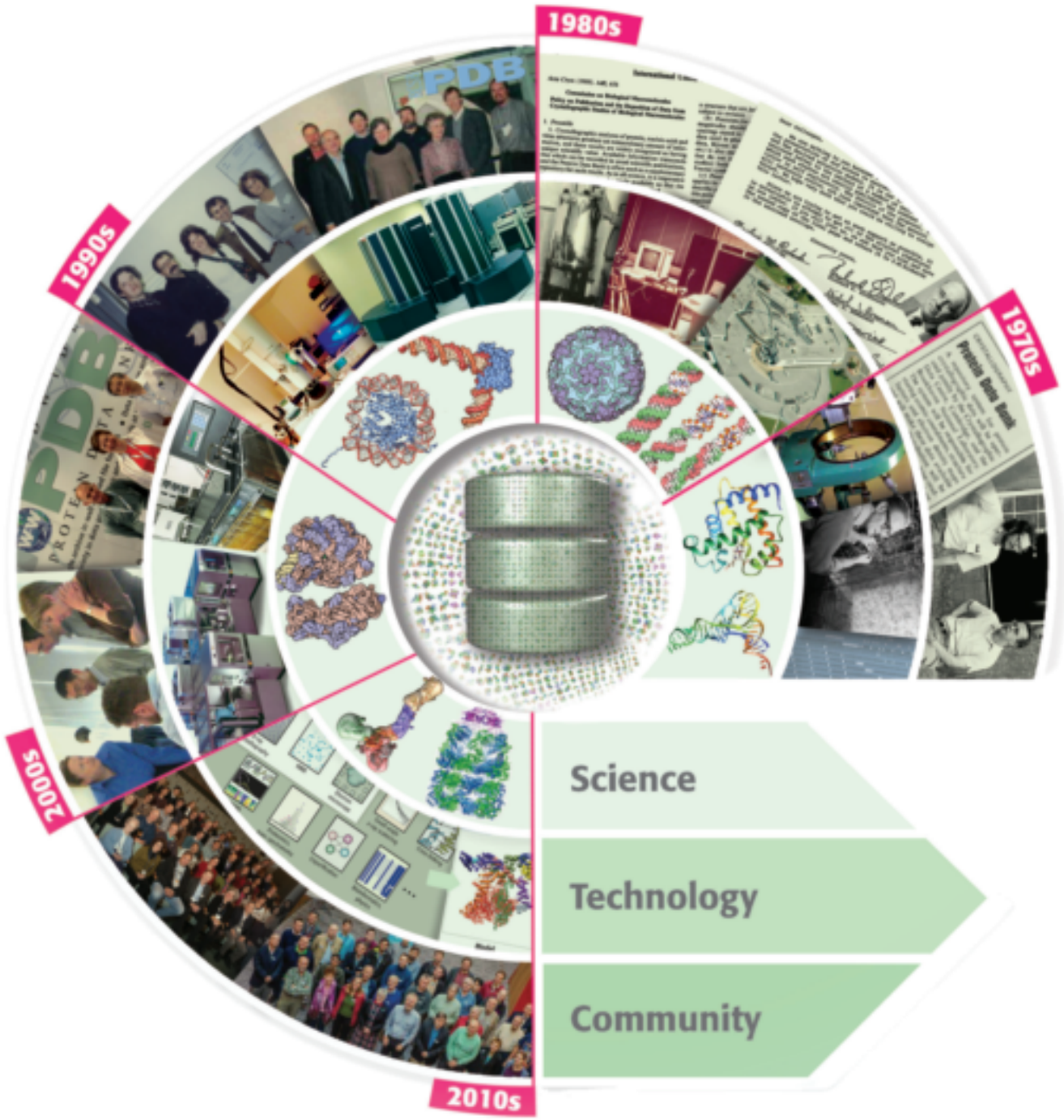
ACA RefleXions

American Crystallographic Association Structure Matters

Number 4

Winter 2017



Annual ACA Meeting in New Orleans Revisited

ACA RefleXions

ACA - Structure Matters

www.AmerCrystalAssn.org

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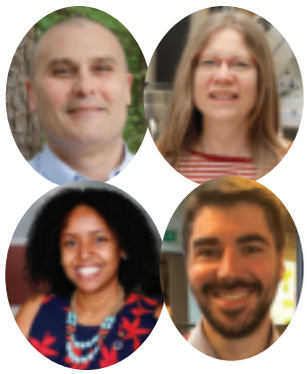

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Deadlines for contributions to *ACA RefleXions* are: February 1 (Spring), May 1 (Summer), August 1 (Fall), and November 1 (Winter)

ACA RefleXions (ISSN 1058-9945) Number 4, 2017. Published four times per year in the spring, summer, fall, and winter for the membership of the American Crystallographic Association, P.O. Box 96, Ellicott Station, Buffalo, NY 14205-0096. Membership in the ACA includes a non-deductible charge of $1.75 from membership dues to be applied to a subscription to *ACA RefleXions*. Periodicals postage paid at Buffalo, New York. POSTMASTER: Send address changes to ACA, P.O.Box 96, Ellicott Station, Buffalo, NY 14205-0096.

Dear Colleagues,

This morning there was frost on the lawn and I could see my breath in the air. I can't believe that Winter is here already. It doesn't seem possible that the year is coming to a close and I am writing my final President's column for ACA *RefleXions*. This quarterly exercise has truly helped to put the year into perspective and when I look back at my ramblings in the first issue of 2017, I'm reminded of how far we've come as a society. When I sat down to type out that first missive, we hadn't yet hired Kristin Stevens and we had many unanswered questions about the shape of the ACA in the post-Marcia era. We've worked hard this year in trying to answer these questions, and having recently returned from the final Council meeting of the year, I can say we are well on our way to a stronger ACA.

That's not to say that all the work is done. Not by a long shot. We still have a website redesign to implement, improvements to our membership database to make, and meetings to reorganize for attractiveness and sustainability. Over the past few months, we've been assessing a variety of options for both the website and the membership database and hope to have some new changes rolling out in the new year. The meeting reorganization team has been working on some pretty exciting changes for the future, too. Suffice it to say that we've continued to pour our time, effort and brain cells into finding ways to make the ACA the best organization for its members.

We've continue working to make *Structural Dynamics* the place to publish our members' research. The special topic issue based on the 2016 *Transactions Symposium* at the Denver ACA meeting was published in May and the special issue, *Ultrafast Structural Dynamics – A Tribute to Ahmed H. Zewail*,was published this past July. The last special topic issue of the year, *Swiss National Center of Competence in Research: Molecular Ultrafast Science and Technology* will be published in the November/December issue. Submissions have increased 28% since 2016 and 85% since the journal was launched in 2014. The editorial board continues to encourage submission of static-dynamic studies for inclusion in the journal. To stay up-to-date with the latest news on *Structural Dynamics* sign up for email alerts on the website at ***aca.scitation.org/journal/sdy***.

Over the latter half of the summer and into the fall, we compiled statistics on our membership and attendance at the 2017 meeting. These can be found on the ACA website under the 2017 meeting page. You'll see that we're doing well for a scientific society, but we still have a long way to go before we reach true gender equality and diversity in our membership. To help us keep better track of the demographics of the ACA, we're adding a few extra questions to the membership renewal and the meeting registration processes. I hope that you'll take the time to answer these questions so we can ensure the ACA is honoring the values expressed in our diversity statement.

Finally, I want to take a moment to thank all the people that took the time to talk or email with me this year. I heard many viewpoints from across the membership which helped me understand what makes people love the ACA, what about the society people find frustrating, and what we can continue to improve for the future. I've had many lively conversations and debates and I want everyone to know that I've appreciated your candor and I attempted to act on as much as I could over this short year. Additionally, it has been a pleasure working with the other members of Council this year. I will be sad to see Past-President Tom Terwilliger rotate off Council and I know Lisa Keefe will do a wonderful job as President in 2018. And of course, it is with bittersweet emotion that we say farewell to Marcia who has been a guiding light for Council and for all the ACA for nearly 30 years. We wish her all the best in her retirement!

Indeed, it has been a challenging and enjoyable year for me as ACA President. I thank you all for giving me the opportunity to serve in this capacity and I wish you all the best of luck in your future endeavors.

Amy Sarjeant

IUCr Meeting and GA 2017 in Hyderabad

The 24th Congress and General Assembly of the International Union of Crystallography was held at the Hyderabad International Convention Centre August 21-28, 2017 and attracted approximately 1,700 attendees from over 70 countries. India had the largest number of participants at 514, followed by the USA with 300. Canada had 26. While the venue was somewhat remote and shuttle service from the conference hotels ran considerably less frequently than one may have expected, the Convention Centre layout certainly served very well for the Congress and General Assembly (GA). The main exhibit hall was large enough to accommodate vendors, posters and lunch, resulting in excellent networking opportunities and booth traffic. The only problem was that the participation in and attendance at education-related sessions was severely underestimated, so that many of those sessions offered standing room only for anyone arriving within a few minutes of the sessions' start time!

Overall, the program presented a great variety of topics, ranging from solid-state chemistry and physics, small molecule crystallography and macromolecular crystallography, to specialized methods like PDF and cryo-EM, to educational sessions and to new developments in instrumentation and analysis methods.

On three evenings, delegates from 47 countries convened to conduct IUCr business. Albania & Kosovo, Tunisia, Singapore and Bangladesh each became Category I members of the IUCr, while the Regional Committee of Crystallographers from Latvia, Tunisia and Ukraine withdrew its membership. The US

delegation consisted of 5 members: Joe Ng (USNCCr Chair), Cora Lind-Kovacs (USNCCr Vice Chair), Amy Sarjeant (ACA President, ex officio USNCCr member), Sue Byram (ACA Treasure, ex officio USNCCr member), and Branton Campbell (USNCCr member). Ilia Guzei (USNCCr member) served as the alternate. The Canadian delegation, was chaired by Louise Dawe (CNCC member), and included Pawel Grochulski (CLS), Tomislav Friščić (CNCC member), and Patrick Mercier (alternate and CNCC Chair).

Bid by USNCCr for IUCr in San Diego in 2023 – it's the WEATHER! Branton Campbell, Ana Ferreras, Amy Sarjeant, Cora Lind-Kovacs, Joe Ng, Sue Byram, Ilia Guzei

During the general assembly, the financial health of the IUCr was discussed as a continuing concern, especially as the revenue from journals has decreased and expenses for special programs have increased. The IUCr has implemented an Associates program *(www.iucr.org/people/associates)* that allows individual crystallographers to become IUCr Associates. The fees are to support continuation of many programs that started during IYCr2014. In return, Associates get access to networking and educational opportunities, discounts to IUCr open access fees, six free articles on Crystallography Journals Online, discounts on the purchase of print copies of the International Tables, and on books from several other publishers.

ACA booth with US National Committee: Ana Ferreras, Bill Duax, Sue Byram, Hanna Dabkowska, Joe Ng,Tom Terwilliger

Happy winners of San Diego trivia contest: Cora Lind-Kovacs, Vijaya Kanthit, Bernadette Fruehann, Karsten Dierks, R. Wiesinger

Other topics discussed included the establishment of the Bragg Award for early career crystallographers. A lively debate about what defines an "early career crystallographer" ensued at the GA, and a subcommittee will work to come up with guidelines to answer this question. The GA also voted in support of the IUCr Executive Committee (EC) adopting a diversity policy to encourage participation by traditionally underrepresented groups.

The GA concluded with votes for new members to the EC and for the location of the 2023 Congress. We are happy to report that Hanna Dabkowska (Canada) has been elected as IUCr Vice President and Graciela Diaz de Delgado (Venezuela) has been elected to the EC as a regular member. Sven Lidin (Sweden) was elected as IUCr President and Luc van Meervelt (Belgium) will serve as Secretary/Treasurer. In addition to Graciela, Jenny Martin (Australia) and Masaki Takata (Japan) were elected to join Wulf Depmeier (Germany), Santiago Garcia-Granda (Spain), and Radomír Kuzel (Czech Republic) on the EC. Marv Hackert (US) will remain on the EC for the coming triennium as Past President.

A major task for the US delegation was the presentation of a bid to host the 26th IUCr Congress and GA in San Diego in 2023. The ACA and USNCCr shared a booth to promote both the ACA and the IUCr bid. Several fliers and table-top signs, prepared by ACA HQ staff and Chief Financial Officer, Narasinga Rao , helped advertise the 2018 Annual Meeting in Toronto, and we were even able to sign up a few new members to the ACA! A special thank you goes to Bill Duax for providing crystallography-engraved glasses that were raffled off among all participants of "San Diego Trivia". The US bid presentation at the GA was certainly one-of-a-kind, as the delegates walked in to "Surfing USA" with inflatable surfboards and beach balls. Unfortunately, visa policies were a major concern for many delegates, and the bid was won by Melbourne, Australia.

Overall, members of the ACA were well represented at the IUCr with many chairing sessions or giving invited talks. We were pleased to be part of the international community of crystallographers and are looking forward to Prague in 2020!

Cora Lind-Kovacs, Sue Byram, Louise Dawe and Amy Sarjeant.

New ACA SIG for CryoEM

It gives me great pleasure to announce that ACA now has a new Special Interest Group for Cryo-electron microscopy (CryoEM). The formation of this new SIG reflects the rapidly growing interest in use of CryoEM methods within the structural biology community, and perfectly coincides with the recent Nobel Prize in Chemistry awarded to CryoEM pioneers Jacque Dubochet, Joachim Frank, and Richard Henderson.

The petition to form the SIG was circulated at the May 2017 ACA meeting in New Orleans and was signed by more than 30 members, with interest subsequently confirmed by email. In September, at Diana Tomchick's request, I submitted the petition materials for consideration by Council, and I also agreed to become the 2018 Chair. As a long-time ACA member who has also been extensively involved over the past decade in developing and maintaining data archives for structures determined by CryoEM (***emdatabank.org***), I am honored to serve in this role. In addition, Rui Zhao has agreed to serve as Chair Elect, and Dominika Borek is serving as Secretary.

Thanks to forward-thinking sponsorships by the Biological Macromolecules and Light Source SIGs, we can already look forward to lots of excellent discussion about CryoEM at the 2018 ACA meeting in Toronto. On July 22 there will be a full day of presentations from CryoEM scientists with morning and afternoon scientific sessions chaired by Wah Chiu (Stanford U) and Lori Passmore (MRC-LMB).

Wah Chiu, Lori Passmore, and John Rubinstein (U Toronto) are also co-organizing a full day pre-meeting workshop on July 20 entitled *CryoEM – A guide to high-resolution structure determination*. The aim of the workshop is to provide a detailed overview of specimen preparation, image processing and building/refinement of atomic models, with focus on high-resolution single particle cryo-EM. Aspects of image processing and modelling will be hands-on with state-the-art programs used by workshop students to process sample datasets.

In short, if you are interested in learning more about and/or using cryoEM for your own research interests, please join our new SIG and plan to come to this year's ACA meeting! There, please also join your new officers at our first official CryoEM SIG meeting to discuss priorities and content for scientific sessions at future meetings.

In recent years, many of the popular CryoEM-based conferences and workshops (e.g., the 3DEM Gordon Research Conference) have become tremendously oversubscribed. Adding CryoEM-based topics to ACA's meeting sessions and activities is a terrific way to expand the conversation and support our members with interest in incorporating this exciting, rapidly developing methodology into their research programs.

Cathy Lawson

New ACA SIG for Best Practices for Data Analysis and Archiving

We are pleased to announce the formation of a new scientific interest group focused on data best practices, with Nick Sauter (Lawrence Berkeley National Laboratory, Berkeley, CA) acting as SIG Chair, John Rose (University of Georgia, Athens, GA) as Vice-Chair, and Suzanna Ward (CCDC) as Secretary-Treasurer.

Data, along with its generation, transmission, immediate storage, analysis, documentation, reproducibility, and long-term curation, has been identified as a key topic of interest by methods developers and scientific end users alike. Issues arising from the collection of terabyte datasets are no longer confined to specialized light sources like free-electron lasers. Rather, modern synchrotron diffraction beamlines are now being equipped for serial crystallography, complete with high-throughput sample delivery and high-frame rate pixel array detectors. Practical and philosophical questions abound. Where should the data be stored, at the light source, or the home lab? Is data compression acceptable, even if it is lousy, and can blank or poor images be thrown away? What are the best algorithms for treating high-multiplicity data from thousands of crystals? The repertoire of inquiry has expanded to include time domain structural work. How should supporting data streams be treated, which might report experimental conditions such as laser excitation, chemical mixing, or temperature jump, along with reaction progress measured spectroscopically? As instrumentation and analysis improve, will it eventually prove useful to model the entire diffraction pattern including the non-Bragg diffuse signal for clues to structural dynamics?

