symmetry of the Vault protein found in certain cellular organelles.

From an early age we have been taught to respond in a very clear and unambiguous way to the question: What are the states of matter? And the answer is, obviously: solid, liquid and gas, right? Aren't we forgetting something? Where do we place the living organisms? The future study of biological processes and the human brain has to include additional concepts besides the molecular components, not in the sense of a 'vitalistic' explanation but including the concepts of 'dissipative structures' and far from equilibrium physico-chemical phenomena. (See the writings of Nobelist I. Prigogine.) Our beloved 'macromolecular structures' represent the parts of this magnificent machinery that make 'life' possible, but we should not ignore the 'fluxes' (nutrients, ions, chemical, electric, and nervous signals, etc.) that make those thermodynamic processes possible. It is at the interface of these two poles that I would like to understand the workings of the human brain.

I always think of opera as a 'dissipative structure' driven by the music and the words. It would disappear without the flow of those two components, no matter how superb the staging might be. Can the components only explain the opera? Are words alone enough to explain the emotions expressed by characters? Is the music alone enough to drive the action? Is music more important than words? Or the other way around? I leave these questions for the reader and the future generations to ponder as we incessantly drive towards an understanding of mental processes in strictly molecular and physico-chemical terms.

Reflections. As I finalized writing these notes, it seemed to me that besides the historical facts and anecdotes a few key points could be relevant to other people's lives and could help them in their decisions and career choices.

Contingency of life. We can plan our lives in a certain path and direction but there is always an element of the unexpected and unplanned that should be seriously considered.

Transforming power of education. I was indeed transformed by the education that I received first in Spain and later in my graduate studies at the University of Texas at Austin, and my postdoctoral years at Purdue University. However, there was a critical difference between the education I experienced in Spain and the one to which I was exposed in the USA. The spirit of many universities in Spain at the time was condensed in the words inscribed at the entrance of some of them: *Sapientia Aedificavit sibi Domun* (wisdom built its house here), implying that knowledge had its house in those buildings and should not go beyond those quarters. I have seen engraved on the stones of the mall at the University of Texas at Austin its mission: *Transforming lives for the benefit of society*. I do think that this second vision is more valuable to help younger generations realize their full potential and enrich the future of human kind.

Instruments vs. results. Our field of research has depended heavily on the labors of many engineers and instrument makers, from the early inventors of x-ray sealed tubes to the enormous number of people involved in synchrotron design, construction and maintenance, and to the instrumentalists now working the development of the x-ray Free Electron Lasers. These colleagues need to be recognized for their ingenuity, creativity and hard work.

What we do matters! Just by the contingency and fragility of life, early this spring our oldest grandson (Mateo, aged 5) was diagnosed with Acute Lymphoblastic Leukemia. The news was devastating for the entire family. Yet with the available treatments, developed in the last decade by dedicated biomedical workers around the world, as well as medicinal chemists, pharmacologists and protein crystallographers in academia and the pharmaceutical industry, the prognosis for a full cure ranges between 80-90%. I could have never imagined that the early research of J. Kraut and collaborators characterizing the binding of methotrexate to DHFR could have any relevance to the therapeutic agents used to treat our grandson. After months of grueling treatment, requiring long hospital stays, Mateo is doing well. I mention all these personal notes to emphasize that *what we do does matter*. Our dedicated work, even if not devoted to any particularly successful cure in the clinic, is complemented by the same devoted work by thousands of other workers in the biomedical fields where breakthroughs are accomplished and lives saved.

I would like to end these biographical notes with my slight addition (in parentheses) to the words of Michael Rossmann: "*There are two reasons why we do research. One is the personal enjoyment of discovery (and the fulfillment of our full potential). The other is the desire to contribute something to the benefit of mankind*." I would like this to be the message that I pass along to the future generations of protein crystallographers and structural biologists.

Spotlight on Stamps: Getting the Lead Out

Galena, a silvery gray mineral that is the natural source of lead(II) sulfide, is widely distributed in the Earth's crust and has been mined since ancient times. It is the most important mineral ore of lead, a heavy metal commonly used in car batteries, ammunition, solder, piping, and radiation shielding. The element is typically obtained by heating the ore in excess air, which converts the sulfide to the oxide (a metallurgical process known as roasting), followed by smelting with limestone and coke. The annual world production of refined lead is now around 11 million metric tons, roughly half of which comes from mining and the rest from recycling scrapped metal, mainly lead-acid batteries. China and Australia are the two top producers of primary (mined) lead, accounting for about two-thirds of the world's output. Significantly, secondary (recycled) lead represents nearly 90% of the refined lead generated in the United States, which was 1.26 metric tons in 2013.

Attractive specimens of galena are featured on stamps from several different countries, including Algeria, Belgium, Burundi, Canada, Kenya, Mexico, Spain, and Uganda. My favorite one is from Peru, illustrated below, since it not only shows the name and chemical formula of the mineral but also the unit cell parameters of its crystalline lattice. As a matter of fact, galena crystallizes in the cubic close-packed (or face-centered cubic) system, with perfectly square faces ($a = b = c$) and mutually perpendicular crystallographic axes ($\alpha = \beta = \gamma = 90°$), and is therefore isostructural to sodium chloride (halite) and other alkali metals and silver halides.

Interestingly, Galena is the official state mineral of Missouri and Wisconsin and also the namesake of several cities across the United States. The best known is perhaps Galena, Illinois, located in the Northwest corner of the state, an area where the mineral was mined by Native Americans for over a thousand years and used in burial rituals. Ulysses S. Grant, the Civil War general, lived in Galena for a few years before becoming the 18th President of the United States (1869-1877). There are also towns named Galena in Alaska, Kansas, Indiana, Maryland, Missouri and Ohio.

Daniel Rabinovich

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John Helliwell Receives 8th Max Perutz Award

John Helliwell, Professor Emeritus of Chemistry at Manchester University, UK, received the 8th Max Perutz award at the 29th European Crystallographic Meeting, which was held in Rovinj (Croatia) from 23-28 August 2015.

John is an ACA member with a rich scientific history, who played a key role in the development of modern crystallography. He pursued his undergraduate studies in physics at York University, with Michael Woolfson and Peter Main, and subsequently trained for his PhD in structural biology in Oxford under the supervision of Margaret Adams. There he received mentorship from Charlie Bugg and Guy Dodson in the laboratories of Dorothy Hodgkin and David Phillips.

In the 1980s, while working at Daresbury, UK, he spearheaded the realization of the first dedicated synchrotron light source instrument for protein crystallography, pioneering the use of synchrotron radiation for the study of macromolecular structures. Since then he has contributed greatly to the expansion of the potential of x-ray crystallography and to solving crucial technical problems, such as phasing.

While his outstanding contributions to the technical aspects of synchrotron radiation has made him well known within the crystallography community, it is his work on crustacyanin that tickled the media's fancy. Crustacyanin is a multimolecular protein complex that, upon binding the pigment molecule astaxanthin, gives lobsters their characteristic deep blue color. John and his group solved the x-ray structure of crustacyanin, shedding light into the mechanisms driving the striking color change that occurs upon cooking. When astaxanthin binds to the native form of crustacyanin, the pigment looks blue; high temperatures unfold crustacyanin and cause release of the pigment, which in its free form has an orange hue. The paper, published in *PNAS* in 2002, got coverage from *Scientific American* that same year, although the details of the problem are still being researched at present.

A prolific author, John has published over 250 articles including peer-reviewed papers, conference proceedings, book chapters and educational and outreach pieces; he has also written an entire book on protein crystallography, entitled "*Macromolecular Crystallography with Synchrotron Radiation*". He was president of the European Crystallography Society from 2006 to 2009, and served as Editor-in-Chief of the IUCr journals from 1996 to 2005, supervising the launch of *Acta Crystallographica* Section E and Section F. He is also on the Advisory Board of the ACA's journal, *Structural Dynamics*. During the years he has travelled worldwide supporting synchrotron facilities and tirelessly promoting x-ray crystallography in conferences, workshops and other outreach events. For all of this and for his impressive scientific achievements, he has been awarded many prizes in the past. Among them the ACA 2014 Patterson Award inspired our first News and Awards article in his honor, which appeared in the summer 2013 issue of *RefleXions*.

Sow-Hsin Chen Awarded 2015 Guinier Prize

Sow-Hsin Chen received the 2015 Guinier Prize at the SAS2015 meeting, which was held in September in Berlin. The Guinier Prize is sponsored by the International Union of Crystallography and recognizes a "lifetime achievement, or a major breakthrough or an outstanding contribution in the field of small angle light scattering".

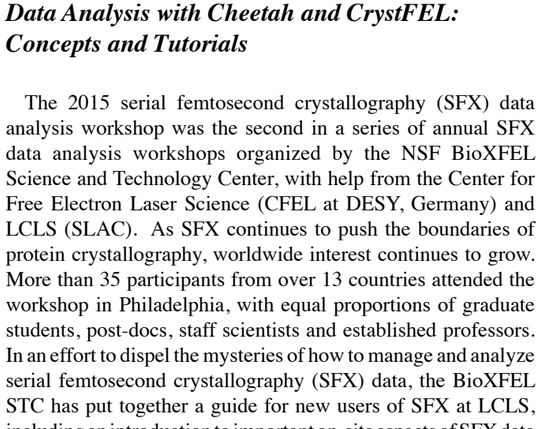
Sow-Hsin Chen is Professor Emeritus of Nuclear Science and Engineering at MIT. During his 50-year career, He has contributed enormously to developing small angle scattering techniques in the field of soft condensed matter physics. His research interests led him to investigate the complex behavior of liquid mixtures, such as micellar mixtures, microemulsions, protein solutions, proteins and surfactants complex solutions. Most recently he explored the dynamics of supercooled water near hydrophobic and hydrophilic surfaces, using a high-resolution quasi-elastic neutron scattering (QENS) technique. In 2005 and 2006, his studies demonstrated the presence of a second low temperature critical point in supercooled water, something that had been previously proposed but never verified.

Chen received his BS and MS in physics from National Taiwan University and from National Tsing Hua University, respectively. He then won a fellowship from the International Atomic Energy Agency, which brought him to the USA. He obtained a second MS in nuclear science from the University of Michigan, and a PhD in physics from MacMaster University, in Canada, under Nobel Laureate Bertram Brockhouse. After post-doctoral training at the Atomic Energy Research Establishment in Harwell, UK, he became a Research Fellow at Harvard University, with another Nobel Laureate, Nicolaas Bloembergen. He then joined the MIT faculty in 1968. Throughout his career, he has been a member of several national advisory boards and review committees, and has acted as a consultant for nuclear programs in developing countries. Moreover, he has published some 400 peer-reviewed publications and a text book, and has trained a big part of the new generation of expert scientists in the field.

Chiara Pastore

ACA Philadelphia: WK.02. Serial Crystallography Data Analysis with Cheetah and CrystFEL: Concepts and Tutorials

The 2015 serial femtosecond crystallography (SFX) data analysis workshop was the second in a series of annual SFX data analysis workshops organized by the NSF BioXFEL Science and Technology Center, with help from the Center for Free Electron Laser Science (CFEL at DESY, Germany) and LCLS (SLAC). As SFX continues to push the boundaries of protein crystallography, worldwide interest continues to grow. More than 35 participants from over 13 countries attended the workshop in Philadelphia, with equal proportions of graduate students, post-docs, staff scientists and established professors. In an effort to dispel the mysteries of how to manage and analyze serial femtosecond crystallography (SFX) data, the BioXFEL STC has put together a guide for new users of SFX at LCLS, including an introduction to important on-site aspects of SFX data collection, which is available here: ***www.bioxfel.org/resources/LCLSdata_overview.*** Following an overview of SFX by BioXFEL STC Director of Science John Spence, the workshop focus was two-fold: firstly, data reduction and hit finding by Cheetah (***www.desy.de/~barty/cheetah***), quickly bringing the almost insurmountable data collection rates to manageable amounts of preprocessed diffraction data from nano/microcrystals, presented by Nadia Zatsepin. Secondly, participants were led through the fundamentals of indexing, merging and evaluating SFX data using CrystFEL (***www.desy.de/~twhite/crystfel/***), a software suite written for high-throughput analysis of serial crystallography data (at X-FELs or synchrotrons), presented by its lead developer, Thomas White (DESY).



John Spence presented on overview of emerging techniques in serial femtosecond crystallography (SFX).

Seasoned crystallographers reflected on the usefulness of the workshop – a highlight of the ACA meeting for some! – reminding them of the early days of crystallography, before GUI's and easy-to-use interfaces, since in SFX details of spot size, shape, Ewald sphere construction and detector dynamic range must

be understood and accounted for to ensure accurate hit-finding and intensity calculation. Since the software is almost entirely UNIX-based and command-line driven, the workshop enabled participants of various experience levels to go from the stage of raw SFX data to a final list of merged intensities to be used for structure determination, and to learn how to obtain metrics to assess data quality.

