Nozomi Ando
2020 Margaret C. Etter Early Career Award
Contributions to ACA Reflexions may be sent to either of the Editors:

Edwin D. Stevens ............................................ edwin.stevens@wku.edu
Paul Swepston ............................................. paulswepston@me.com

Cover: Connie Rajnak
Historian: Virginia Pett
Photographer: Richard Bromund
Copy Editor: Sue Byram

Please address matters pertaining to advertisements, membership inquiries, or use of the ACA mailing list to:
Kristin Stevens, Director of Administrative Services
American Crystallographic Association
P. O. Box 96, Ellicott Station, Buffalo, NY 14205-0096. Membership in the ACA includes a non-deductible charge of $1.75 from membership dues to be applied to a subscription to ACA Reflexions. Periodicals postage paid at Buffalo, New York. POSTMASTER: Send address changes to ACA, P.O.Box 96, Ellicott Station, Buffalo, NY 14205-0096.
Structure Matters

President’s Column

Spring 2020

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 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.

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 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 Presidents’ 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 grateful 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

Vice-President’s Column

Spring 2020

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 ddrose@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 to ACA, I’d like to start with a big thank you to our previous Canadian Representative, Tomislav Frčić. 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, is that 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.cccw2020.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 Fodge 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 allosteric 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 technology had just been equipped with our newest 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 was there. He offered his lab to me, and I moved my lab to Cornell University. Sitting among boxes, we resumed research. The initial location on the beautiful Cornell campus. Sitting next to each diffraction spot told us that the halo scattering was actually something that the field was concerned about, and Peter Moore at Yale University had warned us about the possibility (Polikov & 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 the 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.

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-temperature 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

References

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.

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.

Nozomi Ando - Thinking Outside the Lattice

Diana Tomchick - Scattering Studies of Protein Structural Dynamics

Diana Tomchick
Dept. of Biophysics
Univ. of Texas SW Medical Center
Irving, TX 75061
diana.tomchick@utsouthwestern.edu

Ilia A. Guzei
University of Wisconsin-Madison
2124 Chemistry Depart.
1101 University Avenue
Madison, WI 53706
iguzei@chem.wisc.edu

Gerald F. Audette
Dept of Chemistry
York University
4700 Keele Street
Toronto, ON
Canada M3J 1P3
audette@yorku.ca

Canadian Representative

Ilia A. Guzei
University of Wisconsin-Madison
2124 Chemistry Depart.
1101 University Avenue
Madison, WI 53706
iguzei@chem.wisc.edu

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.
We are accepting nominations for Vice President, Secretary and members to the following committees: Communications, Education, Data Standards & Computing, and Meeting Reorganization / Enhancement. Anyone with suggestions can contact Lisa Keefe keefe@imca-cat.org, Amy Sarjeant Amy.Sarjeant@bms.com, or Bryan Chakoumakos chakoumakobc@ornl.gov.
The extreme hardness of diamonds has allowed crystallographers to study materials at pressures greater than the core of the Earth. Now, the extreme heat conductivity of diamond gives crystallography a new X-ray source without equal: the IμS DIAMOND source. Diamond conducts heat five times more efficiently than any other known material, making it perfect to cool the intense heat loads in a modern microfocus source. This results in a source better than any microfocus rotating anode: higher intensity, stability and reliability, lower power consumption, and no regular maintenance costs.

Contact us for a personal system demonstration.

www.bruker.com/imsd
Argonne to host PDF and Rietveld Course

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 nanoparticles on a wide range of experiments 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.

VERSATILE, POWERFUL, CUTTING EDGE

• One source, two wavelengths
• Much more flux than any microfocus sealed tube
• Curved detector for 150° two-theta coverage per frame
• Hybrid photon counting detector with massive dynamic range
• Best-in-class data quality

The XtaLAB Synergy-DW is a unique, versatile instrument giving you the ability to research a wide range of samples with just one very-high-flux instrument. Whether you are studying biological or chemical systems, weak or strong diffraction or something else, the XtaLAB Synergy-DW with the HyPix-Arc 150° is the cutting-edge solution you need.
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.

Virginia Pelt
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 even-ually 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 with a Grade school mentor who would supervise my research efforts. After about a year Norm was presenting these results in the presence of Verner, who was trained a physicist. He and I calculated atomic distances were estimated in electron diffraction of gases. The work originated around 1930 when very few inter-atomic distances were known. Verner sent me to one of his postdoctoral al 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 UF₆ was apparently unsymmetric, as this seemed to defy the Born-Oppenheimer approx-imation. 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 symme-try of UF₆, but perhaps it was settled in a meeting we had with Prof. Richard Feynman of the Physics Department.

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 fac-tor). 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 cur-rent use! I continued to attend ACA meetings until they got gobbled up by the macromolecular types. I found specialized meetings more useful, an example being Journées des Actinides, a small Euro-pean meeting that brings together chemists and physicists who are inter-ested in the actinides. It is amazing how little chemistry most theoreti-cal physicists know!

