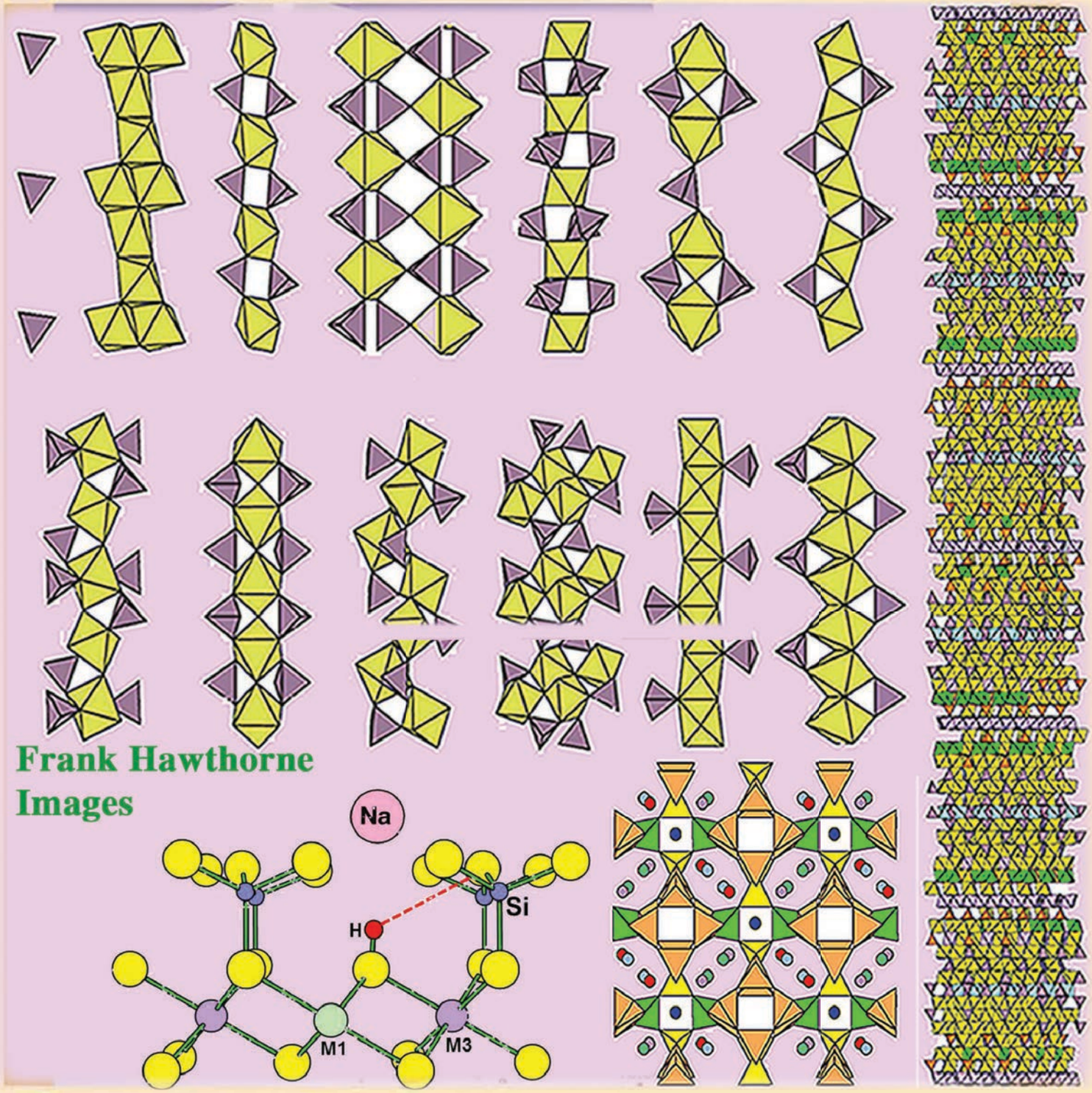
ACA RefleXions

American Crystallographic Association
Structure Matters

Number 2

Summer2018



Buerger Award at Toronto ACA Meeting

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ACA RefleXions

ACA – Structure Matters

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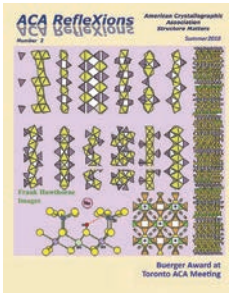
Table of Contents

Lisa Keefe
2018 ACA President



What's on the Cover
Page 8

2018 ACA Award Winners to Be Honored in Toronto

Jason McLellan
Etter Early Career Award

Frank Hawthorne
Buerger Award

Simon Billinge
Warren Award

Nobel Laureate John Polanyi
Keynote Lecturer in Toronto

Contributions to ***ACA RefleXions*** should be sent to the *Editor*:

Edwin D. Stevens ..... edwin.stevens@wku.edu

Cover:	Connie Rajnak	Book Reviews:	Joseph Ferrara
Historian:	Virginia Pett	News & Awards:	Kay Onan
Photographer:	Peter Müller	Puzzle Corner:	Frank Fronczek
Copy Editing:	Sue Byram	Spotlight on Stamps:	Daniel Rabinovich

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

Kristin Stevens, Director of Administrative Services
American Crystallographic Association
P. O. Box 96, Ellicott Station
Buffalo, NY 14205
tel: 716-898-8627; fax: 716-898-8695
kstevens@hwi.buffalo.edu

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President's Column


Lisa Keefe

It's all about structure—ACA aims "to promote the study of the arrangement of the atoms in matter, its causes, its nature and its consequences, and of the tools and methods used in such studies" (By-Laws of the ACA), as well as "to promote interactions among scientists who study the structure of matter at atomic (or near atomic) resolution," (About ACA, ACA website). The American Institute of Physics (AIP), of which the ACA is a member society, is instrumental in promoting our science of structure through a variety of mechanisms, including reporting on significant achievements and discoveries, highlighting science from our annual meeting, supporting our journal Structural Dynamics, advocating for the support of our scientific research, and providing tools and services for strengthening our society. It has become ever more important for scientific societies to be strong voices in promoting science and advocating for support of research. ACA is diligently doing its part.

Publications speak volumes. Central to promoting the science of structure is ACA's journal, Structural Dynamics—a peer-reviewed, open access, online-only journal co-published by ACA and AIP Publishing. Structural Dynamics publishes on all matters structure, from structure determinations to dynamics of systems, whether it be experimental or theoretical. Recent articles have focused on emerging areas of structural research using X-ray free-electron lasers or time-resolved approaches to study surfaces and interfaces, liquids and solutions, materials, and biological systems. Emanating from these new areas of development are innovative instruments, novel methodologies, and elucidation of complex structures and systems. Embracing these exciting areas of structural science, ACA showcases key developments and associated challenges in the Transactions Symposium sessions at the annual meetings. Papers from these Transactions Symposium sessions will be published in Structural Dynamics.

Education and outreach are essential. The ACA Summer School serves to educate the next generation of structural scientists as well as to integrate structural science into complementary areas of research. In addition to supporting the summer school, ACA supports other schools by offering eligible participants a complementary one-year student membership in ACA. Course organizers should contact ACA headquarters for details.

Annual ACA meetings provide numerous opportunities to connect. At the 2018 meeting in Toronto, to complement the scientific sessions are the exhibit show, poster sessions, social events, SIG meetings, and business meeting. All ACA members are encouraged to attend the ACA business meeting at which council reports on the financial status of ACA, presents on accomplishments, and announces news such as the focus of the next year's Transactions Symposium. Planning is underway for the 2019 meeting in Cincinnati / Northern Kentucky; SIGs are soliciting input for session topics and will meet in Toronto to make final decisions. Council is pleased to announce the locations of the following future meetings: 2020 in San Diego, 2021 in Baltimore, and 2022 in Portland, OR.

AIP enriches ACA member's experience. Keep abreast of federal science policy through AIP's FYI—a news and resource center for federal science policy that focuses on the physical sciences. Offerings include free subscription to news weekly (FYI This Week) and monthly (FYI Bulletin), as well as information on the FYI website (under 'Publications' menu) for tracking budgets and bills. AIP provides forums through which the member societies can jointly advocate for support of science. In March, ACA Council leadership and appointed representatives attended the AIP Assembly of Society Officers meeting and Annual Meeting of the Corporation. The focus was on communicating science accurately, advocacy for support of the physical sciences, and strategic planning for long-term sustainability. AIP representatives will attend the ACA meeting in Toronto, meeting with Council and noting science highlights for promotional reporting.

Your continued membership in ACA is vital to the sustainability of ACA. Membership is important for recognitions, nominations, invitations to represent ACA in a variety of capacities both within ACA and in the global community, and AIP, as well as other activities of ACA. Continuous annual support of ACA will enable ACA to provide enriching services for career development, opportunities for highlighting scientific discoveries, and promoting structural science. Coming soon for ACA members is recognition for continued membership in ACA. Regardless of whether or not you attend the annual meeting, please renew your ACA membership annually.

Next year, ACA will celebrate 70 years of promoting structure and facilitating interactions among scientists. ACA is looking to the future. The 2019 annual meeting in Cincinnati / Northern Kentucky will build upon the exciting scientific advances reported in Toronto. As ACA's reach extends into new areas of structural science, so will the ACA website and the structure of the

annual meeting evolve. The design of a new website is underway with a targeted launch date in late 2018. Over the next several years, annual meeting attendees will experience an evolution to contemporary meeting structure as Council and meeting organizers work to implement changes that will enhance the meeting experience. Throughout these processes, your input is welcome. Connect with ACA council. Celebrate 70 years of structural science and participate in the evolution of your ACA for the next 70 years.

Lisa Keefe

RefleXions from Canada

Tomislav Friščić

This is a particularly exciting summer for Canadian crystallographers, as the annual ACA meeting is taking place this July in Toronto, Ontario, whose organization is spearheaded by **Gerald Audette** from **York University** and **Tiffany Kinnibrugh** from **Elmhurst College**. So, I thought it would be appropriate to highlight a few details from this upcoming meeting, with a little bit of input from Gerald. The ACA meeting is his primary meeting every year, and he tells me that all of the sessions look absolutely stunning. However, he is particularly excited by **Cryo-EM sessions Advances in Biological Cryo-Electron Microscopy 1** and **2** (**2.1.4** and **2.2.4**) that represent the new Cryo-EM SIG as of 2018. He also tells me to keep an eye on the Dynamic Crystals session (**1.1.3**) organized by **Louise Dawe** from **Wilfrid Laurier University** and **Dmitriy V. Soldatov** from the **University of Guelph**. Gerald's background on structural biology makes him also especially keen on the sessions on the **Structural Biology of Pathogens** (**3.1.1** and **4.1.1**) and on the **Structural Biology of Inherited Metabolic Disorders** (**3.2.1**). As one last bit, Gerald also mentioned the **Crystallization on the International Space Station** session (**3.2.2**), which will promote STEM among students from local university summer camps by offering a part of the session being open to the public and students. So much from Gerald and, as we are already highlighting sessions, guess it is OK if I also provide a plug for the one on **NMR Crystallography** (**2.1.3**) that I am co-chairing with **Manish Mehta** from **Oberlin College**.