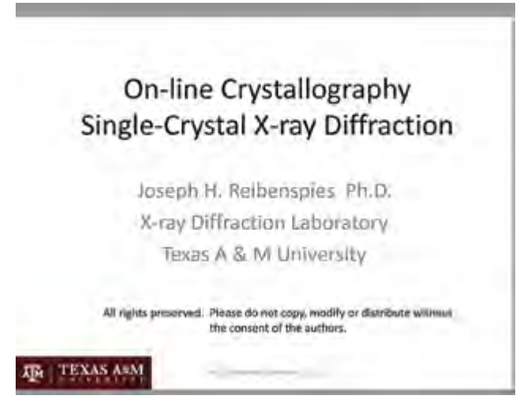
Nadia Zatsepin and Thomas Grant

Net RefleXions

Winter is in full swing. At least in Wisconsin, snow is already on the ground and flip flops have been packed away for warmer times. So there is all the more reason to stay indoors with a cup of hot chocolate and take the time to revisit the fundamentals of x-ray crystallography. In this installment of *NetfleXions*, I will highlight two useful online tutorials for both graduate and undergraduate students that cover the basics any aspiring crystallographer needs to know.

The first tutorial has been built by Patrick J. Caroll (UPenn) and can be accessed at ***http://crystal.chem.upenn.edu/course/index.html***. The tutorial is broken up into eight major topics from *Introduction* to *Structure Refinement*. When you click on one of the topics, you're taken through a series of webpages, each focused on a specific aspect of the overall topic. Through the combination of simple text, pictures, and interactive windows, the tutorial builds your understanding of the theory of diffraction and its applications. The tutorial begins with a brief history of x rays and x-ray crystallography before launching into definitions of unit cells, symmetry, and space groups. Then the tutorial goes through the set-up of an experiment and the mathematics behind the phenomena of diffraction and structural solution. For visual learners, like me, the interactive windows were a real delight. I enjoyed spinning and turning molecules to really see the symmetry elements being discussed in the tutorial. The scope of the material covered was quite broad, but the straightforward language made it accessible.

If you are more of an auditory learner, the tutorial created by Joe Reibenspies (Texas A&M) is a perfect fit for you. This tutorial consists of a series of eight lectures and it can be accessed from ***http://xray.tamu.edu/xscd_course.php.*** Each lecture lasts about an hour and Joe narrates the slide shows with a dash of humor. The lectures cover the entire process of modern x-ray crystallography: from picking the right crystal to publishing the resultant crystal structures. The lectures are comprehensive and detailed. Since sometimes the time constraints of a course do not permit detailed discussion of the publication process for crystal structures, lecture 8 is a great supplement to a crystallography class. In addition, the tutorial outlines guidelines for identifying good quality crystals, which can be incredibly helpful for novice crystallographers.



I hope these two tutorials will help get you, dear reader, through the long winter months. Stay warm!

Anastasiya Vinokur

YSSIG Report

The Young Scientist Special Interest Group (YSSIG) has begun diversifying its activities associated with ACA in the continued growth of the association. In addition to use of the ACA (@ACAxtal) and ACA YSSIG (@ACA_YSSIG) twitter accounts to disseminate crystallographic news and updates, YSSIG is working on protein crystallography projects with local schools near the Denver, Colorado area where the 2016 ACA meeting will be held.

To expand efforts of ACA nationally, I received a generous grant from the American Chemical Society to attend a meeting of the Council of Scientific Society Presidents (CSSP) in Washington, DC. The CSSP is an umbrella organization that unites current and past presidents of scientific organizations that range from Oceanography (Association for the Sciences of Limnology & Oceanography) to Photonics (International Society for Optics and Photonics). The four-day conference consisted of scientific discussions, policy work groups, and informal sessions. Members of the society shared many common interests and concerns including the necessity of increased diversity, the utility of a degree in science, the role of online education in colleges and universities, and open-access academic publishing. I was excited to be able to report that the ACA has begun its own open-access journal *Structural Dynamics*. Other societies were pleased to hear about the journal and mentioned that it will give the ACA increased visibility internationally as well as within our home community in North America.

The academic discussion went into greater detail about the interrelated nature of the scientific societies. Jacqueline Barton (Caltech) delivered a captivating story on how fundamental studies of charge transfer in DNA complexes led to an understanding of how proteins are able to discover and signal for DNA mutations.

Just as DNA is the basis of life, the following sessions gradually expanded from DNA to pollens, to topics of multicellular life (as complex as human psychology). This 'increasing complexity' was capped by a talk from Charles Frank Bolden, Jr. (current Administrator of NASA) on NASA's efforts involving Mars exploration. His talk also involved possible crystallographic studies with postulated experiments examining Mars soil in the next 30 years.

The conference provided me an opportunity to learn of the governance of academic societies, specifically on the financial concerns that scientific societies (and researchers!) are facing in the current environment.

Charles F. Bolden present a ~30 year time line for Mars explorations with key steps (including asteroid redirection and new propulsion technologies) highlighted on route to the 'grand effort' of a manned mission to Mars.

Overall the CSSP meeting exposed me to a wide variety of science and governing styles. A common theme that emerged was that constant selfevaluation was needed to anticipate 'disruptive innovations'. Diversifying the services, audience, and membership of the ACA is a constant effort of YSSIG; accordingly, we are also very much interested in hearing from members how best to improve our sessions and services. We look forward to hearing from the community and meeting with everyone at the 2016 ACA conference.

Martin Donakowski

News from Canada

On October 27 the members of the Canadian National Committee for Crystallography and other interested parties had a teleconference to discuss the moving of the offices of the CNCC from NRC, Ottawa to the Canadian Light Source (CLS) in Saskatoon. A major part of this meeting was a presentation by Nicole Arbour who is a senior advisor to the Government and International Relations Office and Manager of the Grant to the International Affiliations Program (IAP). The CNCC falls under the jurisdiction of the IAP and is required to report to the IAP annually. Arbour introduced the IAP and discussed its function. There are 29 International Unions such as the IUCr, IUPAC etc. that fall under the jurisdiction of the IAP. Currently as a newcomer to the IAP, she is gathering all of the necessary data to highlight the value of the program to government. There are hopes that this reorganization of what was formerly known as the Canadian Science Technology and Innovation Council will engage, in a more active manner, the Canadian Science and Technology Community. One of the goals is to try to include other institutions like the Research Councils, NSERC, CIHR and NRC as well as the Royal Society of Canada and University Associations.

The current make-up of the CNCC is Chair, Patrick Mercier; Vice-Chair, Tomislav Friscic; Executive Secretary, Michel Fodje; Treasurer, Brian Patrick; Past Chair, Jim Britten; Past Secretary, Joe Schrag; Past Treasurer, Marie Fraser; Canadian Representative to ACA, Michael James; Webmaster, Louise Dawe; Recruiter for IUCr Commissions, Lynne Howell; Member from Maritimes, Andreas Decken.

Lastly, I would like to present a brief summary of the Buffalo-Hamilton-Toronto Meeting that was held on November 6, 2015 in Hamilton at McMaster University and hosted by Vivian Saridakis and Gerald Audette from York University. There were 125 registered at the meeting that was sponsored by Art Robbins, Bruker, Fortebio Malvern, BioRad, VWR, TTP Labtech, Rigaku, Formulatrix and Molecular Dimensions. Each year the attendees vote on the topic that will form the basis for the invited presentation.

For 2015 the topic was "Combining X-ray diffraction with techniques such as cryo-electron microscopy (Cryo EM)". The invited speaker for 2015 was Helen Saibil, the Bernal Professor of Structural Biology, Birkbeck College, London. The title of her talk that was presented in the morning of Nov. 6, was "Cryo EM of Pore-forming proteins in the molecular arms race between host and pathogen". Her talk was centered on the pore forming proteins of bacteria and the pore-forming proteins of the immune system.

The afternoon was dedicated to 10 presentations from trainees (graduate students and post-doctoral fellows) from different X-ray crystallographic or cryo EM labs in the Buffalo, Hamilton, Toronto area (even as far east as Queen's University Kingston, Ontario). Above is a photograph of Helen Saibil (on the right) with the 10 presenters in the afternoon session. The planning for the 2016 BHT meeting has already begun. It will be held at McMaster University and will be hosted by Alba Guarné on November 4, 2016.

Michael James

Bruce Willard Brown (1927-2015)

Bruce W. Brown earned both his Bachelor's and Master's degrees in chemistry at the Polytechnic Institute of Brooklyn. His 1949 undergraduate thesis was *Tungsten and Molybdenum Bronzes*, and his 1952 MS thesis was *The Solid State Preparation, Absorption Spectra and Conductivity of Sodium Tungsten Bronzes - Na_xWO_3*. In 1950 he traveled west to the University of Washington in Seattle where he became one of Ed Lingafelter's students when machine computations in crystallography were starting to develop.

His graduate studies were interrupted in 1952 as the New York draft board caught up with him. As a Physical Science Research Assistant, he worked to develop defenses against chemical agents and was an instructor in Chemical Weapons Identification at a junior college. He told the tale of ordering a Weissenberg camera for part of this effort and when the supply house called to find out why it was rejected, he discovered the base receiving officer was the one who returned the instrument and who offered Bruce the explanation "A camera was ordered and any fool could tell that was not a camera!" Bruce also related how he spent countless nights in the Army laboratory during the absence of others because the instruments were very sensitive to line-power fluctuations caused by building elevators, other experiments involving transients, etc.

Returning to Seattle, crystallographic computations were initially made on borrowed equipment (nightly) in the University business office by wiring boards and feeding IBM cards to obtain the required multiplications and sums. Then, the University installed its first computer, an IBM 650, placed conveniently on the fourth floor attic annex of Bagley Hall, the Chemistry building (a direct climb from the basement where our labs and offices were located). This was a card-input, card-output machine requiring an office machine printer to list input or results. Since grant money for Lingafelter's students was very low, a key to the room was acquired and the nightly use continued, requiring a bit of janitorial work at the end of the shift to remove punched tabs, replenish card and paper bins, etc.

TThe computer itself had a magnetic drum as its memory, able to hold 2,000 10-digit numbers. An adjacent room was full of tubes as the drivers for each of these memory bits, but the computer console allowed one to conveniently know when a particular tube had "failed" because it was marginal electronically. Observation of an IBM technician swapping tubes led a few of us to do the same. Unfortunately during the summer of 1957 while one of the below mentioned authors was at Los Alamos, the problem became catastrophic and the entire room of tubes needed attention and replacing.

In 1956 the IBM 650 computer was just being programmed in machine language for high efficiency and speed Since we knew the time the memory drum took for one revolution as well as the time for loading a location, the time required for addition (or other simple arithmetic steps), and that of storing the result to a specific location, it became possible for repetitive functions, such as the trigonometric ones, to make the process efficient with very careful programming. Lyle Jensen, Jim Stewart, Bruce Brown and, Bruno Morosin (the latest addition to the group), were involved in this effort. (Jensen was Lingafelter's first graduate student. He had become a professor in anatomy at the medical school on the edge of the campus, and he had excellent diffraction equipment the group could use when it was free. More important, he was actively pursuing crystallographic problems.). Soon assembly languages, SAP and SOAP became available, followed by FORTRAN. Bruce continued his long involvement in crystallographic computer programming to various degrees even at Portland State. (These computer codes were eventually developed by Jim Stewart, then a chemistry professor at the University of Maryland, into a system of programs, XRAY63, that eventually evolved into the XTAL system.)

Bruce wrote his dissertation, *The Crystal Structures of the Bis-Ethylenediamine Complexes of Nickel (II) Thiocyanate*, and earned his PhD in May, 1961 at the University of Washington.

Bruce accepted a position in the Department of Chemistry at Portland State College (which eventually became known as Portland State University) and remained there until retirement in 1992. During this period, he taught general and analytical chemistry and x-ray crystallography and he developed a series of courses for non-majors in environmental chemistry and chemical safety. He also served a hitch as Department Chair, and then eventually became Assistant Dean of Sciences. He also served on the Chemical Safety Committee for some years.

Bruce was much loved by his students because of his efforts on their behalf while acting as their advisor. He was considered tough and demanding by his students but always fair because it was obvious to them that he had their best interests at heart.

Bruce will be particularly missed by his children, step-grandchildren and other relatives as well as by many who interacted with him over the years. They miss his jokes and photos which have been more recently sent by e-mail'

Bruno Morosin and David McClure

Don Cromer (1923-2015)

Don Tiffany Cromer died on November 11, 2015. He earned his PhD in chemistry at the University of Wisconsin in 1953 and joined the Los Alamos National Laboratory where he remained for 38 years. His major contribution to x-ray diffraction consisted of using Dirac-Slater wave functions to calculate scattering factors, particularly important for heavy atoms. Together with the values for anomalous scattering, especially near L-edges, his work

resulted in some of the most cited research papers in physics in the 1950s and 60s. He was the recipient of the E.O. Lawrence Award for his meritorious contribution in nuclear chemistry, presented by President Nixon at the White House in 1960.