The undergraduate cur-riculum 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 Bueger 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 an-hydrus 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 re-cords of Mozart piano sonatas as played by Wan-da Landeska.

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 arrange-ment 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 “Mar-shed”.

For my graduate studies I applied to and was ac-cepted 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 discour-aged. For personal reasons I chose Caltech.

In 1951 I received my B.Sc. from Caltech and mar-rried 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. 

Verner Schomaker Photograph by John A. Moore, University of Wash-ington, courtesy of AIP Emilio Segre Visual Archives

J. Holmes Sturdivant Photograph courtesy of the Archives, California Institute of Technology

Dick Marsh & Linus Pauling

ACA Living History Project - Jim Ibers

ACA Structure Matters

American Crystallographic Association
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 Freeman family, Hans married 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 function, 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 and at the electron density function. 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 to be 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 audience asked me to define a unique unit cell. This helped prevent confusion in the practice of 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 Riecke 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 Crystal Structures 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 hung in all of our residences. “Day and Night” remains my favorite and is currently hung in my bedroom.

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 XeF4 from Xe, F2, and sunlight.] Earlier Pauling suggested to Caltech’s inorganic chemist, Don Yost, that Xe should form stable compounds but Yost disliked Linux and ignored his suggestion. The sample of XeF4 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 F0, weights were difficult to assign for small F0, and there was no attention given to F0 < 0. Verner had taught us that one never changes the data but only the model. F2 is far closer to the data than F0, and fortunately the ORFALS least-squares program available from Bill Busing and Henry Levy of Oak Ridge National Laboratory allowed one to refine on F2. Thus I put together a suite of programs and the necessary instructions for ORFALS, ORTEP, Carroll Johnson’s thermal plotting program, and FORDAP, the Fourier program Al Zaikin 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.]

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 XeF4 from Xe, F2, and sunlight]. Earlier Pauling suggested to Caltech’s inorganic chemist, Don Yost, that Xe should form stable compounds but Yost disliked Linux and ignored his suggestion. The sample of XeF4 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 F0, weights were difficult to assign for small F0, and there was no attention given to F0 < 0. Verner had taught us that one never changes the data but only the model. F2 is far closer to the data than F0, and fortunately the ORFALS least-squares program available from Bill Busing and Henry Levy of Oak Ridge National Laboratory allowed one to refine on F2. Thus I put together a suite of programs and the necessary instructions for ORFALS, ORTEP, Carroll Johnson’s thermal plotting program, and FORDAP, the Fourier program Al Zaikin 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 Riecke 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 Crystal Structures 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 hung in all of our residences. “Day and Night” remains my favorite and is currently hung in my bedroom.

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.] Meanwhile The Long Island Railroad 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.

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.

At Northwestern I was very happy. I was on the editorial board of Structure, and 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.] Meanwhile The Long Island Railroad 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 program.

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 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 O₂, molecular N₂, NO, SO₂, CS₂, and aryldiazoo compounds, among others.

The research on iron-sulfur chemistry led my group to the very rich chemistry of soluble metal chalcogenides containing modulated selenide chains and ambiguous-valent metal, which was published recently in Angew. Chemie.

Jim Ibers speaking at the Florence IUCr meeting in 2005

grams 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.

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 O₂, molecular N₂, NO, SO₂, CS₂, and aryldiazoo 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 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 O₂, molecular N₂, NO, SO₂, CS₂, and aryldiazoo compounds, among others.

The research on iron-sulfur chemistry led my group to the very rich chemistry of soluble metal chalcogenides containing modulated selenide chains and ambiguous-valent metal, which was published recently in Angew. Chemie.

Jim Ibers speaking at the Florence IUCr meeting in 2005

The research on iron-sulfur chemistry led my group to the very rich chemistry of soluble metal chalcogenides containing modulated selenide chains and ambiguous-valent metal, which was published recently in Angew. Chemie.
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—and 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 article 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

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 voices and writing styles that hit the news in Fall 2016—only a few months before she gave her original lectures. They chose rather to pay respect to as many female scientists 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 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 Crys-
Bill Duax Testimonial

Spring 2020


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 (former Medical Foundation), Buffalo, 1968-1969. Head crystallography department Medical Foundation Buffalo, 1969-1970, head molecular biophysics 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 on 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 has carried out his message of crystallography to Venezuela, Chile, Equador, Brazil, Bolivia, Urugay, 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. I 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 Reviews in 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.
I was first introduced to Bill more than 40 years ago, almost longer than I can remember. Most of all, he has been a great personal friend for me, an exceptional scientist, colleague and gentleman. He has 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 a 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
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 multinational 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 1 to V as the annual dues increase.

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.

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.

The USNC/Cr serves crystallographers residing in the US, regardless of country of origin or immigration status. As chair of the USNC/Cr, I was asked 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 multinational 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 1 to V as the annual dues increase.

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.

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.