I would also like to highlight two Canadian researchers that I have had the opportunity to get to know well over the past years. Although of very different backgrounds and at very different stages in their careers, they are certainly among the most enthusiastic and dynamic contributors to X-ray diffraction, crystallography and crystal engineering in Canada. One of them is the above mentioned **Dmitriy** (**Dima**) **Soldatov**, who is an Associate Professor at the Department of Chemistry, **University of Guelph**. Dima (Figure 1a) has made significant contributions to the understanding and the design of molecular solids based on coordination complexes. He obtained his M.Sc. in solid-state coordination chemistry from the Novosibirsk State University in Russia, and his Ph.D. was performed between the Institute of Inorganic Chemistry of the Russian Academy of Sciences and the Institute of Physical Chemistry of the Polish Academy of Sciences. He moved to Canada in 1999 as a post-doctoral researcher with John A. Ripmeester at the NRC Steacie Institute for Molecular Sciences in Ottawa, before settling in a faculty position at the University of Guelph in 2007. In Canada, Dima has rapidly established a reputation as an expert crystal engineer, pioneering the field of soft materials which, although not inherently microporous, possess a highly flexible structure that can be re-organized to achieve molecular capture and gas sorption. More about this topic can be found in his authoritative review in *J. Chem. Cryst.* **2006**, *36*, 747. Dima's design of such soft supramolecular materials, a term coined by him, was based on ingenious use of coordination bonds to easily assemble molecular complexes whose "wheel-and-axle" shapes prevent them from forming

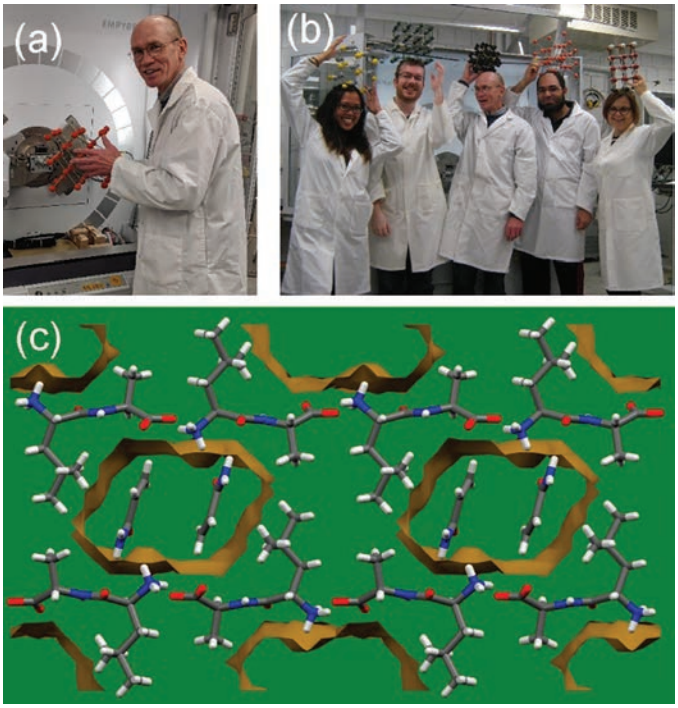


Figure 1. (a) **Dima Soldatov** is in his element in the diffraction lab, handling large crystal structures. (b) The Soldatov group, in good cheer, having fun the way only crystallographers can (left-to-right): **Angel Ho**, **Aaron Smith**, **Dima Soldatov**, **Farukh Ali**, and **Ielizaveta Poloz**. (c) Image of large host-containing voids in the crystal structure of one of the dipeptides being investigated by the Soldatov group.

very stable close-packed crystalline materials. Today, Dima's research group (Figure 1b) has switched focus towards utilizing crystal engineering and solid-state organic reactions to create new ways for valorization of biomass. They are investigating how solid-state assembly of oligopeptides can lead to new types of solid-state reactivity, for example through incorporation of small guest biomolecules (Figure 1c). I am particularly excited by their investigations of thermal reactivity of small peptide crystals, for example the work published in *Cryst. Eng. Comm.* **2014**, *16*, 7196. This research has recently led Dima's team to unravel a simple, efficient methodology to cyclize simple, inexpensive dipeptides, yielding piperazine structure of high value, for example in pharmaceutical chemistry.

Soldatov is a careful and meticulous researcher who is capable of transferring his outstanding knowledge, expertise and, most importantly, tremendous enthusiasm in solid-state chemistry and crystallography to his students. His enthusiasm and dedication have made him an important part of our solid-state and materials community: he is the Secretary of the **Materials Division** of the **Canadian Society for Chemistry** (**CSC**) and for the past two years he has been the central person in organizing the highly popular "Molecular Materials" Symposia at the annual CSC meetings. This Symposium has been tremendously successful in bringing together the top molecular materials and crystal engineering researchers from Canada and abroad, and Dima tells me that the next edition is already being prepared by him, **Kathryn Preuss** and **Stephen Loeb**, for the upcoming 102nd CSC meeting in Quebec City. Dima has been the Executive Editor of the *Journal of Structural Chemistry* since 2006, and he is also a central figure for users of the Cambridge Structural Database (CSD) in Canada, who are indebted to him as the **Director of the CCDC National Affiliate Centre Canada**. This is a position he has held for the last 10 years, distributing licences, helping Canadian users, and generally acting as a voluntary mediator between Canadian crystallographers and the Cambridge Crystallographic Data Centre (CCDC). I also have the pleasure of working with Dima in organizing a recently emerged tradition in Canada – the **Crystal Engineering and Emerging Materials Workshop of Ontario & Quebec** (**CEMWOQ**) meetings, which bring together researchers from all aspects of solid-state sciences, Crystal Engineering and materials chemistry. Along with his colleague Kathryn Preuss, he has organized the CEMWOQ-2 at the University of Guelph and is a permanent member of the CEMWOQ Steering Committee that is helping me organize the upcoming CEMWOQ-5 event in Montreal this July. You can check out how that is going along on the conference webpage: http://friscic.research.mcgill.ca/CEMWOQ5.html and Twitter feed (**@CEMWOQ**).

My second highlight in this column is **Vedran Nicholas** ("**Nick**") **Vukotic**, a rising star who is building his career at the interface of academia and industry. Nick (Figure 2a) and I actually share Croatian origins - he was born a stone's throw away from the old city walls of Dubrovnik (Croatia) before moving to Canada at a young age. He received his Ph.D. from the **University of Windsor** working with Professor Stephen Loeb (who was also highlighted in one of last year's columns) where he was awarded an *NSERC* **Alexander Graham Bell Canada Graduate Scholarship**. His work on incorporating mechanically interlocked molecules (MIMs) into metal-organic frameworks (MOFs) resulted in a number of publications and two landmark *Nature Chemistry* articles. This work (*Nat. Chem.*, **2015**, *7*, 514) was actually highlighted by *Nature* as an important contribution to the field when the 2016 Nobel Prize in Chemistry was awarded for the "design and synthesis of tiny molecular machines." The archetypal compound *UWDM-1* (University of Windsor

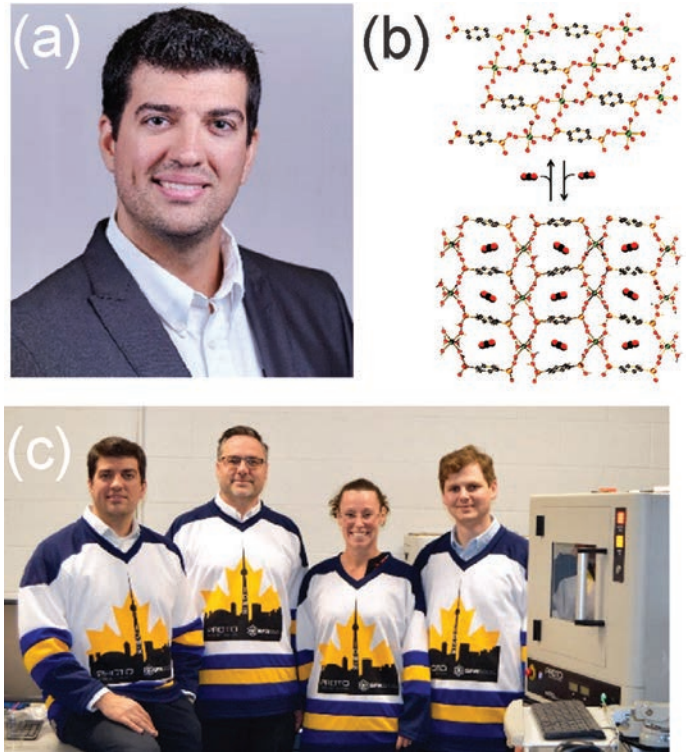


Figure 2. (a) **Nick Vukotic** is having a good day as he just published a paper demonstrating a novel high-pressure cell for a benchtop diffractometer: (b) The work was published in the high-impact journal CHEM in collaboration with the Shimizu group in Calgary (*CHEM*, 2018, **4**, 868) and investigates a CO_2 pressure-induced closed-to-open transformation of a hydrogen-bonded organic framework (HOF). (c) Nick and his team at the instrument manufacturer PROTO Manufacturing Ltd., who was a gold sponsor of the Inorganic Discussion Weekend (IDW) 2017 (left to right): Nick, **Robert Drake** (Sales Manager), **Janet Casey** (Marketing Specialist and Graphic Designer) and **Stanislav Veinberg** (Application Scientist).

Dynamic Material) demonstrated that large amplitude rotational dynamics of a macrocyclic component of a MIM could function inside a MOF, as confirmed by single-crystal X-ray diffraction and H^2 solid state NMR (*Nat. Chem*., 2012, 4, 456).

Nick has so far had an explosive career: he was one of only two Canadians to be awarded the **Ludo Frevel Crystallography Scholarship** by the **International Centre for Diffraction Data** (**ICDD**) in 2011 and 2012; he also received the **Governor General's Gold Medal** - the most prestigious award that can be received by a student in a Canadian educational institution for research excellence and exceptional academic achievement. However, following his Ph.D. Nick decided to pursue a career in industry, joining **PROTO Manufacturing, Ltd.** (**PROTO**), supported by a prestigious industrial **OCE Talent Edge Fellowship**. PROTO is a Canadian-based company that has been providing innovative X-ray diffraction instruments for residual stress, LAUE single-crystal orientation, and powder diffraction. At PROTO, Nick advanced very quickly and is currently the Principal Scientist and Product Development Manager, and his continuing research activities have also landed him into an Adjunct Professor position in the Department of Chemistry and Biochemistry at the **University of Windsor**. Most recently, Nick and his PROTO team have developed the only high gas pressure *in situ* diffraction chamber which can operate with a benchtop powder diffractometer. This system was utilized in a joint publication (*CHEM*, **2018**, *4*, 868, see Figures 2b,c) with Professor George Shimizu at the **University of Calgary** to investigate a pressure-induced closed-pore to open-pore phase transition in a hydrogen-bonded organic framework (HOF) material.

This is all for now – I am looking forward to seeing you all at the ACA Annual Meeting in a few weeks. In the meantime, keep your eye on the Canadian crystallography by following the webpage of the *Canadian National Committee for Crystallography*: https://xtallography.ca/.

See you in Toronto!

Tomislav Friščić

2018 Spring ACA Council Meeting Highlights

Diana Tomchick

The 2018 Spring Council Meeting was held at the Hauptmann-Woodward Institute (HWI) in Buffalo, NY on April 17. Voting members in attendance were President Lisa Keefe, Vice President Joe Ferrara, Treasurer Sue Byram, Past President Amy Sarjeant, Canadian Representative Tomislav Friščić and Secretary Diana Tomchick. Non-voting members in attendance were IUCr Representative Hanna Dabkowska, YSIG Representative George Lountos, Director of Administrative Services Kristin Stevens, CEO William Duax and CFO S.N. Rao. In addition to this meeting, Council held three online Council meetings (one in January, one in March and one in May) to decide various pressing issues, which will also be described below.

The ACA Council was saddened to learn of the recent passing of Judith Flippen-Anderson, who had contributed a lot of volunteer work at many levels for the ACA in the past decades. Lisa Keefe informed the Council members that the new editor of *ACA RefleXions*, Ed Stevens, planned to include contributed obituaries for Judy in the summer edition. Council is also working on plans for members to contribute funds in memory of Judy; stay tuned to *RefleXions* for more information.

Under New Business, John Helliwell has accepted the position, previously held by Charles Carter, as ACA representative to the American Institute of Physics (AIP) Publishing Board of Managers; the new *RefleXions* co-editor is Paul Swepston; the positions of *RefleXions* Copy Editor and "NetRefleXions" contributor need to be permanently filled; the ACA verbally supported the annual March for Science; Council adopted a diversity statement that is now on the ACA web site (see http://www.amercrystalassn.org/diversity-statement); and a membership survey of the ACA is currently in process, with the help of the AIP. ACA Outreach funding will support the following initiatives: financial support for the Summer Course in Crystallography at Notre Dame, June 10-17, 2018; a one-week high-school level workshop at Brookhaven National Laboratory entitled "Structural biology: using crystals and synchrotrons to see the building blocks of life in action"; and annual complimentary student memberships to student attendees of the Modern Methods in Rietveld Refinement for Structural Analysis workshop at the Advanced Photon Source, June 17-22, 2018 and the annual X-ray workshop at the Department of Chemistry at NYU, June 27-28, 2018.

Front row, from left to right: Sue Byram, Joe Ferrara, Lisa Keefe, Amy Sarjeant, Diana Tomchick
Back row, from left to right: Bill Duax, Kristin Stevens, Hanna Dabkowska, George Lountos, S.N. Rao
Photo taken by Kristina Vitale.

