ACA RefleXions

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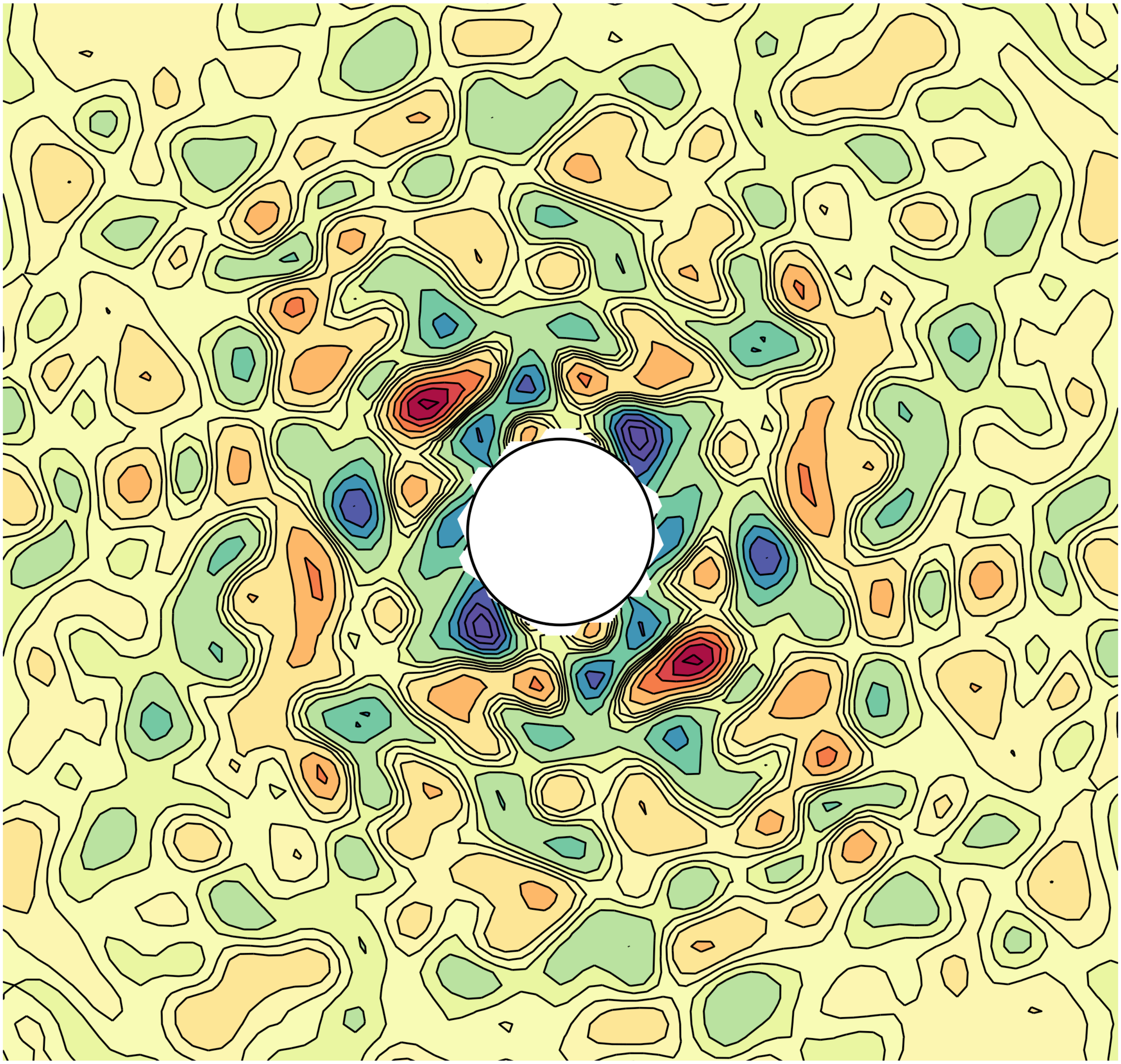
American Crystallographic Association

Structure Matters

Number 1

Spring 2020



Nozomi Ando

2020 Margaret C. Etter Early Career Award

ACA RefleXions

ACA – *Structure Matters*

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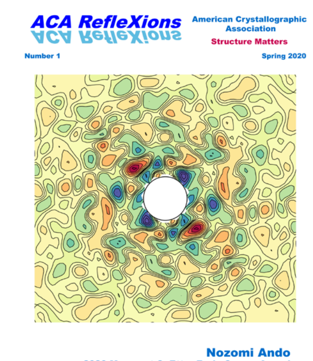
Brian Toby
2020 ACA President



Nozomi Ando received the Margaret C. Etter Early Career Award from the ACA. The cover image is described in Nozomi Ando's article, 'Thinking Outside the Lattice' page 7.

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Brian Toby
President

The ACA: Where from Here?

As I sit down to write this, I have recently returned from our winter Council meeting. (ACA Council used to meet several times per year; to save money we now meet monthly by phone and in person at the Annual Meeting and currently have only one other face-to-face meeting. Why Buffalo in January? That, I am less prepared to explain.) Immediately prior to our January 2020 meeting, we had a full-day workshop led by Robert Nelson, a consultant arranged and paid for by the American Institute of Physics to review the ACA. I have been to more management retreats during my career than I would care to recall, but this one I found of tremendous value. Robert led Council (and two invited guests) through a list of exercises, starting by envisioning ACA in 3-5 years, if we were able to accomplish all that we would want. Over the rest of the day, he took us through a series of additional exercises that encouraged us to think about different goals and priorities. In the end we came up with a list of eight planning tasks for the next ~six months and two longer-term items. I am very grateful to both the AIP and Robert for this.

While the ACA is expecting a deficit for the coming year, we are solvent, at least for the present. Nonetheless, we can foresee that change is needed: Newer generations of scientists expect more value from their professional memberships or they may not join. The increasing cost of our meetings is making it harder for some of our loyal members to attend. The way that crystallography is practiced is changing, with an increasing number of scientists performing the work, but fewer seeing crystallography as their primary professional identity. While the ACA has always been a home for scientists with interests in how atoms or molecules are arranged in matter, the range and power of non-crystallographic techniques for this have grown. For the ACA to continue to be the premier forum where scientists come to present results and educate each other on techniques and instrumentation for all types of structural research, we will need to adapt.

While we face challenges, I do not want to spread gloom-and-doom, as I believe the opposite is true. This is a great time to be involved in structural science. We have better instruments, software and more interesting and important problems than ever before. The world needs our help in solving important challenges, for example in energy generation/storage and in health sciences. One need look no farther than the cell phone in your pocket to see an example for how modern materials have transformed our lives, much of which would not be possible with knowledge gained through crystallography. The ACA is a vibrant family of diverse, motivated and supportive scientists, with many who are generous with their time as volunteers despite significant professional and family obligations. We are also blessed with a small but talented and dedicated staff that keeps us advancing. I am proud to be an ACA member and look forward to where we will be going.

Continuing on (and assuming that only people who will really care about the ACA are still reading, as anyone else has already fallen asleep or skipped ahead), I'd like to pass on some ACA news. With significant disappointment, I need to mention that we were not able to arrange centralized childcare for the 2020 meeting. In our survey on this topic, we heard from less than a dozen interested members and that makes this economically infeasible. However, thanks to Kristin's research in this area, we are now able to list a childcare provider on our conference website, which we hope will be helpful

to ACA attendees. Also, a first for 2020, we have set aside a small amount of funds for need-based travel support for members, which could include consideration for assistive, child- or elder-care costs. Note that this support program compliments the ACA's student travel fellowships and is also separate from requests from session chairs for speaker support. Feel free to contact me at toby@anl.gov.

On a separate subject, having been entrusted by the ACA to lead our society, I am trying to advocate for it as well. One breathtaking chance for me to do that was at the Council for Scientific Society President's December meeting, where I had the chance to introduce myself to Senator Susan Collins (R-Maine), who after my introduction asked me what crystallography was. I was gratified to have her undivided attention to my 30 second answer. For the future, Council has asked the Communications Committee to work on a handout so we can be even better prepared for these events. While in Washington I also had the chance to meet with U.S. National Science Foundation leadership. As you may have heard, the NSF decided in 2019 to stop funding the U.S. National Committee for Crystallography, which used that fund to pay for U.S. participation in the International Union of Crystallography. The NSF did continue to fund U.S. participation in about 20 other international Unions. The reasons given for this were unclear but included words such as "not aligned with the NSF's mission." I wrote to Dr. France Cordova, NSF director, to follow up on this disturbing information. She was unavailable to meet with me due to travel conflicts, but set up a meeting with two senior leaders who report to her. This resulted in a warm and supportive discussion, with some leads for the USNCCr, as well as some interest in the ACA's educational outreach plans.

Finally, I'd like to also open a dialog our membership, by asking what can the ACA provide that will add more value for you to be a member? The ACA is working on a mentorship program, I hope we do more in crystallographic education and a professional certification program is being discussed. One example of a minor change we are offering this year is to allow members to pay next year's membership dues as part of their registration for the 2020 Annual Meeting. I am hoping that for members who receive travel reimbursements, they will be able to also be reimbursed for membership dues. Feedback on how this works would be helpful. While the ACA does not have a budget allowing for a major investment in anything, I'd like to hear ideas from you (I can be reached at toby@ANL.gov) on what the ACA could do to make the society membership more valuable. This could be something that you want or something that you think would draw in that friend you know in the field, who so far has not made the investment by paying dues. Please pass on your thoughts.

Brian Toby

David Rose
Vice-President

While it is dangerous to jump to conclusions based on one month 'on the job', I am encouraged and optimistic about the direction of the ACA. I ran for this position with the intent of contributing to the evolution of our annual meeting: to make it more meaningful and valuable to our members, to broaden the scope of rapidly evolving technologies, to make it more inclusive to members of all backgrounds, career stage, access to finances, and competing priorities such as family commitments.

Discussions have already begun about ideas to make the annual meeting more than a place to meet colleagues and discuss their latest work, important though that is. We will be seeking your input on what would attract you to the ACA meeting over many competing meetings. I know that cost is a major factor: the site-selection committee has been charged with considering all aspects of the cost of attending the meetings, including hotel rooms and accessibility to services. Funding is being arranged to help attendees with caregiving responsibilities or needs (eg. childcare). For meeting content, would more workshops or hands-on sessions in the latest techniques within the core meeting be attractive? Perhaps it would be beneficial to extend our mentorship program further than to trainees to include early- and mid-career scientists, with either round-table or one-on-one consultations. There are so many aspects of being a researcher for which we do not receive any training. What could ACA provide that you are missing in building your career or expanding your abilities, perhaps opportunities that would result in the ACA being on your regular rotation of annual meetings? I'd invite any thoughts or ideas to drrose@uwaterloo.ca or to the ACA office.

Many of us do not attend the ACA meeting every year, for various reasons, and that is understandable. Some ACA members only renew membership when registering for the meetings, and let it lapse otherwise. I want to encourage anyone working in our area of molecular structure to renew annually regardless of meeting attendance. The annual meeting does not happen within a one-year cycle, but involves years of consultation and planning. Evolution of our meeting and our society can only occur with financial stability. Membership is not particularly expensive and those of us in the fortunate position of having discretionary professional allowance funding can often claim full or partial reimbursement. Others may be able to claim a reduced rate based on student, postdoc, retired or unemployed status. Please, even if you cannot join us in San Diego, give serious consideration to supporting your organization annually.