Bruno Morosin and Jim Schirber

Gerson Cohen (1939-2015)

Gerson H. Cohen passed away on July 11, 2015 at the age of 76. He was a scientist his entire life, and worked as an x-ray crystallographer at the NIDDK/National Institutes of Health from 1965-2006.

Gerson was a treasured member of the Section on Molecular Structure in the Laboratory of Molecular Biology, NIDDK, NIH for many years. He was a computer expert when these technologies were just developing and the Laboratory depended on his skills for the early structure determinations. He was sorely missed when he retired.

David Davies

Gerson was a very important contributor to our understanding of the structure of proteins, and a central figure in the design and application of the computer methods used to solve such structures. As a colleague he was always warm, friendly and helpful. His presence has been missed since the day he retired and left the laboratory. We recall him as he was in those days, and hope that memory will be a comfort to his friends and family

Gary Felsenfeld

Contributtors to this issue: Cele Abad Zapetero, Allyssa Adcock, Avni Bhatt, William Booth, Ivana Brekalo, Sue Byram, Chris Cahill, Chelsy Chesterman, Martin Donakowski, Robert Evans, Joe Ferrara, Jeanette Ferrara, Jim Fettinger, Robert Fick, Frank Fronczek, Kamran Ghiassi, Richard Gillilan, Thomas Grant, Anna Gres, David Haas, Kasia Handing, Karina Heffernan, Michael James, Matthew Jensen, Pascal Krote, Alberto Landeros, Dorothee Liebschner, Brian Mahon, Andres Manriquez, Daniel Mast, David McClure, Bruno Morison, Chiara Pastore, Virginia Pett, Daniel Rabinovich, Connie Rajnak, Jim Schirber, Marina Solomos, Anastasiya Vinokur, Huanchen Wang, Kittikhun Wangkanont, Nadia Zatsepin.

Structural Dynamics
co-published by AIP Publishing | ACA

Upcoming special topic issues:

Protein Dynamics – Protein molecules are not static while performing their functions, but dynamic. The range of the motions is highly variable amongst different proteins, ranging from modest side chain rearrangements to very large scale folding/unfolding events. States very far from the crystal structure have shown to be functionally important. Methods for studying these dynamics include X-ray scattering, NMR, electron microscopy, mass spectrometry and various other spectroscopies, calorimetry, and theoretical or computational approaches.

Energy landscape theory and the funnel concept have shown how to relate this well determined structure with the complete protein landscape that is used for folding and function. A static snapshot of a protein produced by X-ray crystallography or NMR is very useful in determining this funneling landscape and therefore for identifying key players in the function. The energy landscape of the conformations defines the capabilities of the protein to recognize its partners or substrates and perform its catalytic, signaling, or structural role in its biological function.
Guest Editors: George N. Phillips, Jr. and José Onuchic

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

The 12th Femtochemistry Conference (FEMTO12 - Frontiers of ultrafast phenomena in Chemistry, Biology, and Physics -

FEMTO12 will bring together scientists from all over the world to present and discuss the most recent advances in femtosciences, including reaction dynamics, coherent control, structural dynamics, solvation phenomena, liquids and interfaces, fast processes in biological systems, strong field processes, attosecond electron dynamics and aggregates, surfaces and solids with contributions from both theory and experiment.

Guest Editor: Jochen Küpper

Soft X-ray in Energy and Time (SXET) – This issue will have reports on the current status and new developments in soft x-ray absorption and emission spectroscopy as well as its resonant processes towards the Heisenberg limit (time versus energy limit). It will feature technical and methodological developments for high energy resolution or ultrafast time-resolved approaches addressing new scientific questions for solid, liquids, gases and interfaces. ***Guest Editor: Emad Flear Aziz***

2016 Changes on the Editorial Board

Franz Pfeiffer and Linda Young completed their terms on the Editorial Board at the end of 2015. We are grateful for their time and efforts that helped us through the initial years of the journal.

We welcome Shaul Mukamel (UC Irvine) to the Editorial Board. Professor Mukamel is an internationally known expert in the field of ultrafast optical phenomena. Among the honors he has received are the Hamburg Prize for Theoretical Physics (2012), the ACS Ahmed Zewail Award in Ultrafast Science and Technology (2015) and election to the National Academy of Sciences (2015). He is co-authored the first paper contributed to *Structural Dynamics* (Two-dimensional x-ray correlation spectroscopy of remote core states , D. Healion, *et. al*, *Struct. Dyn. 1, 014101 (2014)*) and has been a strong supporter of the Journal since its inception. We look forward to his continued contribution as an author as well as a member of the Editorial Board.

Congratulations to Editor-in-Chief Majed Chergui on being Awarded the 2015 Edward Stern Prize

The Edward Stern Prize is awarded for Outstanding Achievement Award bythe International X-Ray Absorption Society (IXAS).

IXAS is an international scientific organization that represents scientists working on the field of structural analysis of molecules, materials and proteins using inner shell excitations induced by x-rays (or electrons). It was officially founded in 1994 following several informal X-ray Absorption Fine Structure (XAFS) conferences in the growing field of x-ray absorption spectroscopy.

Structural Dynamics
co-published by AIP Publishing | ACA

The Edward Stern Prize represents the highest honor given by the Society. Winners are recommended by the IXAS Awards Committee and approved by the IXAS Executive Committee. The IXAS Awards Committee invites nominations from both experimental and theoretical studies of XAFS. The Prize is awarded every third year on the occasion of the XAFS conference to two scientists for lifetime achievements.

Majed Chergui is Professor of Physics and Chemistry at EPFL, where he pursues a variety of ultrafast UV and X-ray spectroscopic studies on chemical and biological systems. Since 2013, he has been founding Editor-in-chief of the journal *Structural Dynamics*, published by the American Institute of Physics (AIP) and the American Crystallographic Association (ACA). With the Edward Stern Prize, the IXAS committee recognizes Majed Chergui "for his pioneering work in the field of time-resolved X-ray absorption spectroscopy.".

Why Publish in Structural Dynamics

Metrics: An average time from submission to publication of ~62 days is highly competitive with many of the journals produced by industry leaders, and an average download per article in 2015 of more than 450 is a clear indication of both high quality of the papers and the wide exposure they have had even in the inaugural year of the journal.

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

Publication Charges & Open Access Fees : Open access is also an "author pays" model. Authors will be assessed an Article Processing Charge of ***USD 2200,*** which covers the cost of publication and allows the author to retain copyright through a Creative Commons Attribution 4.0 Unported license.

ACA members can take advantage of a special discounted article processing charge of USD 1500 when publishing in Structural Dynamics. The corresponding author must be the ACA member (***membership.amercrystalassn.org/***).

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

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The Journal is now indexed in Thompson Reuters databases and our first impact factors will be calculated in 2016.

Alan Turing: The Enigma, by Andrew Hodges, Princeton University Press, Paperback, 2014, ISBN:978-0-691-16472-4-

Even though Andrew Hodges' *Alan Turing: The Enigma* is now thirty-two years old, it is still regarded as one of the most well-researched biographies of Alan Turing. Its relevance prevails despite its age, and the book was the inspiration for the Academy Award-winning film, *The Imitation Game* (which, ironically enough, was heavily criticized for its manifold historical inaccuracies that in no way came from the book it was supposedly inspired by). However, despite *The Imitation Game*'s particular failures, the film's impending release led to a re-release of Hodges' book. The new "movie-tie-in" edition's cover is a scene from the movie, showing Benedict Cumberbatch as Turing from the back, facing his famed Enigma machine. That was about the extent to which the book tied in to the movie.

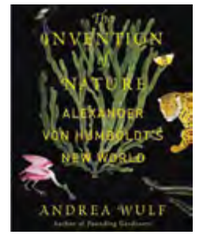
I initially saw the film, which had been well-received by audiences who were willing to ignore—or perhaps unaware of—its historical inaccuracies. After seeing the film, I wanted to learn more, having heard Turing's name mentioned repeatedly in my brief undergraduate career as a programmer. And though I found the book a thrilling and fast-paced read (albeit a bit hefty at 736 pages), I was wildly dissappointed that presumably someone responsible for the making of *The Imitation Game* could have read the exact same book, and come out with the screenplay for said film, particularly because the extreme care with which Hodges' researched and wrote *The Enigma* is ever-present in his prose, which the film idly cast aside. Hodges' sought to provide his audience with a detailed and accurate account of Alan Turing, a brilliant man whose work provided the foundation for modern computing as we know it.

Given the role Turing played in helping the Allies crack the German codes during World War II, one might expect him to have been the subject of myriad biographies, with Hodges' only being one of the many. Yet the top-secret nature of Turing's work meant that for many years his contributions went unrecognized. His universal machine, something we today recognize as a fundamental concept of computing, was ahead of its time. Hodges' biography helped garner recognition both for Turing and the importance of his research in broader cultural circles. And, as I mentioned previously, it provided inspiration for *The Imitation Game,* which despite its inaccuracies made Turing a household name in an age of technology that arguably would not exist without his contributions.

Whether or not you saw *The Imitation Game* and want to learn more or you just have an interest in the history of computing or codebreaking or World War II (or all of the above), Hodges' book is an excellent read, and one that I highly recommend.

Jeanette S. Ferrara, NYU School of Journalism

The Invention of Nature: Alexander von Humboldt's New World, by Andrea Wulf, Alfred A. Knopf, New York, 2015, 496 pp., ISBN-13: 978-0-385-35067-9



Although the subtitle suggests that *The Invention of Nature* is only about the New World, the book covers much more: Humboldt's early life, his trip to the new world, his attempts to visit the Himalayas stymied by the East India Company, a substitute trip to Siberia, his interactions with the scientists of his day, his publications that provided tremendous information to the general public and his later life in Berlin. The epilogue discusses one of the repercussions of WWI—the purge of everything German from many places around the world. Humboldt's current obscurity arises from his Prussian heritage and use of the German language.

I vaguely remember Humboldt as an explorer of South America from my elementary school classes – everyone learned about the Humboldt Current (at least in the US in the fourth grade in 1970). I did not realize the extent of Humboldt's travels nor his contributions to our understanding of nature. As he traveled through South America he took detailed notes and made measurements with all types of instrumentation creating a fascinating picture of the connectivity of nature. He climbed near the summit of Mt. Chimborazo in the Andes, taking measurements all along the way in clothes that were not suitable for even a low ascent. He mapped the plant life as he ascended and ultimately correlated the types of plants he saw rising up the mountainsides with the plants one sees as one heads north from the equator to the pole.

In life Humboldt influenced the likes of Simon Bolivar, Thomas Jefferson, Ralph Waldo Emerson and Henry David Thoreau. He presented results to the Royal Society and published many works for the general public including titles like *Personal Narrative* and *Cosmos*, bestsellers of their day.

The book does not end with Humboldt's death in 1859. After his death, his work influenced the naturalists George Perkins Marsh, Ernst Haeckel and John Muir, all of whom contributed to the creation of the national parks system in the US to preserve nature.

What Humboldt can teach us, as perhaps the first great naturalist, is that everything is connected and has a place and that we need nature to survive.

Joe Ferrara

ACA Philadelphia: WK.04: Small Angle Scattering – Structural Biology and Soft Matter

This past year, 2015, marks the 100th anniversary of the publication by Peter Debye of his now-famous formula describing scattering intensity as a sum of atomic scattering factors (*Ann. der Physik* 416 809-823 (1915)). Since that time, the technique of small-angle scattering (neutrons and x-rays) has been applied to the study of nearly every form of matter. While the foundational physics of scattering is common to all application areas, individual fields have since diverged to develop many specialized tools appropriate to the type of matter under investigation. Biological systems, for example, are weakly scattering systems of finite size, most often studied in dilute monodisperse form where preparation methods are critical to success. Polymers and other soft matter, on the other hand, are often strongly scattering, present in concentrated form, and studied in "as is" polydisperse condition.

As science progresses, the boundaries between structural biology, materials science, and engineering are beginning to dissolve. It is not uncommon now for molecular biologists to be interested in assembly of fibrils that may be non-monodisperse and of nearly macroscopic length, or interested in proteins embedded in nanodiscs or complex lipidic phases. Similarly, the highly developed tools for shape and flexibility analysis developed for biologists may be of considerable interest in the study of synthetic materials. With this in mind, we organized a dual-track workshop aimed at getting soft-matter scientists and biologists in one room for a joint morning session covering the common basics of small-angle scattering. The morning session was followed by two breakout sessions: one devoted to structural biology, the other to soft matter.

Prior to the course, a web site was constructed containing important software installation instructions for students as well as a course schedule, speaker information, and links to tutorial data and online tools. This website will remain active after the course as a general resource for SAS students.