The long-term financial health of the ACA continues to be a focus of the Council. As the ACA CFO, S.N. Rao plans to remain in this position for only a few more years, thus Council has asked him to prepare an investment policy statement for ACA funds. He will present this to the ACA Finance Committee (which consists of the CFO, Treasurer, Director of Administrative Services, a member at large appointed by the Chair and an industrial representative appointed by the Treasurer), which will address the question of who will be responsible for investments of ACA funds after Rao retires.

Much of the work of the ACA is performed by the standing committees (Communications, Continuing Education, Data, Standards & Computing), and also by ad-hoc committees (Finance, Meeting Site Selection, Outreach, Member Experience, and Meeting Enhancement). Council spent a good deal of time discussing how to set specific, measurable goals for these committees. Decisions were made to have the Communications Committee create guidelines to handle requests from outside groups for money to support external events such as workshops and meetings and to have the Finance Committee address such requests and to track how contributed funds were expended. An updating of the duties of the Communications and Education Committees will take place, and the Data, Standards & Computing Committee will be asked to communicate closely with the newly created Best Practices for Data Analysis & Archiving SIG to chart a future path for the two entities. As Judith Flippen-Anderson was a member of the ACA Meeting Site Selection Committee, Council decided that as of 2019, the committee will consist

of the ACA CFO, Vice President, Past President and Director of Administrative Services.

A strategic plan for the ACA was presented at the ACA 2015 General Members Meeting in Philadelphia. As with any organization, strategic planning should be revisited on a regular basis, and so Council has decided that a strategic planning process for the ACA should take place in 2019. Lisa Keefe is investigating the possibility to acquire funds from the AIP via their Venture Partnership Fund to help defray any costs that may be involved for the ACA.

Joe Ferrara reported that the ACA Member Survey is in progress, and results are expected by the Toronto ACA annual meeting. He is still in the decision-making process for the topic of the Transactions Symposium for the 2019 ACA meeting in Cincinnati/Northern Kentucky and is searching for volunteers to be Program Chairs for the 2020 ACA meeting in San Diego.

Tomislav Friščić, the Canadian Representative, highlighted several upcoming Canadian meetings, including the 2018 ACA meeting in Toronto, July 20-24, 2018; the 9th Canadian Chemical Crystallography Workshop (CCCW18) as a satellite meeting of the 101st Annual Meeting of the Canadian Chemical Society in Edmonton, Alberta, May 22-26, 2018; the 8th Annual CLS Mx Data Collection School at the Canadian Light Source in Saskatoon, Saskatchewan, June 4-8, 2018; the 19th Sagamore 2018 Conference on Quantum Crystallography in Halifax, Nova Scotia, July 8-13, 2018; the 5th Crystal Engineering and Emerging Materials Workshop of Ontario & Quebec (CEMWOQ-5) in Montreal, July 16-19, 2018; and the 11th Canadian Powder Diffraction Workshop in Hamilton, Ontario, July 25-29, 2018. Tomislav reported that the Larry Calvert Travel Fund of the Canadian National Committee for Crystallography is in good financial shape and has awarded the first crop of travel awards to Canadian students, postdocs and researchers for travel to crystallography-related conferences.

Hanna Dabkowska presented highlights of IUCr activities, including the provision of $9,000 in support for student travel grants to the Toronto ACA meeting; the publication of 431 pages of abstracts of the 2017 ACA meeting in New Orleans, LA in *Acta Crystallographica,* Volume **A73**; the support for 80 international meetings and schools since January 2016; the selection of Melbourne, Australia, for the 26th IUCr Congress in 2023; the IUCr Newsletter, published since 1993 with Bill Duax as Editor and Patricia Potter as Production Manager has been transferred (since Volume 25, Number 2) to the Chester, England IUCr office; the support of the IUCr Outreach and Education Fund of initiative in Africa, the IUCr-UNESCO OpenLabs and crystallographic schools around the world; the 2018 IUCr Crystal growing competition is now open; and the next IUCr Executive Council meeting will be held prior to the European Crystallographic Meeting in Oviedo, Spain, August 21, 2018.

Highlights of the report from George Lountos, the Young Scientists Interest Group (YSIG) representative, included details about the plans for the YSIG Mixer at the Toronto ACA meeting, which will be sponsored by Bruker and take place at 3 Brewers on Adelaide; TTP Labtech will sponsor a Three-Minute Thesis competition; and the YSIG has sponsored a meeting workshop entitled “Molecular Art and Animation”. YSIG will also host a New Attendees Meeting, which will provide brief introduction to new attendees about the format of the ACA meeting and how they can not only get the most out of the meeting, but also how to become actively involved in the ACA.

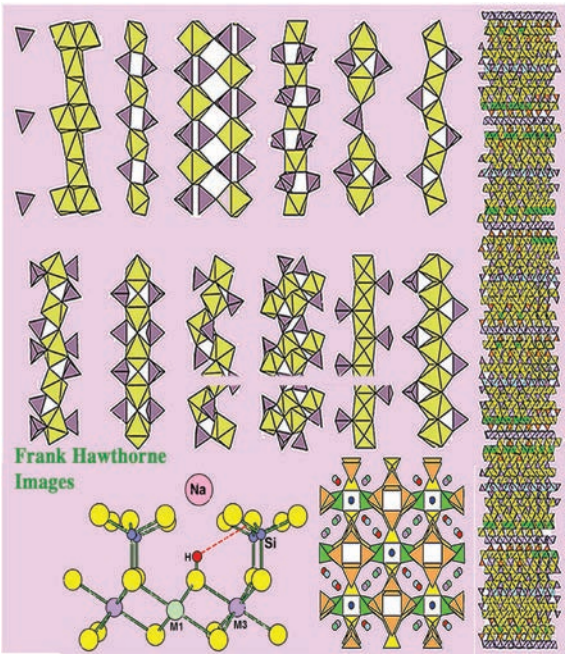
Sue Byram, the ACA Treasurer, noted that the ACA is making progress on reducing expenses and increasing income, with a projected smaller loss in 2018 than in 2017, but this will depend upon total dues-paying membership and attendance at the Toronto ACA meeting. Despite an increase in dues in 2017, the ACA didn’t have a reduction in membership, but a slight gain, which correlated in a leveling off of meeting attendance. Several suggestions were made for activities at the Toronto meeting to encourage continuing membership renewals, including stickers for your meeting badge in Toronto that indicate your length of ACA membership.

For the 2018 annual meeting, Council approved the request of the ACA Annual Meeting exhibitors to close the exhibit space during the noon – 2 PM hours, and to hire a band for the Meeting banquet. The ACA will also present the Warren, Buerger and Etter Early Career Awards, as well as announce the new ACA Fellows.

Preparations for the annual meeting in 2019 in Cincinnati/Northern Kentucky are well underway, and the Program Chairs should soon provide details regarding workshops and the Transactions Symposium. Council approved the ACA Meeting Selection Committee recommendations of San Diego, CA as the 2020, Baltimore, MD as the 2021 and Portland, OR as the 2022 ACA Annual meeting sites.

The next Council meeting will be on Friday, July 20 2018, in Toronto, ON, Canada.

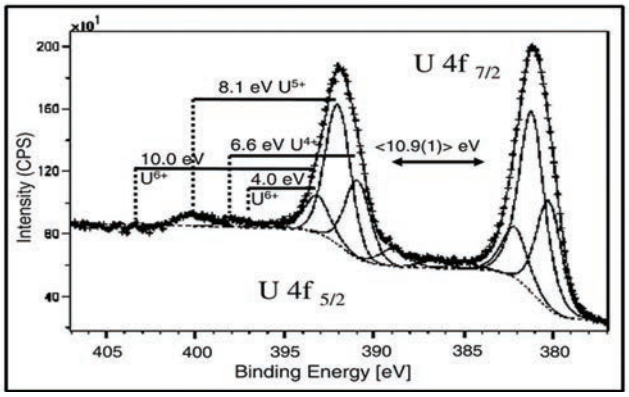
Diana Tomchick



Frank Hawthorne, Distinguished Professor of Geological Sciences at the University of Manitoba, is the **2018 ACA Buerger Award** winner. When asked to provide images of his work, he sent the 4 shown at left plus the curve shown below. The largest image at upper left is described as 'chains of tetrahedra and octahedra in sulfate minerals'; 'the unit cell of carlfrancisite' forms the entire right side of the figure; 'the framework in bohseite' is next along the bottom; and finally: 'the environment of hydrogen in the amphibole structure.'

Frank has received numerous other awards and honors, he is a fellow of the Royal Society of Canada, and was awarded their Bancroft Medal, and their Willet G Miller Medal. He is a recipient of the Carnegie Medal of the Carnegie Museum of Natural History and the Killam Prize in Natural Sciences of the Canada Council. He has been elected a Fellow of the Geochemical Society and the European Association of Geochemistry. He was awarded a Canada Research Chair in Crystallography and Mineralogy, is a Companion of the Order of Canada, and was elected a Foreign Fellow of the Russian Academy of Sciences. Hawthorne was awarded the IMA Medal of the International Mineralogical Association and the Roebling Medal of the Mineralogical Society of America, he was awarded the W. W. Hutchison Medal of the Geological Association of Camada as well as that association's highest honor, the Logan Medal.

Hawthorne's early work focused on structural and crystal-chemical problems of amphiboles. He used several experimental techniques, including X-ray and neutron diffraction, infrared spectroscopy, and Mössbauer spectroscopy. He summarised his results in a 300-page paper on amphiboles, for which he was awarded the Hawley Medal of the Mineralogical Association of Canada.



U 4f5/2 and U 4f7/2 regions of the X-ray Photoelectron Spectrum for a uraninite crystal showing the presence of U in three valence states.

His academic interests include topological and electronic aspects of crystal structures, graph-theoretic and combinatorial approaches to crystal structure, the crystal chemistry of rock-forming minerals, short-range order in minerals, diffraction and spectroscopic methods, microbeam analysis, and solution of unknown mineral structures. His personal interests include English poetry, biography, painting and sculpture, the history of Europe and Central Asia, the history of Science, chocolate and coffee. He is married to the crystallographer Elena Sokolova.

Martin J. Buerger was a mineralogist who made major contributions to crystal growth, morphology of crystals, structure analysis, and phase transformations as well as instrumentation for crystallography. The M.J. Buerger Award was established by the ACA in 1983 and is awarded every three years.

Connie Rajnak

American Crystallographic Association, Inc.
Statement of Financial Position
December 31, 2017 and 2016

Assets	**2017**	**2016**
Cash and Cash Equivalents	$120,057	$100,972
Investments	$1,035,465	$1,104,842
Accounts Receivable	$493	
Bonus and Uncashed Checks	$38,205	
Total Assets	$1,194,220	$1,205,814
Liabilities and Net Assets		
Unearned Revenues	$57,730	$73,876
Other Liabilities	$2,491	$22,133
Uncashed Checks	$22,022	
Total Liabilities	$82,243	$96,009
Net Assets - Unrestricted	$587,936	$585,752
Net Assets - Restricted	$524,041	$524,053
Total Liabilities and Net Assets	$1,194,220	$1,205,814

Restricted Fund Balances

(as of December 31, 2017)

Bau award	$36,494
Buerger Award	$38,978
Dave Rognlie Award	$60,000
Etter Award	$68,909
Fankuchen Award	$71,343
Patterson Award	$48,786
Pauling Award	$38,925
Supper Award	$12,661
Trueblood Award	$40,459
Warren Award	$31,399
Wood Award	$54,211
Student travel Award	$21,876
TOTAL	$524,041

A more detailed report on the ACA finances may be obtained by sending a written request to the ACA office in Buffalo, PO Box 96, Ellicott Station, Buffalo, NY 14205-0906. You may also request this information using the 'contact us' form on the ACA website, or email directly to kvitale@hwi.buffalo.edu.

Candidates for ACA Offices in 2019

The Nominating Committee proposes the following candidates for 2019.