David Rose

Gerald F. Audette Canadian Representative

RefleXions from Canada

As this is my first chance to offer some RefleXions from Canada, I'd like to start with a big thank you to our previous Canadian Representative, Tomislav Friščić. I have some big shoes to fill, and I am grateful for all your hard work over the past several years as the Canadian Rep on Council. Thankfully, you've not gone far, as our new Chair of the Canadian National Committee on Crystallography (CNCC), which brings me to my first RefleXion, that is the resource that is the CNCC site xtallography.ca. I encourage all our Canadian crystallographers to visit the site, learn a bit more of the history of the CNCC and get updates on Canadian crystallographic events and travel opportunities, including funding opportunities or students and PDFs through the Larry Calvert Travel Fund (https://xtallography.ca/index.php/student-funding/). I hope in future columns to have the opportunity to continue the tradition of providing some highlights of the structural science and researchers from across Canada. However, I thought that in order to keep this first column to the point, I would highlight the upcoming Canadian meetings with a crystallographic/structural focus.

As always, we have a number of upcoming meetings that we can look forward to in our upcoming conference/meeting "season". The first meeting is the now annual Canadian Chemical Crystallography Workshop (CCCW20) – May 19-22 in Winnipeg, MB. The 11th CCCW will be held just before the 103rd Canadian Chemistry Conference & Exhibition (May 24-28, 2020;

http://www.ccce2020.ca/), which will itself have numerous talks and posters with structural studies to entice the active meeting participant. Headed up again by the incomparable, incredibly energetic and enthusiastic Louise Dawe, CCCW20 is targeted for grad students and PDFs who would like an improved understanding, both theoretical and practical, of crystallographic structure determination. More information about the meeting, as well as registration, can be found at https://xtallography.ca/index.php/xtal/meetings/cccw20/.

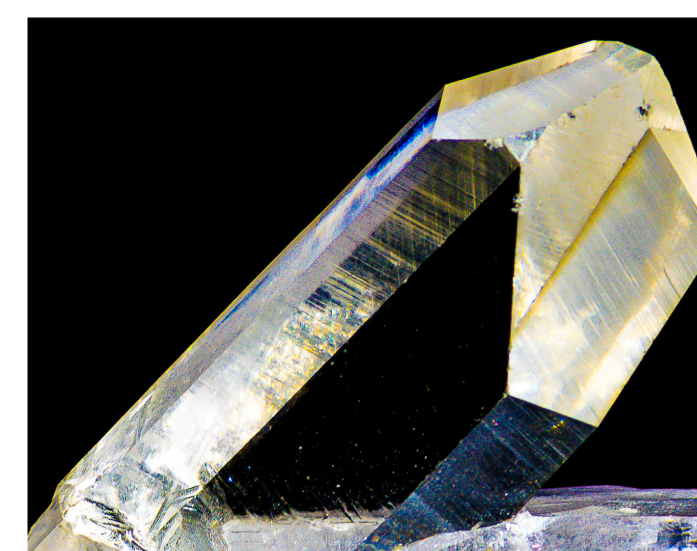
The second meeting I would like to draw your attention to is the 13th Canadian Powder Diffraction Workshop (CPDW13). CPDW13 (https://xtallography.ca/index.php/xtal/meetings/cpdw-13/) is also just prior to the Canadian Chemistry Conference & Exhibition, being held between May 19-22 in Saskatoon, SK as a satellite meeting to the annual CLS User's meeting (May 23, 2020). Organized by Jim Britten, Partick Mercier, Michel Fodge, the list of speakers includes Robert von Dreele (Argonne), James Kaduk (Poly Crystallography), Stefan Kycia (U. Guelph), and CLS locals Feizhou He, Joel Ried, Graham King, Beatriz Moreno, and Gianluigi Button. Combining software orientation, data collection and problem sessions, the CPDW13 looks to be an exciting program!

For the macromolecular crystallographers out there, the Annual MXSchool (https://cmcf.lightsource.ca/school/mxschool/) hosted by the Canadian Macromolecular Crystallography Facility (CMCF) at the CLS, which normally runs in mid-late June, will be taking a hiatus this year to allow for upgrades at the CMCF. Upgrades to the CMCF-ID insertion device, beamline optics and endstation upgrades are planned, as is the installation of an Eiger gM detector, with a move of the Pilatus 6M detector to the CMCF-BM endstation. You can follow the progress of the upgrades on the CMCF site at: https://cmcf.lightsource.ca/beamlines/upgrade-projects/. Michel Fodje assures me that his is only a hiatus, that the MXSchool will return, and that the CMCF plans on supporting the community at local meetings this year.

Of course, the Structural conference season includes the annual ACA meeting (more details are of course found in this edition of RefleXions). This year's meeting, held from Aug. 2nd – 7th in San Diego, looks to have an exciting program around the theme of "Training the Next Generation". This sounds oddly Star Trek-ish to me (I suppose I should go ahead and watch Star Trek Picard!). And this year's IUCr congress and general assembly, the 25th general assembly, is being held in Prague, Czech Republic from August 23rd – 30th, 2020. As always, the program of the IUCr congress looks fantastic. I look forward to meeting many of you at meetings this year!

I hope to provide the community with more highlights of the Canadian Structural and Crystallographic community in future columns and look forward to be a voice for the dynamic Canadian community to the ACA. Please feel free to contact me with suggestions of upcoming events, meetings and people engaging in crystallographic and structural science to highlight. I can be reached by email at audette@yorku.ca, and I look forward to hearing from you!

Gerald Audette



Nozomi Ando Wins NSF Early Career Award

Nozomi Ando was selected by the American Crystallographic Association (ACA) to receive the 2020 Margaret C. Etter Early Career Award (see Winter 2019 RefleXions). The exceptional potential that the ACA honored has been recognized by the National Science Foundation (NSF) and Nozomi has just won an NSF Faculty Early Career Development (CAREER) award.

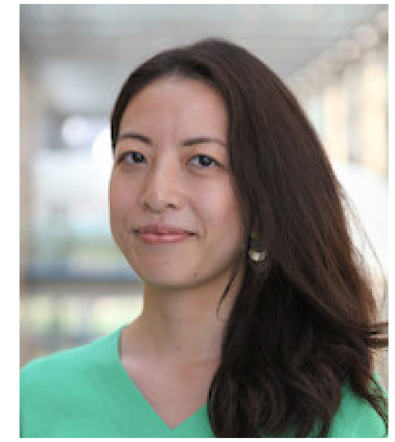
This program "emphasizes the importance [NSF] places on the early development of academic careers dedicated to stimulating the discovery process in which the excitement of research is enhanced by inspired teaching, enthusiastic learning and disseminating new knowledge."

The research work that Nozomi will be pursuing under this grant will apply her interdisciplinary skills, which lie at the intersection of x-ray physics and enzymology, to the challenge of truly understanding the central question of structural biology: how sequence gives rise not just to structure but also to function. The techniques she will use come from many fields, including crystallography, chemistry, biology, physics and statistics.

Her study will be carried out on the ribonucleotide reductase (RNR) family, which performs an essential step in DNA synthesis. This family is of particular interest because it has evolved multiple levels of complex allostery while simultaneously conserving a catalytic mechanism that pre-dates the oxygenation of the Earth.

The goal of Nozomi's educational plan is to promote innovative thinking both within academic research and beyond. She will be doing so in a two-pronged way: she will develop a career-focused seminar series and a modern structural biology course that is focused on filling an educational need. The typical student comes to such a course without familiarity with foundational mathematical concepts. To address this, the new course will foster active learning of both theory and practice.

Thinking Outside the Lattice



Nozomi Ando
Cornell University
Ithaca, NY 14850

It's an honor to receive the 2020 Margaret C. Etter Early Career Award from the ACA. Since 2003, this award has recognized "outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career." I am grateful to the ACA and my colleagues for this recognition and to my mentors who paved a path before me. I am especially grateful to my own mentees for believing in my vision and bringing their talent, creativity, and dedication. My career would not exist without them. This piece, which I am delighted to share as part of ACA's celebration of International Women's Day, is for them and for all young scientists.

A New Hope: The Rise of Diffuse Scattering

There were several pioneering studies on the topic of macromolecular diffuse scattering, but a particularly significant one was that of Caspar, et al. (*Nature* 1988). Using X-ray film, the scientists exposed an insulin crystal long enough to reveal features that were weaker than the bright spots that we commonly associate with diffraction images. These included the broad ring around 3 Å that is often seen with hydrated protein crystals as well as halo-like features emanating from diffraction spots. After subtracting the strongest of these features from the image, a blobby, cloudy pattern emerged. The scientists attributed this signal to the internal motions of the protein molecules by invoking a simple model known as the liquid-like model. The details of the model do not matter as they are not meant to be realistic, but the significance of their work was in establishing a new hope - that we might learn about protein dynamics from crystallography.

To understand what diffuse scattering is, it's instructive to go back to the basics. The goal of crystallography is to determine the position of every atom in a molecule, and we do this by measuring the intensities of the bright spots known as Bragg diffraction. However, we have known for a long time that crystals fluctuate and are imperfect. The probability that an atom is at its average location is in part described by the temperature factor, or B-factor. In last year's spring issue, Eaton Lattman from the Hauptman-Woodward Medical Research Institute wrote a delightfully intuitive way to understand B-factors. In his description, the instantaneous scattering from a fluctuating atom gives rise to a "tipsy walk" in the so-called Argand diagram. Importantly, the end-to-end distance of such a path is shorter than one constructed from a perfectly straight path. The consequence of this is that the amplitude of the scattering is diminished when atoms fluctuate, and from experience, we know this to be true: disorder in a crystal leads to the loss of diffraction spots starting at the outer edges. In other words, the B-factor describes the loss of the Bragg signal due to disorder.

What happens then to the diverted X-rays? For a typical protein crystal, it turns out that only about half of the scattered photons go into the Bragg diffraction pattern. The remainder scatters in all directions, giving rise to a diffuse pattern that is spread out throughout reciprocal space. The Bragg signal, as we know well from crystallography, provides atomic coordinates and B-factors. However, its twin, the mysterious diffuse scattering signal, holds the secrets to how atomic displacements are correlated. Understanding how different parts of a protein communicate is exactly what we so often seek in biochemistry. It was this promise of diffuse scattering that led to a series of attempts to understand this elusive signal. But this proved to be very difficult. Highlights from this period include the work of Wall, et al. (*PNAS* 1997), which was the first study to draw attention to the importance of how we measure this signal.

The Death Star: The Attack of the Phonons

In 2012, a few days before the ACA Meeting in Boston, a number of scientists gathered in Buffalo, NY for the Biodynamics@Buffalo conference. Those who attended may remember why this meeting took place. What mattered to me is that I happened to be thinking about a crystal structure with a striking B-factor pattern from Catherine Drennan's group at MIT (Kung, et al. *Nature* 2012), and immediately after my talk, Sol Gruner from Cornell University gave a talk reminding the community that pixel-array detectors were now available for launching the next assault on diffuse scattering. This was around the time that similar detectors were about to catalyze a revolution in the cryo-electron microscopy field. Structural biology had just been equipped with our newest technology.

Having spent many years in the small-angle X-ray scattering (SAXS) field, the idea of a scattering signal that is orientation-dependent and even harder to measure than solution scattering was extremely appealing to me. When I began my independent career in 2014 at Princeton University, I was lucky that the like-minded Steve Meisburger had just defended his PhD. Based on our interactions at the Cornell High Energy Synchrotron Source (CHESS), I offered him a postdoc position without an interview, and he took the offer without even knowing what the job entailed. The essential part of this story is that the Force was strong in Steve, and like me, he came from a rigorous training in SAXS.

Soon after, we had succeeded in collecting data on crystals of interest. The diffuse signal, however, looked like a mess in 2-D diffraction images. They were smeary and uninterpretable. Were they even real? To address this, Steve mapped the pixel intensities in 3-D reciprocal space. What emerged was a 3-D map that showed that there is indeed information there (Fig. 1a). The messy diffuse signal was connected in 3-D reciprocal space, forming patterns and even displaying symmetry. We named the map, "the Death Star". But we also noticed that a better approach was needed. Clear artifacts could be seen in the map, such as the shadow of the beamstop, which is what made the map look like a Death Star in the first place.