Within the ACA, the long-established Data Standards & Computing Committee has historically provided counsel on subjects related to public access, such as how to craft requirements for data deposition prior to the publication of a crystallographic structure, and how to ensure reasonable access to source code. However, during the 2017 Committee deliberations, it was noted that important subjects related to scientific reproducibility, which are naturally of present concern to the ACA, were already under intense discussion within the larger crystallographic community. For example, the World Wide Protein Data Bank, with its PDBx/mmCIF working group, is currently developing standards for the archival of unmerged Bragg reflection intensities, which will permit, among other aims, the validation of the entire data processing pipeline from integrated intensities to structure. Similarly, the IUCr's Diffraction Data Deposition Working Group has been actively considering best practices for organizing raw diffraction images for long-term retrieval, and at least three web services are offering to accept raw data for deposition. One associated challenge, that must eventually be addressed, is that if the purpose is to support the claims made in published results, the archive must include not only the raw images, but also the workflows, scripts, and code that made the analysis possible.

Considering the breadth of these issues, the Committee asked how the work of the ACA could become more relevant and inclusive, without being redundant with international efforts. The immediate result was our petition to form a new scientific

interest group, so as to draw in the participation of all interested individuals within the ACA. Our focus on data best practices is a notable departure from the central organizing principles of many of the other ACA interest groups, which have coalesced around experimental methods (Light Sources, Neutron Scattering, CryoEM), types of sample (Biological Macromolecules, Fiber Diffraction, Materials, Small Molecules), or particular scientific demographics (Industrial, Service Crystallography, Young Scientists). It is our hope that data, and its association with evolving computational methods, will attract the interest of many ACA members across the entire spectrum of disciplines. We also see a strong educational component to our work. It is right for scientists to question the computation, and to the extent that we can train crystallographers to seek a deeper understanding, and help provide the tools to do so, the new special interest group will have succeeded.

Our immediate plan is to have our first business meeting at ACA 2018 in Toronto, as well as our first scientific session.

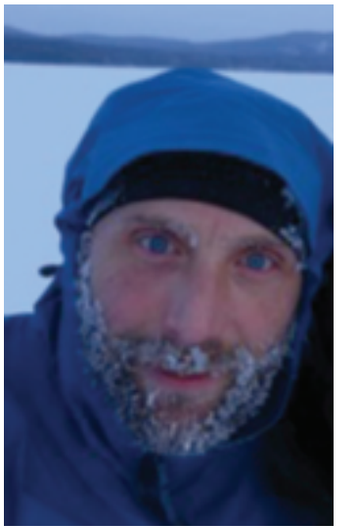
Nick Sauter & John Rose

What's on the Cover

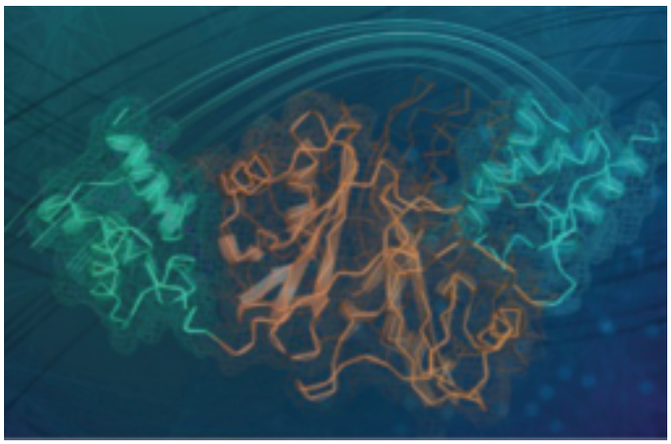
Helen M. Berman (Board of Governors Distinguished Professor Emerita of Chemistry and Chemical Biology at Rutgers, The State University of New Jersey) is the first winner of the ACA's new Dave Rognlie Award. Helen has been a champion of open access data repositories for science. She helped established the Protein Data Bank in 1971 and from 1998-2014, she was the Director of the Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB). The cover picture depicts the synergies of science, technology and community in the evolution of the Protein Data Bank from a small archive of biological structures created and used primarily by crystallographers, to a worldwide data resource used by a diverse community of scientists. The center of the circle is a symbolic picture of the PDB archive. For each decade starting in the 1970's, the figure depicts the types of structures deposited in the PDB (second ring), the kinds of technologies that were used to determine those structures (third ring), and the community driven activities that occurred that enabled the PDB become more useful and accessible (fourth ring).

This is the final postcard from Canada for 2017 and, whilst recovering from insanely cold weather in this part of North America, I am also taking great joy in highlighting an extremely successful young investigator of macromolecular structure and function, ***T. Martin Schmeing*** (McGill University, Montreal, Quebec).

Martin is a Tier II Canada Research Chair in Structural Biology of Macromolecular Machines, and he really loves big molecular machines that make peptides. Having performed his PhD and postdoctoral research on ribosomes with Tom Steitz and Venki Ramakrishnan, co-winners of the 2009 Nobel Prize in Chemistry, Martin's group is pursuing a new research area at McGill University, working on a megaenzyme that makes peptide bonds. These nonribosomal peptide synthetases (NRPSs) are huge microbial enzymes that synthesize their products (*i.e.* NRPs) through amide bond formation between building block monomers. The chemical and biological properties of NRPs make them useful to society as therapeutics (for example, antibiotics, antivirals, anti-tumours, and immunosuppressants) and as natural, "green" chemicals. The impact of NRPSs on human health is remarkable: penicillin has saved millions of lives worldwide; cyclosporin made organ transplantation viable and widespread; cephalosporin is used to fight methicillin-resistant *S. aureus* infections; and daptomycin is a billion-dollar drug, successful against hospital-acquired gram-positive infections. Martin's research is focusing on multiple aspects of the structures and functions of NRPSs, specifically the catalytic event which links substrate amino acids into peptides, and the manner in which these enzymes' domains and modules work together to form a complicated but productive catalytic cycle. Whereas the mechanism through which the precursors building blocks are linked together into the backbone of the NRP product was previously unknown, Martin has developed a novel chemical biology approach to capture complexes of substrate analogs bound to the condensation domain (check out *Cell Chem. Biol.* **2016**, *23*, 331, also highlighted on the journal homepage!). These reaction–competent substrate analogs become covalently tethered near the active site, to mimic covalent substrate delivery by carrier domains. This has enabled determination of co-complexes of the condensation domain for the first time, clarifying a likely role of the catalytic histidine in positioning the substrates for catalysis by nucleophilic attack. Martin has also made a number of other accomplishments in this challenging scientific arena, most notably he characterized important conformational changes in the condensation domain and suggested substrate tunneling through the megaenzymes (*J. Mol. Biol.* **2013**, *425*, 3137), determined the structure of an alternative NRPS domain that can perform both peptide bond formation and peptide heterocyclization to form thiazoline or oxazoline rings, leading to biologically active heterocycle-containing peptides found in therapeutics and diverse natural products. Most recently, Martin's group succeeded in describing the likely catalytic mechanism for such cyclodehydration (*Proc. Natl. Acad. Sci. U.S.A.* **2017**, *114*, 95.)



In a landmark study published in *Nature* (see *Nature* **2016**, *529*, 239), Martin's group recently solved four independent structures of the initiation module of the NRPS that synthesizes the antibiotic gramicidin. This provided fantastic insight into the initial stages of gramicidin synthesis, revealing staggering movements required for synthesis, with both the peptidyl carrier protein domain translocating 61 Å and rotating 75° and the adenylation subdomain rotating 180° in just one of such transitions to transport substrate between two distal active sites. This work provided the so far most complete view of this important type of macromolecular machines, leading to numerous highlights in scientific and general press, such as *AAAS Eurekalert*, *Chemical & Engineering News*, *STAT* and *Newswise*, including the amusing article on "How Getting Proteins to Dance the 'YMCA' Could Yield New Antibiotics". Martin's fantastic and productive career has been decorated by a number of honors and awards. Among his publications, 6 have been published in *Science* or *Nature* and, among other prizes, he is the 2017 recipient of the *New Investigator Award* by the *Canadian Society for Molecular Biosciences*, the recipient of the *2016 Joe Doupe Young Investigator Award by the Canadian Society for Clinical Investigation*, was recently put in a difficult situation by being simultaneously nominated for the *CIHR New Investigator Award* and *Canada Research Chair* position!



An artistic rendering of the 75° swing and a 61 Å movement of the peptidyl carrier protein (PCP) that are a part of the catalytic activity of gramicidin-producing nonribosomal peptide synthetase (NRPS), part of Martin Schmeing's work published in Nature 2016, 529, 239.

Martin's lab continues to rapidly build momentum in NRPS study. He cunningly spent the academic year on sabbatical at UCSD, skipping the arctic weather bomb and brushing up on his cryo-EM (an important part of the upcoming 2018 ACA meeting in Toronto!). This will certainly enable his lab to take an even more multi-technique approach to studying NRPSs. Martin and his lab are keen to keep the insight rolling, so look for more interesting NRPS structures form the group in the near future!

You can always keep up with the most recent work from the Schmeing group at: ***www.med.mcgill.ca/biochem/schmeinglab/Schmeing_Lab_website/Home.htm***

The extremely successful Schmeing group, hard at work.

In other news from Canada I hear that, as a result of continuous addition of new beamlines, the **Canadian Light Source** (CLS) has decided to temporarily turn down the ring current to 220 mA. Overall, this is expected to reduce the flux/brightness at the experimental hutches by around 12%. However, we should not despair as the first steps towards operation in top-up mode should be made as early as May 2018 (maybe just in time for the annual ACA congress?)!

I am very saddened to share the news of passing of ***Ronald George Cavell*** (University of Alberta) this November. He was one of the founding members of the ***Canadian Institute for Synchrotron Radiation,*** the organization that developed the CLS from concept to construction. He was the president of the Institute from 1999 to 2006 and for his vision, leadership and commitment to CLS he was awarded the ***Saskatchewan Distinguished Service Award*** by Premier Brad Wall in 2009. He has left a lasting mark on the chemistry of phosphorus compounds, transition metals and carbenes, and was the inaugural recipient of the ***Alcan Lecture Award by the Chemical Institute of Canada*** in 1979.

2018 will be extremely busy for Canadians, with the next ACA Annual Meeting just around the corner - do not forget to send your abstract for the meeting before the deadline in March! The preparations for the meeting are in a highly advanced stage, guided by ***Gerald Audette*** and ***Tiffany Kinnibrugh*** as Program Chairs, and ***Louise Dawe*** and ***David Rose*** as Poster Chairs. The meeting will open with a Keynote Lecture by ***John Polanyi***, the 1986 Nobel Laureate in Chemistry and the online program announces ***Frank Hawthorne*** **(University of Manitoba)** as the recipient of the Buerger Award, ***Simon Billinge*** **(Columbia University)** as the winner of the Warren Award, while the Etter Early Career Award goes to ***Jason McLellan*** **(Geisel School of Medicine, Dartmouth College)**. Brief biographies of these three outstanding researchers can be found on the meeting webpage, at: ***www.amercrystalassn.org/2018-awards***

I will update you as soon as possible on the details of all other meetings planned in Canada for 2018, which include the *27th Buffalo-Hamilton-Toronto (BLT) Crystallography Symposium*, the *5th Crystal Engineering and Emerging Materials Workshop of Ontario and Quebec* (CEMWOQ-5, to be held in Montreal), the 9th *Canadian Chemical Crystallography Workshop* (CCCW-9, I hear that this meeting will be held at the University of Alberta in Edmonton). Louise Dawe, who is now a member of the IUCr Calendar Committee has very kindly informed me about the upcoming 19th Sagamore 2018 Conference on Quantum Crystallography, to be held 8-13 July 2018 in Halifax, Nova Scotia, with Conference Chairs Chérif Matta (Mount Saint Vincent University) and Paul Ayers (McMaster University). More information on this meeting can be found on the webpage: ***www.sagamore2018.ca/***

Finally, for more information on the activities of Canadian National Committee for Crystallography, including the applications for conference support from the Larry Calvert fund, regularly check the page maintained by Louise Dawe: ***xtallography.ca/***

As I am writing this, the temperatures have sunk to -24 °C and feels like a good time to wrap up 2017. I am very grateful to Martin Schmeing for helping out in the preparation of this wintry postcard. Wishing you all the best in 2018 and see you in Toronto!

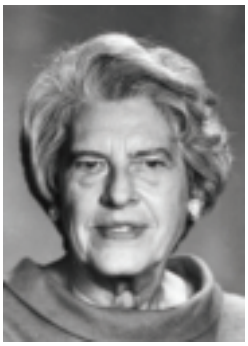
Tomislav Friscic

ACA History Project News

Alexander Wlodawer's Living History in this issue describes a remarkable career. He grew up in Poland, then did his graduate work at UCLA. During his postdoctoral work at Stanford he was part of the group that developed the first synchrotron beamline for protein crystallography. At the National Bureau of Standards he and colleagues constructed a neutron diffractometer for protein crystals, which enabled the joint refinement of X-ray and neutron data to elucidate protein structures. At the National Cancer Institute his group determined the structure of HIV protease and its complexes with inhibitors, which led directly to successful drug design by others. You'll enjoy reading his closing comments about the "Polish Crystallographic Mafia".

Speaking of drug design, ***Thomas Blundell,*** winner of the 2017 Ewald Prize from IUCr, published a review article describing the fruitful exchange between academic protein crystallography and pharmaceutical drug discovery. The link to this article appears online at ACA History / Impact of Structural Science. This page has greatly expanded in the last several months to include links to articles and videos on perovskites (Mike Glazer's Bragg Lecture); a brief history of macromolecular crystallography, featuring 24 Nobel Prize winning crystallographers; a discussion of economic growth resulting from use of X rays (S. N. Rao); and structural information in drug design for Alzheimer's disease (Greg Petsko).

If you missed the IUCr Congress in Hyderabad, you can view the ***Symposium in Honor of Bill Duax*** online at the ACA History web pages. The eight speakers described Bill's life and scientific career, as well as his significant contributions to both ACA and IUCr. Bill was president of the ACA (1986) and president of the IUCr (2002-2005); he has been CEO of the ACA since 1988.



Also online now at ACA History is the biography of ***Rose C. L. Mooney-Slater*** by Frank Fronczek. Rose was the first female X-ray crystallographer in the US. At Sophie Newcomb College in New Orleans where she was a faculty member for 20 years, she mentored future scientists, notably Ruth R. Benerito and Richard Marsh. (See Dick's online Living History for details.) Her career included a Guggenheim fellowship, work on the Manhattan project, and a stint at the National Bureau of Standards where she was instrumental in establishing the crystallography research tradition at NBS/NIST. She was a contemporary of Kathleen Lonsdale, Dorothy Crowfoot Hodgkin and Helen Megaw but her career wasn't as well known until Frank did the necessary research. [Photo credit: AIP Emilio Segre Visual Archives, *Physics Today* Collection]

Virginia Pett, pett@wooster.edu

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I decided to become a scientist rather early on—at the ripe age of four. My mother was a biochemist at the Nencki Institute of Experimental Biology in Warsaw, Poland. One day I offered to Professor Włodzimierz Niemierko, then director of the Institute, my future services subject to successful graduation from kindergarten, school, and university. Little did I know that I would actually accomplish that goal, but, to tell the truth, any thoughts about crystallography were definitely not on my mind then. Moreover, although those promising beginnings took place in Poland, almost my entire scientific career has been connected with the United States, a fact that I attribute to several circumstances.

When I was in high school, I was selected to become a member of the Polish delegation attending a meeting of the American Junior Red Cross on the hundredth anniversary of the establishment of the Red Cross in the United States. Luck was with me: English was not taught in my school, but my parents insisted early on that I study the language, so I did not have much competition in the selection process. That meeting in the summer of 1962 truly changed not only my own life but also the lives of many other participants. A visit to the White House hosted by President John F. Kennedy was truly inspiring (the arrow points to me). A visit to the United Nations headquarters in New York provided an impetus for another young meeting participant, Ban Ki-moon, to become a diplomat and later occupy the most important office in that same building for a decade. My own goal was also set: I would finish my high school and university studies and go to the United States for graduate studies.

When the time came to choose the direction of my university studies, I abandoned the idea of life sciences and decided to study physics. I followed that track for three years until 1966, when I had to select my specialization. That same year, Professor David Shugar started a completely new program in biophysics in Warsaw. I joined its very first class and decided to work on my master's thesis at none other than the Nencki Institute. However, rather than conducting experiments in physics, I dabbled in neurophysiology of vision but quickly convinced myself that torturing cats should definitely not become my future career.