Officers:

Vice-President: Brian Toby & Diana Tomchick
Treasurer: Marie Frazer & Ilia Guzei

Committees:

Communications: Heba Abourahma & Louise Dawe
Continuing Education: Allen Oliver & Corie Ralston
Data, Standards, and Computing: Christina Hoffmann & Eric Reinheimer

To nominate write-in candidates for any office, write to the ACA Secretary: Diana Tomchick, Dept. of Biophysics, University of Texas, Southwestern Medical Center, Irving, TX 75061 (diana.tomchick@utsouthwestern.edu). Letters must be received by September 15, 2018 and must be signed by five ACA members, and include a signed statement by the candidate describing his or her qualifications. Voting will be by electronic ballot. Statements from all candidates will be available on the election website. The voting window will open in October 2018.

Brian Toby - Vice President

Senior Physicist; Group Leader for Computational X-ray Science; APS Chief Computational Scientist; Advanced Photon Source, Argonne National Lab, Argonne, IL USA

Education:

BA in Chemistry, with honors and highest distinction, Rutgers University, 1980, Ph.D. in Physical Chemistry, Caltech, 1986. Research Associate and Lecturer, Department of Materials Science, University of Pennsylvania, 1988-1991.

Professional Activities:

U.S. National Committee on Crystallography, Member (2004-2009), Vice Chair (2009-2011), Chair (2012-2014), US Delegate to IUCr Congress for 2005, 2008, and 2011, Delegation Leader, 2014. American Crystallographic Association, Chair for Neutron, Material Science and Synchrotron SIGs, V.P. Nominations Committee, ACA 2.0 Transition Committee (various years). Organizing Committee of the Denver X-ray Conference, 2008-. International Union of Crystallography: Commission on Neutron Diffraction, 2008-2011; Commission on Powder Diffraction, 2012-2016; Committee on the Crystallographic Information, 2000-2002. Editorial Board, *The Journal of Physical and Chemical Reference Data*, 2007-2015. Co-Editor for *Crystallographic Education, Powder Diffraction* journal (International Centre for Diffraction Data), 2006-. ACA representative on the American Institute of Physics Publications Committee, 2009-2012. Associate Editor, *International Tables for Crystallography, Volume G* (2005).

Research Interests:

Determination of structures of crystalline and partly-crystalline solids, particularly with powder diffraction; structure determination techniques and instrumentation; structure-property relationships in functional materials; materials informatics.

Statement:

I am running for vice president of the American Crystallographic Association because I am very concerned about the future of crystallography. Yes, scientists will continue to perform the structural analyses that are the *raison d'etre* of the ACA – for as far in the future as my crystal ball is calibrated. The results will remain critical to scientific research. However, I wonder if the scientists doing this work will call themselves crystallographers? As in-depth study of crystallographic analysis disappears from our curricula, how will scientists be educated to perform this work? Will the quality of results suffer; will crystallography remain the gold standard? We can flail over the injustice in this, but like it or not, increasingly crystallography is just one of many techniques that domain scientists employ for their research, be it structural genomics, solid-state chemistry or condensed-matter physics. However, since my own crystallographic software generates >500 citations/year, I know there is no shortage of people using crystallography. That will

not change.

If elected, I want to lead the ACA in a discussion on how to best improve crystallographic education. The ACA needs to ensure that there will be a next generation of expert crystallographers in North America, best done I believe by advocating to the organizations that establish scientific policies on the importance of this crystallographic expertise. Likewise, I would also like to see the ACA take a greater role in educating younger scientists in crystallographic techniques. I have taught at the ACA Summer School for most years in the past ~15 and recently became a co-director of the Oak Ridge-Argonne Neutron/X-ray School. In that role, I cannot tell you how many young scientists (or their advisors) have written that they need external instruction because they can't learn enough about diffraction and crystallography at their home institutions. Nonetheless, I can vouch that as valuable as these summer schools are, they can only *introduce* students to crystallography. Anyone working in the field needs to know so much more. Educational outreach can bring new people to the ACA and perhaps even a small revenue stream.

For those who do not know me, an introduction is due. I started in crystallography at Rutgers in 1977 after my freshman year, when crystallographer Joseph Potenza offered me a summer job in single-crystal structure determination. I learned skills there that have served me well: to solving structures with MULTAN, Patterson and difference maps; I taught myself how to find burned-out chips in the CAD-3 that Nonius would no longer service, as well as how to reprogram data collection (in a PDP-8 with 4K of memory!) Building wooden-stick crystallographic models, perhaps not. Based on Joe's advice about the decline in crystallography (even back then), I moved to another field for my graduate work, but was lucky enough to be Dick Marsh's teaching assistant. I was able to move back to my first love — crystallography — when Union Carbide (rest in pieces) hired me to run their corporate powder diffraction lab and sent me to Brookhaven, where I helped Dave Cox get the first dedicated synchrotron powder diffractometer running. Two years later I escaped Carbide to work for Takeshi Egami at UPenn, where I helped pioneer pair distribution analysis for structural analysis, demonstrating the accuracy of the technique and writing the first PDF fitting program for local-structure in crystalline materials. Also while in Philadelphia, I found the other love of my life, psychologist Diane Pies Toby. We then moved to Allentown, for a much happier industrial work experience with Air Products and Chemicals. There I did zeolite crystallography and would have set a record for the most complex structure to be determined from powder diffraction, had APCI then allowed me to publish it. I was later very lucky to be invited to lead the crystallography team at the NIST Center for Neutron Research, where my goal was to make neutron diffraction much more accessible to the community. At NIST, I created the EXPGUI program, which I believe is one of the most cited single-author papers in crystallography. Finally, I moved to Argonne about a dozen years ago, to lead construction of the 11-BM powder diffractometer, personally designing and implementing the mail-in access system that has allowed 11-BM to be the most productive instrument at the APS (likely the world) and has helped synchrotron powder diffraction to become so very widely used. My most recent project has been to help Bob Von Dreele develop GSAS-II, which is the only general-purpose crystallographic software package initiated in the current century. GSAS-II is used for solving and fitting all scale of structures, from perovskites to proteins, from both single crystal and powder diffraction measurements, and using data from lab instruments, synchrotrons, reactors and TOF neutrons, potentially in combination. There, that covers 40 years and ~140 papers (www.researcherid.com/rid/F-3176-2013) in 1 paragraph. It has been quite a ride and a lot of fun!

As a member of the ACA for nearly 30 years, I have the chance to be involved in many ways, serving on a number of committees, organizing sessions, etc. I also served as vice-chair and chair of the U.S. National Committee for Crystallography. For the IUCr, I spent nearly a decade to extend CIF to powder diffraction by creating the pdCIF dictionary. I enticed the journal Powder Diffraction to add a section for educational articles, which I now co-edit. I have gotten a Bronze Medal from the U.S. Dept. of Commerce, the Barrett Award from Denver X-ray Conference and been named a Fellow of the ACA and the International Centre for Diffraction Data.

In closing, while this statement is already too long, I want to end by saying how proud I am to be associated with so many others I admire who also called themselves crystallographers. I think of the Braggs, who welcomed women into their groups in a time when many institutions would not admit them; Von Laue, who risked his career if not life, to speak up to Nazis for Jewish scientists such as Haber and Einstein. I will not go on, but my list of crystallographers/heros is extensive. I am very proud of the ACA's history with diverse leadership from its start, long before this became fashionable.

Without knowing who else is running, from experience I can be sure that the nomination committee has provided another fine candidate; I am confident the ACA will be in good hands. Nonetheless, I see this as a

pivotal time for the ACA to look forward to the future of our field and for us to plan to increase our organization's value to the next generation of scientists.

Diana Tomchick -Vice President

Professor
Departments of Biophysics & Biochemistry
UT Southwestern Medical Center
Dallas, TX 75390, USA

Education:

B.S., Chemistry, Washington State University (1983); Ph.D., Chemistry, University of Wisconsin-Madison (1990), adviser Lawrence F. Dahl; American Heart Association Postdoctoral Fellow, Department of Biochemistry, University of Wisconsin-Madison (1990-1993); postdoc, Department of Biology, Purdue University (1993-1997).

Professional Activities:

Director of The Structural Biology Laboratory at UT Southwestern Medical Center since 2000; member of the ACA since 1986, and ACA Secretary since 2015; member of the International Union of Crystallography Commission on Biological Macromolecular Structure; member of the American Chemical Society since 1985; synchrotron beam time proposal reviewer for the Advanced Photon Source (2011-present).

Research Interests:

The use of structural biology and especially the techniques of X-ray crystallography and cryo-electron microscopy in the study of molecular mechanisms of neurotransmitter release, bacterial pathogenicity, cell signaling and division, and enzymology; improved methods of protein crystallization, data collection and phasing of data from poorly diffracting crystals; improved methods of sample preparation, data collection, model building and validation of molecular models via single particle cryo-EM reconstruction.

My crystallographic experience began with small molecules as an inorganic chemist, and I was a recipient of an ACA student travel award to the 18th IUCr Congress in 1987 in Australia, as well as a recipient of the Patterson Student Poster Prize in 1990. My training eventually led me to my current position as the Director of a campus-wide core facility that provides expertise in macromolecular structure. This position requires significant organizational and financial skills as well as scientific expertise, and for many campus research groups I am the professional "face" of crystallography. In the last two years, my facility is also providing cryo-EM single particle reconstruction services to our campus, so I am also learning some new skills! 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. The ACA provides a critical resource for the molecular structure community to network and keep abreast of scientific and technical advancements, and to educate the next generation of scientists as well as the general public.

Statement:

I am honored to be nominated for ACA Vice President. I have been a member of the ACA for more than 30 years, and always enjoyed attending meetings and renewing friendships, old and new. These meetings have always felt like a scientific home for me. It's exciting and humbling to think about the possibilities to help guide the organization over the next few years.

I believe that the best things the ACA currently provides to its members are 1) a framework for supporting best practices in the elucidation, analysis, dissemination and archiving of structural results; 2) education of the current and future practitioners of the science; 3) celebration of the joys of long and fruitful careers, collaborations and friendships; and 4) advocacy for the importance of structural research to scientists and to the public at large.

As Vice President and eventually President of the ACA, I would continue to support the excellent efforts the society does in pursuing these goals, primarily through the annual meeting, which includes Transactions Symposiums, excellent scientific presentations, educational workshops, awards to senior scientists, ACA Fellows and for student travel and presentations; the sponsorship of the ACA Summer school; the publication of a peer-reviewed journal, Structural Dynamics; the publication of a quarterly newsletter, RefleXions; the support of the ACA History Portal; the ACA web site, which will be updated soon, and also support for various outreach activities. A truly amazing aspect of the ACA is that these activities are primarily organized and supported by the volunteer efforts of the society members. There are wonderful opportunities for professional growth for individual members, including students, through service to the society, and I plan to actively encourage such involve-

ment in the future.

In order to achieve these important goals, as ACA Vice President I would work to assure that the ACA is on a strong financial foundation for the future. Much progress has recently been made by the ACA Council, which approved and is currently implementing a 3-year plan for succession for the ACA Headquarters staff, as former Director of Administrative Services Marcia Colquhoun has retired and Chief Executive Officer William Duax will gradually transition from his duties with the ACA. While this plan has already helped with the financial bottom line for the organization, more work needs to be done to ensure financial stability. S.N. Rao, the ACA Chief Financial Officer, has informed the ACA Council that he will remain as CFO for a few more years, but a replacement needs to be found. I view the identification of a suitable replacement for the ACA CFO as an absolutely critical next step for the ACA Council, and if elected Vice President I would encourage the ACA Finance Committee and to make that a priority.

The explosion of interest in new structural methods in the last five years has and will continue to provide opportunities for the ACA to attract and retain members. By targeting practitioners and students interested in novel molecular structural techniques such as electron diffraction, cryo-electron microscopy, NMR crystallography, small-angle X-ray scattering and other methods while not ignoring the interests of our current members, our annual meetings have retained relevancy and thrived. I believe we should examine the potential for novel joint meeting formats with other societies, and pursue these opportunities if they are beneficial scientifically and financially to the ACA and its members.

In 2015, ACA President Tom Terwilliger presented at the Annual Meeting the Strategic Plan for the society, which had been developed through the input of many members over a span of several years. In the intervening years, due to (understandably!) financial concerns, the Council has been focused on developing and implementing the succession plan for the ACA Headquarters, as well as the tasks of ensuring the normal operation of the society. I believe that it is now time for the ACA leadership to place more emphasis on the implementation of the other key aspects of the ACA Strategic Plan, including career enhancement resources, outreach activities, and member communication resources. I would look forward to finding new and novel ways to fund these activities in order to ensure the continued health of the society.