Our years of SAXS training told us what we needed to do: start over from scratch, focus on collecting the cleanest possible data, and write new data processing software. Steve went onto write an impressive software suite that borrowed techniques from both crystallography and SAXS. It was an incredible mountain to climb, and even then, we faced the problem of interpreting the signal when we would eventually arrive at the summit. Thus, I enlisted the help of Dave Case at Rutgers University who I had initially met at that fateful Biodynamics meeting. In my final year at Princeton, Dave began a year-long sabbatical in my lab and performed a series of large molecular dynamics simulations of protein crystals, which stimulated many important discussions.

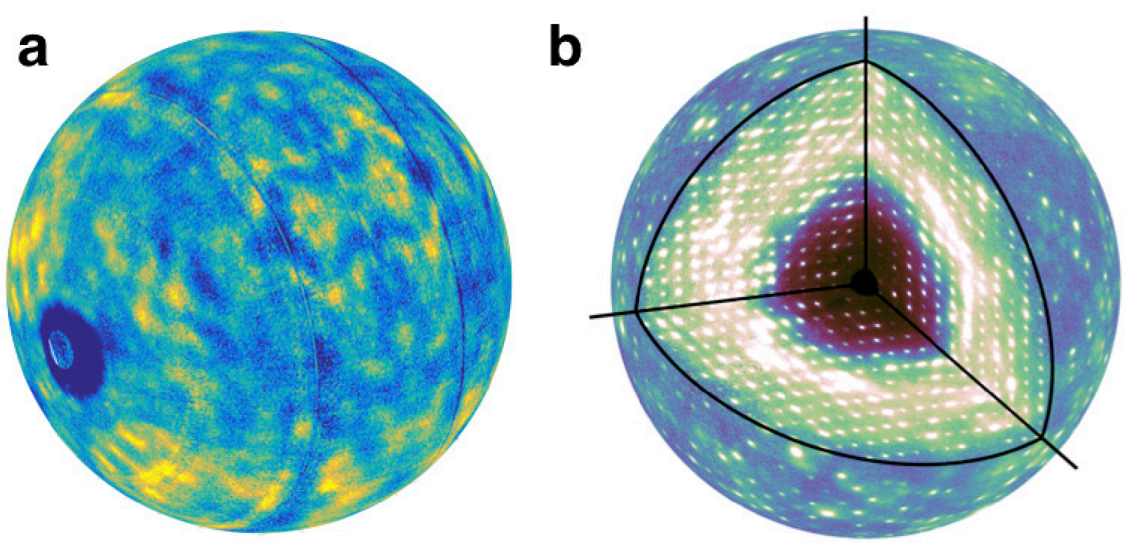


Figure 1. a) Death Star I in 2015. b) Death Star II a few years later (Meisburger, et al., *bioRXiv* 2019).

The end result of this productive year was the 3-D diffuse scattering map of triclinic lysozyme collected at room temperature (Fig. 1b). It was the most detailed map that the field had seen. However, through its beauty, something was glaring at us. Halos. Our experience with SAXS meant that we would obsess over the small-angle features near the diffraction spots, and with the fine detail in Steve's map, we could clearly see halos emanating with a power-law dependence. This was the first sign that the diffuse signal was dominated by thermally excited lattice vibrations, known as acoustic phonons. The phonons cast doubt on our plans. Was there no information about protein dynamics in diffuse scattering? Was all hope lost?

It was time to move, however. The synchrotron had been calling, and so after four great years at Princeton, I moved my lab to Cornell University.

The Return of the Protein

In the summer of 2018, my lab regrouped in a new location on the beautiful Cornell campus. Sitting among boxes, we resumed research. The initial goal of the diffuse scattering field was to extract information about protein dynamics, but we had not yet succeeded. Steve had shown that the halo scattering had distinct 3-D shapes, and he performed simulations to confirm what we had feared: the phonons appeared to explain most of the diffuse scattering intensities. We now had data that showed us the strength of numbers, that is, the number of unit cells. Lattice vibrations meant that atoms separated by many unit cells were correlated, and the signal arising from such correlations was amplified by the large number of unit cells. The contribution of phonons to diffuse scattering was actually something that the field was concerned about, and Peter Moore at Yale University had warned us about the possibility (Polikonov & Moore, *Acta Cryst D* 2015).

Although phonons were not what we were looking for, it was still a major victory that Steve was able to explain most of the diffuse scattering signal in terms of a vibrational model. No other model had come so close to explaining this signal before. Moreover, the closest data points that we could measure next to each diffraction spot told us that atoms were correlated over at least 10 unit cells, and the existence of such long-ranged correlations has significance in the context of protein-protein interactions. This work also told us that strong features like halos should not be subtracted from the Death Star. They must be accounted for but not removed because the act of removing these features corrupts the diffuse scattering signal, and this was in fact how the diffuse signal had evaded us for so many decades.

At this point, we had come a long way, but we had not yet reached the true summit - there was another mountain to climb. Steve planned for his next battle by checking his calculations against another set of data. He calculated the B-factors that we would expect from the lattice vibrations and compared them to the B-factors we obtained from the Bragg data. What he saw was that although lattice vibrations accounted for a large amount of the atomic motions implied by the B-factors, there was still a gap. Could this gap be due to protein motions?

To test this, Steve performed a simulation treating the protein as an elastic network and fit the model to the residual B-factors. Then, he asked whether this model could explain the diffuse scattering. However, we already knew that the diffuse intensities are dominated by the contributions from lattice vibrations. How can we place protein motions and lattice motions on the same playing field? The trick was to return to a fundamental concept in structural biology: the

Fourier Transform. The Fourier Transform, as students learn in my class, tells us how much a certain component contributes to a signal. Hence, Steve carefully calculated the Fourier Transform of the diffuse intensities and produced the diffuse Patterson map, or 3D-ΔPDF as it is known in the materials field. The diffuse Patterson represents the autocorrelation of the difference electron density as a function of distances within the crystal. The key takeaway is that it allows us to detect the contribution of short-ranged correlations that are intrinsic to protein motions over all other correlated motions in a crystal.

The cover art of this issue depicts the prize after the long road to the summit: the experimentally derived diffuse Patterson from our triclinic lysozyme dataset. Shown as a topology map, dark red corresponds to strongly positive values, and dark blue corresponds to strongly negative values. Features near the origin corresponding to the shortest length scales have the largest amplitudes. In agreement with our B-factor analysis, we found that lattice vibrations fail to explain the full amplitudes near the center of the diffuse Patterson map. Steve then calculated the diffuse Patterson from the elastic network model of protein motions, which was fit to the residual B-factors. Remarkably, much of the missing short-ranged correlations appeared. Although there is much more to this story, this was the key finding that we had been waiting for. It was the return of protein dynamics.

Final Thoughts

This story is part of what I will present this summer at the 2020 ACA Meeting. You can read more about it in Meisburger et al. (*bioRXiv* 2019). There were also many other epic battles that were not mentioned. You can learn about the history of the macromolecular diffuse scattering field in *Chemical Reviews* (Meisburger, et al. 2017). I should also mention that I am not the only one known to make Star Wars references in the diffuse scattering field! Be on the lookout for the great works of Mike Wall at Los Alamos National Lab.

Finally, I was asked to write a message for aspiring scientists in celebration of International Women's Day. I am no expert on how to succeed, but I can offer some thoughts:

1. Think big, think outside the box. Be glad to be different. Use feelings of being "different" to propel you to be unique in science. Develop a vision for the future of science.
2. Learn to share and when you're in a position to do so, pay forward. In the wise words of Sol Gruner, "By sharing, you lose some, but you gain more." Use experiences of hardships to help others avoid the same. You can't change the past, but you can change the future. In the end, we all benefit.
3. Do everything in your power to maintain your health – both physical and mental. My current method of choice is hot yoga, which I find more enjoyable than room-temp yoga. Find an activity that works for you, and remember that there is no shame in taking your mental health seriously.
4. Find humor in daily experiences. Maybe write about your day to day experiences in terms of an epic story, like Star Wars.

Nozomi Ando

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The main governing body of the American Crystallographic Association is the Council. The Council, which meets two to three times per year, sets policy and has the ultimate responsibility for the actions of the association. It is composed of a president, vice president, past president, Canadian representative, secretary and treasurer. The membership elects these officers and terms commence on January 1st. The president is elected and serves for three one year terms of vice president, president, and past president, sequentially and is a member of the ACA Council during each one year term. The Canadian representative, the secretary and treasurer are elected for three year terms.

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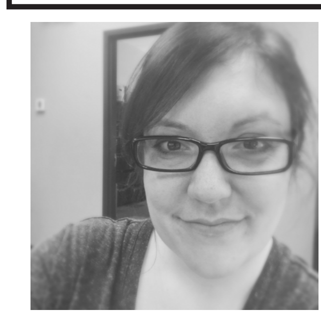

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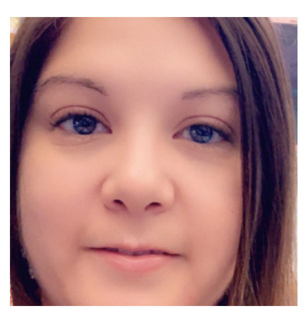

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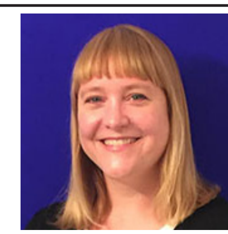

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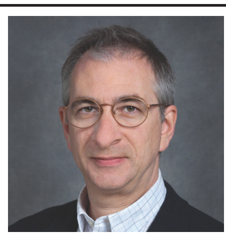

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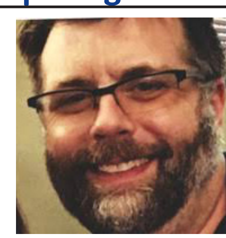

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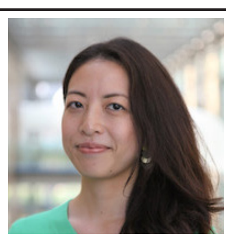

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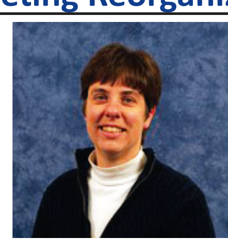

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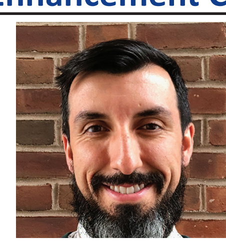

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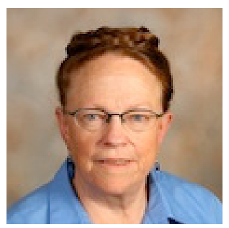

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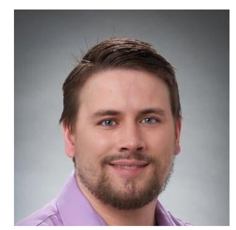

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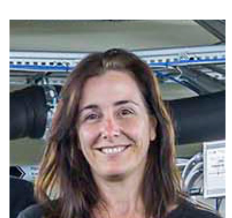

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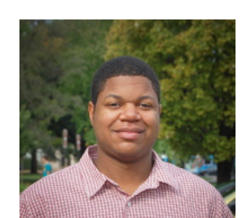

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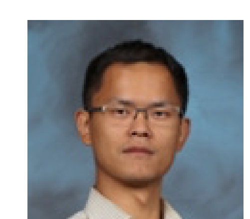

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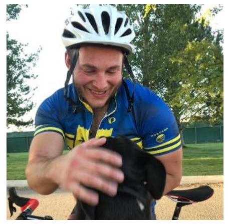


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Argonne to host PDF and Rietveld Course

Sorry - The Course is full.