Jan Ilavsky (APS) began the morning with a joint session lecture entitled *Biology Meets Soft Matter*. **Angela Criswell** (Rigaku) led the first morning tutorial session in how to use the most common software tools (ATSAS) to do basic SAS data processing. As in our previous ACA SAS (2014) Workshop, the important role of laboratory SAXS instrumentation and technique was emphasized with a variety of short lectures under the heading *Do Try This at Home*: **Sergio Rodrigues** (Xenocs), **Peter Worsch** (Anton Paar), and **Angela Criswell** (Rigaku).

After lunch, the group divided for application-specific lectures and tutorials. Students were encouraged to freely migrate between lectures depending upon their particular interests. The biological session began with a general lecture on SAXS and SANS specifics for biology by **Jill Trewhella** (U. Sydney). **Richard Gillilan** (MacCHESS, Cornell), followed with a hands-on tutorial in P(r) calculation and shape reconstruction. **Kushol Gupta** (UPENN) covered the all-important area of sample preparation, with some introduction to the new method of inline size exclusion chromatography coupled with static light scattering (SAXS-SEC-MALS). As an introduction to advanced processing, **Susan Krueger** and **Joseph Curtis** (NIST) conducted a SASSIE tutorial using the new online CCP-SAS platform. Online tutorials offer the advantage that there is no need for software installation on student laptops. The biology track finished with the important *Publishing Data: what you should know* lecture by **Jill Trewhella**. This final lecture gave students some vital tips for safe interpretation of data and good publication practices.

The afternoon soft matter track was led by **Jan Ilavsky** (APS) with assistance from **Kevin Yager** (BNL). Ilavsky began the session with a general lecture on soft matter basics. **Kevin Yage**r next gave an overview of grazing incidence small-angle x-ray scattering (GISAXS), which is becoming a field in its own right. Jan Ilavsky continued with lectures on models, a central component of soft matter data analysis as well as comments on instrumentation. The soft matter track concluded with an in-depth hands-on tutorial of data processing using the Irena package.

Wk.04 was well attended, with 46 participants. Due to strong interest among biologists and limitations of room size, it was necessary to cap attendance for the biology track. We had also hoped to encourage a larger number of soft-matter specialists. All students were provided with lunch, a set of printed course notes, and an *authentic* ACA SAS memory stick containing course notes, tutorial data, and other useful material.

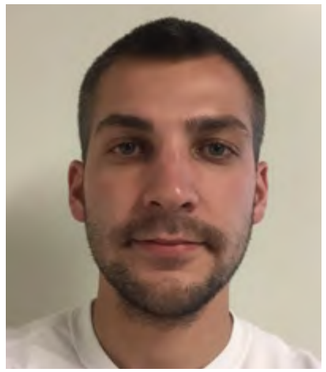
The course website was created with help from CHESS, the Cornell High Energy Synchrotron Source (**Barbara Herman** and **Nika Ablao**) and will continue to remain online as a future resource for SAXS students and researchers. Thanks also to **Kathy Dedrick** and **Irina Kriksunov** for administrative and logistical support. In addition to our speakers, we thank the non-lecturing members of the organizing committee for valuable insight and behind-the-scenes help: **Shuo Qian** and **Volker Urban** (ORNL), **Thomas Weiss** (SSRL), **Zhang Jiang** (APS), **Andreas Keilbach** (Anton Paar).

This training workshop would not have been possible without the generous support and participation of our corporate sponsors: **Anton Paar, Dectris, Rigaku, and Xenocs**.

Richard Gillilan

The following notes were written by the 2015 recipients of travel grants and / or the young researchers selected for the SIG Etter Award Lectures. Many would not have been able to come to the meeting without the financial support provided by ACA members when they generously contribute to the travel award funds.

Kamran Ghiassi: I attended the entire



meeting and gave an oral presentation in the *Important Science from Small Molecule Structures* session. One of the best features of the meeting was the diversity of topics in the field of small molecule crystallography. It was truly a great experience going to so many different talks and posters. I enthusiastically endorse the Etter Early Career Symposium because it gives young scientists a chance to present talks. I am currently a member of the American Crystallographic Association (ACA), American Chemical Society (ACS), and Electrochemical Society (ECS). I plan to continue my membership in these organizations and may add others depending on the direction of my research.

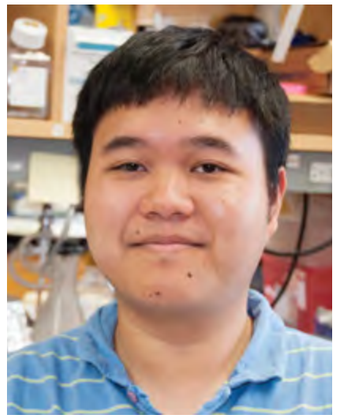
Allyssa Adcock: Being not only a first

time attendee at a national conference, but also a first year graduate student, I was unsure of what to expect. But I had an amazing experience at the meeting in Philadelphia that left me with the desire to become more involved in the crystallographic community.

I was impressed by the welcoming sense of camaraderie at the meeting, as well as by the diversity of the program. After listening to three day's worth of passionate speakers and poster presenters, I left the conference with both with a renewed sense of excitement for my research as well as countless new ideas and opportunities. For future meetings, however, I would enjoy seeing more events similar to the Bruker YSSIG Mixer, e.g. a young scientist lunch or coffee break, where graduate students could have more chances to meet people and develop their networks. I also felt that there were fewer sessions concerning small molecule/inorganic crystallography in contrast to the more prevalent biochemistry-related talks.

In addition to the ACA, I am also a member of the American Chemical Society, and I do plan to continue my membership with both. I am incredibly grateful to the ACA for awarding me a travel grant to attend the meeting and experience the conference, and I look forward to attending next summer's meeting.

Kittikhun Wangkanont (Pun): I am a

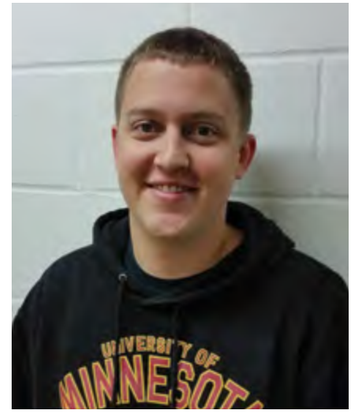


PhD student in the department of chemistry at the University of Wisconsin-Madison. I have been an ACA member since 2012, but 2015 was the first time I was able to attend an annual meeting. I was excited that at my first meeting my abstract was selected for an oral presentation in the *Structural Glycobiology* session, which was directly related to my research on carbohydrate-binding proteins. The meeting covered a broad range of topics that are quite relevant to my own research and helped enrich my scientific experience. The session on data collection strategies was quite informative. Unfortunately, many interesting sessions were happening concurrently. One way to circumvent this issue would be to give speakers an option to present posters as well as talks. That would also maximize personal interactions at the meeting.

Everyone at the meeting was very welcoming, supportive, and willing to talk with younger students. I got a chance to meet and discuss my research with several scientists I had only known through their publications. It was also a great venue for networking with crystallographers from other academic institutions, industry and national laboratories, especially because I am looking for postdoctoral opportunities. I also met and became friends with other students, many of whom I still keep in touch with.

I am also a member of the American Chemical Society (ACS). Although ACS has a lot more presence on campus (something ACA might want to do), the ACS meetings are extremely large and quite impersonal. There is nothing like the YSSIG. Combined with an affordable student membership fee, I will definitely continue my ACA membership and I am looking forward to future ACA meetings.

Matthew Jensen: Every year, my



PI, Carrie Wilmot, takes interested lab members to the annual ACA meeting. This year's meeting in Philadelphia was my second ACA meeting, and it was very beneficial for me. My participation in the poster session, attendance at sessions, and interactions with experienced crystallographers helped my graduate career path immensely. And the Liberty Bell was pretty awesome, too!

The travel grant provided me the crucial opportunity to not only present my research at a national meeting, but to network with my peers and more senior crystallographers. I eagerly anticipate the meeting every year because of the array of new methodologies and crystallographic problem-solving techniques that are presented. These skills help me develop new approaches to my thesis project and show me new ways to think about crystallography. I especially enjoyed listening to talks that strengthened my understanding of the theory behind x-ray crystallography. Constant reminders of principles, such as how the Ewald sphere and reciprocal space interact, helped me to think critically about what is going on during data collection. Posters and talks about new advances in looping and cryo-protection techniques motivated me to adopt new ways of handling my own crystals.

My favorite session was titled, *Play it Cool? Ambient and Cryogenic Approaches*. This session discussed the theory behind how cryo-protection works in macromolecular crystals, as well as offering several new cryo-protection techniques. One noteworthy talk was presented by Doug Juers of Whitman College. He discussed his recent results detailing the use of vapor diffusion based cryo-protectants. The technique utilizes the vapor pressure of short-chain alcohols, such as methanol and ethanol, to drive these molecules into the crystal lattice. This technique interested me the most because it removed the extra handling step of soaking a crystal in a cryo-protectant drop. This step has proven detrimental to one of my crystal types, so I am eager to test Doug's method on my own system.

The poster session was excellent again this year. I always enjoy the opportunity to discuss my project with peers and experts in crystallography. Many people stopped to ask me questions and offer advice. I speak for all graduate students when I say that advice received at a national meeting goes a long way in helping alleviate lab problems! I am very grateful for the opportunity to present my poster and learn from others' posters, too.

Once again, I would like to thank the ACA for the travel award to attend this year's meeting in Philadelphia! Your financial aid helped me learn and grow as a young crystallographer. I can't wait for next year!

Kasia Handing: I appreciate the

opportunity to have participated in the 2015 ACA Meeting. It was the first ACA Meeting that I attended. I loved the atmosphere and how open the people were. It was easy to make connections, talk about science and share experiences. I had the chance to meet many new people, both fellow students and professors that have been some of my scientific role models. I enjoyed the career panel organized by YSSIG. It gave me a broader perspective on possible career paths and an opportunity to ask questions. I hope there will be another session like this at the next meeting. I would say my favorite session was *Standard Practices in Crystallography*. I learned a lot about the most common procedures directly from the best crystallographers. It would be nice if the recordings from these sessions would be made available online for review.

The ACA Meeting was an enriching experience, though I feel that some improvements could be made. The abstracts for the talks should be available in advance for attendees to more effectively plan which sessions to attend. I also feel that topics should not be clumped together, but spread out so that someone with specific interests can attend as many talks about their subject as possible. Another small but crucial component is the severe lack of refreshment options during break times. Hearing several presentations consecutively can make for a long day, and it is pleasant to break up the monotony by chatting with your colleagues while sipping a nice, warm beverage. However, during each break there was only one carboy of coffee for a conference of hundreds.

Currently I'm ACA member and I'm going to continue my membership in the future as well as participate in upcoming meetings.

Marina Solomos: The 2015 ACA

meeting in Philadelphia was my first ACA meeting and it was a great experience. I enjoyed being at a conference that was focused on topics valuable to my research, and it was extremely helpful to meet with leaders in the field and receive feedback during my poster presentation. I appreciated the diversity of the talks and the opportunity to learn about an array of instrumental techniques, in addition to single crystal x-ray diffraction, that might enhance my research.

I returned with a lot of new ideas to try. If I could change one thing, I would suggest there be even more professional development sessions throughout the meeting with people from a variety of careers so that we have multiple

perspectives and opportunities to ask questions.

So far in my graduate school experience, I definitely found the ACA meeting to be one of the most useful (and also the most welcoming) conferences. Everyone I met was friendly, helpful, and willing to discuss any problems with crystallography we had encountered in our graduate research. In addition to the ACA, I am a member of the American Chemical Society and the Materials Research Society, and I hope to continue my ACA membership and attend more meetings in the future.

Brian P. Mahon: The ACA meeting provided me with an opportunity to begin networking for future collaborations and careers. With that said what I found to be most helpful were the poster sessions where I was able to meet a wide range of scientists from different facilities across the nation and the world.

If possible, I would suggest having fewer simultaneous sessions. I am not sure how this would be possible but it would be very helpful as there were several talks I would have liked to attend but could not due to overlapped times.

I am currently a member of the American Chemical Society and the ACA. I do plan to continue my ACA membership beyond this conference.

I think the ACA has done a great job keeping its members informed. I would recommend, if possible, to have more workshops available covering a diverse range of not only novel crystallographic techniques, but also other biophysical and biochemical techniques. This would give students a great opportunity to keep their skill sets current and would help when they need to find jobs.

Anna Gres: I was a first-time attendee

and enjoyed the meeting a lot. From my point of view, it was extremely valuable to hear the opinions of the experts in the field regarding good practices at all stages of solving crystal structures. That is why I enjoyed the talks in the *Standard Practices in Crystallography* and *General Interest* sessions. However, unfortunately for me, those talks conflicted with the *In the Service of Science* and *Biochemistry in the X-ray Beam* sessions. I do realize it is extremely difficult to work on the schedule but my suggestion would be try to avoid overlaps at least within subareas of interest (*e.g.* protein crystallography, small-molecule crystallography, material sciences *etc*.).