Last but not least, I believe that for the ACA to remain relevant and important as a Society, that we must be able to offer solid reasons for scientists to remain members of our group. We have a brand, we are the scientists for whom "structure matters". I would be honored to serve as the next Vice President of the ACA, and to find new ways to promote that brand to a new generation of scientists.

Marie Fraser - Treasurer

Associate Professor
Department of Biological Sciences
Faculty of Science
University of Calgary

Education:

B.Sc. (Honours, Chemistry), Queen's University (1983); Ph.D. with S. Fortier, Department of Chemistry, Queen's University (1987); Alberta Heritage Foundation for Medical Research Postdoctoral Fellow with M.N.G. James, Department of Biochemistry, University of Alberta (1987-90).

Professional Activities:

Member, Accreditation Committee, Chemical Society of Canada (2012- 2019); Member, Canadian National Committee of the International Union of Crystallography (2015-2018), Treasurer (2005-2015); Member, Canadian Macromolecular Crystallography Facility Beamline Team (2013-present); Chair, Biochemistry Program (2013-16), Biochemistry Cluster (2009-11).

Research Interests and Responsibilities:

Structural biology; macromolecular crystallography; enzyme mechanism; protein ligand-binding; protein-protein interactions. Teaching: introductory biochemistry to chemists and kinesiologists; macromolecular crystallography to senior undergraduate biochemists; crystallography at the graduate level.

Statement:

I appreciate the opportunity to express my support for the ACA by running as a candidate for the position of Treasurer. As an undergraduate student, I first thought that the bond lengths we learned in our chemistry courses all came from spectroscopic measurements. Only in third year did I realize that much of what we know about molecular structure comes from the solid state, from crystals. As a graduate student and a postdoctoral fellow, I received an excellent

education in crystallography. Now I consider myself a crystallographer and I rely on the meetings of the ACA and the IUCr - in addition to the literature - to keep current in the field. Serving on the executive of the ACA would give me the opportunity to give back to the crystallographic community in our region.

As a graduate student, I saw the view that crystallography is "only a tool" sweep through chemistry and I now see that view sweeping through the macromolecular field. Many faculty believe that their graduate students do not need to learn crystallography. There is a lot for our students to learn: molecular biology, protein purification, structural biology on top of the soft skills of writing and presenting. However, I think my students who are using crystallography in their research should learn more than what I teach at the undergraduate level, which is how to be an informed user of macromolecular models. My students are to be generators of those models, not just users. A major role of the ACA and the IUCr is education. We need to help both the users and generators of models from crystallography become better informed.

To fulfill this role in life-long education, we need to engage the community of users and generators of crystallographic models. The ACA serves to connect crystallographers primarily through the annual meetings. Most new members join when attending these meetings. Scientists can hold memberships in more than one professional society. I would hope the ACA could keep these new members engaged as crystallographers.

Ilia Guzei - Treasurer

Distinguished Scientist
Chemistry Department
University of Wisconsin, Madison
1101 University Ave
Madison, WI 53706, USA

Education:

M.S. in Chemistry (1992), Lomonosov Moscow State University, USSR.

Ph.D. in Chemistry (1996), Wayne State University, Detroit, MI USA.

Professional Activities:

ACA meeting co-chair (2017), member of the USNC/Cr (2017-), member of the ACA Outreach Committee (2015-), member of the ACA Communications Committee (2014-17), ACA Poster session chair (2011-16), ACA summer school instructor (2012), instructor in short courses in crystallography (2004-), coordinator of several single-crystal X-ray diffraction system users meetings (2001-), moderator of an internet crystallographic forum (2000-), ACA and IUCr workshop and session organizer, Acta Cryst. C co-editor (2005-14).

Research Interests:

Small molecule single-crystal X-ray crystallography, crystallographic education, twinning, non-routine crystallographic experiments, crystallographic software development, ligand steric properties in organometallic compounds.

Outreach Interests:

Organization of the annual WI Crystal Growing Contest for middle and high school students that attracts over 600 participants; management of the WI Space Crystal Mission in collaboration with Center for the Advancement of Science in Space.

Statement:

I thank the nominating committee for choosing me as a candidate for the three-year Treasurer position. Over the last decade I have been actively involved with the ACA, including serving on the USNC/Cr and co-chairing the New Orleans ACA meeting. In particular, serving as the Poster Chair for five years allowed me to meet a lot of the members from different scientific backgrounds and to collaborate with the ACA leadership.

The current CFO and Treasurer have been successful in implementing their vision of getting our organization toward fiscal viability. I intend to sustain this momentum to ensure that the ACA makes wise investment choices, maximizes income, and controls expenses. I believe that the current upward trend on the ACA balance sheet will allow the organization to expand its programs and attract new members, which in turn will strengthen our association. The decline in the membership must be reversed, and Treasurer plays a critical role at this junction.

Whereas I do not have formal financial education, I have been the Treasurer of the WI ACS Local Section since 2017 and in that short time substantially improved its record-keeping, collaborated with the section's executive committee, reviewed financial and tax statements, and established a well-funded outreach grant program. Since 2014 I have been organizing the WI Crystal Growing Contest that requires a commitment to fund-raising and communication with a large number of sponsors and potential donors. I am happy to say the contest has always run at no cost to the participants.

I understand the financial challenges our organization faces and am looking forward to serving as Treasurer in a way that benefits the entire membership.

Heba Abourahma - Communications

Associate Professor
Department of Chemistry
The College of New Jersey
Ewing, NJ 08628, USA

Education:

B.Sc. Chemistry (honours) Saint Mary's University (1997); M.Sc. Chemistry, Ottawa University (1999); Ph.D. Chemistry, University of South Florida (2004); Postdoc University of Iowa (2004-2005)

Professional activities:

American Chemical Society, member, 2000-present; American Crystallographic Association, member, 2005-present.

Research Interest:

Crystal engineering, cocrystals and the application of supramolecular chemistry principles to making functional materials.

Statement:

I am delighted and honored to be nominated to serve on the Communication Committee of the ACA. I have been a member of the ACA for over 10 years. The community feel of the ACA is unparalleled and it is what has kept me a member year after year. The relatively small size of the ACA is conducive to building relationships that last beyond the meetings. Furthermore, the commitment of the ACA to plan quality meetings has been very impressive.

The ACA has supported me and my students over the years and I would be honored to support the association back by taking on a role in the Communication Committee. Being a professor at a primarily undergraduate institution is ideal to reach out to young scientists and to get them excited about science in general and crystallography in particular. If elected, I commit to stand by the ACA's mission to promote and preserve crystallography and further its vision to educate young scientists.

Louise Dawe - Communications

Associate Professor
Chemistry and Biochemistry Department
Wilfrid Laurier University
ON, Canada

Education:

BSc(Hons.) Chemistry, Memorial University of Newfoundland (MUN; 2002); MSc Chemistry, University of Utah (2003), BEd(Int/Sec.), MUN (2003); PhD Chemistry, MUN (2008)

Professional activities:

ACA Service SIG (Chair 2011-2012); ACA Small Molecules SIG (Chair 2012-2013, Secretary 2013-2015); ACA Canadian Division (Chair 2014-2015); 2015 ACA Annual Meeting Program Co-Chair, ACA Nominating Committee (2016-2017); 2018 ACA Annual Meeting Poster Co-Chair; Executive Member and Webmaster for the Canadian National Committee for Crystallography (2015-); Chair of the Canadian Delegation to 24th Congress & General Assembly of the International Union of Crystallography 2017 (Hyderabad, India); Member of the International Union for Crystallography Sub-committee on the Union Calendar (2017-)

Research Interests:

Small molecule X-ray crystallography; supramolecular and coordination chemistry; molecular magnetism; greener synthesis; active learning in undergraduate education.

Statement:

I am honored to have been considered by the nominating committee for membership in the ACA Communications Committee. I attended my first ACA meeting in 2008, where I found my professional "home". The colleagues and friends that I have made through the ACA have contributed enormously to my growth as a scientist. In particular, the "Would You Publish This?" session, held regularly at our annual meetings, has taught me that my colleagues in the ACA want to share their experiences to help others tackle challenging problems.

In turn, I have tried to give back to our association, and the wider crystallographic community. In addition to the official positions that I have held as part of my professional activities, I have been involved in several other ACA and IUCr initiatives, targeted at

communicating crystallography to a wider audience. I was a member of the local organizing committee for the 23rd Congress and Assembly of the International Union of Crystallography (Aug. 2014, Montreal, Canada), where I coordinated outreach activities for the United Nations International Year of Crystallography 2014 (IYCr2014). These activities included organizing public lectures by three international high impact scientists at McGill University, which were attended by over 300 members of the general public. I organized a public display of Jean-Louis Hodeau's panels, Journey into the Crystal at the metro stop of the Montreal Convention Centre. Foot traffic is very high in this area, and over the course of the eight day congress, it is estimated that several thousand people saw this display. I also organized lunchtime screenings of documentaries for the families and guests of Congress attendees, in collaboration with Prof. Juan-Manuel Garcia-Ruiz (producer and host of The Mystery of the Giant Crystals), and with the British Crystallographic Association (for the production Hidden Glory: Dorothy Hodgkin In Her Own Words.) I was a member of the ACA's task force for IYCr2014. In this capacity I worked with a sub-group of crystallographers on outreach to youth, and organized with Dr. Amy Sarjeant and Dr. Christine Beavers, a North American Video Contest on crystallography. In my capacity as the program co-chair for the 2015 ACA meeting, I again teamed with Prof. Garcia-Ruiz to organize two additional outreach activities for delegates and their families: 1) We displayed the poster exhibit CRISTALES; and 2) We held a lunchtime screening of The Mystery of the Giant Crystals, with a question-and-answer session which I chaired, and hosted by Prof. Garcia-Ruiz.

On International Women's Day 2018 (March 8) I had the unique and exciting opportunity to remotely connect with a high school class to discuss crystallography, science, and post-secondary expectations. This plays into my vision to make a contribution as a member of the Communications Committee, by building off some of the outreach initiative started by the ACA IYCr2014 taskforce, and some of my more recent experiences. If elected, I hope to include a notable outreach component to my activities with the Communication Committee.

Allen Oliver - Continuing Education

Research Professor
Dept. of Chemistry & Biochemistry
University of Notre Dame
Notre Dame, IN 46556

Education:

BSc in Chemistry (1993); MSc in Chemistry (1994), PhD in Chemistry (2000) Waikato University, New Zealand; Post-doctoral fellow (2000-2002) UC Berkeley.

Professional Activities:

Co-organizer ACA Summer Course in Chemical Crystallography; co-editor Acta Crystallographica C; program chair ACA 2013; served on Small Molecule, Service and General Interest Groups as secretary and chair; served on ACA Communications Committee; Secretary of the Pittsburgh Diffraction Society; developed a short course in crystallography with Pontificia Universidad Catolica de Chile.

Research Interests / responsibilities:

Chemical crystallography, crystallographic education, facility management.

Statement:

It is an honor and privilege to be nominated for a position on the Continuing Education Committee. My interest in serving on the Continuing Education Committee stems from my participation as a crystallographic educator. I currently serve as one of the co-organizers of the ACA Summer Course in Chemical Crystallography. The primary mandates of the Education Committee are: selecting awardees for travel scholarships to the ACA conference; vetting proposed workshops that take place at the ACA Conference and expanding professional development within the community. I believe that with my experience in similar matters associated with the summer course I have a solid understanding of the needs of the committee. For the ACA Summer Course, I am directly involved with selection of scholarship awardees, planning the curriculum that includes a number of workshops, and developing networking opportunities for the course attendees. These are directly translatable skills to the mission of the Continuing Education Committee. I have previously served on the Communications Committee, as Chair and Secretary for

several SIG's within the ACA and as a program chair for the ACA annual conference. I feel that with this prior knowledge I have a broad insight into the needs of the community and have worked with committee members at all levels and will bring that knowledge and expertise to the position.

Corie Ralston - Continuing Education

Head
Berkeley Center for Structural Biology
Molecular Biophysics and Integrated Bioimaging Division,
Lawrence Berkeley National Laboratory
Berkeley, CA, USA

Education:

BS Physics, University of California at Berkeley. PhD Biophysics, University of California at Davis, advisor: Dr. Stephen Cramer. Post-doctorate work at the Albert Einstein College of Medicine, New York, advisor: Dr. Mark Chance.