The Structural Science group at the Advanced Photon Source (APS) of Argonne National Laboratory will host its first "X-ray Powder Diffraction and Pair Distribution Function Data Analysis Course," which will be held from June 29 to July 2, 2020, at the APS. The course will be exercise-oriented, aiming to provide participants hands-on training on analyzing powder XRD and PDF data for small molecules and materials, to take advantage of mail-in access to diffractometers at the 11-BM, 11-ID-B and 17-BM beamlines. Instruction will be provided by APS staff. The registration fee is $60 per person, and attendees will be responsible for paying their travel, lodging and meal costs. Registration and course details can be found at https://www.aps.anl.gov/Structural-Science/SRS-Courses. Applications will be accepted on a first-come basis until the class is full. Non-US nationals are encouraged to apply early as site access may require additional advance arrangements.

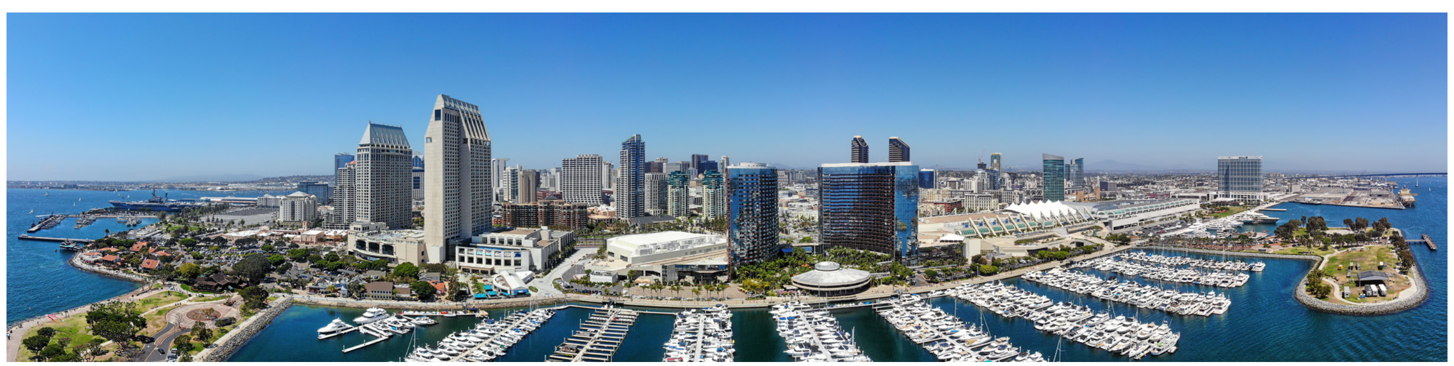
70th Annual Meeting of the American Crystallographic Association

AUGUST 2-7, 2020 | SAN DIEGO, CALIFORNIA

ACA 2020
American Crystallographic Association
August 2 - 7, 2020 • San Diego, CA
TRAINING THE NEXT GENERATION

Scientists interested in molecular and materials structure with specialties in biology, chemistry geosciences, materials science and much more will converge on the San Diego waterfront in August 2020 for exchange of scientific research and technique know-how for the 70th Annual Meeting of the ACA. For 2020, the meeting will have the overall theme of "Training the Next Generation". Session topics will expand well beyond traditional single-crystal and powder X-ray diffraction techniques to include next-generation methods and facilities such as cryo-EM, micro-electron diffraction, and advanced capabilities at national synchrotron and neutron sources. The conference also seeks to empower the next generation with session content balanced between new scientific results and education on how to perform similar work.

San Diego is a city on the Pacific coast of California known for its beaches, parks and warm climate. Immense Balboa Park is the site of the renowned San Diego Zoo, as well as numerous art galleries, artist studios, museums and gardens. A deep harbor is home to a large active naval fleet, with the USS Midway, an aircraft-carrier-turned-museum, open to the public.



Schedule/Sessions | Workshops | Awards

Keynote Speaker | Program Team | Hotel Info

Member Registration | Non-member Registration | Important Dates

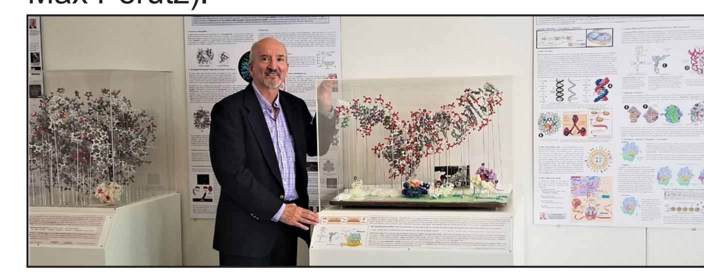
ACA History Project Update

In this issue of *ACA RefleXions* **Jim Ibers** presents his Living History, describing his scientific journey. During his graduate work at Caltech he became "hooked on crystallography" and he made many contributions to X-ray diffraction methods both theoretical and practical as he migrated to Shell (Emeryville, CA), Brookhaven National Laboratory, and Northwestern University. His research emphasizes inorganic chemistry and solid state chemistry. Among other honors he received the American Chemical Society Award in Inorganic Chemistry and the ACA Buerger Award; he was elected to the American Academy of Arts and Sciences and to the U. S. National Academy of Sciences.

The Latest Additions to ACA History online are biographies of Kathleen Lonsdale and **Helen Megaw**. Lonsdale is famous for her many contributions to science, including her "definite proof, from an X-ray point of view," that the phenyl ring in aromatic compounds is planar. Her 1936 book *Simplified Structure Factor and Electron Density Formulae for the 230 Space Groups of Mathematical Crystallography* was completely handwritten! See a sample page online.

Helen Megaw was an inorganic crystallographer who was famous for her studies of ferroelectricity and of perovskites. Here is her photograph superimposed on the perovskite structure in the background. It was she who proposed that the Festival of Britain (1951) use designs based on crystallography for textiles, carpets, tablecloths, and other objects. She recruited Lonsdale, Bragg, and Hodgkin to provide these patterns.

As an example, two ties owned by Jenny Glusker are shown above. Both represent contoured Patterson maps (left, insulin, contributed by Dorothy Hodgkin; right, horse hemoglobin, contributed by Max Perutz).



Marvin Hackert (UT-Austin) has made a 22-foot long display of molecular models and posters in a hallway frequently on the route for tour groups. The models are kept dust-free in display cases built in the carpentry shop, and with each ball-and-stick model there is a smaller 3-D ribbon diagram and an accompanying poster that explains the biochemical importance of the molecule. In the photo the model at left is hemoglobin. Marv is standing by a large model of t-RNA. Included in the case are smaller 3-D printed models of DNA; a nucleosome core particle; a t-RNA synthetase complex; and a model of the small ribosomal subunit with three bound t-RNAs and the large ribosomal subunit with growing polypeptide exiting the peptide channel. This public display is an excellent way to explain and publicize what structural scientists do!

Virginia Pett

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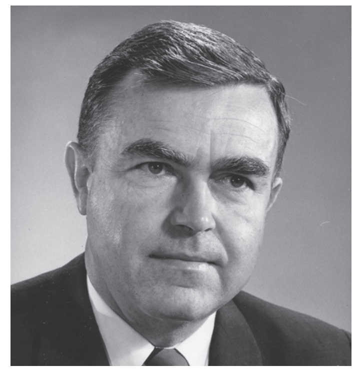
To start at the beginning, I was born in Los Angeles and lived in California for the first 25 years of my life. Early on I wanted to become an archaeologist, then an astronomer, then a chemist. So I applied to Caltech, my neighborhood school for science and engineering, and was accepted after a grueling three-hour written examination. Before the first quarter of school began I was required, as were all 160-admitted Freshmen [no women in those days], to attend a one-week orientation camp on Santa Catalina Island. The most important message I took away was the Caltech Honor Code for all undergraduates. In its simplest terms: You can't cheat in Science because you will eventually be found out. I have adhered to that Code as a husband, a father, a scientist, a teacher, a research director, and all others I have dealt with.

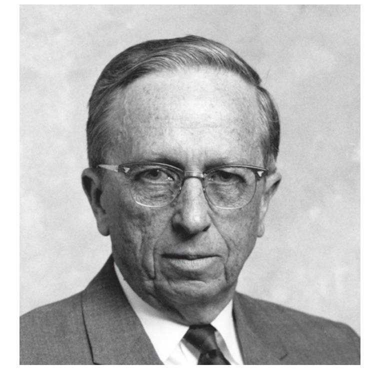
I did surprisingly well academically in the first school quarter and thus was required to find a mentor who would supervise my research efforts. After talking to several Professors I chose to work both in the library and in the laboratory for Prof. Norman Davidson. Norm was interested in optical properties of metal ions in mixed oxidation states. After about a year Norm ran out of funding (National Science Foundation (NSF)), but he told me to see Dr. David Shoemaker of the Pauling group. I found a door in the basement of Crellin Laboratory with the name "Schomaker" on it. The office was dark, but I knocked and Prof. Verner Schomaker let me in. I told him I was an undergraduate looking for a lab position. Verner, who got his degree under Linus Pauling, was interested in electron diffraction of gases. The work originated around 1930 when very few interatomic distances were known. Verner sent me to one of his postdoctoral researchers, Ken Hedberg. I worked for Ken for several years. One day when I was talking to Verner in his always dark office, he mentioned that he was troubled by experimental evidence that UF_6 was apparently unsymmetric, as this seemed to defy the Born-Oppenheimer approximation. By this time the Schomaker group had a French postdoctoral researcher, Jean Hoerni, who was trained a physicist. He and I calculated complex amplitudes for electron scattering. I don't recall if we ever resolved the issue of the symmetry of UF_6, but perhaps it was settled in a meeting we had with Prof. Richard Feynman of the Physics Department.



Verner Schomaker

Photograph by John A. Moore, University of Washington, courtesy of AIP Emilio Segrè Visual Archives

In an ensuing discussion in Verner's dark office he noted that the Fourier transform of the wave function is the atomic scattering factor (form factor). This was 1954 and I attended my first ACA meeting in Cambridge, MA where I found that I was presenting these results in the presence of Dr. G. W. Brindley whose form factors were in current use! I continued to attend ACA meetings until they got gobbled up by the macromolecular types. I find specialized meetings more useful, an example being Journées des Actinides, a small European meeting that brings together chemists and physicists who are interested in the actinides. It is amazing how little chemistry most theoretical physicists know!



J. Holmes Sturdivant

Photograph courtesy of the Archives, California Institute of Technology

The undergraduate curriculum at Caltech was fixed by your Deity and Caltech President Prof. Robert A. Millikan. As a result I took an "elective" course in X-ray crystallography from Prof. J. Holmes Sturdivant. These days you can't get near an X-ray beam on a diffractometer; in those days we centered the crystal in the collimator with mA and kV turned down. Unit cell determinations were usually obtained from a Laue camera but the instrument of choice for data collection was a Weissenberg camera. A Buerger precession camera was available, but was rarely used. Estimation of intensities was done visually, by packing the Weissenberg camera with multiple photographic films separated by very thin Cu sheets. As an intensity standard I made up a film strip from multiple beam exposures. The material I chose to examine was ceric iodate monohydrate, probably because its crystals were a pretty yellow color! It was not the wisest choice for two reasons: it had a large unit cell for those days and it was anhydrous until Don Cromer at Lawrence Livermore Laboratory identified a water that I had missed. In any event I was hooked on crystallography. I estimated intensities at night while listening to records of Mozart piano sonatas as played by Wanda Landowska.