At that time, many young people in Poland became very active politically and secret groups were discussing how to improve socialism to the point that it would actually deliver on its promises. Major political upheavals took place during and after March 1968, which strongly encouraged me to emigrate. Although I was already accepted to a graduate program in neurobiology at the University of Iowa, I also applied for doctoral studies at two universities in California, UCLA and Caltech. The major impetus was geography: I was a mountain climber, and realized in time that there were no mountains in Iowa. I later discovered that my application to Caltech was never considered, since I had been unable to send them the $10 application fee. However, I was not only accepted to the Molecular Biology program at UCLA but also awarded a stipend. Thus, it was not Iowa, but California, and not neurobiology, but molecular biology. The only problem was how to get there.

Due to some rather obscure American regulations, I could apply for a refugee U.S. visa only in Italy. Therefore, I went to Rome, filed visa applications, and waited. In a serendipitous development, I was hired as a completely unqualified technician in a laboratory in the Istituto Superiore di Sanita. The head of the laboratory was Rita Levi-Montalcini, who some years later became a Nobel laureate, and the area of study was a small protein called nerve growth factor (NGF). I became completely fascinated by this hormone that directs the growth of neurons. Of course, it was not at all clear to me that this would become important much later.

I came to Los Angeles in the summer of 1969 and started my graduate studies the day after my arrival. That same year, a young scientist named David Eisenberg moved from Caltech to UCLA to become an assistant professor. I became one of his first graduate students. David decided to establish at UCLA a new area of investigation, namely protein crystallography. It was barely a decade since the first protein structures had been determined by Max Perutz and John Kendrew, and only a few places in the world were engaged in such studies. I certainly did not plan on becoming a crystallographer when I started my graduate work, but I was very quickly converted and realized that this should be the field of my specialization.

For the next 4 years, I tried to solve the crystal structure of rabbit muscle aldolase, but there was no structure by the time I was ready to write my thesis. However, it was still possible at that time to graduate without solving a protein crystal structure and by publishing only a single paper—thus, Ronald Reagan's signature was finally placed on my Ph.D. diploma (he was then the governor of California). While at UCLA, I tried to interest David in NGF, but he did not bite.

My next move was to look for a postdoctoral position. Brian Matthews at the University of Oregon must have learned that my Ph.D. thesis presented little experimental data, so he very politely turned me down. My luck somehow prevailed, however: I contacted Eric Shooter, a professor at Stanford University and one of the major players in the NGF field. Eric became interested and promised to support my quest for the structure of this protein, but since he did not have funds to support me, he made a deal

with Keith Hodgson, who at that time was starting a project to utilize synchrotron radiation as a source of X-rays for protein crystallography. Thus, I could work on both methods development and structure determination.

The summer of 1974 was the most successful period in my career as an experimental crystallographer. I crystallized not only NGF but also two other proteins, L-asparaginase and monellin. At that time, just crystallization of a protein alone was sufficient for a full publication, even in *Proceedings of the National Academy of Sciences*. However, the development of a synchrotron beamline as a source of X-rays was a much slower project, and I did not have any equipment to collect X-ray diffraction data at Stanford. I ended up flying regularly to Oregon, so Brian Matthews was stuck with me despite his earlier decision.

Nevertheless, my main project at Stanford was the development of the first synchrotron beamline for protein crystallography. That work was directed by Keith Hodgson, with further participation by Margueritte Yevitz Bernheim and a graduate student, James Phillips. We were joined by Julia Goodfellow (now Dame Julia) a year later. To say that our facilities were primitive is to overestimate the true state of affairs. Our only detector was an Enraf-Nonius precession camera that could be used with Polaroid films for alignment or with multiple packs of radiology films for "data collection." In the photo Keith Hodgson (with his back turned) and I were installing a precession camera in the hutch at the Stanford Synchrotron Radiation Lightsource in 1975.

We used this beamline to collect diffraction data for proteins such as NGF, L-asparaginase, azurin, and rubredoxin. Most crystals of these proteins were too small to provide measurable diffraction with standard laboratory X-ray tubes, so we considered the use of synchrotron radiation to be quite successful. Experiments involving rubredoxin, performed with Lyle Jensen and his colleagues at the University of Washington were particularly important, since we tuned the wavelength to match the absorption edge of iron, thus maximizing the anomalous signal. We were quite pleased to see even by the naked eye that there were differences between the intensities of Friedel mates (the central projection in the space group *R*3 is non-centrosymmetric). Those very early experiments clearly proved that the tunability and high intensity of the synchrotron X-ray beam would ultimately revolutionize protein crystallography.

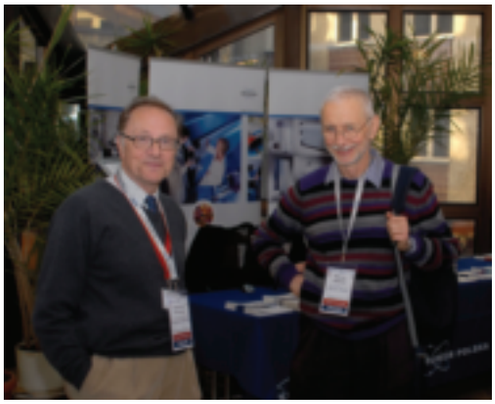
Running experiments was exhausting, since the beam was dumped every two hours and it was necessary to adjust the camera after every fill. My longest single experiment took six nights and five days, with sleep possible in—at most—two-hour increments (on the floor, under a table). We felt pressure to get some positive results before others would beat us to it and, by mid-1976, we finally published our preliminary results in *Proceedings of the National Academy of Sciences*—just in time, since the results from Deutsches Elektronen-Synchrotron (DESY) in Hamburg came out soon thereafter, and another group in Novosibirsk was also developing a protein crystallography beamline.

My next move was in 1976, to the National Bureau of Standards (NBS, now the National Institute of Standards and Technology) in Maryland. My main project was to construct a neutron diffractometer capable of measuring data from protein crystals. To a large extent, progress was due to two colleagues with very extensive knowledge of neutron technology, Antonio Santoro and Ted Prince. They came up with the idea of building a flat-cone diffractometer utilizing a 1-meter-long linear detector and helped me with writing the operating software. I was later joined by my first postdoctoral fellow, Lennart Sjölin, who very successfully continued the process of software development. My predecessor, John Norvell, had already grown crystals of ribonuclease A (RNase A), the largest having a volume of 100 mm^3; thus, the course of action for the next eight years was set.

Lennart and I initially concentrated on the determination of the crystal structure of RNase A based on neutron data alone, but we quickly realized that this might not be the best way of proceeding. However, discussions with Wayne Hendrickson, with whom I would meet quite regularly during the Washington Crystal Colloquia—organized by no less than a future Nobel laureate, Jerome Karle—led us to adapt Konnert and Hendrickson's program PROLSQ for joint X-ray and neutron refinement. This approach allowed us to publish quite significant data on the protonation states of residues such as histidine and on amide hydrogen exchange. Subsequently, we decided to investigate another small protein, bovine pancreatic trypsin inhibitor (BPTI). In retrospect, our BPTI work was much more important than our RNase A work, as BPTI became a prototype for the development of macromolecular NMR and for computational methods interpreting the folding, structure, and dynamics of proteins. Since BPTI was originally studied in Munich, I established a very fruitful collaboration with the future Nobel laureates Robert Huber and Hans Deisenhofer. X-ray data personally collected by Robert, merged with our neutron data, were used for joint refinement, leading to the first truly atomic-resolution (1 Å) protein structure to be deposited in the Protein Data Bank (PDB). The structure of the even-smaller protein crambin was refined earlier but deposited later by Martha Teeter.

A few years after my move to the NBS, I attended the 1978 Congress of the International Union of Crystallography in Warsaw. There I met Tom Blundell, one of the top British crystallographers of the second generation. Tom and I discussed the NGF stalemate in considerable detail and came to an understanding: his laboratory would take over the project, but I would be kept in a supporting role. That agreement held for the next 13 years—that was how long it took to finally determine the structure of this very small protein. The results were worth it, though: the structure, published in *Nature* in 1991, elucidated a newly discovered fold

that included a cystine knot, later found in many other important proteins. Tom held his part of the bargain and I was included as a co-author of that paper, even though by then we were more competitors than collaborators.



Another important event in my career that could be traced to attending a scientific meeting took place in 1986. I participated in a Congress of the European Crystallographic Association in Wroclaw, Poland, where I met a distinguished Polish crystallographer, Professor Zofia Kosturkiewicz, who suggested that I accept her former student Mariusz Jaskólski as a visitor to my laboratory. Indeed, Mariusz came to the U.S. a year later, and we then started our very successful collaboration that continues until today and that has resulted so far in more than 40 joint publications. In the 2011 photo above, Mariusz and I are at a Multi-Pole conference in Warsaw, Poland.

My move to the National Cancer Institute (NCI) was an indirect result of Joel Sussman's sabbatical at the NIH. Joel worked closely with us on structural investigations of DNA duplexes containing unpaired bases and spent lots of time in our laboratory. In 1986, he told me about a plan to start a structural biology laboratory at the NCI in Frederick, Maryland, and encouraged me to apply for a group leader position (he himself applied for the position of a lab chief). However, Joel ultimately decided to accept the position of the director of the PDB (then at Brookhaven), and George Vande Woude, the head of the Frederick program, offered me the lab chief position. I accepted and moved to Frederick in 1987, with Irene Weber assuming a group leader position, and with Ron Rubin joining us as a group leader a little later.

The moment of transition between the NBS and NCI happened when my laboratory became engaged in a new and exciting research area, namely structural investigations of retroviral proteases (PRs). Inactivation of HIV PR was shown to prevent viral particles from maturing into their infective form, thus making HIV PR a potential target for antiviral drugs. However, genuine proteins from HIV-1 were very difficult to come by at that time. As is often the case, the start of the project was quite fortuitous—through my introduction to Jonathan Leis, who at that time worked at the Case Western Reserve University in Cleveland, Ohio. Jonathan had been working for a long time on biochemical characterization of various retroviral proteins and had successfully purified milligram quantities of PR from Rous sarcoma virus (RSV, now usually called avian sarcoma virus, or ASV). We immediately decided to investigate its three-dimensional structure as a stand-in for the structure of the much more medically important enzyme encoded by human immunodeficiency virus type 1 (HIV-1).

Crystals of RSV PR were grown by Maria Miller within a month of receiving the protein. Derivatization of the crystals with a uranyl compound, an excellent anomalous scatterer of CuKα radiation, yielded a single-site derivative (which marked, as it later turned out, the active site) that enabled the proper choice of the space group enantiomorph and helped in setting some additional derivatives in common origin and handedness. J. K. Mohana Rao and Mariusz Jaskólski were crucial participants in that phase of the project. The electron density map, based on multiple isomorphous replacement phases from the four best derivatives, allowed us to trace the main chain of the dimeric molecule, and the atomic model of RSV PR was complete in October 1988.

As soon as the first RSV PR model was complete, Irene Weber built a homology model of the HIV-1 enzyme. The model looked very plausible: it had all the features of the template, with differences limited to the loop regions. The structure of RSV PR was published in *Nature* in early February 1989. A week later, in the same journal, the crystal structure of HIV-1 PR was unveiled by Manuel Navia, Paula Fitzgerald, and co-workers from Merck Sharp & Dohme, and that same week, Irene's model was published in *Science*. After the first burst of joy, suddenly there was consternation because the crystal structures of the RSV and HIV-1 PRs, while similar in the basic features, also showed some perplexing differences, especially in the C-terminal region of the molecules. Whereas the RSV PR model had a clear α-helix, the HIV-1 PR structure had a straight β-strand, and the topology of the dimer interface was completely different. Instead of the interlaced termini with three inter-subunit β-sheet connections found in the RSV PR, the HIV-1 PR crystal structure had a hairpin with only one area of inter-subunit contact, and a disordered N terminus. The latter difference was not trivial; rather, it had profound consequences for the dimer stability and for the PR's ability to excise itself from the viral Gag-Pol fusion polyprotein synthesized in the infected cell. Moreover, the question about the correct features of retroviral PR was not purely academic, because an accurate HIV-1 PR model was badly needed for a structure-guided design of inhibitors that might be developed into AIDS drugs.

The dilemma of which HIV-1 PR model could be resolved only by experiment, but the main question was how to obtain the protein. Help came from Stephen Kent, then at the Caltech, who was pioneering the methodology of protein synthesis using a purely chemical process. He and Jens Schneider quickly sent us 0.2 mg of chemically synthesized HIV-1 PR, enough to grow a few crystals. Our molecular replacement calculations had to rely on Irene's model of HIV-1 PR, as the coordinates of the Merck structure were not made available. However, more material was needed to produce heavy-atom derivatives, because it was critical to obtain phase information experimentally, to avoid model bias, and to produce an independent model of the protein. More protein was also needed for cocrystallization trials with inhibitors. The Kent group set a precedent by producing for us, within a period

of just two weeks, milligram quantities of HPLC-purified enzyme for successful crystallographic studies. The definitive structure of the HIV-1 PR apoenzyme, showing its agreement with the RSV PR-derived model, was published in *Science* in August 1989.

The next goal was to determine the structure of HIV-1 PR in complex with inhibitors. The first such inhibitor, MVT-101, was provided to us by Garland Marshall (Washington University). Cocrystals with the synthetic enzyme grew overnight, and we were able to complete and publish the structure of the complex four months after the publication of the structure of the apoenzyme. It is worth stressing that the coordinates of the synthetic HIV-1 PR:MVT-101 complex were deposited in the PDB in April 1990 and, for the two most critical years, were the only ones freely available to all researchers worldwide who were working on the design of specific retroviral PR inhibitors, although we were not directly involved in such efforts. The first HIV-1 PR inhibitor to become a drug, Saquinavir (Ro-8959), was developed by Roche and approved for clinical use in December 1995. It is generally recognized that determining the structure of HIV-1 PR has been the springboard for the development of successful rational drug design strategies not only in that particular case but also for other pharmacological targets, taking the idea from a flimsy dream to practical reality.

With very significant participation by Alla Gustchina, who had studied the structure of pepsin in Moscow and was thus well acquainted with aspartic proteases, we continued to study retroviral PRs from other sources, such as FIV, EIAV, XTLV, and XMRV. Our focus was on models of potential resistance to anti-HIV drugs, as well as on the function of these enzymes in carcinogenic viruses.

My involvement with atomic-resolution protein structures also happened through serendipity. In the mid-1990s, Fred Dyda and I convinced the NIH management to create a facility for our institution at beamline X9B at the Brookhaven synchrotron. However, having access to the beamline was clearly not enough; we needed someone who could professionally operate it. Here, luck was with us: Zbyszek Dauter, who for almost 10 years had worked at the EMBL DORIS beamlines in DESY Hamburg, was persuaded in 1997 to move to Brookhaven. This was a significant loss for the European crystallographic community but a clear win for us, since Zbyszek has many talents and has been known for years as not only a great crystallographer but also a superb collaborator. Since he excels at working at the resolution of 1 Å and beyond, engaging him in projects that involved studies at atomic resolution benefited us tremendously. Many such projects have been completed through our collaboration during the last 20 years.

It is not a coincidence that many names mentioned in this memoir are Polish. Although I never explicitly tried to find collaborators in that country, my contacts in Poland resulted in several scientists visiting my laboratory, and some staying for many years. Additionally, many distinguished crystallographers with Polish roots are very active and successful around the world. Thus, the "Polish Crystallographic Mafia" came into existence—in addition to my colleagues mentioned above, it also includes many others. Wladek Minor, well known as a co-author of the HKL3000 package, has been particularly involved in our efforts to maintain and enhance the quality standards of macromolecular structures deposited in the PDB. Years ago, I was involved in the first crusade to make deposition of atomic coordinates of published structures mandatory—it is hard to believe today that, at that time, many prominent protein crystallographers were fervidly opposed to such a policy. However, it became the law of the land, followed some years later by the requirement to deposit experimental structure factors as well. In the last few years, we have become, together with some other colleagues who do not claim any Polish roots, self-appointed policemen monitoring the PDB, plucking rotten apples and rectifying less-severe errors of selected structures. I think that these efforts may ultimately turn out to be quite important, since the presence of bad apples in the PDB bushel is guaranteed to cause serious problems in meta-analyses, in particular by biasing projects that might lead to the creation of new drugs. Other efforts of the Mafia included the organization of meetings entitled Multi-Pole Approach to Structural Science, as well as editing the latest textbook of protein crystallography. One indication of our success was that Mariusz Jaskólski and I received in 2015 the first-ever Polish-American Scientific Collaboration Award given by the Foundation for Polish Science and the American Association for the Advancement of Science. We were very proud of being selected in a highly competitive contest encompassing all fields of science. My photo taken during the award ceremony was used for the cover of a special edition of the Polish journal *Postępy Biochemii (Advances in Biochemistry)*, for an issue celebrating my 70th birthday. That issue included reviews and primary research articles by my mentors, students, and collaborators.