Research Interests:

Macromolecular crystallography beamline development, X-ray footprinting beamline development.

Statement:

I am very pleased to be considered for a position in the Continuing Education committee for the ACA. I am a strong believer in continuing to learn and grow at all stages of life, and would be happy to try to expand the Continuing Education efforts of the ACA. I believe this effort is critical for maintaining the general knowledge of macromolecular crystallography methods and theory. I began my professional career as an MX beamline scientist in 2001, and I watched as the beamline user base became increasingly less versed in crystallography data collection methods and crystallographic theory through the years. Our national crystallography beamlines and the software infrastructure for structure solution have become so automated that it is no longer necessary to possess knowledge about crystallography theory in order to solve a protein structure, and generally the technical expertise for crystallography has shifted to the beamline scientist. In some ways, this trend is positive because it frees the biologist to focus on the scientific problem at hand, rather than on details of data collection strategies and structure solution. However, I believe it is important to maintain a base of knowledge in crystallography. The ACA Continuing Education Committee can fill this role, promoting courses for undergraduates, graduate students, post-docs, and PIs new to the field. I also believe that in today's world, scientists must learn to communicate their science to the general public in an accessible way. I believe the ACA can offer courses in scientific presentations at all levels, from the general public to other scientists in the field.

Christina Hoffmann - Data, Standards, & Computing

Lead Instrument Scientist
Neutron Spallation Source
Oak Ridge National Lab
Oak Ridge, TN 37831, USA

Education:

Professional Activities:

Research Interests:

Statement:

No Candidate Statement was received from Christina Hoffman, despite multiple requests.

Eric Reinheimer - Data, Standards, & Computing

Western Regional
Account Manager
Rigaku Oxford Diffraction
The Woodlands
TX 77381, USA

Education:

BS Chemistry (2000), MS Chemistry (2002), California State Polytechnic University, Pomona; Ph.D. (2007), Texas A&M University with Prof. Kim R. Dunbar; Post-doc (2007-2009), California Institute of Technology with Prof. Douglas C. Rees; Post-doc (2009), Université de Rennes I with Prof. Marc Fourmigué.

Professional Activities:

Member of the American Chemical Society (1999-2004; 2007-Present); Member of the American Crystallographic Association (2002-2004; 2009-Present); Member of the Royal Society of Chemistry; Member of the Editorial Boards of the journals Crystallization Process and Technology, Crystal Structure Theory and Applications, Structural Chemistry and Crystallography Communication and Cogent Chemistry; Instructor at ACA Chemical Crystallography Summer School (2014-2017).

Research Interests:

Assisting anyone, including students, postdocs and faculty members with a structure fascinates me still to this day! Personally, my research interests include utilizing hydrogen and halogen bonding to perpetuate photochemical reactions and thermal expansion in the organic solid-state and the array of supramolecular interactions in Lewis Acid/Base co-crystals and how such interactions may be exploited for stabilizing energetic compounds or in the detection of nerve agents. Additionally, I'm interested in the condensed matter physics and physical properties of chalcofulvalene-based organic metals, superconductors and hybrid materials demonstrating conducting, magnetic and optoelectronic properties.

Statement:

First and foremost, I wish to thank the nomination committee for putting my name forward to serve as a member of the ACA Data, Standards and Computing Committee. This is a position in which I would be very honored to serve.

Ever since I solved my first structure almost twenty years ago, I've been fascinated by X-ray Crystallography. To this very day, I remain excited whenever I see a new structural model reveal itself on my computer screen. Having been blessed by various mentors over the years who've taught me the value structure determination has in garnering a fundamental understanding of the analyzed materials, I've come to appreciate the importance of data standardization in all aspects related to the process of structure determination and reporting. While ultimately resolving a new structural model is the most exciting, strict attention to detail and how those underlying details are disseminated are the cornerstones upon which structural science can continue to make an impact in the understanding of fundamental processes across various scientific disciplines.

With the daily proliferation of new structures being reported, rigorous adherence to standards whereby the data and the context of that data can be understood is critical. From a pedagogical standpoint, at least within the context of peer-reviewed publications, how the structural data are reported and the context of that data is just as important as how a student may have synthesized their compound, purified their protein or above all grew that crystal to produce that seminal result. With so many students learning how crystallography can benefit their scientific understanding, new crystallographers should also learn that developing good practices on how that data is reported and catalogued is essential to crystallography as a whole. The data formats are there thanks to the continued efforts of the database organizations, software groups and instrument manufacturers; however the oratory the crystallographic community has with each of these entities must continue to not only maintain high data standards, but to also teach the next generation of crystallographers what those standards are and should continue to be.

It is truly a wonderful time to be a structural scientist! With the advent of new technologies related to Cryo-EM, SAXS, sources, detectors and computing, the science of structure elucidation is poised to continue making a strong scientific impact for a long time to come. With the advent of these technologies and the discoveries being made by them, it is essential that high data and computing standards be upheld. As it has always done, the ACA has maintained a critical role in establishing those standards and will most assuredly continue doing so for many years to come.

From the Editor's Desk

The Spring 2018 issue of *ACA RefleXions* was my first effort as a new Co-Editor, and there has been a very steep learning curve. I expected that I would make some blunders, and I am thankful to those with sharp eyes who have reported them to me.

First, under the section on Scientific Interest Group (SIG) Officers, I omitted the officers of the two newest SIGs, the Best Practices for Data Analysis & Archiving SIG and the Cryo-Electron Microscopy SIG. Their current officers are now listed below. The CryoEM SIG is off to an exciting start with full day of scientific sessions at the Toronto ACA Meeting scheduled for Sunday, and a workshop on CryoEM high-resolution structure determination on Friday. The Best Practices SIG also has a scientific session scheduled for Monday morning. Descriptions of the new SIGs were published in the Winter 2017 issue of *ACA RefleXions* (p. 4).

On page 8 of the Spring 2018 issue, an incorrect address is given for Joseph Ferrara. His correct address is given on page 9. Also, on page 10 of the Spring 2018 issue the name of Paul Sanschagrin, a member of the Data, Standards, and Computing Committee, was mispelled (it was spelled correctly in his email address).

On page 31 of the Winter 2017 issue, the title above the picture of Joe Ferrara implies incorrectly that he has been elected as President. The ACA Election Results table to the left of his picture correctly states that he has been elected Vice President for 2018. Joe will serve as ACA President in 2019.

We are pleased to announce that Sue Byram has agreed to join the staff of *ACA RefleXions* as Copy Editor, replacing Jane Griffin. Also, due to an injury, Paul Swepton has resigned as Co-Editor.

Ed Stevens

Index of Advertisers

Best Practices for Data Analysis & Archiving SIG Officers

Nicholas Sauter, Chair 2018
Molecular Biophysics
& Integrated Bioimaging
Lawrence Berkeley National Lab
1 Cyclotron Rd, MS 33-345
Berkeley, CA 94720
nksauter@lbl.gov

John Rose, Chair-elect
Biochemistry & Molecular Biology
University of Georgia
B204B Life Science Bldg
120 Green St
Athens, GA 30692
jprose@uga.edu

Suzanna Ward, Secretary-Treasurer
CCDC
12 Union Rd
Cambridge, CB2 1EZ, UK
ward@ccdc.cam.ac.uk

Cryo-EM SIG Officers

Catherine Lawson, Chair 2018
Center for Integrative Proteomics
Research
Rutgers University
174 Freylinghuysen Rd
Piscataway, NJ 08854
cathy.lawson@rutgers.edu

Rui Zhao, Chair-elect
Biochemistry & Molecular Genetics
University of Colorado, Denver
MS 8101 12801 E 17th Ave Rm 9108
Aurora, CO 80045
rui.zhao@ucdenver.edu

Dominika Borek, Secretary
Chemistry Department
U. of Texas Southwestern Medical Ctr
5323 Harry Hines Blvd.
Dallas, TX 75390
dominika@work.swmed.edu

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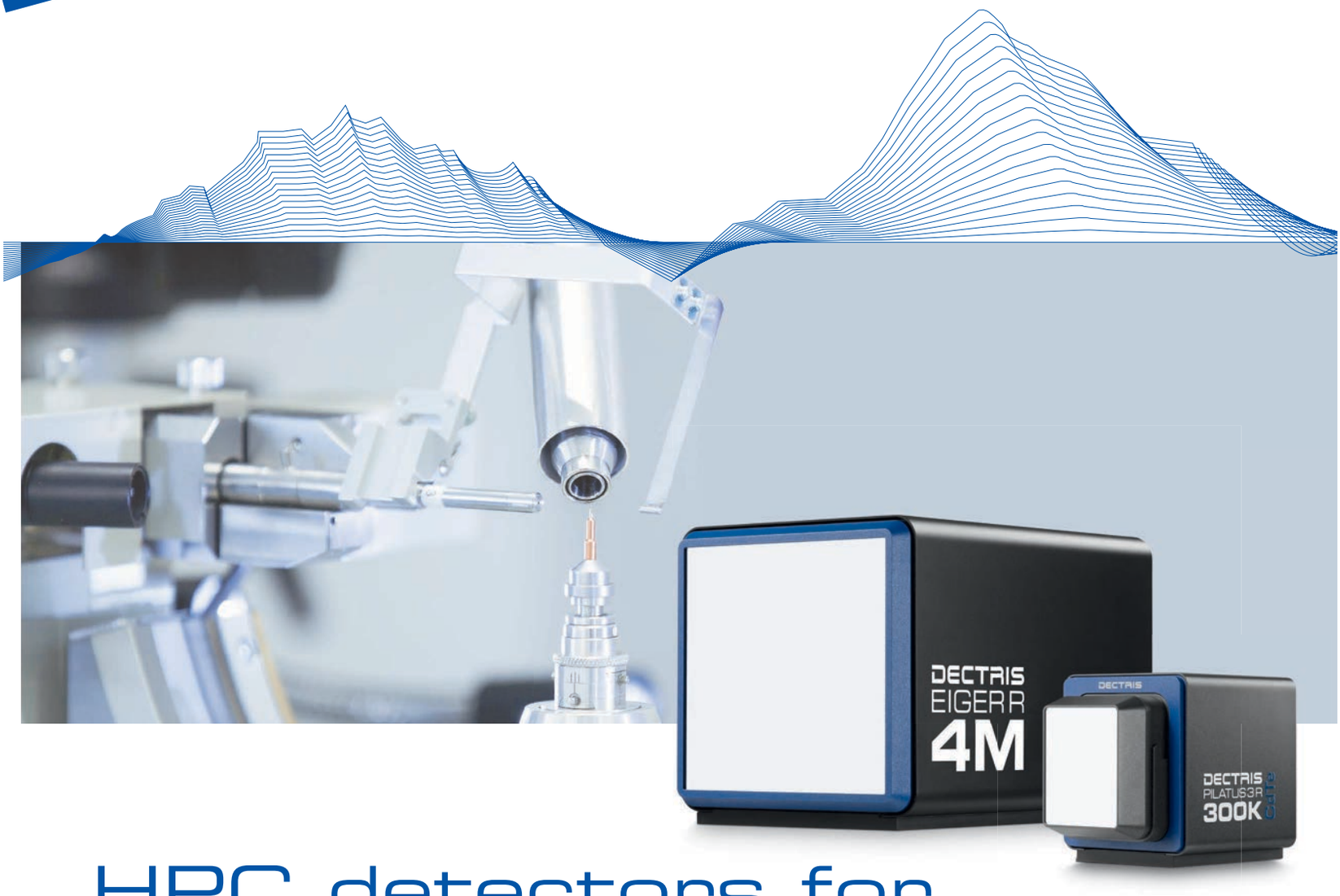