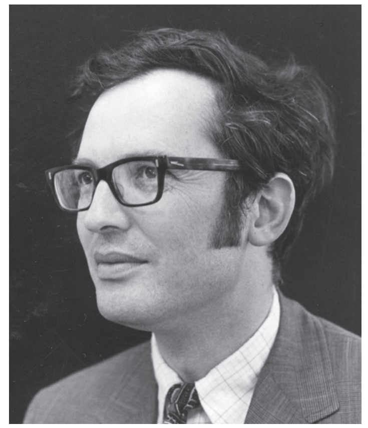
Verner and his associates had realized the "B" in IBM stood for Business and they devised the "M-card system" for calculating Fourier syntheses that depended on IBM sorters, tabulators, and mergers. These devices were on the second floor of Throop Hall and were used by the Caltech Business Office. An arrangement was worked out for me to use these devices at night. Except for the occasional moth getting caught in the tabulator the calculations went smoothly. I was able to calculate a three-dimensional Fourier synthesis of ceric iodate. Failure to find that it was actually a monohydrate was perhaps the first, but certainly not the last crystallographic error I would make. Speaking of errors reminds me of Dick Marsh, another member of the Pauling group. Dick's main pastime, when he was not working on a project for Pauling, was finding errors in the literature. The victims were "Marshed". I eventually got "Marshed".

Dick Marsh & Linus Pauling

For my graduate studies I applied to and was accepted by the University of California, Berkeley, and Caltech. (Remember as an Angelino it was my impression that there was nothing much East of the Sierra Nevada Mountains, including Ivy League schools!) Ken Hedberg urged me to go to Berkeley as going to the same graduate school as one's undergraduate school was strongly discouraged. For personal reasons I chose Caltech.

In 1951 I received my BSc. from Caltech and married Joyce, my high school sweetheart. For the next three years she was employed in downtown Los Angeles and supported us while I was in graduate school. After receiving my Ph.D. in 1954 we went off to Melbourne Australia on a 1-year NSF postdoctoral fellowship to work with Lloyd Rees and John Cowley at CSIRO on electron diffraction of solids. The year in Melbourne was an amazing experience. My colleagues at CSIRO introduced Joyce and me to sherry, great Australian wines, and many overnight stays and local side trips. We even managed a rail trip across the Nullarbor Plain to Perth and a cruise ship back. We also hitchhiked to Sydney to see Hans Freeman, a fellow graduate student at Caltech. Hans, Joyce, and I hitchhiked to Canberra and then parted and Joyce and I hitchhiked back to Melbourne. Despite all of this John Cowley and I managed publication of a ferric chloride/graphite compound. That publication has been highly cited. Incidentally for those who knew the Freemans we would see Hans and his wife many years later in Adelaide for a week enjoying Wagner's Ring Cycle. Shortly thereafter we were saddened by Hans's death.

1955-1961: Shell. With Verner's help I had secured employment in Dave Stevenson's group at Shell Development Company in Emeryville, California. Emeryville is just across the Bay from San Francisco. Shell was interested in better characterization of solids and that was where I fit in. Overall the group was concerned with testing new instrumentation to prevent other Shell laboratories from buying instruments they did not need. My colleagues in Dave's group were very generous with their time: Jerry Swalen taught me to program in FORTRAN; Bob Snyder et al. devised the use of oil to facilitate the X-ray examination of air- and water-sensitive crystals. Ed Smutney showed us the wonders and apparent sins of North Beach in San Francisco! In my spare time I wrote a number of crystallographic papers: among others, estimates of standard deviations of observed structure factors and of the electron density from intensity data, a variety of new atomic form factors, including relativistic ones, anharmonic oscillations of nuclei, and tables of atomic scattering amplitudes for electrons (in volume 3 of *International Tables for X-ray Crystallography* (1962)). This last effort was co-authored in 1959 with Boris Vainshtein of the Soviet Union and was carried out on an IBM computer available at IBM San Francisco. In 1959 the U.S. was engaged in a "Cold War" with the Soviet Union! Dave Templeton at UC Berkeley noticed my crystallographic papers and asked me to apply for an assistant professor position at Berkeley. I told him "No" as I was very happy at Shell. Shortly thereafter Shell at Emeryville fell apart as a result of a reorganization at Royal Dutch Shell. It is interesting to contemplate what might have ensued if I had said "Yes" to Dave Templeton!



Walter Hamilton

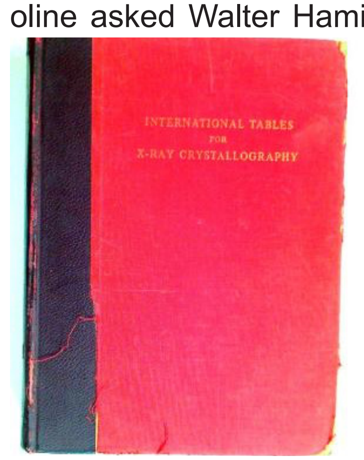
Courtesy of AIP Emilio Segrè Visual Archives, Physics Today Collection

1962-1964: Brookhaven National Laboratory, Upton, New York. Again with Verner's help I ended up at Brookhaven as a Senior Chemist. Joyce and I sold our home in Kensington in the Berkeley hills and ended up with enough cash to buy a lovely two-acre lot and home in Bellport along the south shore on Long Island, New York. I joined an excellent Chemistry Department and was especially pleased that it included Walter Hamilton, a colleague of mine from Verner's group at Caltech. Also in the Department was Sam LaPlaca, who collected X-ray data on a primitive diffractometer. In contrast the neutron diffraction facilities at the graphite reactor were state of the art and I took advantage of them to study O-H-O bonding. Shortly after my arrival, at a seminar there was excitement over the report of xenon tetrafluoride, the first stable rare-gas compound. Someone in the back of the seminar room said he had repeated the synthesis following the announcement of its discovery. [One can prepare XeF_4 from Xe, F_2, and sunlight]. Earlier Pauling suggested to Caltech's inorganic chemist, Don Yost, that Xe should form stable compounds but Yost disliked Linus and ignored his suggestion. The sample of XeF_4 started the LaPlaca, Hamilton, and Ibers adventures in crystallography. We solved the structure by using open-source software.

I did not like some of the computer programs in vogue at that time, as one was forced to refine on F_o, weights were difficult to assign for small F_o, and there was no attention given to $F_o < 0$. Verner had taught us that one never changes the data

but only the model. F_o^2 is far closer to the data than F_o, and fortunately the ORFLS least-squares program available from Bill Busing and Henri Levy of Oak Ridge National Laboratory allowed one to refine on F_o^2. Thus I put together a suite of programs and the necessary instructions for ORFLS, ORTEP, Carroll Johnson's thermal plotting program, and FORDAP, the Fourier program from Al Zalkin at Lawrence Berkeley National Laboratory. These all compiled nicely on the Brookhaven CDC 3600 computer. One cannot say enough for the great contributions the National Laboratories have made to crystallography, especially with the availability of open source software. [As a historical note, Edward Hughes in the Pauling group in 1941 was the first to apply the least-squares technique to the refinement of crystal structures.]

Around 1961 Kathleen Lonsdale became General Editor for a projected four volume revision of *International Tables for X-ray Crystallography*. Overall, Caroline MacGillavry and Gerard Rieck were in charge of Volume III, Physical and Chemical Tables, that included X-ray and electron diffraction scattering factors and a variety of largely mathematical details. [Some of you may remember "The Red Books" with their lousy bindings.] Caroline asked Walter Hamilton and me to edit Volume III. It was there that the genesis of the book *Hydrogen Bonding in Solids* by Hamilton and Ibers (1968) occurred. I took the opportunity to express to Caroline my interest in drawings by M. C. Escher, a fellow Dutchman. She provided contact information. Escher was taken by surprise and indicated that he never sold fewer than four prints at a time. Some of you may remember the prints I ordered as they have hung in all of our residences. "Day and Night" remains my favorite and is currently hung in my bedroom.



"The Red Books"

I don't remember why I was there but around 1962 I attended a meeting of about 12 people in the French Alps overlooking Lake Geneva. In attendance were Martin Buerger, Jose and Gabrielle Donnay, and several high-level theorists, including Hans Wondratschek. The purpose of the meeting was to organize the space group information for the new International Tables. I, as the "pci" — the practicing crystallographic idiot — made two important contributions. I kept the theorists from making "c" the sole monoclinic symmetry axis and I had them include the necessary information to define a unique unit cell. This helped prevent crystallographers who collected limited data sets from collecting half the data twice. Incidentally, the "b" axis as the symmetry axis, was chosen by the mineralogist Grose in the 18th century who characterized diverse crystals and provided their axial ratios.

1965: Northwestern University. Although I was very happy at Brookhaven it was situated in the middle of nowhere with nothing much but duck farms to the East of the Hamptons. Our lovely two-acre lot and home in Bellport were great but our dog joined packs and attacked the postman and we dared not let our cat outside. Also, setting up a laboratory at Brookhaven to do preparative chemistry would have been difficult. Although to the West was New York City with all its attractions, getting there involved The Long Island Railroad, where I use the term "railroad" euphemistically. Joyce and I were very interested in cultural events, especially the theatre. Thus when I was approached by Iowa State University as a possible replacement for Bob Rundle, who was retiring, I was tempted, but Ames was not my idea of an environmental improvement. [Larry Dahl took the Ames offer.] Somehow Northwestern got wind of the possible Ames offer and countered with one of their own. Evanston, and especially Chicago, were civilization and a full-professor offer from Northwestern was an easy choice.

As this is an "ACA Living History" I have up to this point concentrated on crystallographic matters, although I warn you that I do not consider myself to be a crystallographer but rather an inorganic chemist. To emphasize this point, since joining the faculty at Northwestern about 9% of my publications have been in *Acta Cryst.*, whereas about 33% have been in *Inorg. Chem.*

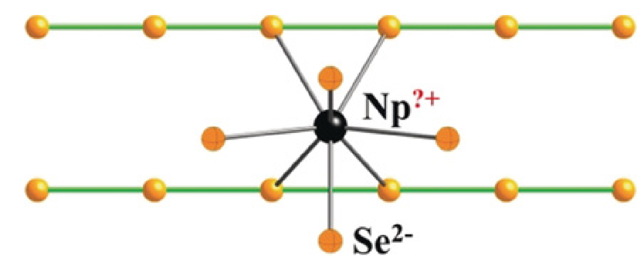
As part of my start-up package at Northwestern I purchased a brand-new four-circle Picker diffractometer. For computing, Northwestern had a CDC 3600 computer so I simply brought the program suite I had at Brookhaven and compiled the programs at Northwestern. If more computing power were needed we had overnight access to the CDC 7600 at Lawrence Berkeley Laboratory. The Picker was controlled by punched cards and then paper tape. To collect data efficiently I wrote something akin to the traveling salesman problem. I was fortunate to have an electronics shop available to fix encoder problems. We devised a cold stream to cool crystals. It worked reasonably well, but far better when Jean-Jacques Bonnet, a postdoctoral researcher, supplied a glass transfer tube from his glassblower in Toulouse. Overall this setup for the Picker worked very well probably for about 20 years, but was quickly abandoned by my group once the Nonius version of a four-circle diffractometer became available.

Jim Ibers speaking at the Florence IUCr meeting in 2005

As I had one of the few diffractometers in 1965 I collaborated with a number of chemists to solve a variety of structural problems. It was evident to me and to Larry Dahl that solving the crystal structure was the fastest way to characterize a compound. This fact was later "discovered" by Al Cotton. Concomitantly my research group began to produce compounds often involving phosphines, especially triphenylphosphine. Common sense dictates that if you know something better than you can determine it crystallographically you should make use of it. This led me to write a group refinement program for phenyl groups. It also led my group into hydrides, molecular O_2, molecular N_2, NO, SO_2, CS_2, and aryldiazo compounds, among others.

In the United States research projects are driven by available funding. The research detailed above was largely funded by the NSF. But our interest in molecular oxygen compounds enabled me to secure National Institutes of Health (NIH) funding. The ensuing research was largely organic chemistry! The group made a variety of porphyrins, delved into porphyrin oxygen chemistry, made synthetic analogues of known protein molecules, and began an ongoing collaboration with Dick Holm on iron-sulfur chemistry.