I would like to think that being invited to write this memoir does not indicate that my scientific life is over—I certainly hope this is not the case, since quite a few projects are still a long way from being completed. I have been blessed with having excellent mentors, with being able to work in well-equipped laboratories, and, most importantly, with having superb collaborators, who were principally responsible for whatever successes my laboratory could claim. I am very grateful to all those already identified, and to the many individuals whose names I did not have a chance to mention. Thank you all!

WK.01: CSD Workshop - Communication and Innovation

The Cambridge Structural Database (CSD) continues to grow at an increasing rate, passing the milestone of 890,000 entries before the 2017 ACA meeting. In recent years, as the rate of crystal structure publication and the overall number of structures grows, we have made targeted improvements to the ease of communication of crystallographic information and the effective use of the data through automated and innovative approaches.

The morning session, presented by ***Paul Sanschagrin*** (CCDC US), focused on an introduction to the CCDC and the CSD, followed by the crystal structure deposition and curation workflow. This helped the attendees understand how to provide structures, what depositors should consider during the process, and how CCDC adds value during the curation process. One of the key points Paul covered was the ability to publish structures directly through the CSD as a CSD-Communication. This led into a discussion of the various methods for accessing CSD data, including the web-based *Access Structures service*.

After a brief break, the workshop shifted to looking at the best methods for communicating crystal structures and structural information. This included an introduction and hands-on work to explore various techniques for generating high-quality graphics, graph set figures, and files for 3D printing. A brief demo of some Tips and Tricks for *ConQuest* and *Mercury* was also presented.

The afternoon session, also presented by Paul Sanschagrin, focused on enabling attendees to start using the CSD Python API. After a brief introduction to Python and the CSD Python API, participants were unleashed to tackle a series of increasingly more complex problems. The material introduced a basic script, how to interact with *Mercury*, and some additional tasks, and then ended with attendees being presented with several scientific challenges that could be approached using the CSD Python API.

We were excited to see that most attendees took part in the full workshop, learning to communicate crystal structures more effectively and getting technical with some Python programming. We're sure they'll take back what they've learned and be able to apply it to their own work.

Paul Sanschagrin and Peter Wood

WK.04: Research Data Management

This Workshop, organized by the IUCr Diffraction Data Deposition Working Group, covering all aspects of Research Data Management, comprised two plenary sessions and an accompanying technical session (see accompanying report by Herbert Bernstein). The two plenary sessions were entitled (i) *What every experimentalist needs to know about recording essential metadata of raw diffraction data* and (ii) *Research data policy mandates and requirements on principal investigators*. The technical session addressed the increasing challenge to raw data archiving posed by high data measurement rates at today's synchrotrons; it also described prospects for enhanced computer hardware and software developments to address these challenges.

Workship speakers left to right:- John Helliwell, Peter Meyer (seated), Simon Coles, Wladek Minor, Marvin Hackert, Herbert Bernstein, Andrew Allen, Marian Szebenyi, Loes Kroon-Batenburg and Brian McMahon.

John Helliwell (U. Manchester, UK) introduced the purpose of the Workshop as: capturing current best practice with processed and derived data across the widest possible range of IUCr Commissions; defining for each type of experiment the essential metadata for complete understanding and reuse of archived raw diffraction data; and tracking continuing technical challenges and opportunities in managing large raw data volumes and rates.

Marvin Hackert (U. Texas at Austin, IUCr President) described the role of the IUCr in the global hierarchy of policy-making bodies interested in scientific data management, and introduced the considered response of the IUCr (***www.iucr.org/__data/assets/pdf_file/0011/125687/OpenData_crystallography_web.pdf)*** to a recent international Data Accord on *Open Data in a Big Data World* (***www.icsu.org/publications/open-data-in-a-big-data-world***). Of particular importance was the need for the discipline to ensure that efforts to make research data more findable, accessible, interoperable and re-usable (the so-called 'FAIR Principles') did not compromise data quality or the ability to archive data in a sustainable way.

In response, ***Marshall Ma*** (U. Idaho, Co-Chair CODATA Task Group on Coordinating Data Standards among Scientific Unions) described the multi-disciplinary perspective of CODATA, the ICSU Committee on Scientific Data. He emphasized that a key tenet of Open Data was to be *as open as possible, as closed as necessary,* and that there is a need to evolve policies, practices and ethics around closed, shared, and open data. He also explained how the Task Group he is co-chairing is working towards a Commission on Data Standards for Science to address this need in an international and interdisciplinary way.

Herbert Bernstein (Rochester Institute of Technology) emphasized the need to capture metadata associated with x-ray diffraction images so that they could subsequently be fully interpreted, especially for the purpose of re-use. Improvements in detector speed and resolution continue to push data acquisition rates to the limit, and managing the capture and integration of essential metadata with rapidly acquired images is technically very challenging. However, efforts to convert the existing metadata descriptions of the previous-generation imgCIF format to a form compatible with the newer HDF5/NeXus files offered the best way to ensure that this was achievable.

Loes Kroon-Batenburg (U. Utrecht, Netherlands) presented a range of case studies of real data sets where incomplete metadata characterizing the experimental arrangement prevented many software packages from properly interpreting and indexing the diffraction images. In many cases the missing metadata (*e.g.* concerning the beam center or orientation of the instrumental axes or both) could be inferred from close analysis and manual interpretation of the images. However, in her sample survey of cases derived from macromolecular crystallography raw diffraction data archives, the lesson is that, extrapolating to the large scale, huge numbers of images are being collected at the moment with insufficient detail to permit their easy re-use.

Marian Szebenyi (Director, MacCHESS, Cornell U) in her talk on *Research data management at CHESS* described the recent implementation of the *CHESS DAQ*, a large more centralized system with separate storage for raw data, metadata, and general user data. Operationally there are nightly incremental backups and full archiving at the end of each CHESS running cycle. Raw data are kept on-line for a few weeks and off-line for several years. Limited metadata are stored in the diffraction image headers. It was emphasized that data belong to the users, who are responsible for any depositions in on-line repositories.

Andrew Allen (NIST) described *Metadata for small-angle scattering measurements*. This presented a diversity of challenges embracing x rays and neutrons, and in turn spallation and reactor neutron sources. The nature of the sample was also stressed as an important challenge for metadata recording. Andrew concluded with a summary of the international efforts to address these challenges.

Stephen Burley (Director, RCSB Protein Data Bank, Rutgers U) described the PDB's overall data management architecture and its increasing provision for archiving unmerged intensities. The PDB does not itself archive diffraction images, but their uniform OneDep deposition system provides access to all nodes of the WorldWide PDB that can link to archives of images stored elsewhere through a registered Digital Object Identifier (DOI) obtained by a depositor *via* an archive external to the PDB.

Wladek Minor (U. Virginia) described one such archive, the *Integrated Resource for Reproducibility in Macromolecular Crystallography* (***www.proteindiffraction.org***), that he maintains under the NIH *Big Data to Knowledge* initiative. Currently holding over three thousand openly available diffraction experiments and almost twice as many diffraction data sets, this project includes among its goals the development of tools for automatically extracting and curating diffraction images and

associated metadata, in particular to allow later reprocessing of the diffraction data as methods for structure determination improve; the creation of a web-based system for semantic searching, analysis, and data mining of appropriate subsets of diffraction images and associated metadata; and the creation of a repository for diffraction data that did not yield an x-ray structure with the currently available methods.

Simon Coles (U. Southampton, Director of the UK National Crystallographic Service, 'NCS') described *administration, raw diffraction data, structure factors and coordinates* at the NCS. This included the experiences gained from many years in e-Science applications (*i.e.* the eCrystals project ***ecrystals.chem.soton.ac.uk***). Raw diffraction data are also preserved but only available on request. The need for the UK Service to combine laboratory information management and a data repository led to the system called *Portal*.

Peter Meyer (Harvard Medical School, Chief Curator for the SBGrid Databank) described the role of the Databank as a data publication and data dissemination system to preserve diffraction data sets supporting published structural biology crystal structures. A set of REST application programming interfaces supports reprocessing pipelines. Data citation support and reference manager integration were briefly mentioned.

The wider aspects of research data were addressed within the context of the IUCr's newly established *Committee on Data* (*CommDat*), which will continue to track raw diffraction data management, but will also have significantly wider terms of reference. These include: preservation of raw diffraction data and associated metadata, identified by DOIs; data mining within individual and across multiple databases; data and software development; data and instrumentation; data policy drivers coming from policy makers (*e.g.* funding agencies); data type domains (discrete *versus* diffuse, *i.e.* continuum, scattering); data and e-Science; data and data publishing (*IUCrData*; recommendation of editors for *IUCrData*; linking of data to articles in IUCr publications; new article categories involving data); and data repositories. In the final discussion, in part stimulated by considering these wider aspects, issues raised for immediate consideration included: the importance of open-source software in maintaining the transparency of numerical processing; and the reproducibility crisis in general in science.

In summing up there has obviously been great progress in provision of archives for raw diffraction data. Several are now available in Australia, Europe, and the US with a strong role also evident at the centralized neutron and x-ray facilities as well as the role of university repositories such as at the University of Manchester provided for its research staff. There has also been good progress on defining metadata in the various IUCr Commissions' areas. Thirdly, there is a widening range of raw diffraction data re-use by researchers, leading to improved understanding of current apparatus limitations such as inadequate knowledge of the center of the diffraction pattern in various cases, as well as in the current laboratory practices and data analyses. There is clearly strong interest in all aspects of Research Data Management for macromolecular crystallography.

John Helliwell & Brian McMahon

WK.04: Technical Subsession: For synchrotron- and XFEL-based macromolecular crystallography (MX), high source brightness and the new generation of pixel array detectors raise big data, high-performance computing (HPC), and high-performance networking issues in Research Data Management for high data-rate MX. This technical subsession, organized by ***Herbert Bernstein*** (Rochester Institute of Technology) and ***Robert Sweet*** (Brookhaven National Laboratory) with the cooperation and assistance of the WK.04 organizers, occupied the last two hours of the Workshop.

Jean Jakoncic (NSLS-II, Brookhaven National Laboratory) reviewed the impact of more brilliant synchrotron beamlines, faster sample handling, high-speed pixel array detectors, and highly automated data processing on the data rates and volumes for MX, taking us from doing a structure in the 1990's requiring hours to weeks, to doing a structure today requiring seconds to hours. Using the NSLS-II AMX and FMX high-brightness microfocusing beamlines with Dectris Eiger 9M and 16M hybrid pixel array detectors, the problems being faced and solutions being deployed in dealing with High Data Rate Macromolecular Crystallography (HDRMX) at various facilities for handling of a thousand crystals per day, generating more than 1GB/s of data per beamline and up to 30 TB per day per beamline, even allowing for sample mounting delays, were discussed.

Henry Gabb (Intel Corp.) discussed recent computational hardware and software approaches to providing the HPC support needed to deal with MX data arriving and needing to be processed in near real time. The Intel(R) Scalable System Framework (SSF) describes an integrated approach to providing computational, memory and networking resources. The Intel Software and Programming Tools Ecosystem for HPC describe compilers, libraries and support software that helps in making use of modern hardware, especially in doing parallel computations.

The discussion at the end of the workshop was lively, especially considering the late hour and the need to get the attendees to the reception. There is clearly strong interest in the technical aspects of Research Data Management for MX.

Herbert Bernstein

WK.02: CrysAlis and OLEX2: From Raw Data to Publication

At the ACA meeting on in New Orleans, ***Carla Slebodnick*** (Virginia Tech), ***Charlotte Stern*** (Northwestern U), ***Eric Reinheimer*** (Rigaku Oxford Diffraction), ***Brandon Mercado*** (Yale), and ***Horst Puschmann*** (OlexSys) led a workshop that covered features in the *CrysAlis*^{Pro} and *Olex2* software suites. The workshop was attended by nearly 30 people and generously supported by Rigaku Oxford Diffraction.

The workshop was divided into modules, each of which offered practical examples with real data. The day began with Carla presenting two perspectives on the same data. First, she demonstrated the automatic processing features of *CrysAlis*^{Pro} and structure solution/refinement features of *Olex2*. She then led the attendees (Photo 2) through the same data manually to familiarize them with both software packages. In the next module, Eric guided workshop participants through importing data from other vendors into *CrysAlis*^{Pro} and subsequent processing data. In the final session before lunch, Charlotte used the just-processed data to further demonstrate structure solution and refinement in *Olex2*, emphasizing helpful tools that streamline disorder modeling. Charlotte also covered features in *Olex2* that help prepare the crystallographic files for dissemination.

CrysAlis*^{Pro}*/Olex2 workshop instructors. L-R: Horst Puschmann, Eric Reinheimer, Brandon Mercado, Carla Slebodnick, Charlotte Stern

After lunch Brandon presented a tutorial on a twinned data set, and then the attendees worked through the data individually with the help of instructors. Horst, whose plane was delayed for a day coming from England, finally landed in New Orleans with just enough time to race to the Hyatt and present additional examples of disorder modeling in *Olex2*. Horst also encouraged us (including those of you reading this summary!) to search *Olex2* on *YouTube* for video tutorials. The instructors (Photo 3) appreciated the feedback from participants and enjoyed interacting with them over the course of the conference.

Brandon Mercado, Charlotte Stern, Eric Rheinheimer, Horst Puschmann, Carla Slebodnick

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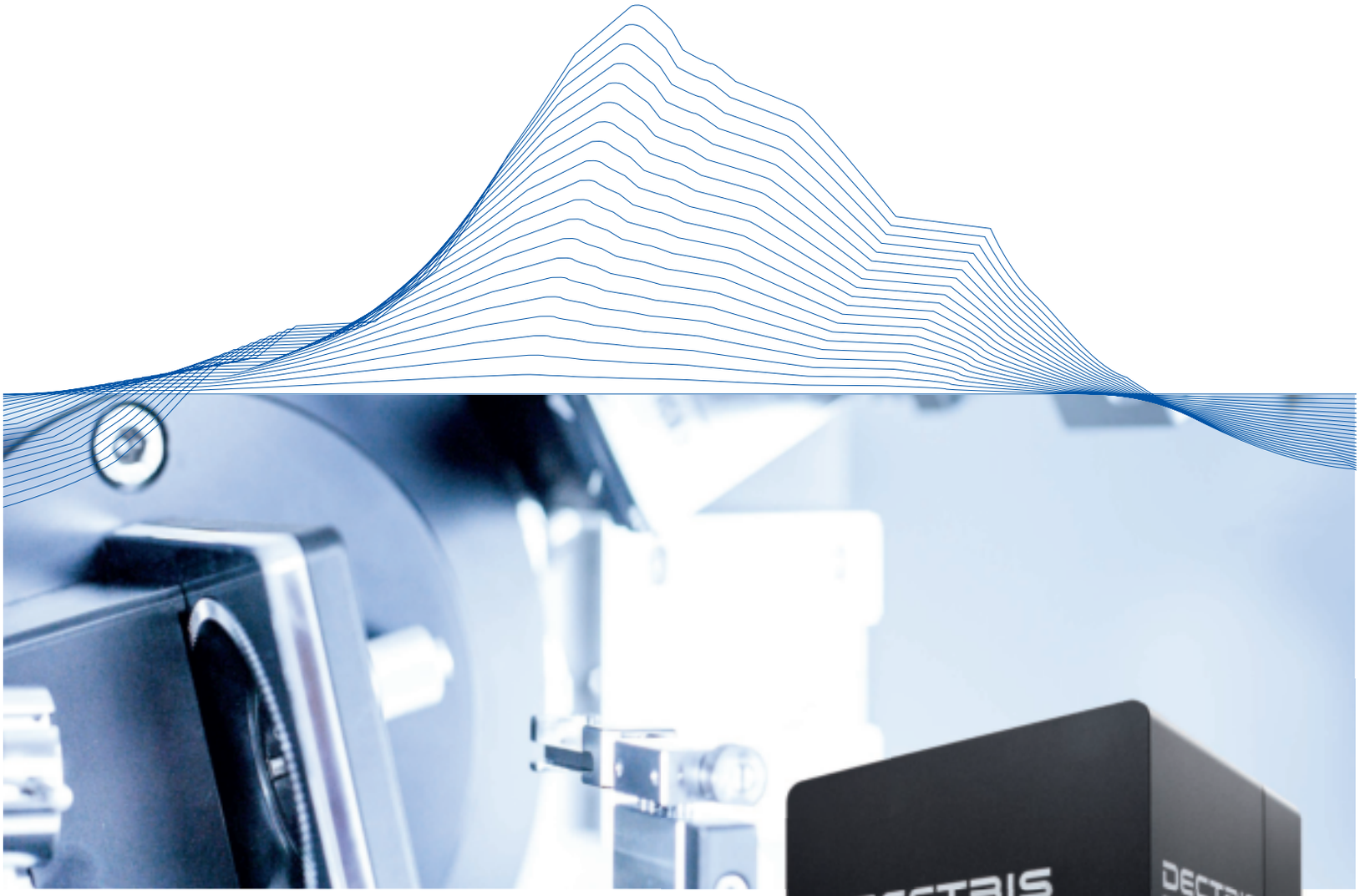

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Cinnabar and the Color of Life

Vermilion, a bright red or scarlet pigment originally made from powdered cinnabar and later synthesized from its constituent elements, is the common mineral form of mercury(II) sulfide (HgS) and has been widely used in art and decoration since antiquity. It was used in sacred rituals since the time of Buddha and it symbolizes life, immortality, and good fortune in traditional Taoism. It was applied as a cosmetic in Ancient Rome and to paint the walls of the most lavish residences of illustrious citizens, such as the renowned Villa of the Mysteries in Pompeii. Vermilion, either natural or synthetic, has also been used for centuries in Chinese carved lacquerware, to embellish important manuscripts during the Middle Ages, and it is the red color of choice often seen in the paintings of Renaissance masters such as Leonardo, Titian, Raphael, Rubens, and Botticelli.