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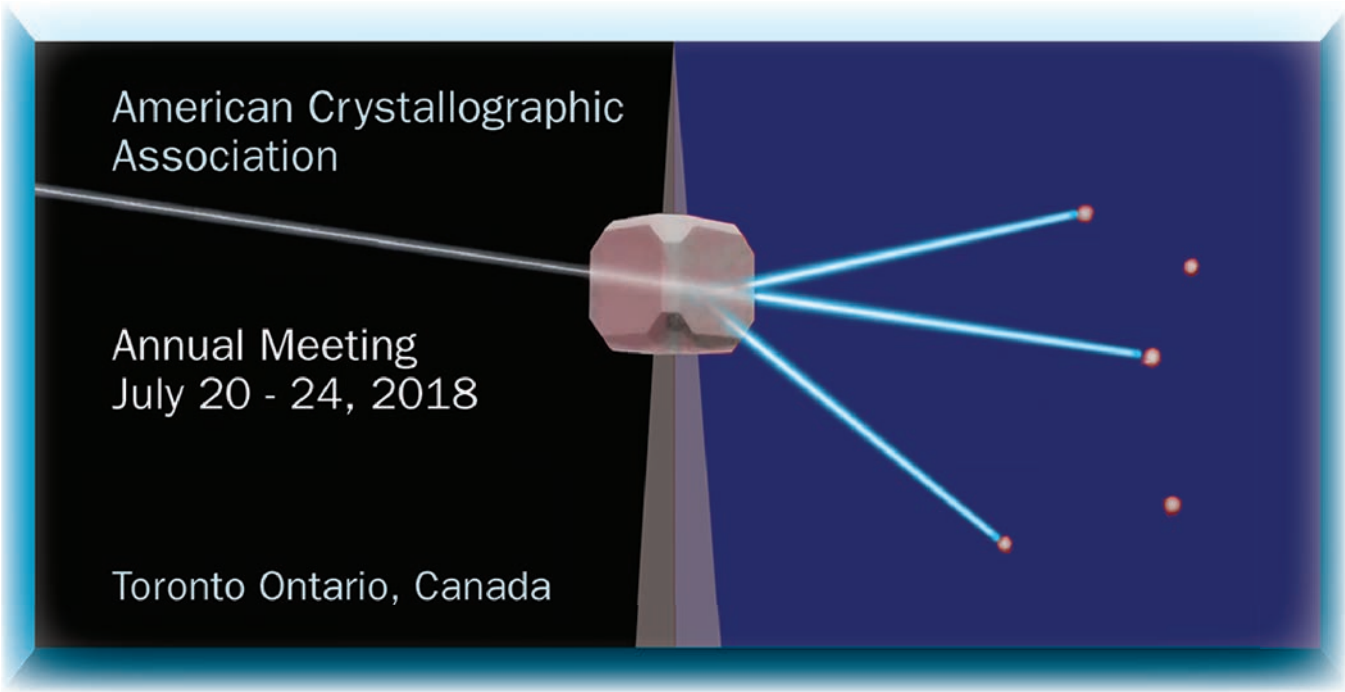
Structural Dynamics Poster Prize Awarded

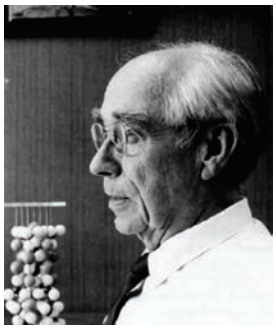
The journal *Structural Dynamics*, copublished by the ACA and AIP, sponsored a poster prize at the March 2018 BCA meeting. The award winning poster, titled "Structural studies on the concerted conformational dynamics of a catalytic loop and C-terminal domain in an archaeal amino acid decarboxylase," was presented to **Chellam Gayathri Subash** of IIT Madras, shown with John Helliwell, chair of the judging committee.



ACA History Project Update

Judith Flippen-Anderson originated the idea for the ACA History Project in 2010. She sought to preserve the history of crystallography through "Living History" memoirs published the in ACA RefleXions magazine. Since then, the Project benefitted greatly from her thoughtful advice, as it expanded to an online mission to present the history and impact of crystallography. We will sorely miss her incisive intelligence and her passionate support of the ACA.

Helen Megaw, whose biography by Mike Glazer appears in this issue, was a crystallographer-mineralogist. When the Mineralogical Society of America presented her with the Roebling Medal in 1989, Bob Newnham commented, "Along with Kathleen Lonsdale and Dorothy Hodgkin, Helen Megaw is one of the grand old British school of women crystallographers who serve as role models for many of us – men and women alike." Megaw made important contributions to our understanding of hydrogen bonding and ferroelectric transitions; she is best known for her work with feldspars and perovskites. The background to her photo is the perovskite structure for which she is famous.



The Martin J. Buerger Award was established by the ACA in 1983 to honor **Martin J. Buerger**, Professor Emeritus of M.I.T. and University Professor Emeritus at the University of Connecticut. The Award will be presented to Frank C. Hawthorne at the Toronto meeting in July 2018.

Buerger was a mineralogist who made major contributions to many areas of crystallography. He invented the X-ray precession camera, and in 1944 he published *The Photography of the Crystal Lattice*, a detailed description of the theory and practical use of the precession camera for examining single crystals. A detailed obituary describing his life and work is now online at the ACA History web pages, along with his own account of the founding of the ACA.

An ongoing effort for the ACA History Project is to include crystallographers like Megaw and Buerger who worked in the last century by publishing online obituaries that previously appeared in ACA RefleXions. **Vanessa Reitz**, Webmaster for the ACA History pages, will be adding these as they become available from the ACA office.

Virginia Pett
pett@wooster.edu

Contributors to this Issue

Heba Abourahma, Louise Dawe, Marie Fraser, Jeanette Ferrara, Joe Ferrara, Frank Fronczek, Mike Glazer, Ilia Guzei, Christina Hoffmann, Lisa Keefe, Allen Oliver, Kay Onan, Virginia Pett, Corie Ralston, Connie Rajnak, Eric Reinheimer, Ed Stevens, Brian Toby, Diana Tomchick

Helen D. Megaw (1907 - 2002)

By Mike Glazer

2018

http://www.newulsterbiography.co.uk/index.php/home/viewPerson/1919

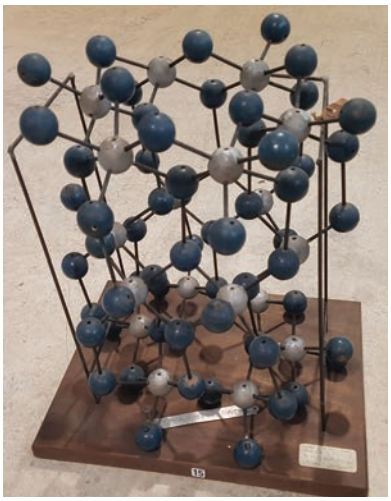
It was during the IUCr Congress in 1969 at Stony Brook that I first met Helen Dick Megaw. I had been spending a great year in the Chemistry Department at Harvard working in the research group of Jack Gougoutas together with his students Les Lessinger and Jon Clardy. I needed now to consider what I would be doing in the future. I liked the USA very much and was thinking of making my career there. Now, Helen, who was a member of staff at the Cavendish Laboratory, Cambridge, UK, had received some funding to employ a postdoctoral assistant, and my old PhD supervisor, Kathleen Lonsdale, had suggested to her that she should try to persuade me to come and work with her. Helen's field of interest was in perovskite structures but at that time I was more interested in organic molecules. To be frank, I had never got on well with inorganic chemistry and didn't think I would ever be able to understand their structures. But Helen was obstinate and kept trying to persuade me to work with her. I think it was at the clambake on Fire Island that I finally gave in and agreed to move back to the UK. I have never regretted that move because I was soon to discover that my "boss" was a very remarkable person from whom I would learn a great deal. So who was Helen Megaw?

Well, she was born on June 1st, 1907 into a very distinguished and influential Northern Irish family. Her father, Robert Dick Megaw, was a famous Chancery Judge in the High Court of Justice of Northern Ireland and an Ulster politician. In addition, her uncle, Major-General Sir John Wallace Dick Megaw, was a director of the Indian Medical Service, while one brother built the Mersey tunnel (in Liverpool), the Dartford tunnel (London), the Victoria underground line (London) and Battersea (London) power station. Another brother, Sir John Megaw was a Lord Justice in the Court of Appeal, and one of her sisters researched diet and health in the 1930s and marriage laws in Uganda in the 1950s. A most extraordinary family background.

Helen was born in Dublin, Ireland, where she attended the Alexandra School from 1916 until her family moved to Belfast in 1921 just before the partition of Ireland. After a brief period at the Methodist College, Belfast she went to Roedean School, Brighton, England from 1922 until 1925. One of her aunts was secretary to the Mistress of Girton College, Cambridge (one of the only two Cambridge Colleges for women) and Helen's ambition was to study there. She won an exhibition to the College in 1925 but for financial reasons decided to go to Queen's University, Belfast. The next year she won a scholarship and this time it proved possible for her take up a place at Girton. Originally, she had intended to read Mathematics, but she had enjoyed Chemistry at school and on her teacher's advice she opted for Natural Sciences so that she could study both Science and Mathematics. She thought that the regulations required her to study three subjects and she planned to study Chemistry, Physics and Mathematics. However, her Director of Studies, Miss M. B. Thomas, explained that she was required to study three experimental subjects (Mathematics being an optional extra) and she advised Megaw to choose Mineralogy as her third experimental subject. Had Megaw known that she could have chosen Geology instead of Mineralogy she would have opted for Geology and, in all probability, she would not have become a crystallographer! She achieved a Class I in Part I of the Natural Sciences Tripos in 1928. She then specialised in Physics, obtaining a Class II in Part II in 1930. When Ernest Rutherford at the Cavendish Laboratory told her that there was no opportunity for her to do post-graduate work in the Physics department, Miss Thomas suggested that she approach Professor Arthur Hutchinson whose Department of Mineralogy had a strong crystallographic tradition. So it was that she became a research student under the renowned, and some would say infamous, John Desmond Bernal, investigating the thermal expansion of crystals, and the atomic structure of ice and the mineral hydrargillite (a hydroxide of aluminium). One of Bernal's students at the same time was the young Dorothy Crowfoot, later to become famous as the Nobel Prize winner Dorothy Hodgkin, and Helen and Dorothy became firm friends.

Bernal was a stimulating influence on Helen and happily confirmed her interest in crystals. Her choice of Crystallography was a wise one, because it was

the one scientific discipline then, thanks principally to W.H. and W.L. Bragg, that had already established itself as a place in which both men and women could engage on an equal basis, and she never, or rarely, was aware of any form of discrimination. She started work on the structure of the mineral hydrargillite, a form of $Al(OH)_3$. Below I show a photograph of a model of its structure, which I have in my Crystallography collection in Oxford. Although rather rough, having seen better times, I have kept it because it was her first crystal model and it was constructed with help from Dorothy Hodgkin in 1934.



Her main Ph.D. work with Bernal was a study of the crystal structures of ice. Helen's accurate and demanding work on ice and heavy ice showed that the hydrogen atoms were involved in bonding between two oxygens. She and Bernal surveyed the known structures of hydroxides and of water, and concluded that there were two types of hydrogen bonds. In one type, found in ice, the hydrogen oscillates between two positions, each being closer to one of the oxygen atoms than the other. In the other type the hydrogen is bonded more strongly to one of the two oxygen atoms. In honour of her discoveries of the nature of ice, an island in Antarctica was named Megaw Island in 1962.

On another matter, it is often said that it was Bernal who suggested that X-ray photographs of biological crystals could be taken by encapsulating them in a mother-liquor in a glass tube. However, I recall that Helen told me that she had given the idea to Bernal first, as this was the technique that she had already mastered for her work on ice.

In 1934 Helen spent a year with Professor Hermann Mark in Vienna and then moved to work briefly under Professor Francis Simon at the Clarendon Laboratory, Oxford. This was followed by two years of school teaching before taking up a position at Philips Lamps Ltd in Mitcham in 1943. It was here that she worked out the crystal structure of a very important industrial material, barium titanate, which is used in capacitors, pressure sensitive devices and in a variety of other electrical and optical applications. This material, which crystallizes in the so-called perovskite structure, belongs to the class of materials known as ferroelectrics, originally discovered around 1935. Because of its strategic military importance much of the work was secret, and Helen was only allowed to publish her work on the structure provided she did not mention its useful properties! This structure is so famous and important that Helen's name is permanently associated with it and with perovskite structures in general. In the ferroelectrics community, Helen's contributions are particularly recognised, and her book *Ferroelectricity in Crystals* published in 1957 was the first of its kind and soon became a classic text.

In 1945, she moved to Birkbeck College London, once again to work with Bernal, and in the following year, she was appointed to a post in the Cavendish Laboratory, Cambridge, where she remained for the rest of her scientific life. A second book followed years later entitled *Crystal Structures: A Working Approach*, a fine text that illustrates well her unique approach to describing the architecture of crystals. Her later detailed studies of the structures and phase transitions in $KNbO_3$, $NaNbO_3$, $LiNbO_3$, and Ca_2NbO_7, including the change in atomic vibrations near a transition temperature, have contributed much to the understanding of the structural basis of ferroelectricity.