An appealing thing was the exhibition where there was an opportunity to learn more about latest techniques available for crystallographers.

I am a member of American Chemical Society and American Crystallographic Association and I plan to continue my membership in both societies. Among other things, I really enjoy the ability to follow recent news in the field and see potential career opportunities.

At the ACA meeting, I presented a poster that received positive feedback from other attendees and won a Linus Pauling poster prize! Attendance of the talks gave me broader insights into the overall world of crystallography and on current developments in the field. I enjoyed being able to network and discuss my work with other graduate students and even some principal investigators from all over the world. I am now looking forward to sharing my work at other scientific events!

Andres J. Encerrado Manriquez: My

participation in this conference was made possible by the great support received from my university and the organizers of this conference (ACA). It was a wonderful and very rich experience, I had never thought of the field of crystallography as a really big one, or at least not as popular as astrophysics or particle research for which presentations usually fill up large auditoriums. But now, hearing all these wonderful researchers and learning about their current projects, the methods and tools they are using, and interacting with the great developers of software and hardware such as Bruker, MiTeGen, and Rigaku, among others, showed me just how broad and comprehensive crystallography is.

I found Philadelphia to be a magnificent city full of history and culture and it was exciting to engage other students and professors in fascinating conversations both inside and outside of the conference, and to catch a nice warm breakfast at the same table with brilliant scientists who might still be thinking of ways to perfect their art of crystal manipulation or techniques for analysis and understanding of complex protein arrays. Luckily I was allowed to participate more actively during one of the sessions by taking the session photos. What a great way to spend an evening; doing what you like and getting a little bit of cash on the side to eat with later.

My only regrets are that I could not attend the presentations that overlapped with one another and there are no video recordings of every session that would allow one to review the material and possibly get in contact with the presenter.

This has been one of the most wonderful experiences in my life, I will never forget my first participation in an ACA conference and the wonderful people that I had the pleasure to talk with.

Pascal Krote: When I was notified

that I was to give a talk at the 2015 ACA meeting, I immediately felt nervous. I was a brand new ACA member and I was the only person in the program talking about electron diffraction. How would my talk be received at the meeting? My jitters immediately left when I learned that I would receive the Etter Lecture Award from the Light Sources SIG. It was very gratifying to know my work was of interest to the Light Source community. I ended up with a 10-minute time slot at the end of the *Early Career* session. It was challenging for me to present my work, a novel technique, and my findings in that short period of time. Nonetheless, my talk was well received by my enthusiastic audience. I was thankful for their praise and constructive feedback.

The venue was an ideal place for a scientific meeting. It offered ample space for concurrent sessions. My one grievance is that I found the concurrent sessions running over 5 days a bit overwhelming. There were a lot of interesting topics to sort through, especially for a first time attendee. It may be helpful if SIG officers generate recommended schedules for the meeting.

I enjoyed all of the sessions I attended. I learned a great deal from Zbignew Dauter's and Miki Senda's talks on data collection strategies. They shared many helpful approaches and they were very engaging speakers. I took copious notes at the *Communicating Science* session, where the speakers gave helpful tips on writing and presenting to audiences outside one's field. Also, I really enjoyed Charlie Carter's talk on the structural biology of the origin of life. I will certainly remain an active ACA member so that I can participate in future meetings and take advantage of the many opportunities members receive.

Thank you to Marian Szebenyi and the rest of the Light Sources SIG for nominating me for the Etter Lecture Award. It made my first ACA meeting memorable, and much more affordable!

Robert Evans: For the second year

in a row, I eagerly looked forward to the ACA meeting, and it did not disappoint! The ACA conference is, for the Wilmot Lab at the University of Minnesota, the "big event" conference of the year. Our PI, Carrie Wilmot, sets high expectations for our posters and participation, and after we return home from the conference each attending lab member is given an opportunity in a special lab meeting to present on topics that we found to be of particular interest. This year two of our lab members, Matt Jensen and myself, were awarded travel grants to attend the ACA meeting. It was very exciting and an honor to receive that e-mail, and Carrie was very pleased that two from her lab were recipients, and she expressed her pleasure, "Two in one year! That's fantastic!"

This year I was especially interested in sessions and posters involving crystallization and crystal handling methods, and in particular, enjoyed learning about random microseed matrix-seeding (rMMS), a cryo-protection protocol that uses alcohol via vapor deposition, a simple device for keeping crystals humid during harvesting, and the physics of diffraction with respect to flux, temperature, icing, cryo-protecting, and so much more. In short, it was a veritable smorgasbord of new methods to try. I could hardly wait to get back to my lab.

The appeal of the ACA's annual conference goes deeper, however, than excellent presenters; I found the exchanges of ideas at the poster sessions to be equally engaging and edifying, not only when I was viewing posters, but also when I was presenting my own work. ACA attendees (students, PIs, and vendors alike) are tremendously helpful and willing to suggest new angles for solving a problem. I am very grateful for the input of many of the attendees, and would like to give a "shout out" of thanks to the Rigaku team for a very enlightening discussion about rMMS. Many of these representatives (from many of the sponsoring companies at the conference) are more than competent sales people, they are full-fledged scientists with substantial experience in crystallography. I was surprised and pleased by the amount of time all of the ACA corporate representatives were willing to spend on me, even after learning that I was a student. I am "a bit" older than most graduate students, and so the various people staffing the booths tend to mistake me for someone with a budget. It is somewhat humorous to watch their faces when they learn that I am a student, but they always continue on bravely, even after learning I'm not in the market for a new whatever. I truly appreciate the time the vendors take to answer questions and to teach.

I hope to see you next year in Denver!

Robert Fick: Attending the ACA

national meeting was really a great experience that benefitted me on many levels. Presenting my research as a poster, I was able to interact with the diversity of attendees and received feedback on my project from both small molecule and macromolecular crystallographers, which led me to see my project from more than just my own paradigm. Visiting other posters, one can see the true breadth of problems that can be explored by crystallography, especially with many of the problems that were explored outside the realm of structural biochemistry that I have been engaged in for my thesis research. I was also able to take in a wide variety of talks, learning about new instrumentation to improve data collection and software modifications that will help to better refine that data. I also sat in on talks concerning chemical syntheses, as well as the macromolecular crystallography more familiar to me. Several different specific techniques caught my eye, with the use of ionic liquids as a possible way to favor crystallization over protein precipitation, something I may need to explore in my attempt to grow large, single crystals for neutron crystallography. Another talk was applicable to a fellow lab member: this concerned the ability to bind a polynucleotide substrate covalently to an enzyme through the use of a controlled linkage as a way to obtain a substrate-bound structure.

The city of Philadelphia was quite the enjoyable location as well, with the local food scene an excellent reason to wander into the city in the evening.

Dorothee Liebschner: This was the

second time that I attended an ACA meeting, and I really enjoyed it. I had the opportunity to present a talk which was followed by an interesting discussion and I obtained many helpful comments afterwards. Overall, the meeting was a booster for me: I learned new things from talks outside my specialization and I got new insights from presentations in my research field. In particular, I enjoyed the session *Standard Practices in Crystallography: Data Collection Strategies*. The talks were followed by interesting discussions by experts of the field. For a young researcher, it is educational to hear their comments and learn from their experience. Apart from enjoying the science, it is also nice to meet friends and former colleagues. And of course, the meeting is a great opportunity to make new friends and to extend my professional network.

I think the meeting was well organized. However, in some rooms, it was difficult to see the slides from seats further away.

I am currently a member of the Protein Science Society of Japan (PSSJ). If my future career brings me to North America, I will consider joining the ACA.

William Booth: My first ACA conference

was good experience. It felt good to be around people who understand your work, and actually seem excited about it. I really liked how adamant the YSSIG is about the importance of networking, and how much interest they have in the development of young scientists. I do wish there was a little more interaction between junior and senior crystallographers. There is a wealth of knowledge, among the seniors, that could benefit us greatly as we begin our careers. Grad students/ post-docs also share a responsibility in putting forth the effort to make new contacts. A possible solution, for a later conference, could be a "Conference Buddy", where a junior crystallographer(s) is paired with a senior crystallographer for a day. Overall, I enjoyed my time in Philadelphia, and look forward to many more conferences as a member of the ACA.

Avni Bhatt. As this was my first national

conference and my first experience with the ACA, I was extremely excited to present my research and learn from others. It was excellent to hear lectures by both students and leaders in the field in the same session.. One of my most memorable experiences was being able to meet some of the brilliant minds in crystallography. The interdisciplinary poster sessions facilitated excellent opportunities for new collaborations in a relaxed environment. I appreciated the casual yet professional atmosphere, as I believe that it is important for scientists to be able to crossover between work-oriented and friendly conversations. I fully intend to remain a student member of the ACA, and am eager to further my knowledge of techniques through workshops and lectures at the 2016 meeting. "

Chelsy Chesterman: I was very excited

to be able to attend the ACA Annual Meeting and honored to be able to give two oral presentations. I obtained a wealth of constructive feedback and I am very grateful for both the student travel award and the surprise speaker travel award that defrayed some of my travel expenses.

I was really impressed with the diversity of talks at this meeting and I thought that the effort to include education-focused sessions was extremely valuable to graduate students and post-docs. I also really enjoyed many of the one-on-one conversations that I had during the poster sessions. If I could do one thing to improve the meeting, I would highlight the plenary sessions in the meeting program more clearly by giving them a larger space/ larger font and potentially including a short description. I missed the plenary sessions the first time I skimmed through the meeting schedule and I think these keynote sessions deserve extra attention.

I joined the ACA in order to attend this meeting and I plan to continue my involvement with the organization in the future. I have volunteered to help with an YSIG sponsored session next year and I am really looking forward to getting more involved. I feel the ACA provides a great opportunity for young crystallographers to network and expand their awareness of crystallography research in North America.

Ivana Brekalo: As a recipient of an

American Chemical Society 2015 Travel Grant, I had the pleasure of attending the 65th annual ACA meeting in Philadelphia. Since this was my first time participating at any ACA meeting, I didn't know what to expect, but I hoped it would be an excellent opportunity to meet new people, get advice on my research, and learn a great deal of chemistry. Now that it is over, I realize that it far surpassed my expectations.

The chance to attend a Rietveld refinement workshop before the conference, as well as some very engaging discussions at the poster session I was in, helped a lot in my pursuit to learn structure solution from powder diffraction data. All the sessions in the fields of materials chemistry and crystal engineering (my primary interests) were exceptionally well organized, with wonderful speakers, and the *Standard Practices in Crystallography* sessions on data collection were very educational. Additionally, I got exposed to the intriguing fields of protein crystallography and electron diffraction techniques, which I had never studied in detail, but found to be very interesting. Even the sessions not directly related to crystallography, such as the evening session on diversity and the *Communicating Your Science* session, were a real treasure trove, offering interesting perspectives about the roles that scientists have which are not strictly related to their own research.

Of course, the social side of the conference was not lagging behind; with the opening reception, the YSSIG mixer, the awards banquet, and SIG meetings all serving as opportunities to meet very interesting people. I was especially pleasantly surprised by the strong presence of young scientists in all areas of the meeting, as well as the attention and help offered to us. Everyone in the meeting was extremely nice and welcoming, which is a wonderful thing for a first time attendee! I didn't know almost anyone prior to coming to the meeting, but left with memories of inspiring people and new friends. That feeling of community, almost family, is maybe the biggest reason why I look forward to coming to the ACA meetings in the future.

Karina Heffernan: This year's ACA

meeting in Philadelphia was the first national meeting that I have had the chance to attend and overall I was very pleased with the experience. First off, I enjoyed the size and general feel of the meeting, it was both small and welcoming. I would repeatedly see the same attendees, which made it easier to introduce myself and establish connections. Second, I was very happy with the organization of the sessions, I found that I was able to attend almost all of the talks I was interested in with very little overlap. By now, I have had the chance to attend other national meetings besides the ACA and I have found the ACA conference better organized than these meetings. Therefore, I can come up with no real suggestions for improving the annual ACA meeting. As for professional societies, I am currently a member of the ACA as well as the Geological Society of America, I do intend to keep my memberships with both of these professional organizations.

Huanchen Wang : The 2015 ACA

meeting in Philadelphia was a great experience for me in multiple respects: it offered both a depth and breadth of crystallographic topics, as well as the newest developments in techniques. Attending lectures, presenting my work and discussing with poster presenters refreshed my mind and extended my understanding of the field. I plan to integrate some ideas we discussed into my research. Also, I really appreciated talking with different vendors to learn the impressive things that they had done to improve the ease of this technique as well as the quality of the results. Another thing I would like to emphasize is that it was one of few conferences where you could meet with experts to discuss the trends of x-ray crystallography.