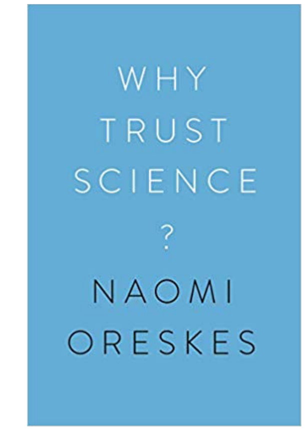
The research on iron-sulfur chemistry led my group to the very rich chemistry of soluble metal chalcogen anions (NSF), examples being the $[AuTe_7]^{3-}$ anion and the $[(Te_4)M(\mu-Te_4)M(Te_4)]^{4-}$ anions, M = Cu, Ag. In the last decade my interests have turned to solid-state chemistry, in particular to research into the solid-state chemistry of the actinides (U and Np). This research was supported by the Department of Energy - Basic Energy Sciences (DOE) and comprised my support from about 2007 until I elected to cease accepting new graduate students. However, it continues in collaboration with two former postdoctoral researchers, Adel Mesbah (France) and Jai Prakash (India). An example of this work is "$NpSe_2$: a New Binary Chalcogenide Containing Modulated Selenide Chains and Ambiguous-Valent Metal", which was published recently in *Angewandte Chemie*.



Overall it is a fun journey through a plethora of problems and curiosities. My many students, postdoctoral researchers, visitors, and research collaborators continue to make this possible. To them I dedicate this History.

Jim Ibers

Editor's Note: *Among the Awards and Honors Jim Ibers has received are the American Chemical Society Award in Inorganic Chemistry, American Chemical Society Award for Distinguished Service in the Advancement of Inorganic Chemistry, the Linus Pauling Medal, the California Institute of Technology Distinguished Alumni Award, and the Martin J. Buerger Award of the American Crystallographic Association. He has been elected to the American Academy of Arts and Sciences and to the U. S. National Academy of Sciences.*



Why Trust Science?

By Naomi Oreskes
ISBN: 9780691179001

Naomi Oreskes' Why Trust Science? is the book version of a series of lectures the scientist and science historian gave at Princeton University in Fall 2016. For those not fortunate enough to have attended the university's Tanner Lectures on Human Values, the book contains not only the text of Oreskes' two lectures, but the four commentaries given at the time by distinguished members of other fields. It also includes Oreskes' reply to her commentators.

Although Oreskes gave her original lectures over three years ago, the content and context of her work is as relevant as ever. One critical thing to remember when reading is that the title of her book is not Should We Trust Science?, but rather Why Trust Science?, and in this book, Oreskes details exactly that, using specific examples to illustrate a larger issue plaguing the American zeitgeist as the first decade of the twenty-first century comes to a close.

Oreskes answers her titular question eloquently in the first chapter, "Why Trust Science?: Perspectives from the History and Philosophy of Science." Her second chapter, "Science Gone Awry," is where things get interesting. It implicitly addresses the question of "should we trust science?," since, as Oreskes demonstrates, sometimes science does get it wrong. Her examples—the Limited Energy Theory, rejection of Continental Drift, eugenics, the link between hormonal birth control and depression, and dental floss—illustrate an important point. Sometimes, science gets the facts wrong, plain and simple. And sometimes, science gets it right, but the powers that be manipulate the perception of scientific discovery in the eyes of the general public.

One critical example Oreskes visits in the book that gets revisited by her commentators is that of climate change. A significant proportion of climate change research in the past decades has been funded by none other than the petroleum industry. Indeed, as I am writing this, oil and gas giant ExxonMobil is headed to court in New York over claims that the company misled investors regarding the planetary impact of climate change as caused by overuse of petroleum-based products and transportation. At this stage in the game, climate change denial seems futile in the face of the mounting evidence to the contrary—but thanks to decades of false information perpetuated by big oil conglomerates with a significant conflict of interest, the damage, both to popular perceptions of the problem and to the planet itself, is largely irreversible.

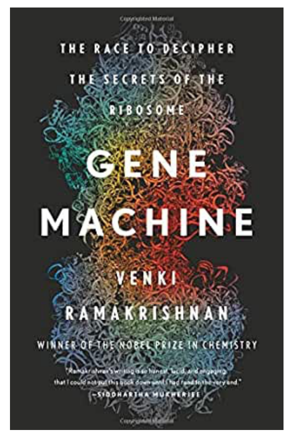
Oreskes does not address the Big Sugar scandal that hit the news in Fall 2016—only a few months before she gave her original lectures. But that instance—where sugar manufacturing corporations paid Harvard University researchers to downplay the negative health effects of sugar consumption in published works—further illustrates a similar point.

Science, like any discipline, can be distorted and skewed by the lens through which its findings are viewed. Nazi scientists took Charles Darwin's theories of evolution and natural selection to a eugenics extreme. Their abuse of Darwin's survival of the fittest research was abominable—but it does not and should not detract from the heft of his original contributions to the field of evolutionary biology.

Before discounting any scientific research, or even before believing every newly published paper out there, one should consider the context of the facts being presented.

Oreskes book is highly academic, both in diction and tone—indicative of the book's origins as a series of lectures at a top university. She makes multiple references to her other published works throughout the book, including Merchants of Doubt, and after having read Why Trust Science?, I find myself inclined to give them a read.

By Jeanette S. Ferrara, MA



Gene Machine: The Race to Decipher the Secrets of the Ribosome

Venki Ramakrishnan, Basic Books, New York, 2018, 288 pages, ISBN: 978-0-465-09336-6.

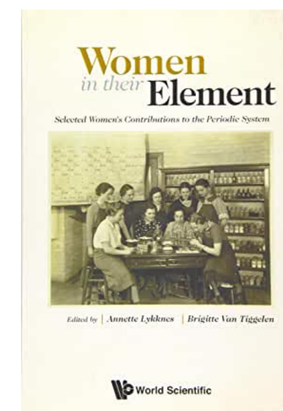
This book came to me through a recommendation by Alex Wlodawer. The author, now at the Medical Research Council Laboratory for Molecular Biology in Cambridge and President of the Royal Society, is one of the recipients of the 2009 Nobel Prize in Chemistry "for studies of the structure and function of the ribosome". The author shared the prize with Tom Steitz of Yale University and Ada Yonath of the Weizmann Institute. Both figure prominently in the story that the author tells us.

This is a memoir not an historical account so you will see some subjectivity in the account. Having said this, the author has provided a wonderful personal account of his quest to first find himself then the structure of the 30S ribosomal subunit and then an understanding of how the ribosome produces proteins. The author does a great job of naming names and giving credit to everyone involved in the heroic effort not just in his labs but labs around the world. The story begins with the author's arrival in 1971 at the University of Illinois. The author takes us with him from Oak Ridge, to

Brookhaven, to the University of Utah and finally the LMB.

There is a short digression at the beginning of the book, Chapter 3, that describes single crystal X-ray diffraction, the method that that has provided a significant portion of the structural information about the ribosome thus far. A second digression takes place in Chapter 15 in which he discusses the seeming randomness of the Nobel selection process and the unfairness of the limit of three persons.

Review by Joe Ferrara



Women in their Element: Selected Women's Contributions to the Periodic System

Edited By Annette Lykknes and Brigitte Van Tiggelen
ISBN: 978-981-120-768-6

Women in their Element is a delightful homage to many of the unsung heroines of The Periodic Table (and several of the sung ones as well). Each of the book's 38 chapters contains the story of a female scientist whose research contributed to our understanding of the elements as presented on The Periodic Table.

A different contributor authored each entry, and the diversity of voices and writing styles mirrors the diverse women discussed and the nature of their contributions. As the editors explain in the introduction, their goal was not to provide a comprehensive guide, as one would require much more than 500-odd pages. They chose rather to pay respect to as many female scientists with ties to The Periodic Table as possible. Every entry provides brief biographical information to orient the reader in the respective scientists' time and place, as well as a more detailed summary of her research and its critical role in shaping our knowledge of the elements.

Quite a few well-known names make an appearance, such as Marie Curie and Lise Meitner. But the majority of the women are lesser known--though they certainly should not be. Because each entry is fairly succinct, the reader only gets a brief glimpse into the lives and discoveries of these women. Fortunately, each entry ends with a list of references the author used when writing it--and this list often includes other, more in depth biographical works--allowing the reader to further pursue at their leisure.

By Jeanette S. Ferrara, MA

William L. Duax
A Friend and Colleague

By Dr. S. Narasinga Rao, CFO, American Crystallographic Association Inc. , Financial Counselor, IUCR , Dean Emeritus, Dr. Joe C. Jackson College of Graduate Studies and Research , Professor Emeritus, Department of Physics and Engineering, University of Central Oklahoma, Edmond, Oklahoma and Ex-Governing Board Member, American Institute of Physics

I am pleased and honored to write a brief article on William Leo Duax, popularly known as Bill Duax and in short as "Bill". Bill Duax was born on April 18, 1939 in Chicago, Illinois, to William Joseph and Alice B. (Joyce) Duax.

As everyone in crystallographic community knows, Bill has been CEO of the American Crystallographic Association for more than 30 years. I have had the pleasure of working closely with Bill as a treasurer for six years and then as Chief Financial Officer of ACA and have served in such capacities since 1986 on the ACA council for 34 years. Bill was instrumental in moving the ACA office in Buffalo at the Hauptman - Woodward Medical Research Institute where he still serves as Herbert A. Hauptman Distinguished Scientist and also as a Professor of Biophysics at the structural biology department at the State University of New York at Buffalo.

Bill began his career at ACA as a member, officer, president and executive officer. He quickly found his footing and not only became a valuable member of our team but started to take over in areas that weren't even on his job description. Jokes aside, Bill's work acumen was second to none, always serious about his deadlines, his tasks for the day: "laid out on little yellow post it notes stuck all over his desk"... and was a sporty team player...in the true sense of the word!

Bill Duax is an American biologist, researcher, Fulbright scholar Council for International Exchange, 1987; Grantee, National Institutes of Health, since 1971; recipient of Special Merit award Institute Arthritis and Metabolic Diseases, National Institutes of Health, 1987-1903, Distinguished Alumni award, St. Ambrose College, 1983, Clinical Ligand Assay Society Distinguished Scientist award, 1994.

Bill received his Ph.D., degree in Physical Chemistry, from University of Iowa, Iowa City, Iowa, in 1967. An Honorary Doctor of Science Degree was conferred upon Bill in 1999 by University of Lodz, Poland.

After getting a Ph.D.from Iowa, he was a Postdoctoral research fellow at Ohio University, Athens, 1967-1968. Research associate Hauptman-Woodward Medical Research Institute (formerly Medical Foundation), Buffalo, 1968-1969. Head crystallography department Medical Foundation Buffalo, 1969-1970, head molecular biophysics department, 1970-1988, associate director research, 1983-1988, research director, 1988-1993, executive vice president research, 1993-1999, vice president, 1998-1999, H.A. Hauptman Distinguished Scientist, since 2000.

Bill as a person, is a complex organic structure whose structure cannot be solved easily. It is not two or three dimensional, but multi-dimensional. There are no known structure-solving techniques for a multi-dimensional Bill, no Nobel Prize winning direct methods even. The only way one could analyze Bill and understand him is by close association with him.

Bill has carried out his message of crystallography to Venezuela, Chile, Equador, Brazil, Bolivia, Uraguay, Peru, Paraguay, Guyana, Columbia, and India to mention not all but a few. Thus, he is not only an American Crystallographer but he is a Global Crystallographer. His interest in minorities and less developed countries is noteworthy. As a member of ACA council he always fought for making Latin American Crystallographers and African Crystallographers to be associated with ACA and make the Latin American Crystallographic Society an affiliate of the ACA. To support crystallographers from these countries to attend ACA meetings he has come forward to donate his personal money.