The postage stamps that illustrate this note feature specimens of cinnabar, which belongs to the trigonal crystal system and typically occurs as thick tabular or slender prismatic crystals or as granular to massive incrustations. Classic localities include the mines of Almadén in Spain and Idrija in Slovenia, both of which operated for centuries but are now open only for tourism. Cinnabar is also the most common mineral ore from which elemental mercury is obtained, with close to 90% of the world production (an estimated 4,500 metric tonnes in 2016) originating from China and the balance from Mexico, Kyrgyzstan, Peru, and other countries.

Despite the well-known toxicity of mercury and its compounds, the element is still used in certain applications due to its unique properties, especially its high density, low melting point, and electrical conductivity (it is, after all, the only liquid metallic element at room temperature). For example, mercury cells have been used in the chloralkali industry since the late 19th century to generate chlorine and sodium hydroxide, even though environmental concerns in recent decades have led to the implementation of alternative methods that rely on ion-permeable materials. Other current applications of mercury include fluorescent lighting and dental amalgams, but these are also been increasingly replaced by safer light-emitting diode (LED) technologies and the use of ceramic composites, respectively. Thus, it is ironic that an element that was once associated with long life and good luck now appears to be doomed to practical extinction in the foreseeable future.

Daniel Rabinovich

The following notes were written by a few of the 2017 recipients of travel grants and/or the young researchers selected for the SIG Etter Award Lectures. They were asked to comment on their personal experiences at the meeting: the venue, the events for young scientists, the overall program and their own presentations and whether or not they are (and plan to continue to be) ACA members. Many would not have been able to come to the meeting without the financial support provided by ACA members when they generously contribute to the travel award funds.

Madiha Nisar: The 2017 ACA annual meeting offered intriguing and enlightening presentations by many crystallographers, which gave me deeper insights into the current trends in the field. The meeting covered a wide range of topics (such as small molecule crystallography, advances in data collection, NMR crystallography, etc.) giving me the choice of attending the sessions that best fitted my research interests. It was good to hear talks from industrial people, as well as academics.

One highlight for me was the talk by Sir Fraser Stoddart on how crystallography helped toidentify the mechanical bond in chemistry. The personal recollections of his career was engaging, poignant and very motivational. It was interesting to find out that the path to a Nobel Prize may have several downs, as well as ups.

I had the opportunity to present my own research *Pharmaceutical Cocrystals of 11-Azaartemisinin with Enhanced Properties* in an oral preview session chaired by Daniel Mast and later in an evening poster session, where I got valuable feedback from several experts in the field of crystal engineering. Meeting people who had been just names in the reference sections of papers was very exciting! It was also delightful to be approached by other poster presenters with suggestions and encouraging comments on my work.

Coming all the way from Hong Kong the award of a travel grant made my attendance of the ACA meeting possible. I will always be extremely grateful for the opportunity it has afforded me. As a first-time attendee it is worth mentioning that the YSSIG session was a great platform to meet other young researchers in this field, whilst learning more about the structure and activities of the ACA. Overall I had a wonderful time in New Orleans and am looking forward to being an active participant in future ACA events!

Bradley Miller: This summer in New Orleans was my first time attending an ACA meeting. I am truly grateful for the support I received that helped offset my travel costs. As a macromolecular crystallographer, it was humbling to meet so many other crystallographers who were willing to share their expertise with a young scientist. I also appreciated the opportunity to present my research and learn how I can engage undergraduates at Bryn Mawr College in structural biology research. It was great to listen to and talk with other researchers on how they get their students involved in crystallography. I am already excited about next year's meeting in Toronto!

Trudie Venter (left): Being South African is an interesting experience and we face various challenges, one of which is interaction with the global scientific community. Attending international meetings are not as simple as hopping on a bus or train and traveling to a neighboring country. I was therefore thrilled to hear that I would receive travel support to attend the ACA meeting in New Orleans, setting foot on American soil for the first time. My visit kicked off with a very instructive workshop on the use of *CrysAlisPro* and *Olex2*. The amiable style of presentations allowed for social interaction as well as intellectual stimulation and already the networking aspect of conference attendance could be observed. My highlight of the conference was definitely Saturday after I finished my presentation when I was approached by a colleague from Missouri State University on the subject of possible collaboration. After all, isn't this what these events are for? The proceedings ended on a high note at the conference dinner, where deep discussions were held with new Canadian friends over glasses of wine. I can say with complete honesty that the 43 flying hours and total transit time of 64 hours was completely worth it, and would like to extend my gratitude to the sponsors who made this possible.

Alice Brink (right): The ACA meeting in New Orleans during May 2017 was a fantastic event highlighting the research developments associated with crystallography, primarily in the US as well as worldwide. The location in the Hyatt Regency Hotel, was centrally situated, easily accessible by streetcar for those wishing to experience a bit of New Orleans life and legends, including the famous beignets. The meeting began with the workshops covering several subjects applicable to small-molecule, protein

crystallography and data management. The Plenary lecture, presented by Sir Stoddart (2016 Nobel Laureate) was filled to capacity and followed by the opening reception which catered mouth-wateringly to a diverse assemblage of appetites. The rest of the week continued with parallel sessions covering a broad collection of research fields. This raised the conundrum as to how one may attend multiple lectures scheduled for the same time? Dynamic positional disorder is feasible for crystals but sadly, not for the crystallographer. I wish to thank the ACA for hosting this meeting and for the spirit of education which permeated the discussions. Questions, problems and possible solutions were continuously raised for the purpose of knowledge expansion. The well-planned program allowed for valuable discussions across diverse fields. The meeting was well worth the 48 hour transit required to attend from South Africa.

Soumya Govinda Remesh: I had the opportunity to present a talk in the Hybrid Methods – BioSAXS session, chaired by Greg Hura and Michal Hammel. The feedback and insightful discussion that followed my talk were very useful particularly since I am writing a manuscript to publish the results. It is always very helpful to have opinions from experts in the field before the peer-review process begins which I think is what such meetings are all about.

Of the various sessions, the *Cool Strcutures* and *Intergrative Approaches to Strcutural Biology* sessions were of particular interest to me. Additionally, the YSIG meeting was very informative and useful for me as a young researcher. I also enjoyed networking with accomplished seasoned scientists, new post-docs like myself and graduate students. There were great discussions about science and also career development both in the hallways and at poster sessions which for a first time attendee like myself implied a welcoming atmosphere. I guess though, the wedding in the exhibition room surely stands out as the most memorable event of ACA 2017!! I am a member of ACA and definitely plan to continue my membership as well as be more involved in organizing future meetings.

Remembering Isabella Karle

Isabella Karle (1921 - 2017), retired from the Naval Research Laboratory (Washington, DC) after more than six decades there, passed away on October 3, 2017, at the age of 95, from a brain tumor. Early on Isabella was told by a teacher that chemistry was not a "proper field for girls" but she went on to become a member of the National Academy of Sciences. She received the 1988 Gregori Aminoff Prize from the Royal Swedish Academy of Sciences, the 1993 Bower Award and Prize for Achievement in Science and, in 1995, received the National Medal of Science. What follows are remembrances from several of her colleagues.

Jenny Glusker: Isabella Karle was a gifted scientist who was very active in determining crystal structures and advancing our understanding of chemical and biochemical reactions and their control. She also willingly made herself available to help anyone having difficulties with direct methods of phase determination.

Isabella's family was Polish-American and Isabella did not speak English until she went to grade school. However this did not cause her any problems and she rapidly excelled in classroom tasks, consistently at the top of her class. Her interest in studying chemistry and an excellent teacher of that subject led her to BS, MS and PhD degrees in physical chemistry by 1944 at the University of Michigan. This was done under the fine tutelage of Lawrence Brockway. In 1942 she married a fellow student, Jerome Karle, who was seated in the adjacent desk during studies. They were a devoted couple, married for 71 years.

Then came the time for Isabella to find a research position, not so easy for women in those days. However, she had very good credentials and was an excellent experimentalist, as shown when she worked for a short time at the University of Chicago on one part of the Manhattan project. The aim was to use chemical techniques on small lumps of impure plutonium oxide to obtain very pure plutonium chloride. This would be a step in the production of pure plutonium metal, the "new element discovered beyond the first 92." The chemistry of plutonium was not known at that time. Any equipment she needed had to be made by her in the laboratory, but fortunately she was a talented glassblower. Her description of this work on plutonium derivatives reminded me of the way Marie Curie worked in the laboratory to purify radioactive materials. It was as if Isabella had said to herself "I need to tackle this scientific problem, what techniques are available to help me do it?" and when she found out what they were she would solve the problem. In this case she worked with silica tubes that she had made, filled with crude plutonium oxide and chemical reactants, and inserted them in a hole in a large block of copper that was heated to high temperatures of 800 to 900 degrees Centigrade. After many experiments under difficult conditions, she ended up, triumphantly, with bright green crystals of plutonium chloride ($PuCl_3$) that she passed on to the physics branch of the Manhattan project.

Isabella approached direct methods in the same way, to the delight of her husband Jerry, who won the Nobel Prize for his work on them. She worked hard to find how to run direct methods correctly and then was able to help others. In fact, because of her contribution to the use of the method, Jerry felt she should share in the honors he received. Isabella, however, was just pleased to use and teach about direct methods. She pointed out that "I do the physical applications, he works on the theoretical. It makes a good team. Science requires both types."

Isabella was then able to use direct methods to study the structures of chemicals derived from, for instance, interesting creatures such as brightly colored frogs found in the tropical South American jungles. Her determinations of the chemical formulae of these compounds increased our understanding of their modes of action and how these modes might be controlled. She provided a knowledgeable intermediary between scientists trying to use the method and not having much luck and those who used mathematics to show how to do it but were frustrated that they did not know exactly how to use the method on crystallographic diffraction data. Now direct methods have been successfully incorporated in computer programs and three-dimensional results can come quickly.

Isabella also observed many of the courtesies that have made it so pleasant to be a scientists in this area. She came faithfully, with her husband, to all ACA meetings and added significantly to the smooth running of the meeting, calming an anxious Jerry when, in the olden days, members claimed they had difficulties using direct methods. She demonstrated the connection between the mathematical formulae and ways of handling phases for the measured structure factors. We often went to her for advice to get the method working for us. Not only was she a great scientist, she was a great teacher. She was also a good friend. She often phoned me to check that we were not working on the same structural problems. We never were but it was so nice that she asked. She also provided me with very helpful advice on raising children while doing a full-time job. She had plenty of experience with her three scientific daughters, Louise, Jean and Madeleine. My daughters greatly appreciated some of her suggestions.

Isabella also served as ACA president (1976) and left very useful information for future presidents such as how to make sure each committee does as asked. This took extra work on the part of the president before, not just during ACA meetings, but the results were constructive.

I am sad that Isabella is no longer with us and will miss her

pleasant smile and interesting conversation, but I am proud to have known her and celebrate here her great contributions to molecular structure determination and her mentoring of early users of X-ray crystallographic methods.

Lou Massa: Isabella Karle was a remarkable scientist and a remarkable person who lived her own version of the American Dream: her parents were Polish immigrants to this country, and Polish was her first language until she went to school at the age of five or six. She was a great student all her life earning her BS, MA and PhD all before the age of 23. While studying at the University of Michigan, she met her future husband Jerome Karle in a physical chemistry lab. Their meeting was facilitated by the fact that they were seated next to each other alphabetically by surname; her maiden name was Lugoski.

Jerome and Isabella's mutual love of science cemented their relationship. They both earned their PhDs under Lawrence Brockway, a student of Linus Pauling. They worked in the field of electron diffraction, which would come to influence their work years later in the field of x-ray diffraction.

Almost immediately after completing their PhDs, they both went to the University of Chicago where they worked separately on the Manhattan Project. Among Isabella's many fascinating stories about that work is one about an occasion when she saved the lab from a potential catastrophe. The scientists carried portable radiation detectors, and one day Isabella noticed her detector going off beside the Coca-Cola vending machine, the type that dispensed soda directly into paper cups. As it turned out, the man who came to refill the machine needed to replace a hose in the machine and hastily grabbed one that had been exposed to massive amounts of radiation from a nearby laboratory. Because she spoke up, no one wound up drinking radioactive soda that day.

Isabella contributed to the field of Plutonium chemistry as a precocious recently minted PhD in her early twenties. She designed her own elaborate glassware to conduct her studies of plutonium chlorides for the Manhattan Project.

Isabella Karle's Curious Crystal Method, Story by Antonia Massa (@antoniabmassa), Photo credit: Rey Lopez a Washington, DC-based photographer, (narrative.ly/isabella-karles-curious-crystal-method .)

Perhaps her greatest contribution to science was to show that crystal structures could indeed be solved using the mathematical methods developed by Jerome Karle and Herbert Hauptman, work for which the two men eventually received the Nobel Prize. Isabella's meticulously designed x-ray experiments provided the all-important evidence needed to prove that their mathematical equations did work.

Those were the days long before you could buy computer-controlled x-ray diffractometers to measure intensities over the whole scattering sphere with electronic high accuracy. She was resourceful, borrowing an x-ray tube source and constructing an experimental arrangement to collect data. Her experimental design included use of the human eye to estimate the relative intensities registered upon photographic film. Imagine the confidence and the intellectual courage behind such an effort.

And the result was that she solved structures that no one else could. It took decades for science to widely accept that she could do this, but finally they did. That laid the groundwork for Jerome and Herbert's Nobel Prize for the mathematics. Though Isabella did not win the Nobel, she collected many other awards. She kept right on with her science, becoming one of the most important crystallographers of her generation. The prizes and accolades she racked up included the highest science award a US citizen can obtain, the National Medal of Science, which was presented to her in person by President Bill Clinton in 1995, in a ceremony held at the White House. She also received the Aminoff Prize, the highest honor in the field of crystallography. She was awarded multiple honorary doctorates, and published more than 300 scientific papers.

Isabella is revered as one of the greats of her generation. Only part of her greatness is as a scientist of historic importance. She managed to be a dedicated wife for more than 70 years and loving mother to three wonderful, accomplished daughters all while working at the highest levels of American science. Isabella will rightly be remembered by history for the greatness of her science. Those who knew her will also be remembering her humility and humanity. We loved Isabella, and she affected us deeply.

Connie Rajnak: I admired Isabella for a long time. She used to come to ACA meetings along with her husband Jerome and she welcomed me when I was a novice crystallographer and needed support. I was disappointed when Jerome shared a Nobel Prize with Herbert Hauptman that did not include Isabella. She should have shared that prize because she was the one who actually solved structures and made direct methods work. Jerome was strictly theoretical.