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ACA Election Results

Council Officers

Vice President
Amy Sarjeant
Treasurer
Sue Byram

Standing Committees

Communications
Jim Fettinger

Continuing Education
Danielle Gray

Data and Standards
Joe Ferrara

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Biological Macromolecules
Chair-elect: Eric Montemayor
Secretary: Rama Madurapantula
General Interest
Chair-elect: Clara Slebodnick
Secretary: Allen Oliver
Industrial
Chair-elect:Andrew Brunskill
Secretary: Richard Staples
Light Sources
Chair-elect: Pawel Grochulski
Materials Science
Chair-elect: Paul Forster
Neutron Scattering
Chair-elect: John Greedan
Powder Diffraction
Chair-elect: Olaf Borkiewicz
Service Crystallography
Chair-elect: Alex Filatov
Secretary: Brandon Mercado
Small Angle Scattering
Chair-elect: Kushol Gupta
Small Molecules
Chair-elect: Stacey Smith
Secretary: Danielle Gray
Young Scientist
Chair-elect: Vicky Doan-Nyguyen

Canadian Division
Chair-elect: Paul Boyle

Vice-President - Amy Sarjeant

Outreach and Education Manager, Cambridge Crystallographic Data Centre, Piscataway, NJ

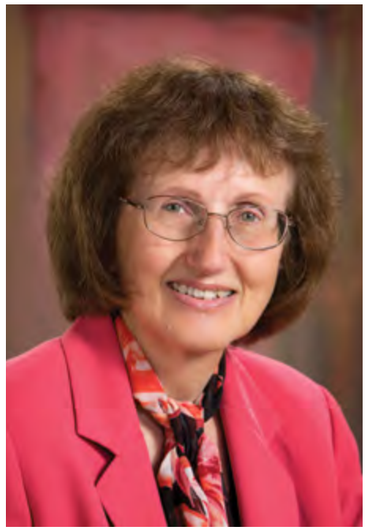
Statement: Think back to when you first joined the ACA. Was it last year or seemingly a lifetime ago? Now, as you read my statement and the others of those fortunate enough to be running for Council or Committee positions, take a moment to consider what drew you to the ACA and what has kept you here. For myself, and I suspect for many of us, I came to the ACA searching for a professional home, a place where, as a crystallographer, the trials and tribulations of my work would be understood and where I might find inspiration. Ask any crystallographer what he or she thinks of the ACA and almost universally you will hear what a tight-knit community this is, how helpful other crystallographers are, and what fun it is to be part of such an organization. Where else can a first-year graduate student present her research in the same session as the authors of her textbooks? In what other society might an undergrad feel free to strike up a conversation with his idols over coffee at a poster session? These interactions are what make the ACA such a vibrant and essential organization to our science.

There is much talk these days of dwindling membership and a lack of relevance in the ACA. It is true that we are at a critical period in our existence. How can we attract new members and keep the ones we have? What do we need to do to stay relevant in the ever-changing landscape of crystallography and scientific research in general? These are hard questions to ask and even harder to answer. We must face these challenges head on and continue moving forward in order to provide the same environment to the next generation of crystallographers that drew us into the ACA in the first place.

I firmly believe that one of our biggest responsibilities as a society, and perhaps the best tool we have for staving off these challenges, is to promote crystallographic education. As a co-organizer of the ACA Small Molecule Summer School for the past four years, I have seen first-hand how little crystallography is taught, even in major research institutions. While it is certainly true that solving a crystal structure today is a far easier task than it was 50 years ago, the science of diffraction is anything but routine. However, if we cannot change the way we educate young scientists about our craft, if we cannot impress upon them how useful, changeable and exciting crystallography is, we risk losing the foundation of our society.

The swell of interest in promoting crystallography to the general public that began last year with the IYCr should provide us with the momentum we need to grow and improve the ACA. I have had the pleasure of being involved with organizing a video contest for K-12 students as a way to bring crystallography into the classroom on that level. It was a joy to see how young children responded to the ideas and theories of crystallography and it is clear that we can do more to spark interest in our science at such a young age. At the IUCr Congress in Montreal last August, I orchestrated a mentoring event for young crystallographers. The overwhelming interest in this Young Observers program highlighted the great need for mentoring the newest members of the crystallographic community. As a member of the ACA Council, I will seek to promote our society and our science through mentoring, education and outreach – both to the general public and through other scientific communities. The road ahead of us is challenging, but I welcome the opportunity to walk it with you.

Treasurer - Susan K. Byram



Business Manager of Crystallographic Systems, Bruker AXS, Madison, WI

Statement: I love crystallography and the people in crystallography, and I want the ACA to thrive. The ACA Treasurer has specific duties, including working with staff on day-to-day operations, reviewing monthly reports, and presenting the Financial Report annually, as well as coordinating with the AIP and the USNCCr. I expect we should also coordinate with other member societies. I have scaled back to part-time at Bruker and feel I could devote time, expertise and energy to give back to ACA, which has meant so much to me over my entire working career. As a member of ACA Council, the treasurer should seek input from our membership and work with ACA Council to present a stable vision for our future. I have hands-on experience in single crystal, powder and polymer diffraction and will try to engage all our research communities and all our vendors. Further, I believe we need some innovative methods to attract and engage new members from all our geographic groups in Canada, the USA, Latin America and beyond. ACA already does an outstanding job of educating budding crystallographers in our science. I believe scientific societies such as ACA should also be educating our political representatives and funding committees about why our science is necessary and important. I believe the financial basics of maximizing income and controlling expenses to achieve our strategic goals can guide us as we go forward.

James C. Fettinger
Communications

Department of Chemistry, Univerity of California, Davis, Davis, CA.

Statement: I am pleased to have been elected to the Communications Committee. While I have been a member of the ACA for nearly 25 years I have not served on any committees so this will be a first for me.

Whenever I have given a talk to the general public at one of our local high schools, junior high's or even at the elementary school level the students are usually awed at what x-ray crystallography is capable of showing them. University talks to graduate chemistry classes are similar. It's as though x-ray crystallography is something new, not over 100 years old, so it's fairly clear that our area of expertise is not well presented to the general public or in general chemistry classes.

It's also apparent that our local schools chemistry classes don't really have any time allotted for learning x-ray crystallography or anything related to structural chemistry so if this is a nationwide problem it may be an area that the Communications Committee may consider for the future now that the IYCrystallography has ended.

As an amateur videographer for the past nearly 25 years, I have gained quite a bit of experience videoing a wide range of activities and then editing for content and feel this will be complementary among the tasks assigned this committee.

Helping the committee in their endeavors towards promoting our conferences with the local media and the general public would be quite illuminating.

Danielle Gray
Continuing Education

Director of the G.L. Clark X-ray Facility, School of Chemical Sciences, University of Illinois, Urbana, IL

Statement: It is an honor to have been elected to the Continuing Education Committee. Knowledge of the fundamentals of the crystallographic technique seems to be disappearing more and more with each new generation of chemists. Instrumentation with shutterless data collection and auto solve are allowing the rapid collection and analysis of vast numbers of crystal structures with little effort. Because of these and other advances, a casual user can collect and solve a structure with little to no formal training. Consequently, the technique is often relegated to being a 'black box' where little understanding is necessary as long as the desired structure solution is obtained. Unfortunately this also leads to a lack in understanding of the power and limitations of the experiment. Without a grasp on the fundamentals, how are inexperienced practitioners who use crystallography to support their research supposed to diagnose problems in their structures or assess the reliability of the structure solutions?

As chemistry advances so does the complexity of the structure solutions being

sought. Now more than ever we need a push for crystallographic education at both the undergraduate and graduate levels. It is essential that a comprehensive crystallographic education be taught to the next generation of crystallographers so that not only can our knowledgebase be maintained, but emerging techniques can be expanded upon to improve research goals. 2014 saw the International Year of Crystallography (IYCr) come and go. During the year many workshops, outreach programs, and educational opportunities highlighted the importance of crystallography to science in the past, present, and future. Let us not halt the educational momentum built up over the past year and continue to not only highlight the importance of crystallography but illuminate the fundamental principles of the technique. Developing and maintaining quality educational programs like the ACA Summer School and continuing to support workshops for both inexperienced and experienced crystallographers will go a long way to improving the overall knowledgebase of current and future crystallographers and scientists. I plan tp build upon the momentum of the IYCr and work to facilitate educational opportunities for the crystallographic community.

Joe Ferrara
Data, Standards & Computing

Deputy General Manager, Product Marketing and R&D, Rigaku Oxford Diffraction. Deputy Director, X-ray Research Laboratory, Rigaku Corporation

Statement: I came to this candidacy in a rather unorthodox manner; I was asked by a colleague to take their place as a nominee. I live for challenges, so I decided to run. I have been a member of the ACA since I joined Molecular Structure Corporation (now Rigaku) in 1988. Over the years I have been an active participant in the development of the hardware and software tools that crystallographers use every day. This experience gives me a unique perspective that will benefit the Data, Standards and Computing Committee. My knowledge base spans all fields of x-ray science and allows me to apply what I learn in one area to another. For example, recent discussions with colleagues suggest the next step in improving the publication and review process is the production of an executive summary of the very comprehensive PDB validation report akin to the IUCr CheckCIF report for small molecule structure validation. An executive summary would highlight the features of the structure that might prevent publication. Such a scheme would make it much easier for non-scientists doing crystallography to submit more polished structures and make it easier for reviewers to catch errors.

Cont'd from page 35

If I could suggest one change to improve the meeting, perhaps there could be a clearer program to distinguish between small-molecule crystallography and macromolecular crystallography. Although the mobile application helped me a lot to set up an itinerary, I still struggled traveling between sessions and the mixed posters.

I plan to attend more ACA meetings in the future.

Daniel Mast: I received an Etter Student

Lecture award from the Powder Diffraction SIG for my presentation on the *High Pressure Behavior of Technetium Metal* at the ACA2015 Meeting in Philadelphia this summer. This was my first ACA Meeting and first oral presentation at a national conference. I had a great experience presenting in the Etter Early Career Symposium and interacting with crystallographers from a wide range of backgrounds. Throughout the meeting there were many opportunities for a young scientist such as myself to discuss science, job hunting, work climate, and any number of other topics with experienced members at every level of leadership. Having previously attended an ACS meeting, this was a new experience in a smaller, more intimate community.

After this meeting and a number of other IUCr events that I have attended since beginning my graduate studies I intend on staying active in the ACA. I hope to see a more pronounced presence from the high pressure crystallography community at future ACA meetings.

Alberto Antony Venancio Landeros: I am working towards a masters in biochemistry, specifically in structural biology, at the Instituto de Biotecnología, under the supervision of Enrique Rudino-Pinera, at Universidad Naciónal Autonoma de México.

This was my first meeting specializing in crystallography, and it was amazing to meet and share experiences with other people using similar approaches or techniques. It was also exciting to meet people working in completely different areas, many of which I had never even heard of. Hearing their presentations, sharing their experiences, and discussing how to solve problems, both theirs and mine, provided me with unforgettable memories.

I also had the opportunity to talk with experts using techniques that could complement my current project, and we are now working on a collaboration (that started in Philadelphia) that is opening a framework for future work.

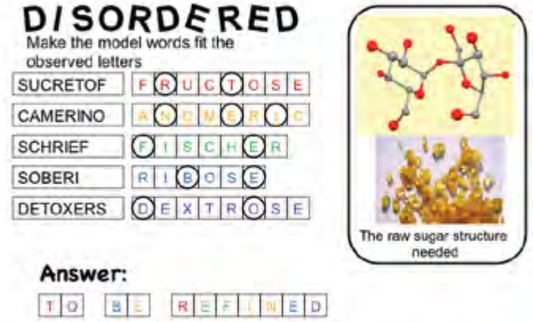
It would have been impossible to attend all the talks at the meeting, I could have attended more if there had been at most 3 simultaneous sessions - 2 would have been better. In my opinion, 4 was too many.

I am currently a member of the ACA and IUCr

Puzzle Corner

***Guest Crossword Puzzler Sought*:** HELP! For some time, I have wanted to have a crossword puzzle with crystallographic words and clues in *RefleXions*, but if there is anything worse than my ability to work crossword puzzles, it is my ability to construct them. I hope that some reader who is a crossword aficionado will step forward to collaborate with me in this endeavor. If you are that person, please contact me, and we can work together on it.

In this issue are the solutions to the previous ***DISORDERED*** and Crystal Connections puzzles, new puzzles of both types, and mention of those who successfully solved the previous ones. As always, I will be pleased to see your solutions (*ffroncz@lsu.edu*) and your ideas for future puzzles.