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.
SUSAN BYRAM (2021)  
Bruker AXS  
5465 E. Cheryl Parkway  
Madison, WI 53711  
Phone: 608-276-3041; Fax: 608-276-3006  
E-mail: susan.byram@bruker.com

AINA COHEN (2020)  
Stanford Synchrotron Radiation Lightsource - Structural Molecular Biology  
SLAC National Accelerator Laboratory  
2575 Sand Hill Road, MS 99  
Menlo Park, CA 94025  
Phone: 650-926-3125  
E-mail: acohen@slac.stanford.edu

WAYNE HENDRICKSON (2022)  
Columbia University  
Department of Biochemistry and Molecular Biophysics  
630 West 168th St.  
New York, NY 10032  
Phone: 212-305-3456  
E-mail: wayne@utl.cumc.columbia.edu

ASHFIA HUQ (2022)  
Industrial Crystallographer  
Phone: 630-986-7321  
E-mail: ashfia.huq@gmail.com

MANISH MEHTA (2021)  
Oberlin College  
Chemistry and Biochemistry  
Science Center N276  
Oberlin, OH 44074  
Phone: 440-775-8359  
E-mail: MANISH.MEHTA@oberlin.edu

MITCH MILLER (2022)  
Rice University  
Department of Biosciences  
6500 Main St.  
Houston TX 77030  
Phone: 713-348-3913  
E-mail: mitchmi@rice.edu

JOSEPH TANSKI (2021)  
Vassar College  
Department of Chemistry  
124 Raymond Avenue, Box 601  
Poughkeepsie, NY 12604  
Phone: 845-437-5731  
E-mail: jotanski@vassar.edu

EX OFFICIO VOTING MEMBERS

President, ACA  
BRIAN H. TOBY (2020)  
Argonne National Laboratory  
Advanced Photon Source  
9700 S. Cass Ave, Bldg. 401/84192  
Argonne, IL 60439  
Phone: 630-252-6488; Fax: 630-252-3222  
E-mail: brian.toby@anl.gov

Treasurer, ACA  
ILJA GUZEI (2019)  
University of Wisconsin-Madison  
2124 Chemistry Department, 1101  
University Ave., Madison, WI 53706  
Phone: 608-263-4694  
E-mail: iguzei@chem.wisc.edu

IUCr Past President  
MARVIN HACKERT (2020)  
Associate Dean of Graduate Studies  
University of Texas at Austin  
110 Inner Campus Dr., G0400, Main 101  
Austin, TX 78712  
Phone: 512-232-3604; Fax: 512-471-6135  
E-mail: m.hackert@austin.utexas.edu

EX OFFICIO NON-VOTING MEMBERS

JEFF LENGYEL  
Cambridge Crystallographic Data Centre  
1411 Grandview Ave., Apt 304  
Pittsburgh, PA 15211  
Phone: 740-361-2658  
E-mail: lengeyi@cdsft.ccm.ac.uk

MARK RODRIGUEZ  
(ICDD Representative)  
Sandia National Laboratories  
P.O. Box 5800, MS 1411  
Albuquerque, NM 87185-1411  
Phone: (505) 844-3683  
Fax: (505) 844-9781  
E-mail: marodri@sandia.gov

JIM CISTON  
(MSA Representative)  
The Molecular Foundry, National Center for Electron Microscopy Facility  
Lawrence Berkeley National Laboratory  
One Cyclotron Road, MS 72-150  
Berkeley, CA 94720  
Phone: 510.495.8072  
E-mail: jciston@lbl.gov

KRISTIN BENNETT  
KB Science, LLC  
Charles Street Station, PO Box 140343  
Boston, MA 02114  
Phone: 202-841-1621  
E-mail: KBennett@KBSCIENCE.com

BCST Co-Chair:  
SCOTT COLLICK  
DuPont

BCST Co-Chair:  
JENNIFER SINCLAIR CURTIS  
University of California, Davis

STAFF

ANA FERRERAS  
Senior Program Officer  
Phone: (202) 334-1697  
E-mail: aferreras@nas.edu

The National Academies of Sciences, Engineering,  
and Medicine Board on International Scientific  
Organizations  
500 Fifth Street, NW, Keck 546  
Washington, D.C. 20001  
Tel: (202) 334-2807; Fax: (202) 334-2231

ACCA ADVISORY BOARD
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 numbers 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.
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

BLASELIA JREATSAN MOCCTHIK AMBERN YOMONE PLEESHT YDUJ

Rearrange the letters in the following

DI SORDE RED

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

TIVYRAG INEPTOR VECCTON CHOSKEN GRUBOPUS

Answer:

Female crystallographers use the letter X for their

Answer:

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 – ffronzc@lsu.edu
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, minimize crystal-to-crystal variability, and minimizes risks of crystal frosting, damage and loss.

Learn More About NANUQs Installation at UCSFs Macromolecular Structure Group.
NeXtal joins a leading lineup of Structural Biology Companies as the newest member of the Calibre Scientific Family.

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 Lattner, 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.