It was natural that when I had a sabbatical I selected Isabella to work with at NRL (the Naval Research Laboratory). She showed me how symbolic addition works and gave me a booklet that describes it. I liked the way she always published every structure she solved and did her best to find something interesting about it. When my 11 months at NRL were almost up she took me home with her and we talked with Jerome (Jerome and I share an interest in the piano but I couldn't persuade him to play anything). She then she rowed me around the lake just adjacent to their property and had a fine time talking about everything under the sun. I told her

about my daughter's brush with breast cancer but she didn't mention that she was a breast cancer survivor herself.

After my sabbatical, I used to send her a birthday letter to which she always responded with a handwritten letter. After I married Stan I sent her an abbreviated version of our Christmas letter every year and she would respond similarly.

Jean Karle Dean: My mother's endless enthusiasm for crystal structure solving and relating 3-dimensional structure to function is why I became interested in crystallography. When I was a child, before computer graphics, I would sometimes help her plot calculated electron density on large sheets of rolled white paper held open on the dining room table by brass candlesticks. By age 18, I was operating an early version of an automatic diffractometer in her lab. Decades later when my workplace purchased me my own diffractometer, I was amused when the installer recommended that I start with a crystal of known structure to teach myself how to use the instrument and to solve the structure. I politely did not say anything and proceeded directly to crystals of interest of unknown 3-dimensional structure.

My mother was always interested in how structure related to function and the importance of intra- and intermolecular hydrogen bonding as well as other attractions between molecules. Earlier in her career, she would get very annoyed when short-sighted editors did not want to publish packing diagrams.

My mother had a natural instinct for solving crystal structures that allowed her to determine the crystalline structure of some of the largest molecules solved by direct methods, generally polypeptides. She also greatly enjoyed her collaborations.

In Stockholm, I was seated next to Nobelist Glenn Seaborg at a sit-down meal at the American Embassy. He told me that he could not understand why my mother was not sharing the 1985 Nobel Prize in Chemistry with my father, Jerome Karle, and Herbert Hauptman. I took that as an immense compliment to my mother's scientific contributions.

Sue Byram: Mrs. Karle was one of the pioneers in the solution of single crystal structures. I knew her over many years, particularly through visiting the Laboratory for the Structure of Matter at the Naval Research Laboratory in Washington DC from the 1970's to the present. She was a hands-on practical user of my company's single crystal diffractometers and we were immensely proud of providing hardware and software which we hope assisted in her important work. She was always eager to use the latest tools which would assist her in solving many difficult structures.

I just re-read the really nice words from the retirement ceremony of Isabella and Jerome Karle in 2009, where it was stated:

"Isabella Karle is one of the pioneers in the area of small molecule structural biology who developed the method on which so many important concepts in peptide structure and function were corroborated. Without her pioneering contributions to this field, much of the wonderful work that followed would not have been possible. Mrs19Karle's early research concerned the structure analysis of molecules in the vapor state by electron diffraction. In the fifties, her research was directed toward crystal structure analysis. She developed practical procedures based on the theoretical work developed by her husband in the Laboratory for the Structure of Matter at the NRL for the determination of phases directly from the measured intensities of x-ray reflections. These practical procedures have become adopted world-wide and have been essential to the explosive output of crystal structure determinations that are indispensable to the solution of problems in a number of scientific disciplines: chemistry, biochemistry, biophysics, mineralogy, material science, pharmaceuticals, drug design and medicinal chemistry, for example."

The whole Karle family is part of the wider crystallographic community and we treasure that. I recall many stories about the family, children included, attending many ACA and IUCr meetings. I started attending ACA meetings in the early 70's and have enjoyed seeing the Karle's at many of them. Indeed, Mrs. Karle was ACA president in 1976, exemplifying her love and devotion to our science. Most recently, I spoke with their daughter, Louise Karle Hanson and her husband Jon Hanson at the August 2017 IUCr meeting in Hyderabad, India. Mrs. Karle was both a distinguished scientist and a lovely human being.

Robert Henry "Pete" Bragg (1919 - 2017)

Robert Henry "Pete" Bragg, professor *emeritus* in the Department of Materials Science and Engineering in the College of Engineering at UC Berkeley, passed away on October 3, 2017, at the age of 98. He joined Berkeley in 1969, one of only six African-American faculty members on the campus. He chaired the department from 1978 – 1981.

Before earning his PhD, Bragg became an expert at x-ray crystallography and x-ray diffraction while working at the Portland Cement Association Research Laboratory. He went on to earn his PhD at Illinois Institute of Technology, working under his mentor Leonid V. Azaroff. Following receipt of his PhD, he worked for nine years on carbon-based materials at Lockheed Martin Missiles & Space Company.

The current Chair of the Materials Science and Engineering Department, Mark Asta, said "Professor Bragg pioneered the use of X-ray based techniques to characterize the structure of complex materials, particularly those containing light elements that had traditionally been relatively 'transparent' to these methods." Besides being a professor at Berkeley, Bragg was a principal investigator in the Materials and Molecular Division of Lawrence Berkeley National Laboratory. He served as an adviser to the U.S. Department of Energy, the Naval Research Laboratory, the National Science Foundation and the National Institute of Standards and Technology.

Ludo Frevel Scholarship Recipient

Through its Crystallography Scholarship Fund, known as the Ludo Frevel Crystallography Scholarship Fund, the International Centre for Diffraction Data (ICDD) awards scholarships to aspiring crystallographers. Because crystallography is such an interdisciplinary discipline the recipients of these scholarships come from many branches of science. This year ACA member ***Ivana Brekalo,*** PhD candidate in Chemistry at Georgetown University, is one of ten scholarship recipients. She is studying *Solid State Synthesis and Templation of Metal Organic Frameworks,* that is, mechanochemical synthesis of different porous and host-guest materials. She has used macrocyclic templates in the solid state to synthesize previously unknown zeolitic imidazolate frameworks and has shown the templation of a specific topological motif. She is currently working on the solid state synthesis of cryptophanes and different metal-organic frameworks.

Facilities to Enhance Research Opportunities

European X-ray Free Electron Laser (EuXFEL): After 10 years of planning and construction and 1.5 billion dollars, the world's third - and by far most powerful - X-ray Free Electron Laser is open for experiments in Hamburg Germany. This European XFEL offers x-ray pulses that are a million billion times brighter than the sun. The creation of XFEL facilities has led to opportunities to overcome the limitations of traditional crystallography in which crystallized samples are necessary. A team of scientists from Arizona State University, led by Alexandra Ros,is the first US group to have access to this facility and they are working on a microfluidic system that will deliver droplets of biomolecule crystals in a fashion that will allow each of the x-ray shots to hit a fresh crystal without the requirement of using large amounts of precious crystals.

ALS-ENABLE: The National Institutes of Health has awarded 6.5 million dollars to Lawrence Berkeley National Laboratory to integrate existing synchrotron structural biology resources to better serve researchers. The center will be based at the Lab's Advanced Light Source (ALS) and will be called ALS-ENABLE. It will bring together four groups of scientists who have individually facilitated access to crystallography and small angle scattering technologies on eight ALS beamlines. Besides providing three core technology operations – rapid response crystallography, high quality and high throughput small angle x-ray scattering and specialized crystallography – there will be user training and outreach. There will also be a consolidation of web tools that have been developed independently to make them more accessible to users.

Kay Onan

CESTA 2017 - A Study of the Art of Symmetry

There is a chasm of understanding that separates the proverbial "scientist" and the general populace. Most people have no clue what actually goes on behind closed rooms full of people with white lab coats and blue nitrile gloves. Research is conducted and published, only shared with other scientists, and the cycle continues. I have sought avenues that attempt to break this cycle, and this past summer I happened upon a peculiarly interesting project. The premise was simple: two chemists, two sculptors, and two engineers work collaboratively (under time and budget restrictions) to create and install a piece of science-art. I had the opportunity to take part in this experiment and would like to share my experience.

For the past two years, Jessica Hoover (Department of Chemistry at West Virginia University) has explored the intersection of chemistry and art. To satisfy the outreach component of her NSF funding, she chose to think outside the box and created the CESTA (Community Engagement of Science Through Art) program. Each year the CESTA team is tasked with creating a piece of public art that engages the community with chemical theory. The program does not simply benefit the community via the installation of a new piece of art, through which science is experienced from a different perspective; it also empowers participants with skills of cross-disciplinary collaboration, public communication (both verbal and non-verbal), and translating ideas into built, three-dimensional space.

Object D4h, an installation completed by the CESTA program team at West Virginia University (or WVU), summer '17.

Almost immediately after meeting the team, we began brainstorming. Our ideas spanned the chemical spectrum: wave-particle duality, electron transport chains, crystal packing, and synthetic pathways. No idea was too ambitious. Our brainstorming sessions were diverse in scope. We visited nearby museums and spoke to educators and curatorial staff about effective display techniques and how to promote public interaction. There were late nights with take-out where we made prototypes for a variety of our favorite pitches. We spoke with university members about location and installation. I personally spent a lot of time behind a glue gun and rotating structures in Mercury. After much deliberation, chemical symmetry and kinetic art became our foci.

Now that we had a concept, our problem shifted to maintaining theoretical integrity while applying the principles of making and design. Each time we grew close to a consensus on *what* we wanted to make, the list of barriers changed. What material was most functional? How would it be installed? Was it safe for/from the public? Did it accurately portray chemical theory?

The optimum perspective view of Object D4h, allowing the viewer to visually combine the three freestanding forms into a singular object.

Fueled by the inspiration of a binuclear organometallic molecule synthesized in the Hoover lab, a sculpture started to take form. The focus remained on symmetry, specifically point group theory, and the materials were chosen based on their function and aesthetic rendering of the intangible. The piece was to be composed of three, freestanding, kinetic sections. The team separated the object to reward viewers who explore the perspective of the object, allowing the three pieces to coalesce into one when viewed from a precise angle. Supports became rotational axes. Cut steel and acrylic became σ_h and σ_v reflection planes, dazzling when seen horizontal, but revealing sharp and intricate symmetry when experienced head-on. Stylistic choices like iridescent paint and light-diffusing acrylic accent the piece and draw in potential audiences. And, thus, *Object* D_{4h} was born.

But, the piece's impact extends beyond the tangible. A webpage was created in conjunction with the installation to allow curious individuals the opportunity to explore symmetry further. The website includes more images of and insight into *Object* D_{4h}, as well as more detailed descriptions of symmetry operations, complete with *.gif* images which illustrate symmetry operations. During the piece's residency and beyond, I hope that *Object* D_{4h} serves as an inspiration to artists, scientists, and general viewers alike.

Object D_{4h} remains on display at the Evansdale Library on the WVU Evansdale Campus. To find out more about the project and sculpture, visit ***cestasymmetry.wordpress.com***. Special thanks to team members Trevor Bryson, Cornelius Hugo, Umida Urjanova, Eric Schreiber, and Bridget Stamp. Additional thanks our mentors: Jessica Hoover, Jason Lee, and Todd Hamrick. The CESTA program will run for a minimum of 2 more years.

Side on view of Object D4h in the Evanston Library. Visitors are welcome to circumnavigate the piece in order to explore symmetry operations from different perspectives.

Owen Phillips (PhD candidate at Georgetown U)

Annual Statement of Ownership, Management, and Circulation

1. Publication Title: ACA Bell/Gross
2. Publication Number: 1958-9945
3. Filing Date: September 27, 2017
4. Issue Frequency: Quarterly
5. Number of Issues Published Annually: 4
6. Annual Subscription Price: $1.75
7. Location of known office of Publication is: 700 Ellicott Street, Buffalo, NY, 14203
8. Location of Headquarters or General Business Office of Publisher: PO Box 96, Ellicott Sta., Buffalo, NY, 14205
9. Full Names and Complete Mailing Addresses of Publisher, Editor and and Managing Editor: Publisher: ACA C/O 700 Ellicott Street, Buffalo, NY, 14203; Editor: Judith Flippen-Anderson, 3521 Lancelot Way, Annandale, VA 22003; Managing Editor: Thomas Koetzle, 35 Arties Dr., Dix Hills, NY 11746
10. Owner: American Crystallographic Association, Inc.
11. Known Bondholders, Mortgagees, and Other Security Holders Owning or Holding 1 Percent or More of Total Other Securities: None
12. Tax Status: Not Changed During Preceding 12 Month

15. Extent and Nature of Circulation			Average No. Copies Each Issue During Preceding 12 Months	No. Copies of Single Issue Published Nearest to Filing Date
a. Total Number of Copies (Net press run)			1300	1300
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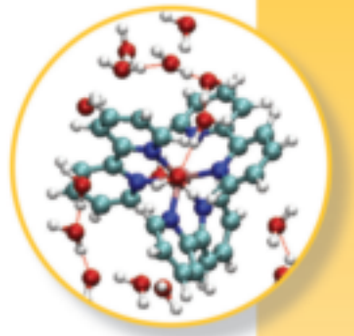
16. Publication of Statement of Ownership will be printed in the Winter 2016 issue.
17. I certify that all information furnished on this form is true and complete.
(signed) Marcia Colquhoun for American Crystallographic Association, Inc.

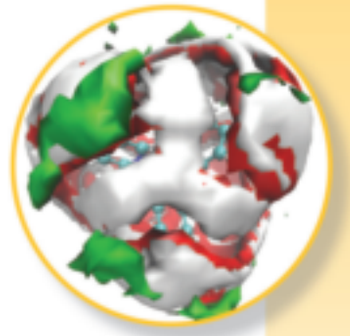
Femtosecond few- to single-electron point-projection microscopy for nanoscale dynamic imaging
A. R. Bainbridge, C. W. Barlow Myers, W. A. Bryan
Structural Dynamics **3**, 023612 (2016)
DOI: 10.1063/1.4947098

Ultrafast structural dynamics of the orthorhombic distortion in the Fe-pnictide parent compound BaFe2As2
L. Rettig, S. O. Mariager, A. Ferrer, S. Grübel, *et al.*
Structural Dynamics **3**, 023611 (2016)
DOI: 10.1063/1.4947250



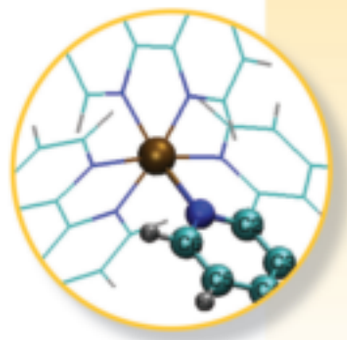
Free electron laser-driven ultrafast rearrangement of the electronic structure in Ti
E. Principi, E. Giangrisostomi, R. Cucini, F. Bencivenga, *et al.*
Structural Dynamics **3**, 023604 (2016)
DOI: 10.1063/1.4935687

Solvation structure around ruthenium(II) tris(bipyridine) in lithium halide solutions
Ida Josefsson, Susanna K. Eriksson, Håkan Rensmo, Michael Odelius
Structural Dynamics **3**, 023607 (2016)
DOI: 10.1063/1.4939898



Investigating vibrational relaxation in cyanide-bridged transition metal mixed-valence complexes using two-dimensional infrared and infrared pump-probe spectroscopies
Karla M. Slenkamp, Michael S. Lynch, Jennifer F. Brookes, Caitlin C. Bannan, *et al.*
Structural Dynamics **3**, 023609 (2016)
DOI: 10.1063/1.4943766

Effective doublon and hole temperatures in the photo-doped dynamic Hubbard model
Philipp Werner, Martin Eckstein
Structural Dynamics **3**, 023603 (2016)
DOI: 10.1063/1.4935245



Structural Dynamics is a peer-reviewed, open access, online-only journal that highlights research articles on structural determination and dynamics of chemical and biological systems and solid materials, enabled by the emerging new instruments (e.g. XFELs, high harmonic generation, electron sources, etc.) and new experimental and theoretical methodologies.

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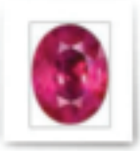

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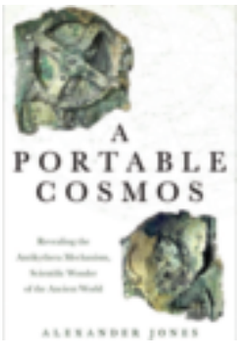

A Portable Cosmos: Revealing the Antikythera Mechanism, Scientific Wonder of the Ancient World by ***Alexander Jones***, Oxford University Press, New York, 2017, 312 pages, ISBN 978-0-19-973934-9

When we think of the wonders of the ancient world, architectural feats like the Pyramids of Giza and the Lighthouse at Alexandria in Egypt come to mind. But the Antikythera Mechanism was, or rather is, a wonder of the ancient world as well—but a scientific one.