Previous Crystal Connections – Cities where at least 3 ACA meetings have been held:

1) On the whole, I'd rather be in ***Philadelphia*** *(purportedly, but not actually on the gravestone of W.C. Fields, 1962, 1988, 2015)*

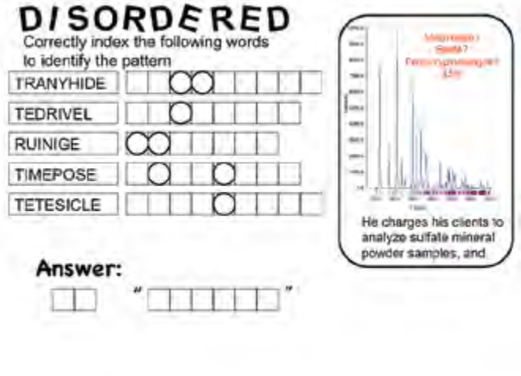
2) Surname of the last husband of Martha Dandridge Custis – ***Greater Washington*** *(1951, 1960, 1982 at NBS Gaithersburg, MD, 1998 Crystal City, VA)*

3) Packenham's last fight: Battle of ***New Orleans*** *(1970, 1990, 2011 & 2017)*

4) The song "Razzle Dazzle" is from this Broadway musical – ***Chicago*** *(1951, 2004, 2010)*

5) "Breaking Bad" setting – ***Albuquerque*** *(1972, 1993, 2014)*

6) ***Honolulu*** Lulu: 1963 Jan and Dean hit song *(1979, 2006, 2013)*



While it is likely clear to all that these were sites of ACA meetings, no reader correctly provided the "at least three" detail. **Ilia Guzei** (Dept. of Chemistry, University of Wisconsin) was the first to provide the solution to the ***DISORDERED*** puzzle. Here is the new Crystal Connections:

Crystal Connections #5 – What do the answers to these clues have in common?

1) "Grassfields" in Portuguese

2) "POW City" or "City of Bridges"

3) Gave element 97 its name

4) The old state capitol is "pathetic", and should never have been built in this otherwise honorable place, according to Mark Twain in *Life on the Mississippi*

5) Located far above Cayuga's waters

6) Irving Berlin wrote patriotic songs at Camp Upton here

7) Home of Lemont Quarrymen baseball team is near here

Send me those answers and comments!

Frank Fronczek – ffroncz@lsu.edu

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Jason Benedict

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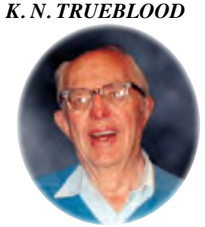

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Friday July 22 - Tuesday July 26, 2016

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Deadlines:

Abstracts: March 31, 2016

Travel Grant Applications: March 31, 2016

Advance Registration: May 31, 2016

Hotel Reservations: June 28, 2016

Abstracts accepted online only
40% of all talks will be from contributed abstracts

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Workshop I

The CSD Python API: A Foundation for Innovation
Organizer: Peter Wood

Workshop II

Computational Approaches to the Structural Modelling of Biological Macromolecules using Small-Angle Scattering
Organizers: Kushol Gupta and Adam Round

Workshop III

Serial Crystallographic Data Analysis with Cheetah & CrystFEL
Organizers: Tom Grant and Nadia Zatsepin

Workshop IV

Magnetic Structure Analysis by Unpolarized Neutron Diffraction Techniques
Organizers: William Ratcliff and Ovidiu Garlea

Workshop V

SHELX Workshop: Small Molecule & Solid State Chemistry / Macromolecules
Organizer: George Sheldrick

Award Symposia

Trueblood Award in honor of Axel Brunger

Fankuchen Award in honor of Elspeth Garman

Bau Neutron Diffraction Award in honor of Benno Schoenborn

Margaret C. Etter Early Career Award in honor of Jason Benedict

Transactions Symposium

Structural Dynamics

Organizers: Jason Benedict & Arwen Peters

Meeting logo designed by John Aspinall

Microsymposia

General Interest Sessions:

Poster Preview, Chairs: Louise Dawe, Bill Duax
Using Standard Tools & Methods in Non-standard Ways, Chairs: L. Dawe, A. Yakovenko, SIGs: Service, Canada
Standard Practices II, Chairs: Peter Mueller, SIGs: GIG, Service, SmMol
Diversity & Inclusion, Chairs: Krystle McLaughlin, Lisa Mueller, SIGs: BioMac, YSSIG
Etter Early Career Session, Chairs: Martin Donakowski, Stacy Vinokur, SIG: YSSIG
General Interest I & II, Chairs: Stacey Smith, Graciela Diaz, SIG: GIG
Industrial Research for Young Scientists, Chairs: Richard Staples, Edward Pryor, SIGs: Industrial, YSSIG
Career Development, Chairs: Martin Donakowski, George Lountos, Elise Blankenship, SIG: YSSIG
Engaging Undergraduates I, Chairs: Joe Tanski, Rachel Powers, SIGs: GIG, SmMol
Engaging Undergraduates II, Chairs: Bruce Foxman, Kraig Wheeler, SIGs: GIG, Service, SmMol, BioMac
Things we no longer need to know, Chairs: Carla Slebodnick, Charlotte Stern, SIG: Service

Small Molecule Sessions:

Mineralogical Crystallography, Chairs: Nichole Valdez, Aaron Celestian , SIGs: SmMol, Industrial, SAS, NMP
Structure Property Relationships, Chairs: Pete Wood, Christine Beavers, SIGs: Industry, SmMol, YSSIG
Would you Publish This?, Chairs: L. Dawe, Danielle Gray, Brian Dolinar, SIGs: Service, SmMol, Canada, YSSIG
Advances in Supramolecular Chemistry I & II, Chairs: H. Abourahma, K. Wheeler, SIGs: Industrial, SmMol, NMP
Cool Structures, Chairs: Xiaoping Wang, Karah Knope, SIG: SmMol
Making Sense of Diffuse Scattering, Chairs: J. Britten, C. Hoffman, SIGs: SmMol, Industrial, Canada, NMP

Biological/Macromolecular Sessions:

Structure Based Drug Design, Chairs: Barry Finzel, Chelsy Prince, SIGs: BioMac, Industrial, YSSIG
What to do with SAS Data / Software on SAS, Chairs: Alex Hexemer, Adam Round, SIGs: SAS, BioMac,
Hybrid Method approaches for structural biology, Chairs: A. Howard, S. Qian, SIGs: BioMac, Canada, SAS, LS
Molecular Machines, Chairs: Eric Montemayor, Aaron Robart, SIG: BioMac
Crystal Sample Preparation, Chairs: Surajit Banerjee, Iva Chitraker, SIG: BioMac
Cryo Electron Microscopy Techniques, Chairs: Sangita Sinha, SIGs: BioMac, Canada
Hot Structures I & II, Chairs: B. Goldsmith, D. Lodowski, K. Stanek, George Lountos, SIGs: BioMac YSSIG
Structural Enzymology, Chairs: Carrie Wilmot, Katarzyna Handing, SIG: BioMac

Light Source Sessions:

Opportunities from New and Improved Sources, Chairs: Bob Sweet, Sean McSweeney, SIG: LS
Surfaces and Interfaces, Chairs: Marian Szebenyi, Kevin Yager, SIGs: LS, SAS
Multiple Crystal Techniques, Chairs: Steve Ginell, Ana Gonzales, SIGs: LS, YSSIG
Radation Damage, Chairs: Gerd Rosenbaum, Elspeth Garman, SIG: LS

Materials Sessions:

The Next 100 Years of Powder Diffraction, Chairs: Brian Toby, Andrey Yakovenko, SIGs: NMP, YSSIG
Magnetic Structure of Complex Materials, Chairs: Branton Campbell, Anna Llobet, SIGs: NMP, SAS
Crystallography in Solid State Chemistry, Chairs: Kirill Kovnir, Danny Fredrickson, SIG: NMP
Novel Measurements for Emerging Science, Chairs: Katie Page, Joe Reibenspies, SIGs: NMP, Fiber, SAS
Fiber Diffraction, Chairs: Joe Orgel, Paul Langan, SIG: Fiber
in-Situ and in-Operando Methods, Chairs: Ashifa Huq, Vicky Doan-Nguyen, SIGs: NMP, LS, YSSIG
Small Angle Scattering with Resonant X-rays in Broad Spectrum, Chairs: Cheng Wang, Wei Chen, SIG: SAS
SAS and Integrative Approaches to Complex Structures, Chairs: K. Gupta, J. Ilavsky, SIGs: NMP, SAS,

Transactions Symposium – Structural Dynamics

Organizers: **Jason Benedict** (University at Buffalo; *jbb6@buffalo.edu*) and **Arwen Pearson** (Universität Hamburg, Germany; *arwen.pearson@cfel.de*)

This transactions symposium will focus on the rapidly growing area of structural dynamics of both chemical and biological systems, as well as solid materials. This resurgence has been driven both by developments in x-ray sources as well as by new approaches for sample delivery, data collection, and processing.

The speakers will present recent work on both equilibrium and non-equilibrium dynamics involving time-scales from seconds to femtoseconds. As well as scientific highlights, the symposium will also include case studies and cutting edge advances in methodology.

As this symposium will produce papers for a special issue of *Structural Dynamics* we will make a particular effort to recruit speakers willing to present work that has not yet been published elsewhere, as well as encouraging a subset of speakers to submit review articles that summarize advances in their sub-field (i.e., structural biology, chemistry, and materials).

General Meeting Information

Obtaining a VISA: Advanced planning by foreign travelers is critical. For those travelers who will requre a VISA: ***applications should be made at least 90 days in advance of the travel date. For further information contact: the U.S. Department of State (http://travel.state.gov/content/visas/en.html).***

Staying Green: All attendees will receive a hardcopy of the Program Book, but the full set of abstracts will only be available online. We are not planning to have a meeting bag, so if you would like one you should remember to bring your favorite from an earlier meeting.

Hotel Information: 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 competetitive 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 this commitment, which also brings with it free meeting space that 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.

Financial Support: Travel support will be available for young scientists. Applications should be made by the abstract deadline – March 31, 2016.

The meeting 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 of Crystallography.

Registration Fees

Category	Early	Late (after May31)
Members		
Regular	$505	$705
Retired	$200	$300
Post doc	$255	$355
Student (grad or undergrad)	$200	$300
Non- Members		
Regular*	$705	$955
Post doc*	$355	$455
Student*	$290	$390
Guest	$ 65	$ 65
Banquet	$70 ($35 students)	
Networking Mixer	$30 (free for students & post-docs)	

Workshops will be held on FRIDAY and the costs vary - check the meeting website for up-to-date information

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

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

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

The Networking Mixer to be held on Sunday, July 24th will be free for registered students and post-docs. All others - $30.00.

Register online or download forms to register by fax or mail.
www.amercrystalassn.org/2016-mtg-homepage
Questions: aca@hwi.buffalo.edu

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

Call for Nominations - 2017 Awards

2017 A. Patterson Award: Established in 1980, this award recognizes and encourages outstanding research in the structure of matter by diffraction methods, including significant contributions to the methodology of structure determination and/or innovative application of diffraction methods and/or elucidation of biological, chemical, geological or physical phenomena using new structural information. The Award consists of a $1,500 honorarium and reimbursement of up to $1,500 for travel expenses to accept the award and to deliver the award lecture at the ACA annual meeting (Selection committee: J. Helliwell (Chair), A. Brunger, W. Hendrickson, A. Sarjeant, Ton Spek, J. Britten, M. Nespolo, and Vivian Stojanoff.)

2017 Margaret C. Etter Early Career Award: To recognize outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career. The Award consists of a $1,000 honorarium and a plaque. The winner is also expected to present a lecture at the ACA annual meeting.

E. A. Wood Science Writing Award The award is named in honor of Elizabeth A. Wood, President of the ACA in 1957, and author of science books for lay readers. Persons who have written books or articles that bring science to the attention of a wider audience are eligible. Successful nominees need not be crystallographers or scientists and 'writing' could include artistic efforts, museum displays, etc.

The deadline for nominations for the 2017 Awards is April 1, 2016.

2016 ACA Fellows: Serves to recognize a high level of excellence in scientific research, teaching, and professional duties, but also service, leadership, and personal engagement in the ACA and the broader world of crystallography and science. Our Fellows program celebrates the excellence of our own members from within the ACA, and promotes their recognition worldwide to constituencies outside of the ACA, such as their employers, other scientific societies, and the government. See ***www.amercrystalassn.org/aca-fellows*** for information on the nomination procedure. ***Nominations for 2016 ACA Fellows are due by February 28, 2016.***

2017 ACA Offices and Committees: In the fall of 2016 we will elect a new Vice-President, Secretary, and one person to each of the ACA Standing Committees (Continuing Education, Communications, and Data, Standards and Computing). Suggestions are due by February 15, 201. Members of the nominating committee are Ward Smith, Martha Teeter and Louise Dawe.

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

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

New ACA Award to Honor the Memory of David Rognlie

David (Dave) Rognlie was a dedicated and much loved member of the crystallographic community, interacting over many years with a large number of scientists through his activities as owner of Blake Industries which sold diffractometer equipment including Huber equipment. In 2013, he sadly passed away and funds have been donated to establish a triennial ACA award in his memory.