On a personal note, when I started as an ACA treasurer in 1989, I started with only $ 80,000 in total assets of ACA that included operating, meeting and award accounts. There were no individual award accounts. All awards were combined in total assets. At Bill's suggestion and with his cooperation, I was able to research where the different awards were, and when they were started so that we could identify to a certain degree different amounts in various award categories. Bill and I also thought that it would be easier if all awards were with the ACA so that we could monitor and administer them. This way, all designated ACA awards will be managed and awards issued by ACA. As CEO, Bill contacted different corporations and companies each year to raise funds to support the ACA Annual meeting program, often raising anywhere from $50-$60,000 each year.

As an example, after many deliberations, I found out that Fankuchen Award was with Rensselaer Polytechnic Institute in New York and they had no idea what to do with it. No single individual was responsible to monitor it. Rensselaer was good enough to transfer the funds that they were holding to the ACA . Bill and I were able to review the records and identify several awards that were situated in several different places. Bill was a visionary to help me organize and put several things in place for ACA. I also had the opportunity to work with him and others, especially, Judith Flippen-Anderson in organizing, budgeting and executing utilizing funds for IUCR congress and General Assembly in 1996 at Seattle.

In Mark Twain's words, Bill Duax is: "The Global man of Crystallography, of fabulous research and fabulous enthusiasm, of somersault splendor, complex structures and functions, of genii and giants and great humor, of humility and sincerity, of dedication to teaching of crystallography and the taught, of integrity, commitment, dedication, teaching and training high school students at the Hauptman-Woodward Research Institute in Buffalo in the United States, leader and promoter of talents in minorities, youth, and research, of inspiring scientists in the land of a thousand crystallographers, and around the globe and of several fields, in the cradle of the Crystal Structures, Grandfather of legend, Great-grandfather of tradition, of wonderful purity, childlike and profoundly stubborn with the moldering antiquities of the rest of the scientists—the one soul under the sun that is endowed with an imperishable interest for crystal lovers and connoisseurs, for lettered and ignorant, wise and fool, rich and poor, bond and free, the one man that all people desired to see and interact."

Bill's accomplishments and achievements include 225 Invited lectures in over 30 countries, 285 Reviewed manuscripts in national and international scientific journals, 45 Review Chapters in Books on Steroid hormone biochemistry ion transport, Antibiotics and X-ray Crystallography, author of 4 Books and 425 abstracts at scientific meetings.

Bill has served as CEO of ACA since 1986. He was program chair for the 17th IUCR Congress and General assembly in Seattle, WA in 1996 and was President of IUCR from 2002-2005, served as and also a member of IUCR commission on Structural Chemistry (IUCR-CSC). Bill also served

as News Letter editor for IUCR from 1993-2017. His scientific interests and hobbies include but are not limited to Bioinformatics, proteomics and Genomics, Ion Transport Antibiotics and Toxins, Crystallography in South America, Crystallography in Central America, IUCR newsletter, American Crystallographic Association, High School Apprentice Program at HWI, Steroid Chemistry, Biochemistry, Photography and Somersault.

Bill has retired as CEO of ACA effective December 31, 2019. He will be sorely missed, by me, and I think I can speak for all who know him and those that had the joy to work alongside of him all these years: Bill will not be forgotten. The above are a few photos of Bill with crystallography pioneers

and Nobel Laureates. He was mainly responsible for bringing eight Nobel Laureates in Crystallography to an ACA meeting in Philadelphia in 1988.

It has been a great pleasure for me to work with Bill so closely on the ACA Council for 30 years. I am personally very happy that we have been able to build the ACA assets from $80,000 to nearly more than a million now, of which nearly half a million is endowed for awards and the balance is in the reserves which has been my goal from the time I became the treasurer in 1989.

The following is a tribute to Bill Duax written by Dr. Alex McPherson at my (Narasinga Rao's) request for the "Symposium on Bill Duax ": at the IUCR Congress and General Assembly held in Hyderabad, India in 2017.

In honor of Bill Duax

To my colleagues and friends in the vast crystallographic community, It is with great pleasure that I offer this brief testamonial for the distinguished, yet always humble, Bill Duax, on the occasion of this symposium. I greatly regret not being able to be there in person and shake Bill's hand and slap him on the back, so I hope these few words will add a mellow note to those happy procedings. I can think of few other scientists who have contributed so much and are so deserving of the recognition you are bestowing upon him. He is truly an exceptional scientist, colleague and gentleman. Most of all, he has been a great personal friend for almost longer than I can remember.

I was first introduced to Bill more than 40 years ago when I was a post doctoral fellow at MIT, and Bill was developing what was to become the finest laboratory in the world in the area of x-ray crystallography of steroids at the Buffalo Medical Foundation (now Hauptman-Woodward). Under his leadership, his group of scientists achieved international renown; not only for their structural investigations, but for the methodologies and mathematical approaches they developed.

Under Bill's leadership, the Buffalo Medical Foundation crystallographers, I think it is fair to say, also became the world's leading institution, and certainly most innovative laboratory, in the development of direct methods. Those methods, bold and controversial at the time, have come to dominate conventional small molecule x-ray crystallography, and have in more recent times had a profound impact on macromolecular research as well.

Bill's active mind didn't rest on these successes, however, and in the 1980's, while still maintaining primacy in mathematical approaches to structure determination, he moved his laboratory in the direction of protein crystallography. As might have been anticipated from their past accomplishments and their intellectual strengths, the group was enormously successful in this field as well.

Bill's scientific achievements and his many published contributions to the field of x-ray crystallography are distinguished, respected, innovative, and a matter of public record. They need no extensive review here. What may not be so evident, and something which must be made crystal clear (pun intended), is Bill's unmatched contribution to the organization and nurturing of both the American and the International crystallographic community. In my view, Bill is the savior, and this is no exaggeration, of the American Crystallographic Association, and he is the most remarkable ambassador to the international crystallographic community that we have ever had.

Bill personally took control of a faltering ACA, a society with dwindling membership, unattractive to young scientists, and increasingly losing any

sense of vision. He completely turned the organization around, gave it new purpose, new direction, attracted new members, and in the end transformed it into one of the most significant, vital, and active scientific societies in the United States. I have never before, or since, known of anyone to do so much for a scientific community as Bill did for the X-ray crystallographers of America.

Finally, it cannot be emphasized enough, what an outstanding friend and representative Bill has been to the international body of crystallographers. In many parts of the world, I am convinced, Bill Duax means American crystallography. He is admired, respected, and personally liked by probably more scientists in more countries than any other man I know. Just as he restored the ACA to health and vigor, so has he promoted the importance of crystallographic research world wide. He has put, if you will, a human face on American scientists.

I very strongly, and with deep sincerity, applaud your honoring Bill Duax at this conference and, from a distance, wish him the best in life. He has been an inspiration as an exceptional scientist, colleague and a trusted friend. He is rich with honor.

Alexander McPherson
Professor Emeritus
University of California, Irvine

Mark Beno Receives Posthumous AAAS Fellow Distinction for Lifetime Achievements

Mark Beno, a senior chemist at the Argonne National Laboratory who died suddenly in 2019, has posthumously received the AAAS Fellow Distinction for Lifetime Achievement. This award honors scientists of diverse accomplishments, "including pioneering research, leadership within a given field, teaching and mentoring, fostering collaborations and advancing public understanding of science." Mark Beno is a worthy recipient of this award.

Mark did pioneering work on the crystal structures of superconductors, solving the crystal structure of the high temperature superconductor YBa2Cu3O7. His seminal paper was published in 1989 and the results continue to inform the field of high temperature superconductors today.

Mark spearheaded the design, construction and operations of the Basic Energy Sciences Synchrotron Radiation Center (BESSRC) beamlines at two sections of the Advanced Photon Source (APS). His expertise led to his being asked to help establish the scientific programs coming on line as the APS was moving to operation. He became the BERSSRC group leader and then moved with his group to the now X-ray Science Division (XSD) in 2003. He held a number of leadership roles within the APS XSD, twice serving as its interim division director.

Mark was well-known for the time he spent on the APS experimental floor, walking around talking with all the staff and users about their projects. Because of his knowledge of science, and of the APS in particular, his advice was always being sought and generously given. His interest was not just in the advancement of chemistry but in the advancement of science in general.

Mark's research produced more than 190 publications and resulted in three awards from the Department of Energy's Basic Energy Sciences, Division of Materials Sciences, for Outstanding Scientific Accomplishment.

About the U.S. National Committee for Crystallography (USNC/Cr)

Greetings from the U.S. National Committee for Crystallography (USNC/Cr), the current members of which you can find listed below. As current chair of the USNC/Cr, I was asked to write a short article for RefleXions to introduce the wider ACA membership to the purposes and activities of our committee, as well as some of our current challenges. I would like to briefly put into perspective how the USNC/Cr fits into the network of crystallographic organizations and bodies representing crystallographers.

If you are reading this news piece, you are likely familiar with the American Crystallographic Association (ACA), which is a remarkable multi-national professional organization, primarily serving crystallographers from the US and Canada, which do not have separate national crystallographic associations.

The International Union of Crystallography (IUCr) is a global umbrella organization that brings together crystallographers from all over the world. The IUCr currently has 53 "adhering bodies" (member nations), most of which represent individual countries, but a few of which represent groups of smaller countries. There are also four Regional Associates of the IUCr, which include the ACA (representing most of North America), AsCA (Asian Crystallographic Association; representing Asia and Australasia), ECA (European Crystallographic Association; representing Europe and Africa) and the newest member, LACA (Latin American Crystallographic Association; representing Mexico, Central and South America). The IUCr publishes crystallographic journals (e.g. *Acta Crystallographica* family), maintains the *International Tables for Crystallography*, publishes an extensive collection of books on crystallographic topics, supports global education initiatives, awards prizes, establishes crystallographic guidelines and standards through its numerous scientific commissions, and maintains a World Directory of Crystallographers (see https://www.iucr.org/people/wdc, and make sure you are included). Similarly, each regional associate also hosts regional crystallographic meetings, supports education and outreach, awards prizes, publishes journals etc. There are considerable informal interactions between the IUCr, its members and regional associates each year.

An adhering body does not interact directly with the IUCr, but rather forms a national committee for this purpose. For example, in the US, the National Academy of Sciences (NAS) is the adhering body to the IUCr, and many other international scientific unions. The NAS organizes US national committees to serve as liaisons between our scientific communities and these international unions. In this way, the US National Committee of Crystallography (USNC/Cr) is charged to represent the interests of US crystallographers to the IUCr, where "US crystallographers" refers to any crystallographers residing in the US, regardless of country of origin or immigration status.

Every 3 years, the IUCr hosts an international meeting; the next one will be held in Prague, Czech Republic, August 22-30, 2020. At these meetings, delegates from the adhering bodies convene a General Assembly for transacting IUCr business, including elections, bylaw changes, selection of future meeting sites, etc. Apart from the guarantee that a representative of each region must sit on the IUCr executive committee, the regional associates do not have formal representation within the IUCr. Rather, the authority to vote and transact business lies with delegates of the 53 adhering bodies of the union, where the number of delegates (and votes) of an adhering body is commensurate with its membership category, which ranges from I to V as the annual dues increase.

The USNC/Cr selects and sends US delegates to the IUCr General Assembly, and nominates US scientists as IUCr officers, members and chairs of the 20 scientific commissions of the IUCr, and as editors of IUCr journals. The USNC/Cr has also been very active in both organizing and supporting crystallography-related education and outreach

opportunities, and has worked to communicate the need for international standards in crystallographic education and the analysis and dissemination of crystallographic data.

Over the past 75 years, the US has played a leading role in the activities of the IUCr, and contributed much to the remarkable success of international crystallographic standards and infrastructure. Six of the past 23 IUCr Presidents have been prominent US scientists. At present, roughly 17% of the 200 journal editors/co-editors and 400+ scientific commission members and consultants of the IUCr are from the US. The US is currently one of only three category V members of the IUCr (in addition to the UK and Russia), which means that we have 5 delegates (and votes) in the General Assembly.