Considered to be the world's oldest analog computer, the Antikythera Mechanism consists of over 80 fragments of bronze. Sponge divers discovered it in a shipwreck off the coast of the Greek island of Antikythera in 1901 (hence the name). But the sponge divers had no idea that the lumps of bronze they had uncovered were part of a portable cosmos, a means by which the ancient Greeks tracked and studied the movements of the universe. The Antikythera Mechanism simulated the motions of the stars and planets as the Greeks understood them to move, betraying the advanced nature of the astronomical sciences in the classical era.

Thanks to modern technology like radiographic tools and surface imaging, modern scientists have been able to painstakingly piece back together this ancient artifact, revealing many of the device's secrets.

Jones details the history of the Antikythera Mechanism, as well as the details of its discovery and the efforts of researchers to unlock its secrets. He leaves no stone unturned, carefully and methodically answering every possible question the reader might have before it even occurs to the reader to have the question.

A Portable Cosmos is an interesting, thoughtful read, and I highly recommend it for anyone with an interest in the classics, astronomical sciences, or the history of computing.

Jeanette S. Ferrara

I have been focused on a number of recent titles that analyze current events so I am a bit behind on my reviews of science oriented books. Here is what I've read the last few months.

Al Franken, Giant of the Senate by ***Al Franken,*** Hachette Book Group, Inc. New York, 2017, 416 pp, ISBN-13:978-1455540419.

Al Franken has not been funny since he became a politician--at least on purpose--until now. Here Senator Franken describes growing up in the Minneapolis suburb of St. Louis Park, becoming a comedian and making it at *Saturday Night Live*, becoming a United States Senator and finally a description of his time on the Hill. Interspersed in the narrative are the trials and tribulations we all face as Americans. *Note added in proof: Al Franken is now an ex-Senator as a a result of sexual misconduct. While the book is still a good read, paying for a copy now would effectively condone bad behavior. You should borrow an existing copy instead.*

This Fight Is Our Fight: The Battle to Save America's Middle Class by ***Elizabeth Warren***, Henry Holt and Co., New York, 2017, 352 pages, ISBN-13: 978-1250120618

Senator Warren describes her life growing up in Oklahoma with her mother as breadwinner, getting into college, dropping out to have a family, then going back to school and ultimately becoming a lawyer. She had been teaching law for nearly 35 years when she was elected Senator in 2012. Senator Warren's book focuses on the issue she has tried to address as a United States Senator: trying to provide the lower classes with the tools to advance in society as she was able to do so.

The Colder War: How the Global Energy Trade Slipped from America's Grasp by ***Marin Katusa***, John Wiley & Sons, Hoboken, 2015, 272 pages, ISBN-13:978-1118799949

This book was recommended to me by a colleague. It describes, in detail, Putin's rise to power and the slow but gradual takeover of the world energy markets--oil, gas and uranium--by the Russian Federation. This book predates the 2016 election but one can see how the need to maintain momentum in dominating world markets, eg thinking sanctions would be reduced by selecting a pro-Putin candidate and interfering in the 2016 election.

Devil's Bargain, Steve Bannon, Donald Trump and the Storming of the Presidency, by ***Joahua Green,*** Penguin Press, New York, 2017, 288 pp, ISBN-13:978-0735225022

This is a short biography of Steve Bannon. It follows him from his early years in Catholic schools, to his time in the US Navy, and his work at Goldman-Sachs. Then it details his career in television and movie making, his tenure at Breitbart News and ending with his appointment as Chief Strategist. The author also provides a history of the relationship between Bannon and President Trump and explains how Bannon was instrumental in restricting the campaign to help Trump with the 2016 election. *Note added in proof. A new book titled "Fire and Fury" by Michael Wolff was released on January 5th. Look for a review of this title here in three months.*

What Happened by ***Hillary Rodham Clinton***, Simon and Schuster, New York, 2017, 512 pp, ISBN-13:978-1501175565

You will either agree wholeheartedly with Secretary Clinton's analysis of why she lost the 2016 election or you will vehemently disagree. There is a lot of discussion about family and friends which could have been left out to focus more on the facts of the 2016 election. A volume two of this book will probably come out once the Mueller investigation is complete and Clinton's arguments about Russian meddling in the election are verified.

Joe Ferrara

ACA Election Results

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Diana Tomchick

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Krystle McLaughlin

Education
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Data and Standards
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Chief Science Officer, Rigaku Americas Corp., The Woodlands, TX; Deputy Director, X-ray Research Laboratory, Rigaku Corporation, Tokyo, Japan.

Statement: I have been a member of the ACA since I began my career as a professional crystallographer with Molecular Structure Corp. in 1988. As a member I have been active in the ACA by voting regularly and attending, exhibiting and presenting at ACA conferences over the years. I did not become active beyond being a member in good standing until 2011. At that time Judith Flippen-Anderson, co-editor of *Reflexions*, asked if I would provide some book reviews. With that I became the *Reflexions* Books Editor. However, I did not become truly active until 2014 when the annual meeting attendance dropped to a level we had not seen in decades. At that point in time I decided that I needed to become part of the solution; it was time to take action to improve the annual meeting and the ACA itself. Since then, I have been an active member in the Data Standards and Computing Committee, the 2019 Site Selection Committee, and the ACA 2.0 Transition Committee.

The ACA is undergoing profound changes. In the early 2000s we had over 2200 members; we now have just over 1000 members.

Past-presidents Chris Cahill and Tom Terwilliger began, and current president Amy Sargent is overseeing, a transition in the management of the organization that was precipitated by the retirement of Marcia Colquhoun and Bill Duax's preparatons to retire. As part of this transition we need to carefully align the business aspects of the ACA with the needs of the membership. To me, this means having the appropriate number of staff running the ACA on a day-to-day basis and ensuring the organization fulfills the needs of the membership.

The ACA's investments have been growing under the management of CFO S.N. Rao. These investments provide the funds that endow our awards and are important to the standing of the ACA as a scientific society. The ACA needs to take over management of the investments in preparation for Rao's retirement. Rather than leave the investments in the hands of a single person I would organize a committee, answerable to the Council, to manage the investments through a low-cost investment firm, such as Vanguard.

The big question that needs to be answered: what can we do about increasing our membership? Every year, I see a lot of the same faces at the annual meeting. This indicates to me that we are not bringing enough young people into the ACA. We need to have a membership drive to increase the rolls. Here, I think we can learn some lessons from our sister society, the BCA, which nearly doubled their membership when Elpseth Garman became their president. Her method was very simple; provide a chance for an annual meeting registration for every 10 new members brought in. The difficult task will

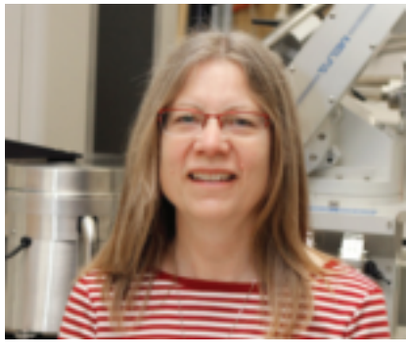
be keeping the new members, and there are a lot of smart people in the ACA that can help. Once we bring in more members, we will have more resources to improve the membership experience.

I feel that I am highly qualified for the position of vice president and eventually president of the ACA. I began studying crystallography as a graduate student at Case Western Reserve University in 1984. Thirty-three years later I am still practicing crystallography and still learning. In 1988 I joined a small company called Molecular Structure Corporation (MSC). MSC was bought by Rigaku in 1996 and I have been with Rigaku since that time. I have been part of, or led, the team that brought many tools for crystallography to the market. This required me to stay in touch with the community and foster many long-term relationships. As a manager in a large company I am required to consider the fiscal consequences of any technical decision I make.

In my spare time I train as a firefighter, for which I am certified at the basic level in Texas. I have been a member of the same all-volunteer department, a 501(c)(4) organization, for almost 25 years. In addition to meeting the training requirements, I have served on the department's Executive Committee for all but 4 years. For the last 15 years I have been Treasurer. My responsibilities as Treasurer include creating budgets, managing the disbursement of all the taxpayer and non-taxpayer funds within prescribed budgets, and interacting with Emergency Services District commissioners, auditors, Texas Workforce Commission and the IRS.

These experiences have taught me how to work with people and achieve difficult goals. I believe I can effectively lead the effort to restore the ACA to the organization it once was: a family of scientists who love their chosen field and enjoy the camaraderie of like-minded professionals.

Diana R. Tomchick - Secretary



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

Statement: It has been an eye-opening and fascinating opportunity to serve as your ACA Secretary for the last 2.5 years. In addition to the typical duties of preparing meeting minutes, the ACA Secretary is a voting member of the ACA Council. In consultation with the ad-hoc Long-Range Planning Committee, the ACA Council has approved a 3-year plan for succession as long-serving Director of Administrative Services Marcia Colquhoun and Chief Executive Officer William Duax step down from their duties. While this plan will help with the financial bottom line for the organization, more work needs to be done, including developing strategies for cost reduction (to the ACA and to members) at meetings and methods to attract and retain members. Targeting practitioners and students interested in novel structural techniques such as electron diffraction, cryo-electron microscopy, tomography and other methods while not ignoring the interests of our current members is one of my goals.

Professionally, I work at a graduate-level biomedical institution as the Director of a campus-wide core facility that provides expertise in determining macromolecular structures. This position requires significant organizational skills as well as scientific expertise, and for many campus research groups I am the professional "face" of structural biology. Perhaps my most important role is as an educator, as I provide expertise in current methods to members of the campus community through the classroom and individual consultation on structural projects, and ensure best practices in the publication of results. The ACA provides a critical resource for members to network and keep abreast of scientific and technical advancements, and to educate the next generation of scientists as well as the general public. As Secretary I will work diligently to support the efforts of the organization as well as the other officers and various committee chairs in furthering these goals.

Krystle McLaughlin - Communications

Assistant Professor, Chemistry Department, Vassar College

Statement: I am enthusiastic about the opportunity to serve on the Communications Committee. This Committee plays a vital role in showing ACA members, others in the scientific community, and the public all of the excellent work and events coming out of the ACA, and I am excited to be a part of that. As an educator, I am very passionate about communicating and generating interest in science as well as discussing issues in science and society.

Since attending my first ACA meeting as a graduate student, I have been pleased to be part of such a vibrant community of scholars. For the past several years I have enjoyed working to support and grow the ACA. For example, through a partnership with the AIP Society of Physics Students I helped start a student symposium and a new undergraduate poster prize to encourage and excite undergraduates to attend the ACA annual meeting. I also worked to introduce the Diversity and Inclusion Session at the ACA meeting, where we highlight research and strategies on diversity issues from crystallographers in our community. Additionally, through online platforms such as blogs, newsletters and social media platforms like Twitter, I actively engage with the wider scientific community on a regular basis and will

enjoy helping ACA expand its reach in these areas. I look forward to continuing to support the ACA, and as a part of the ACA Communications committee I believe I can continue to help ACA grow, adapt and expand.

Peter Wood - Continuing Education

Senior Research & Applications Scientist, Cambridge Crystallographic Data Centre, Cambridge, UK

Statement: I am pleased to serve on the Continuing Education Committee and very much welcome the opportunity to be involved. Education has always been a strong interest of mine right from the beginning of my postdoctoral career. I've been involved with a number of crystallography schools targeted at postgraduates over the last 8 years, but particularly the biannual advanced crystallography school held in Durham, UK. The experience of tutoring PhD students in the nitty-gritty details of the math, physics, chemistry and symmetry underpinning crystallography for 7 full days is hard work, but incredibly fulfilling! It's always exciting to talk through the concepts with a fresh new batch of students, to hear different perspectives/backgrounds and to refresh my own knowledge.

I've also been involved in organizing and running educational workshops at a wide range of academic crystallography meetings over the last decade (including the ACA). These kinds of workshops are extremely helpful for both academic and industrial scientists - to be able to expand one's knowledge and skills in a particular area at a conference you are already going to be attending. When you are tight for time and travel budget, making the most out of the one or two conferences you can attend is even more important. This of course means that it should be a strong focus for the Continuing Education Committee to keep abreast of developing and emerging techniques to ensure that the workshops being planned are appropriate, current and of strong interest to the community..

In recent years I've also become more interested in the presence and impact of crystallography in undergraduate education in schools and in public outreach. I think we, as a community, have a responsibility to continue to communicate the benefits of crystallography and, in particular to help to integrate crystal structures into undergraduate chemistry courses. Compared to other experimental techniques, crystallography and crystal structures are strangely underrepresented in undergraduate chemistry.

I've been coming to ACA meetings since 2007, organizing workshops, speaking and chairing sessions; always enjoying the experience, the science and the atmosphere. Despite not being based in the US myself, I've always felt warmly welcomed into the ACA community and I look forward to serving that community as a part of this committee..

Paul Sanschagrin - Data, Standards & Computing

User Application Scientist, Cambridge Crystallographic Data Centre, Piscataway, NJ

Statement: I am honored to serve on the ACA Data Standards and Computing committee. As someone who has spent his career utilizing structural data as a basis for research, I am keenly aware of the importance of data standardization, both of the data itself and of the metadata that provides context to the data. This is a time when not only is the amount of chemical structural data, crystallographic data and data from other techniques, growing at a significant rate, the amount of data from other connected scientific fields is exploding. The possibility of connecting the structural data to this other data holds promise for enabling scientists to discover deep insights into biological processes, materials properties, and many more important areas. Key to this data synthesis is the ability to understand the content and context of the data, both for humans and computers. In the crystallographic community, we are fortunate to have a long history of uniform data formats including CIF, PDB, mmCIF, and PDBML. Therefore, it is key to continue to maintain these standard formats and to work with database organizations, software developers, and instrument manufactureres to ensure the community's needs are met. It is also important to consider where future data may come from that is not be well covered under existing formats, such as x-ray free-election lasers or Cryo-EM, fields that may also be relevant to structural chemistry and biology. In addition to considering the structural data, which may be considered the results of the experiment, it is becoming more apparent that having the raw data, at least structure factors but perhaps even the x-ray images themselves, can have significant advantages as refinement and other data processing methods improve. This poses significant challenges in terms of reading the data in proprietary or obsolete instrument formats, storage sizes, and network bandwidth issues.

We must also consider the potential for the widespread use of large-scale computing through cloud services, such as Google Cloud, Amazon Web Services, and Microsoft's Azure, as well as through shared systems such as XSEDE. Having uniform standards for data, including metadata for providing context for the data itself, is especially key where users from various organizations and research groups may be utilizing the same datasets. The ACA can, and already does, play a significant role in maintaining data standards and it is key that it continues to play a role.

2018 Award Winners

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Simon Billinge

Etter Early Career
Jason McLellan

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Charles Carter
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Jon Clardy
Joseph Ferrara
James Golen
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Ronald Hamlin
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Marie McKenna
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Matthew Whitley

Ned Seeman (in memory of Brian Craven)

Puzzle Corner

For this issue, we have a new **Crystal Connections** puzzle, the solution to the previous one, the solution to the Nobel laureate word-search puzzle by **Guest Puzzler** ***Joe Ferrara***, and mention of those who provided solutions to previous puzzles..To date no solution has been submitted for ***Crystal Connections #12***

Crystal Connections #13

What do the answers to these clues have in common?

1) "And farther below _____ _____ takes in what Lake Erie can send her."

2) (Fibonacci number following 610) + 6! + 19^2 - 4^3 + 5

3) Irish spelling of *loch*

4) 553.3 meters tall, completed in 1976

5) Members of species *Cyanocitta cristata*, in a yarn by Mark Twain from *A Tramp Abroad*

6) Published the structure of rubber in 1954

7) Earnest Hemingway wrote for this newspaper around 1920.