The award is intended to embody Dave's values and personality: His generosity of spirit, optimism, selflessness and unstinting desire to help others to succeed in their endeavors. Dave played a particular role in the x-ray synchrotron community, but had broad and wide-ranging interests in the science and the people doing it across all spectra. The award will be for any meritorious discovery or advance in structural science by someone at any stage of their career. However, it is not intended to be a "lifetime achievement award" but for a particular discovery or development.

Name of the award: The David G. Rognlie Award

Details: Awarded every third year. The winner will receive an honorarium of $3000 and up to $1500 expenses to attend the ACA meeting to present a lecture covering the discovery or development that led the their selection.

The Award will recognize an exceptional discovery or technical development of particularly high impact in any area of structural science, to be awarded at any stage of a scientist's career without prejudice based on age, gender, ethnicity or race.

The first Award will be made in 2017 at the ACA meeting in New Orleans, LA. Forms for submitting nominations can be found at ***www.amercrystalassn.org/documents/ACAnomNEW.pdf*** and are due by April 1, 2016 . The selection committee is made up of Simon Billinge (Chair), Bobby Barnett and Denny Mills.

2016 Dues are Due: Please renew promptly and remember to support your favorite ACA Award Funds. ***NOTE: It is possible to renew online***

www.AmerCrystalAssn.org

The CCDC Celebrates the 800,000th Entry in the Cambridge Structural Database

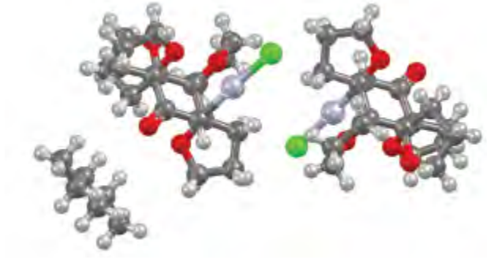
In October of 2015 the Cambridge Crystallographic Data Centre (CCDC) announces that the Cambridge Structural Database (CSD) has passed the milestone of 800,000 expert-curated experimental crystal structure entries with the addition of a novel metal-organic paddle-wheel structure from researchers in Spain. They issued the following press release to highlight reaching this milestone.

The CSD is the world's only comprehensive and up-to-date knowledge base of crystal structure data. It is an essential resource used every day by scientists worldwide for drug discovery, materials science, formulations studies, and structural chemistry research and education.

The CSD's 800,000th entry is a metal organic copper structure (CSD refcode: TUWMOP), published by Khaled Hassanein, Oscar Castillo, Carlos J. Gómez-García, Félix Zamora and Pilar Amo-Ochoa in *Crystal Growth and Design*. Knowledge of this structure, coupled with the wealth of structures in the CSD, will inform the design of new materials, and will be used to predict new crystal structures and validate x-ray data.

Pilar Amo-Ochoa, from the Autonoma University of Madrid (UAM), Spain, said, "We are delighted that our structure, tetrakis(μ-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)acetato)-bis(dimethyl sulfoxide)-di-copper(ii) dimethyl sulfoxide solvate, is the 800,000th entry in the database. We use the CSD in order to know the number of structures containing paddle-wheel type copper(ii) units with ligands of biological interest. Being able to have access to and share the very latest novel metal organic structures with the world is fundamental to our understanding of these frameworks and complexes."

"The remarkable growth of the CSD is testament to the ongoing commitment of the crystallographic community to share their results to benefit scientists everywhere," commented Colin Groom, Executive Director of the CCDC. "Fifty years on from the first crystal structure collection we are reaping the benefit of this unique data resource by learning more and more about the wonderful interplay between molecular conformation and molecular interactions."

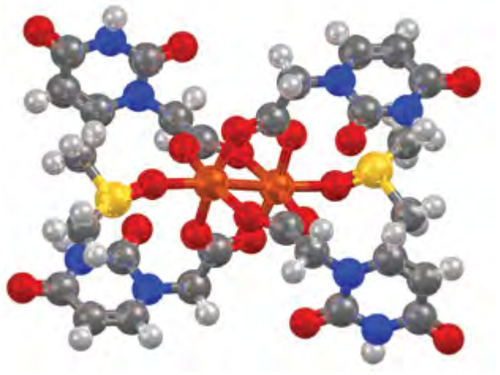


The 200,000th entry is refcode VAVFAZ: ***http://dx.doi.org/10.5517/cc3rb5b***:

Leo A. Paquette , David G. Bolin , Marshall Stepanian , Bruce M. Branan , Uppuluri V. Mallavadhani , Jinsung Tae , Shawn W. E. Eisenberg , and Robin D. Rogers, *J. Am. Chem. Soc*., 1998, 120 (45), pp 11603–11615

Robin Rogers, Editor, *Crystal Growth & Design* added, "I have always been a big fan of the power of the CSD and what it brings to the scientific community, and indeed was very pleased when my own structure was celebrated in 1999 as the 200,000th structure in the CSD. One of my primary goals in founding *Crystal Growth & Design* with the ACS has been to forge strong collaborations with the CCDC. I am delighted that one of our papers contains the CSD's 800,000th entry and I will continue to work for seamless cooperation between our authors, reviewers, and readers and the invaluable services provided by the CCDC."

The Manager of the Cambridge Structural Database, Suzanna Ward commented, "It is exciting that the 800,000th entry has been shared through the CSD so soon after we hit ¾ million entries. This demonstrates both the sheer number of crystal structures published annually in scientific articles as well as the growth in otherwise unpublished structures being shared through the CSD as Private Communications."



The structure of the CSD's 800,000th entry can easily be viewed online at ***dx.doi.org/10.5517/cc1jj92f***

Khaled Hassanein, Oscar Castillo, Carlos J. Gómez-García, Félix Zamora, Pilar Amo-Ochoa, *Crystal Growth and Design,* 2015, DOI: ***10.1021/acs.cgd.5b01110***

About the 800,000th entry: This particular structure is a di-copper paddle wheel with four bridging uracil-1-methylcaboxylato ligands and two dimethyl sulfoxide molecules occupying the apical positions. These dimeric entities are able to involve the entire uracil residue in base pairing interactions to provide supramolecular sheets. Di-copper paddles have been used since ancient times as pigments and fungicides and are today used in organic syntheses as catalysts or oxidizing agents. A simpler copper paddle wheel structure, namely copper acetate monohydrate, was critical in the development of modern theories for antiferromagnetic coupling. Uracil is one of the four nucleobases in the nucleic acid of RNA and it was originally discovered by Alberto Ascoli in 1900.

ACA Summer Course in Chemical Crystallography

www.acasummercourse.net

June 12th – June 19th, 2016

University of Notre Dame

Important Dates:
Applications to the Course – starting January 2016
Acceptance Notifications – March 2016
Registration Deadline – May 1st 2016

The week-long course will be offered from June 12 to June 19, 2016, at the University of Notre Dame in South Bend, Indiana, USA. South Bend is about 80 miles east of Chicago, IL and 100 miles north of Indianapolis, IN. The course will emphasize both theoretical and practical aspects of all 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 prefaces for the course.

The course is planned to accommodate a total of 30 attendees. In previous years there has been a broad demographic of attendees from both the U.S. and abroad with affiliations in academia, government and industry. Anyone interested in the course is encouraged to apply. The course faculty will consist of at least 10 experienced crystallographers with backgrounds spanning corporate to industrial to academia. Tuition will be set at $350 for undergraduate/graduate students and postdoctoral scholars, $550 for faculty and $850 for industrial affiliates. Housing will be available on-site at Notre Dame for approximately $450 for the entire course for double occupancy. A wide variety of dining options are available on campus and nearby within walking distance.

Tuition scholarships will be available to approximately 15 eligible graduate and undergraduate students based on the student's scientific ability and expected benefits obtained from the course. Latin American attendees are encouraged to apply to the course. There are two full travel scholarships available to Latin American attendees. Primarily the course is a graduate level course; however, applications from strong undergraduates will be considered. The organizers wish to encourage international students to apply.

Instrumentation at the University of Notre Dame that will be available for the course includes single crystal diffractometers operating both molybdenum and copper radiation and powder diffractometers. Computer support will be provided by the University with computing resources allocated to each student. All common-use crystallographic software (SHELXTL, GSAS/EXPGUI, FullProf, CRYSFIRE, CRYSTMOL, OLEX-2, shelxLe, TOPOS) and databases (CSD and ICDD) will be available for use.

The course registration form and additional information regarding the course are available at the course website: http://www.acasummercourse.net. On-line applications to the course will be available from early January, 2016 at the course website. International attendees may be accepted early to assist in preparation time for travel visa applications.

Allen Oliver, Amy Sarjeant and Charlotte Stern, Organizers.
Course Website: http://www.acasummercourse.net

NORTHWESTERN UNIVERSITY

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APRIL 2016

3-12 **Macromolecular Crystallography School 2016** Sao Carlos, Brazil, See **www.ifsc.usp.br/mx2016**

4-7 **BCA Spring Meeting**, Nottingham, United Kingdom. Contact Stephan Bryant, **steph.bryant@hg3.co.uk**

10-14 **Powder Diffraction and Rietveld Refinement School**, Durham, UK. Contact: **ivana.radosavljevic@durham.ac.uk**

19-22 **Crystallization: Focus on Micro and Nano Crystals and High Throughput Methods**, SLAC, US Contact Silvia Russi, **srussi@slac.stanford.edu**

24-29 **RapiData 2016. 18th Annual Course**, Stanford, CA Contact Ana Gonzalez at **ana@slac.stanford.edu**

29-1 **Protein Structure, Dynamics and Function**, Providence, RI **Structural-Biology@brown.edu**

MAY 2016

27-5 **High-Pressure Crystallography, 49th Erice Course**, Erice, Sicily, Italy. See **http://crystalerice.org/2016/**

27-5 **30th Meeting of the European Crystallographic Association**, Basel, Switzerland. See **ecm@congrex.com**

29-3 **ISC Granada 2016. 5th International School on Crystallization: Drugs, Foods, Agrochemicals, Minerals, New Materials (ISC2016)**, Granada, Spain. Contact: **isc@iscgranada.org**

JUNE 2016

6-9 **IWPCPS-17: International Workshop for Physical Characterization of Pharmaceutical Solids**, Winter Park, FL. Contact Angeline Rehfeldt by email (google IWPCPS-17 for the site).

19-26 **Structural and Biophysical Methods for Biological Macromolecules in Solution**, Suwon, Korea. Contact: **sarah.marshall@embl-hamburg**

24-29 **9th K.H. Kuo Summer School of Electron Microscopy and 2016 Kuo Symposium on 3D Cryo-EM Molecular Imaging**, Beijing, China. Contact: **hongweiwang@tsinghua.edu.cn**

26-1 **7th European Charge Density Meeting**, Warsaw, Poland. see **ecdm7@chem.uw.edu.pl**

26-1 **26th Goldschmidt Conference**, Yokohama, Japan. Contact: **gs2016@gmt.jtb.jp**

JULY 2016

3-8 **ICCBM-16. 16th International Conference on the Crystallization of Biological Macromolecules** See **www.iccbm16.org/**

6-8 **BBS2016. British Biophysical Society Biennial Conference**, Liverpool, UK. Contact: **enquiries@bbs2016.co.uk**

4-8 **3rd International School on Aperiodic Crystals**, Antwerp, Belgium. Contact **joke.hadermann@uantwerpen.be**

10-14 **American Conference on Neutron Scattering**, on board the *Queen Mary*, Long Beach, CA. Contact: **info@mrs.org**

17-21 **16th IUBMB Conference**, Vancouver, BC, Canada. Contact Grit Schoenherr, **IUBMB2016@icsevents.com**

22-26 **ACA 2016** Downtown Sheraton, Denver, CO Program Chairs: Amy Sargeant & Eddie Snell. See: ***www.AmerCrystalAssn.org***

21-25 **12th International Congress of Cell Biology, Prague**, Czech Republic. Contact the Congress Organiser: **www.cscb.cz**

AUGUST 2016

21-24 **12th International Conference on Biology and Synchrotron Radiation (BSR)**, SLAC, Menlo Park, CA. See: **conf-slac.stanford.edu/bsr-2016/**

22-23 **International Conference on Structural Biology**, New Orleans, LA Hilton NO-Airport Hotel. Contact: **structuralbiology@conferenceseries.com**

28-1 **30th Meeting of the European Crystallographic Association**, Basel, Switzerland. Contact: **ecm@congrex.com**

SEPTEMBER 2016

11-15 **MOF 2016 -5th International Conference on Metal-Organic Frameworks & Open Framework Compounds**, Long Beach, California. See **mrs.org/mof-2016/**

25-2 **3rd European Crystallography School, (ECS3)**, Bol, Croatia. See **3rdeuropeancrystallography-school.weebly.com/**

OCTOBER 2016

17-19 **International Conference on Applied Crystallography**, Houston, Texas. See **crystallography.conferenceseries.com/**

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