In the past, dues for US membership in the IUCr, delegations to IUCr General Assemblies, and some other USNC/Cr activities, have been supported by a grant from the National Science Foundation to the NAS. Unfortunately, support for the USNC/Cr was not included in the most recent 5-year NSF grant to NAS, so that we must now explore alternate funding options or risk losing our membership and involvement within the IUCr, and the tremendous benefits that this involvement brings to US science. If you know of potential avenues for such funding, whether from federal agencies or other organizations, the USNC/Cr would be happy to receive your input.

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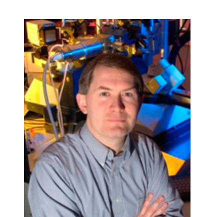

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CORA LIND-KOVACS

Puzzle Corner

For this issue, we have several puzzles on the theme of women in crystallography, including a Crystal Connections, a DISORDERED puzzle, and a word search puzzle by Guest Puzzler Joe Ferrara, containing the names of 32 female crystallographers. How many can you find? Extra credit for providing the names of the nine women pictured in the DISORDERED puzzle. Solutions to previous puzzles and the names of those who provided them are also given.

Crystal Connections #17:
Find the answers to these clues and how they are connected.

1) Yes ______, there is a Santa Claus.
2) Inverted _______ A U.S. Stamp with a Curtiss biplane printed upside down.
3) 523 ______ is a minor planet with orbital period 1870 days, discovered in 1904.
4) A religious Christmas song.
5) A 1976 horror film starring Sissy Spacek, based on a Stephen King novel.
6) M. C. Escher carved blocks of _____ to make periodic prints.
7) To take legal action against.
8) A 1983 horror film about a Plymouth Fury with a bad personality.
9) Mythological creature, part eagle, part lion.
10) Queen Elizabeth, Mister Lincoln and Peace are classic varieties of this.
11) To sway unsteadily.
12) Disguised herself as Ganymede in As You Like It.
13) A historically black university in Washington D.C.
14) LDL stands for _____-density lipoprotein.
15) Suite: ______ Blue Eyes, 1969 song by Stephen Stills
16) 1470 _______ is an outer main-belt asteroid discovered in 1938

DISORDERED

Rearrange the letters in the following

BLASELIA	☐◯◯☐◯☐☐☐
JREATSAN	◯☐◯☐☐◯☐☐
MOCCTHIK	☐◯◯◯☐☐☐☐
AMBERN	☐☐◯◯☐◯
YOMONE	☐◯◯☐☐☐
PLEESHT	☐☐◯☐☐☐◯
YDUJ	☐☐◯◯

Female crystallographers use the letter X for their

Answer: ☐☐☐☐ ☐☐☐ ☐☐☐☐☐☐☐☐☐☐☐

32 Women

word search puzzle

L C H E R Y L S T E V E N S S N D C O R A L I N D
I R E V X Q F K C H G R N W B O R D E N L A C Y W
N W I N N I E W O N G N G X E X G K L Z A J S T Y
D J U D I T H F L I P P E N A N D E R S O N W I J
A J J P E B I N N M A D E L E I N E J A C O B S A
H A J O L W K J Z L X L P D J W I M D O F D F J N
A N T M S K F C X C O N N I E R A J N A K R B K E
N E E H P Z Y X C V T D V R R N U E K K E O V F G
N R F E E O U T D O R O T H Y H O D G K I N I I R
I I Q G T V X C K Y T Q T M R G R J S L L N R K I
C C O W H A V M N N T O A E V N R U D F A T G A F
K H K K G B Q W A C M R T G W E L O G M F E I B F
E A P Q A V N E M L Y E N J T G E N R I O L N X I
L R A B R T J D I B E A Q T Y L I E W D D I I L N
E D T D M R C W N T H W E N R D B S N G L Z A N E
A S Y F A L E A A Z K T N A D N R A C U H A P F J
N O W S N I S H E A E E K O E E I U F Y Z B E X U
O N Y A R U T I N R J A C L F M Z A X L I E T F L
R M T R S R S R A S L Y E I O M V B X I K T T J I
A K A T A S U G K L N H N Z M E Q C D A L H Q D A
D C Q M E J R H E N T N O C R P Q A S U D W B I C
M P H J N A D B E U E N Z N F V H I Q F L O W V H
A P N A M U A P O J D W M T V M L J O P W O X E A
N A R S B S C H R I S T I N E D U N H A M D P Z N
Y F I S I M A R I L Y N O L M S T E A D K B Q R J

DISORDERED

These words have drifted apart.
Reassemble them to obtain high quality

TIVYRAG	G R A V I T Y
INEPTOR	P R O T E I N
VECCTON	C O N V E C T
CHOSKEN	S O H N C K E
GRUBOPUS	S U B G R O U P

The team of astronauts who grow crystals in orbit call themselves…

Answer: THE SPACE GROUP

Solution to Crystoquote #6

While I did not know Dick Marsh well, I can testify that he mentored my career, from afar, with his careful work on the corrections, and some amazingly careful structural work, very often with a message for learning a new thought or trick!
Bruce Foxman

Frances Bernstein provided the solution to the space station DISORDERED puzzle. John Bollinger provided the solution to Crystoquote #6.

As always, I will be pleased to see your solutions and also your ideas for future puzzles. Volunteer Guest Puzzlers are especially welcome!

Frank Fronczek – ffroncz@lsu.edu

March - Aug 2020

10th Workshop on Structural Analysis of Aperiodic Crystals	12th Mar 2020 - 15th Mar 2020 (Bayreuth, Germany)
Better with Scattering: SAXS/WAXS Workshop for Nano Materials	16th Mar 2020 - 19th Mar 2020 (Berlin, Germany)
3rd LACA School on Small Molecule Crystallography	26th Mar 2020 - 29th Mar 2020 (Mexico City, Mexico)
Powder Diffraction and Rietveld Refinement School 2020	29th Mar 2020 - 2nd Apr 2020 (Durham, United Kingdom)
Microscope Operation Workshop at Pacific Northwest Center for CryoEM	6th Apr 2020 - 17th Apr 2020 (Portland, OR)
British Crystallographic Association Spring Meeting	6th Apr 2020 - 9th Apr 2020 (Leeds, United Kingdom)
Canadian Chemistry Conference & Exhibition	24th May 2020 - 28th May 2020 Winnipeg, Canada
17th European Powder Diffraction Conference (EPDIC17)	26th May 2020 - 30th May 2020 (Šibenik, Croatia)
ACA Summer Course in Chemical Crystallography	31st May 2020 - Jun 6 2020 (West Lafayette, IN)
Sixth European School (ECS6)	5th Jul 2020 - 11th Jul 2020 (Budapest, Hungary)
ACA 2020	31st Jul 2020 - 7th Aug 2020 (San Diego, CA)
Twenty-Fifth Congress and General Assembly of the International Union of Crystallography	22nd Aug 2020 - 30th Aug 2020 (Prague, Czech Republic)

Macromolecular Structure Group at UCSF Takes Delivery of a MiTeGen NANUQ™ Advanced Cryocooling Device

On January 22nd, 2020 the Macromolecular Structure Group (MSG) at the University of California, San Francisco (UCSF) took delivery of their order for a MiTeGen NANUQ™ advanced cryocooling device for biomolecular cryocrystallography. With NANUQ™ installed, users at MSG have access to advanced sample cryocooling for use with their research using crystallography.

"MSG focuses on the study of macromolecular structure, function, and interactions through the varied research tools of biochemistry and biophysics, including X-ray Crystallography and SAXS, Electron and Light Microscopy, NMR, Mass Spectrometry, and Molecular Biology. The facility is utilized by over one hundred graduate students and post-docs from thirty-one independent research groups representing seven departments at UCSF." Source is https://msg.ucsf.edu/

MiTeGens NANUQ™ Advanced Cryocooling Device for Biomolecular CryoCrystallography is designed to enable users to obtain great diffraction data from their crystals. It provides researchers with complete control during cryocooling and eliminates the damage-causing mechanisms commonly associated with slow cooling rates and hand plunging of crystals. NANUQ™ allows crystallographers to maximize data quality, maximize throughput, minimizes crystal-to-crystal variability, and minimizes risks of crystal frosting, damage and loss.

Learn More About NANUQs Installation at UCSFs Macromolecular Structure Group.

Lee Daniels joins CCDC's growing North America team

The CCDC, world-leading experts in structural chemistry data, software and knowledge for materials and life science research and application are pleased to welcome Dr Lee Daniels to their growing North America team.

CCDC compile and distribute the Cambridge Structural Database (CSD), a certified trusted database of fully curated and enhanced organic and metal-organic structures, used by researchers across the globe. Their cutting-edge software empowers scientists to extract invaluable insights from the vast dataset, informing and accelerating their research & development.

Juergen Harter, CEO of the CCDC said; "We're so pleased to welcome Lee to the team. His wealth of knowledge from 30 years in both academic and commercial crystallographic roles will be invaluable in supporting our research partners and users, and continuing our dedication to advance chemistry and crystallography for the public benefit around the world."

The CCDC will host its first user group meeting of the year in Cambridge, MA on April 24 – bringing together users from industry and academia to discuss the latest developments and future projects. The event is free for users. Register at www.ccdc.cam.ac.uk/events to secure a place.

CCDC advancing structural science

NeXtal joins a leading lineup of Structural Biology Companies as the newest member of the Calibre Scientifc Family.

NeXtal

See what's NeXt for NeXtal!

We are excited to share the news that Calibre Scientific has added another name to its expanded offering of structural biology solutions with the acquisition of NeXtal Biotechnologies and its full line of crystallization products. Over the past few years, our parent company Calibre Scientific, has been hard at work building a robust portfolio of structural biology companies to better serve the life sciences community. Anatrace, Microlytic and Molecular Dimensions, are just three of the members they've added to their growing family since 2013.

As a pioneer of protein crystallization screens and plates, NeXtal will no longer be a product line of Qiagen. NeXtal is a standalone company whose continued focus will be to simplify and accelerate the process of protein crystallization. Not only will NeXtal's long-proven crystallization screens and prized EasyXtal crystallization plates be available, NeXtal is committed to innovation with the development of new products and ideas to add to its crystallization legacy. To learn more about our new corporate sibling and fulfill all your future NeXtal needs, visit nextalbiotech.com.

Questions? NeXtal has your needs covered, reach out to us at customerservice@nextalbiotech.com

Florida State University/Rigaku Symposium and Workshop on X-Ray Crystallography and Diffraction

The first Rigaku Symposium and Workshop on X-ray Crystallography organized in collaboration with Prof. Michael Shatruk at Florida State University took place January 24-25. More than 70 students attended, including 25 students from neighboring institutions such as the University of Florida, the University of South Carolina and Mississippi State University.

The afternoon of the first day was devoted to plenary lectures from researchers invited by Prof. Michael Shatruk: **Prof. Angus Wilkinson**, Georgia Institute of Technology; **Prof. Corey Thompson**, Purdue University; **Prof. Weiwei Xie**, Louisiana State University; **Prof. Susan Latturner**, Florida State University. Two presentations were then given by Rigaku applications scientists: Dr. Akhilesh Tripathi (powder diffraction) and Dr. Pierre Le Magueres (single crystal diffraction).

On the second day, X-ray data collection and processing workshops were carried out, using the local Rigaku diffractometers at Florida State. Dr. Akhilesh Tripathi led the session on powder diffraction while Dr. Pierre Le Magueres did the same for single crystal diffraction.

Following a set of introductory sessions on the dual source Synergy-S, about 40 students gathered in a conference room for a live demonstration. Dr. Le Magueres remotely connected to the FSU diffractometer's control computer and showed all the steps of a single crystal crystallography analysis using CrysAlisPro: sample screening, pre_experiment, strategy calculation and data collection. The morning session ended with a run of manual data processing in CrysAlisPro. A similar workshop was run concurrently by Dr. Akhilesh Tripathi for general purpose X-ray diffraction on the SmartLab at FSU.

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