Solution to Crystal Connections #12 - *Crystal habits*

1) Deck ***prism***: for transmitting natural light below deck in sailing ships

2) Full-page illustration; scute - ***plate***

3) "Well I headed for Las Vegas, Only made it out to ***Needles***"

4) Highest symmetry hexahedron - ***cube***

5) ***Pyramid*** of the Moon, Teotihuacan

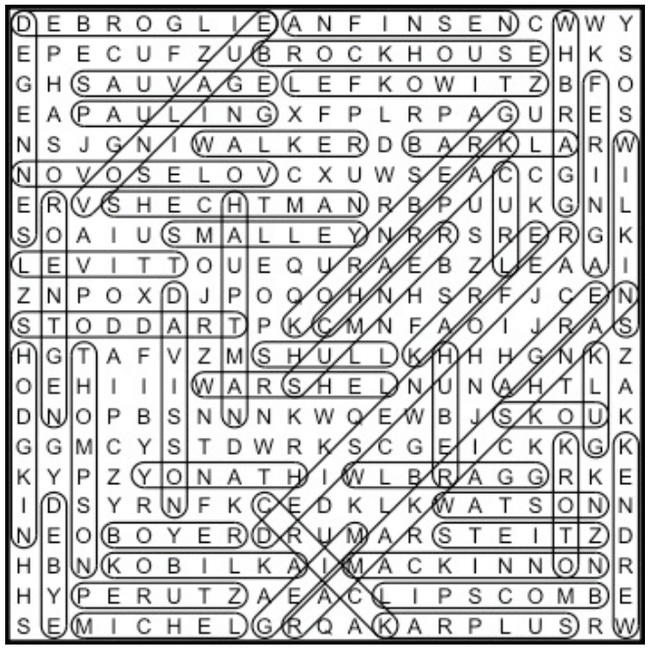
6) A one-person hot air balloon; type of rail car - ***hopper***

7) The Doric temple at Segesta is thought to have never been completed, since these are not fluted - ***columns***

8) ***Blade*** Runner: 1982 movie based on *Do Androids Dream of Electric Sheep*?

9) The ***Wedge***: *Prelude and Fuge in E Minor*, J.S. Bach; a golf club

10) A 3-ball in the Manhattan L_1 Metric, Taxicab geometry - ***octahedron***

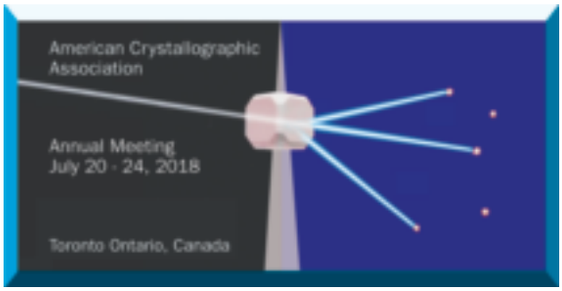


The 52 Nobel laureates associated with crystallography in Joe's word-search puzzle are:

Agre,Anfinsen,Barkla,Boyer,Brockhouse,Charpak,Crick, Curl, Davisson, DeBroglie, Debye, DeGennes, Deisenhofer, Feringa, Geim, Hauptman, Hodgkin, Huber, Karle, Karplus, Kendrew, Klug, Kobilka, Kornberg, Kroto, Lefkowitz, Levitt, Lipscomb, MacKinnon, Michel, Novoselov, Pauling, Perutz, Ramakrishnan, Roentgen, Sauvage, Shechtman, Shull, Skou, Smalley,Steitz,Stoddart,Sumner,Thompson,VonLaue,Walker, Warshel, Watson, WHBragg, Wilkins, WLBragg, Yonath. See solution above.

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

Frank Fronczek – ffronc@lsu.edu



ACA TORONTO

Friday, July 20 - Tuesday, July 24, 2018

Sheraton Centre Toronto Hotel

Travel Grant Application Deadline: March 31, 2018

www.amercrystalassn.org/2018-ys-travel-funding

Abstract Deadline: March 31, 2018
Early Registration Deadline: May 31, 2018
Hotel Reservation Deadline: June 18, 2018

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

www.amercrystalassn.org

Abstract submission - Meeting registration - Full call for papers
Sponsorship opportunities
Information for exhibitors

Program Chair - Gerald Audette
audette@yorku.ca

Program Chair - Tiffany Kinnibrugh
kinnibrught@gmail.com

Posters Chair - Louise Dawe
ldawe@wlu.ca

Posters Chair - David Rose
david.rose@uwaterloo.ca

OPENING SESSION KEYNOTE SPEAKER

John Polanyi - 1986 Nobel Laureate in Chemistry

WORKSHOPS

Cryo-EM – A Guide to High-Resolution Structure Determination
Molecular Art and Animation in 3D
X-Ray Crystallography: Structure Preparation, Electron Density and Solvent Analysis
Applications of Small Angle Scattering to Structural Biology: An Introduction
Rietveld Refinement and pdf Analyses of in situ X-ray Scattering Data within GSAS-II

EDUCATIONAL SESSIONS & YSIG EVENTS

3-Minute Thesis Session
YSIG Orientation and Networking Mixer
Career Development Session
Engaging Undergraduates with Crystallographic Research
Diversity & Inclusivity Session

ACA AWARDS

Buerger Award honoring Frank Hawthorne
Warren Award honoring Simon Billinge
Margaret C. Etter Early Career Award honoring Jason McLellan

SESSIONS

Transactions Symposium – Shining a Light on Structure-Based Drug Design
Structural Dynamics – in Honor of Philip Coppens
Special Sessions in Honor of Dick Marsh
Crystallography on the International Space Station
Advances in Biological Cryo Electron Microscopy
Structural Biology of Pathogens
NMR Crystallography
Neutron and X-ray Scattering of Correlated and Quantum Materials
Dynamic Crystals as Molecular Materials
Mineralogical Crystallography

Toronto meeting logo by Harris Media Group

Transactions Symposium – Shining a Light on Structure-Based Drug Design Organizers: ***Stephen Soisson*** **and** ***Vincent Stoll***

Meeting participants working in the area of protein crystallography, cryo-electron microscopy, and with an interest in drug discovery will have an opportunity to learn from experts how cutting-edge technologies are being applied to next-generation drug discovery. Unique facets of industrial structural biology will be highlighted in the course of discussing small-molecule hit-finding efforts, such as fragment-based drug discovery, and the integration of structural and computational approaches to facilitate structure-based drug design. The role of structural information in "new" modality discovery such as vaccines, biologics and peptides will also be discussed. Unique opportunities to increase the breadth and scope of structural impact in drug discovery will be presented in context of new methods to access traditionally challenging targets such as ion channels and GPCRs, and how next generation synchrotrons, XFELs, and serial data collection techniques could play key roles in the future.

General Meeting Information

As the 2018 ACA Meeting is taking place outside of the US, advanced planning by all travelers is critical. Research should be completed on the documentation needed to access Canada and what is needed to return to your country of origin.

The following links may be helpful:

www.cbp.gov/travel/us-citizens/canada-mexico-travel)

travel.gc.ca/returning/travelling-to-canada)

www.cic.gc.ca/english/visit/apply-who.asp)

Meeting Invitation: To request a letter of participation from ACA contact the Meeting Registrar at ***aca@hwi.buffalo.edu***.

Staying Green: All attendees will receive a hardcopy of the Program Book, but the abstracts will only be available online.

Hotel Information: The entire meeting will be held in the Sheraton Centre Toronto Hotel. FREE in-room internet is included.. We are able to offer discounted room rates due to a commitment to contract for a minimum number of sleeping rooms at this hotel. If we do not fill these blocks, financial penalties will be incurred. This ultimately impacts the health of the ACA. Staying at the conference hotel also helps keep future registration fees lower.

Room rates, in Canadian dollars, are $199 for one or two people, per night (plus tax.). A special rate of $169 CAN is available for students and post docs only. Room sharing can make these rates even more reasonable – use the e Room Sharing feature under accommodations on the meeting web site at ***www.amercrystalassn.org/2018-accommodations***.

Registration Fees

Early until May 31, 2018

Members		
Regular	**$545**	**$745**
Retired	**$240**	**$340**
Post doc	**$290**	**$390**
Undergrad Student	**$235**	**$335**
Graduate Student	**$235**	**$335**
LOCAL* Students - one day	**$100**	**$100**
Non- Members		
fees include a one year ACA membership		
Regular	**$745**	**$1035**
Post doc	**$390**	**$490**
Undergrad Student	**$325**	**$425**
Graduate Student	**$325**	**$425**
Guest	**$ 65**	**$ 65**
Guest banquet ticket	**$ 70**	**$70**
Networking Mixer (May 28)	**$30 (free for students & post-docs)**	

EACH REGISTRATION FEE INCLUDES THE BANQUET ON TUESDAY, JULY 24 - but you must indicate participation when submitting registration

LOCAL* : a student registered at a college or university that is located within 150 miles of the city of Toronto
Anyone registering as a student or postdoc must include documentation of status with the registration form.

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

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

Register online or download forms to register by fax or mail.
www.amercrystalassn.org/2018-meeting-homepage
Questions: aca@hwi.buffalo.edu

Special Discounts Available for Attenting Both ACA Toronto and Aperiodic Crystals 2018 (see following page for informtion)

Financial Support: Travel support will be available for young scientists. Applications for travel support should be made by March 31, 2018. For additional information see ***www.amercrystalassn.org/2018-young-scientists***.

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

Call for Nominations - 2019Awards

2019 I. Fankuchen Award: To recognize contributions to crystallographic research by one who is known to be an effective teacher of crystallography. There are no geographic or age restrictions. The honoree delivers a lecture to the Association and at the recipient's home institution or at another institution of the recipient's choice. The Award consists of $2,500 and up to $2,500 in travel expenses to attend the Annual Meeting. Awarded every three years. Established in 1971 in memory of Dr. I. Fankuchen, Professor of Physics at the Polytechnic Institute of Brooklyn from 1942 to 1964. (Selection committee: ***L. Marks (Chair), Louise Dawe, Paul Langan and Brian Toby.***)

2019 Margaret C. Etter Early Career Award: To recognize outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career. The Award consists of a $1,000 honorarium and a plaque. The winner is also expected to present a lecture at the ACA annual meeting.

2010 K. Trueblood Award: To recognize exceptional achievement in computational or chemical crystallography. The award is established in memory of Professor Kenneth N. Trueblood, UCLA 1949-1998, who was a major force in the early use of computers and the development of crystallographic computer programs. He applied these programs to the examination of chemical and molecular details of many structures at the frontiers of research. His contribution to the famous work on vitamin B12 is one example. Professor Trueblood was a leader in the development of techniques for analysis of anisotropic motion and was also a superb teacher and a lucid author. Established in 2001, the award will be given every three years and consist of an honorarium of $1,500 and up to $1,500 in travel expenses to accept the award.(Selection committee: ***Michael James (Chair), Lee Daniels, Greg Petsko, and Claudia Rawn.***)

2019 Bau Neutron Diffraction Award: The award is in memory of Professor Robert Bau, University of Southern California (1969-2008) and President of ACA in 2006. A much beloved teacher and mentor, Professor Bau made major contributions to the development of the technique of single-crystal neutron diffraction and to its applications in chemical and biomacromolecular crystallography. Established in 2010 and presented triennially, this award will recognize exceptional research achievement in neutron diffraction and consists of an honorarium of $1,500 in cash and reimbursement up to an additional $1,500 for travel expenses to accept the award and to deliver the award lecture at an ACA annual meeting. Selection committee: ***The deadline for nominations for the 2019 ACA Awards is April 1, 2017.***

2019 ACA Offices and Committees: In the fall of 2018 we will elect a Vice-President, Treasurer, and one person to each of the ACA Standing Committees (Continuing Education, Communications, and Data, Standards and Computing). Nominating committee: ***David Rose, Tom Terwilliger and Christine Beavers .*** Suggestions are due by February 15, 2018

2019 ACA Fellows: Serves to recognize a high level of excellence in scientific research, teaching, and professional duties, but also service, leadership, and personal engagement in the ACA and the broader world of crystallography and science. Our Fellows program celebrates the excellence of our own members from within the ACA, and promotes their recognition worldwide to constituencies outside of the ACA, such as their employers, other scientific societies, and the government. See ***www.amercrystalassn.org/aca-fellows*** for information on the nomination procedure. ***Nomination forms for 2019 ACA Fellows can be found at www.amercrystalassn.org/documents/ACAnomNEW.pdf and are due by February 28, 2018.***

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

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

2018 Dues are Due

Please renew promptly and remember to support your favorite ACA Funds.

Please note: In an effort to reduce costs, you will now have the option of receiving ACA RefleXions in different formats. Select 'digital' to be sent a link to a PDF of the current issue or select 'hard copy' to continue receiving a hard copy by snail mail.

It is now possible to renew online at membership.amercrystalassn.org

Special Discounts Available for Attenting Both ACA Toronto and Aperiodic Crystals 2018

The 9th Conference on Aperiodic Crystals will be held at Iowa State University (Ames, Iowa) July 8-13, 2018. This triennial meeting is the flagship meeting of the IUCr Commission on Aperiodic Crystals (CAC) .To encourage participation at both meetings, both the ACA and Aperiodic 2018 are offering discounted fees for those who register for both meetings.

If your register for both meetings: Aperiodic 2018 registrants will receive $100 off the registration fee . and ACA registrants may register at the regular rate. Differences between early and late registration still apply and you must register separately for each conference.

Organizers will cross-check lists to ensure registration and payment for both conferences. Fees must be paid no later than one week before each respective conference.

American Crystallographic Association, Inc.

ACA Summer Course in Chemical Crystallography

www.acasummercourse.net

June 10 – June 17, 2018

University of Notre Dame

Organized by: Allen Oliver, Charlotte Stern, Christos Malliakas and Amy Sarjeant

Important Dates:

Applications Accepted – starting January 2018

Acceptance Notifications – March 2018

Registration Deadline – April 15 2018

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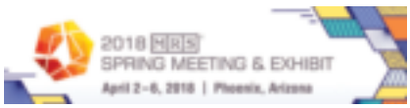
NORTHWESTERN UNIVERSITY

MARCH 2018

1-14 **Cryoelectron Microscopy**. Cold Spring Harbor, NY
https://meetings.cshl.edu



APRIL 2018

2-6 **MRS Spring Meeting & Exhibit**. Phoenix, AZ
http://www.mrs.org/fall2018

10-13 **BCA Spring Meeting**. University of Warwick, UK
http://ww.bcaspringmeetings.org.uk

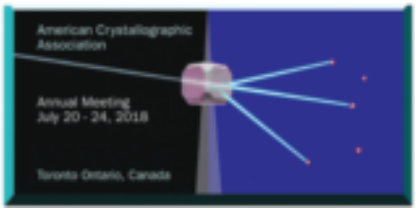
22-27 **RapiData 2018**. Menlo Park, CA
http://smb.slac.stanford.edu/rapidata/rapidata-2018

JUNE 2018

1-10 **51st Erice Course: Electron Crystallography** &
52nd Erice Course: Quantum Crystallography. Erice, Italy
http://crystalerice.org

JULY 2018

20-24 **ACA 2018 Annual Meeting**. Toronto, ON, Canada
http://www.AmerCrystalAssn.org



24-28 **ACNS-2018**. College Park, MD
https://www.mrs.org/acns-2018

AUGUST 2018

19-24 **XXVII International Materials Research Congress**. Cancun, Mexico
http://www.mrs.org/imrc-2018

22-27 **31st European Crystallographic Meeting**. Oviedo, Spain
http://ecm31.ecanews.org

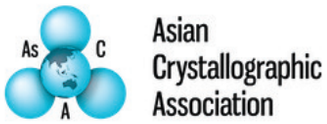
OCTOBER 2018

3-5 **III Meeting of the Latin American Crystallographic Association**. Valparaíso, Chile
https://cristalografia.cl/3rdlacameeting

15-30 **X-ray Methods in Structural Biology**. Cold Spring Harbor, NY
https://meetings.cshl.edu

DECEMBER 2018

25-30 **AsCA 2018**. Auckland, NZ
http://asca.iucr.org



JULY 2019

20-24 **ACA 2019 Annual Meeting**. Covington, KY
http://www.AmerCrystalAssn.org

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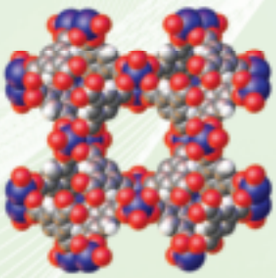
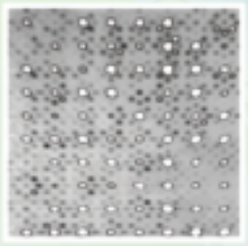
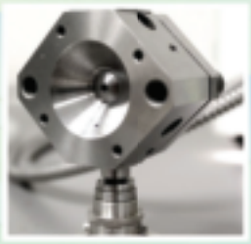


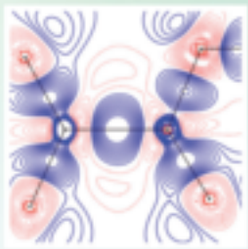
MOFs



Incommensurates

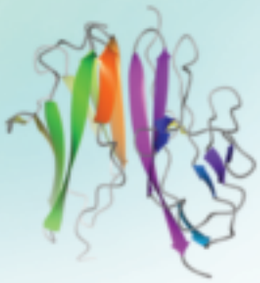


High Pressure



Charge Density

In situ



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