The Cavendish Laboratory was under the leadership of the Nobel Laureate Sir William Lawrence Bragg, and as a result Helen found herself at a place where many important and well-known crystallographers would pass through. She was there during the exciting double-helix days of Crick and Watson and the research by Perutz and Kendrew on haemoglobin and myoglobin. However, she remained loyal to her chosen field of mineralogy and inorganic crystals. The photograph below shows Helen with some members of staff and students at the Cavendish around 1968. (Front row: unknown, A.D. Yoffe, Helen Megaw, Will Taylor, Sir Neville Mott, Jane Brown, Mick Brown. Back students: R. Thornley, unknown, C.N. W. Darlington.)

In addition to her interest in the structures of ferroelectrics, by suggestion of William Hodge Taylor (often known simply as WHT), her immediate supervisor at the Cavendish Laboratory, she took up an interest in the crystal structures of feldspars. These complicated materials make up most of the earth's and moon's surface, and are therefore of great significance in earth sciences. The first structure determination had been carried out by WHT before the war, but such is the complexity of this class of materials, there remained a great deal of unknown science to discover. Feldspars are alumino-silicates with the general formula AT_4O_8 where A is most commonly calcium, sodium or potassium and T represents aluminium and silicon present in the correct proportions to balance the charges on the A ions and the oxygens. Thus, albite has the formula $Na(Si_3Al)O_8$, anorthite $Ca(Si_2Al_2)O_8$ and orthoclase, $K(Si_3Al)O_8$. The plagioclase feldspars form a chemical series whose formulae may be written $Na_{1+y}Ca_y(Si_{3-y}Al_{1+y})O_8$ or more simply An_yAb_{1-y} where Ab is albite and An anorthite. Plagioclase compositions appear homogeneous when examined using an optical microscope; there is no evidence of separation into domains of different feldspar phases. However, X-ray diffraction patterns in the composition ranges $An_{30}Ab_{70}$ to $An_{70}Ab_{30}$ show diffracted beams, called 'non-Bragg' reflections, that cannot occur in perfectly ordered crystals. Megaw, in three papers published in the *Proceedings of the Royal Society* in 1960, showed that the arrangement of 'building blocks' in these crystals was disordered. She used diffraction theory to relate the positions and intensities of the non-Bragg reflections to the probability of the occurrence of fault planes in the structure and to the orientation of these planes within the structure. Knowledge of the detailed structural state of a plagioclase specimen is important because it allows the temperature of crystallization and the subsequent thermal history of the rock in which it occurs to be deduced. One of her discoveries in connection with felspars illustrates a special and unique ability. Helen could visualize crystal structures entirely in her head. She never used computers but instead was able to see the atomic arrangements. For instance, if one asked her what a particular structure looked like down a specific direction she would think for a few moments and then draw it! Thus, she identified a special structural feature in felspars involving rigid tilted tetrahedra which she likened to a "crankshaft". By cooperative tilting this crankshaft can be closed up or extended relatively easily. As a consequence, the distribution of Al and Si in the tetrahedral sites has only a small effect on the bulk moduli of plagioclase felspars.

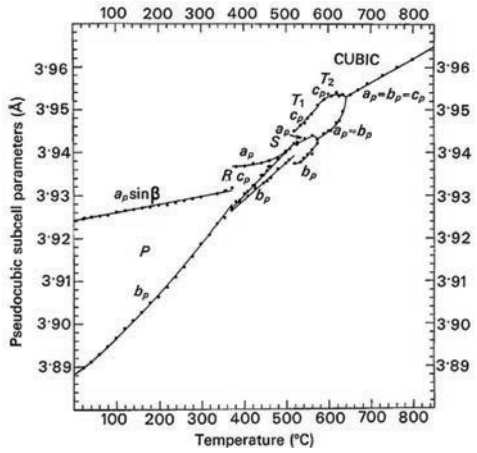
In the years after the war, the economic situation in Britain was dire and recovery was slow. This was a time of much gloom and depression. The government decided that the nation's spirits would be lifted by holding a special festival in 1951, the Festival of Britain. This was to create a series of country-wide events pointing to the future, with a large exhibition on the South Bank of the Thames in London. (The only remaining building from that exhibition today is the Festival Hall.) Helen had the idea that designs based on Crystallography could be used as decorations throughout the Festival site. She got several crystallographers, including Bragg, Lonsdale and Hodgkin to join in with creating the designs, which were then submitted to the Council of Industrial Design. These were then used in for the textiles and other materials used at the Festival of Britain, including in the foyer of the Regatta Restaurant. The carpets, curtains and table cloths, the knives and forks, glasses and so on – all were decorated with features based on crystal structures. Below I show one of the popular textiles produced based on Helen's structure of afwillite and a tie that I possess with Dorothy Hodgkin's insulin structure. Today, many of these objects are kept at the Victoria and Albert Museum in London; more information can be found in the Art and Design archives at http://www.vam.ac.uk/__data/assets/pdf_file/0015/250125/megaw_aad_1977_03_20141020.pdf . I can strongly recommend the beautiful book *From Atoms to Patterns* by Lesley Jackson, where the whole story has been recounted with many excellent photographs of the crystallographic designs.

In 1958 Helen was invited to Penn State by Ray Pepinsky and she took the opportunity to attend the ACA meeting in Ann Arbor to present a paper on KH_2PO_4. She reported later:

After it, Pepinsky, in the discussion, made a criticism so fierce that the chairman said he thought I should have the right to reply at the end of the session. Though very grateful to the chairman, I was not seriously worried. I was confident that my own ideas were right, and thought Pepinsky was quite wrong. But I remember that later someone

in the audience said to me, "Are you still going to State College?" Well I went to State College, and spent a very enjoyable summer. It was worth the opportunities it gave me to travel, see something of America, meet people and see other labs, rather than for any work I actually did there!

In her last few years at the Cavendish, starting in 1969, she and I worked together, initially on the study of phase transitions in the perovskite $NaNbO_3$. This had a sequence of at least seven different phases depending on temperature. She had already produced a graph of the lattice parameters as a function of temperature based on earlier work, and much of it was guesswork. My job was to build an X-ray camera with a reliable high-temperature system. With this I was able to derive a quite accurate sequence of phase transitions, which in the event was very close to Helen's original "guesswork". As a result, I earned Helen's respect and ensured that we continued to keep in touch even long after she retired. As I explained in an earlier article (in ACA Reflexions, Summer 2017) this led on to my own major contribution to the tilting of octahedra in perovskites. I have always been indebted, therefore, to Helen for pushing me toward trying to understand the geometry of perovskites.



In 1972 Helen retired to her home in Ballycastle, County Antrim, Northern Ireland to pursue her other interest, gardening, although she maintained her interest in ferroelectrics and continued to act as a journal referee.

In 1989, Helen became the first woman to be awarded the prestigious Roebling Medal of the Mineralogical Society of America. Bob Newnham (Penn State) wrote at the time:

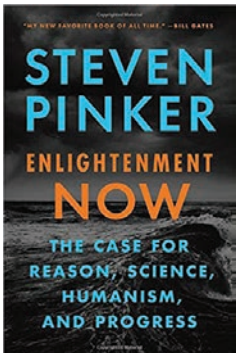
A number of American crystallographer-mineralogists were trained at Cambridge, and all of us remember her meticulous style of teaching symmetry and crystal chemistry. Crystal Structures – A Working Approach*, her last book, published in 1973, contains many of the concepts and interesting home problems presented in her classes. She had a kind heart and a patient way with students that cause many of us to look back with great fondness on our days at the Cavendish. Along with Kathleen Lonsdale and Dorothy Hodgkin, Helen Megaw is one of the grand old British school of women crystallographers who serve as role models for many of us – men and women alike. I am proud to have been one of her students.*

http://www.physicshistory.org.uk/women/Pioneers/MHD.htm

In 2000 at the age of 93 she was awarded an honorary degree at Queen's University, Belfast. In a citation for the honorary degree in 2000, Professor Ruth Lynden-Bell recalled those early days of crystallography research:

It is difficult for us to imagine the scientific environment in the nineteen thirties. It was a time of depression with little money and few jobs. Science departments were much smaller and more intimate. X-ray crystallography was a new science which attracted a number of young women such as Dr. Megaw who became distinguished scientists. In those pioneering days preparation of crystals and collection of data was more difficult and more skilled than it is today. Another big difference, which today's graduates may find hard to imagine, was that there were no computers and the tedious and detailed calculations which lead from the brightness of spots on a photographic plate to a three-dimensional crystal structure were all done by hand. Dr. Megaw was one of the pioneers in this field.

Helen died in Ballycastle on February 26th, 2002 at the great age of 94.



Enlightenment Now: The Case for Reason, Science, Humanism, and Progress, by Steven Pinker, Penguin Random House, New York, 556 pages, ISBN: 978-80525427575

Steven Pinker's latest work, Enlightenment Now, provides an optimistic outlook on the current state of world affairs. According to Pinker, all is not doom and gloom—and he spends 453 pages elucidating as to why. But the book isn't solely a response to the seemingly Earth-enveloping cloud of despair many Americans have felt since the 2016 election. Pinker himself declares in the preface: "this book is not about the forty-fifth president of the United States and his advisors. It was conceived some years before Donald Trump announced his candidacy, and I hope it will outlast his administration by many more."

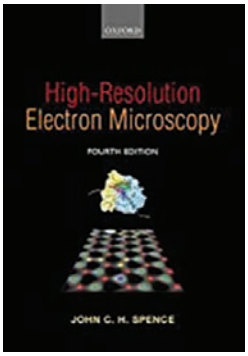
Pinker appeals to Enlightenment-era philosophy—the idea that reason, science, and humanism can solve man's problems—as he addresses various aspects of modern society that are indeed improved, historically speaking (and don't worry, if you don't really remember what the Enlightenment was, Pinker spends part one of the book, so titled "Enlightenment" filling you in). Life expectancy is higher, people are healthier, generally wealth is more widespread and inequality less profound, people are generally happier—you get the idea. And you don't have to take Pinker's word for it—the book is chock-full of graphs and tables, visual representations of well-sourced data proving Pinker's points.

While certainly enlightening (pardon the pun), Pinker's book reads more like an interesting textbook than a work of popular science nonfiction. This is not a bad thing, but it definitely feels geared toward a narrow, highly-educated audience: those "liberal academic elites" who were both baffled and devastated by the outcome of the 2016 election (you don't throw around words like "metastasizing," "abeyance," and "vicissitudes" if you want to reach a broad audience—even The New York Times has an 8th grade vocabulary rule). Despite Pinker's claim that the book is not a direct response to the Trump presidency, in many ways it feels like one—a reassurance that all is not lost to those for whom reason dictated that Trump could not win, and even a year and a half into his presidency, still cannot grasp how he did (Russian election meddling aside, Trump did and does still have a fair amount of supporters, unless Putin paid people individually to show up at all those rallies).

One bone to pick with Pinker*: on page 252, in the chapter "Quality of Life" (which falls under progress), he starts a paragraph with "As a feminist-era husband I can truthfully use the first-person plural in celebrating this gain"—the gain he is referring to is the invention of the washing machine, and the freedom it gave women to join the workforce and pursue other interests, aside from just hand-washing laundry day-in and day-out. Given the widespread reverberance of the #MeToo movement across dozens of industries—including academia—and the media storm that A-lister Matt Damon faced after he was questioned about Harvey Weinstein and qualified his response with one of those "as a father of four daughters"—someone should have taken this line out. It casts a somewhat unpleasant pall—certainly a highly-educated academic like Pinker, who not so subtly digs at Trump throughout the book, should be clever enough not fall into such a classic pitfall. Advice for all: anytime you catch yourself, in writing or out loud, qualifying yourself "as a _____"—just don't.

*Pinker also makes reference to Woody Allen as "the modern avatar of anxiety" and includes dialogue from one of his films—again showing a profound lack of awareness to the current #MeToo movement.

Jeanette S. Ferrara, MA



High-Resolution Electron Microscopy, Fourth Edition, by John C. H. Spence, Oxford University Press, Oxford, 2017, 432pp., ISBN: 978-0-19-879583-4

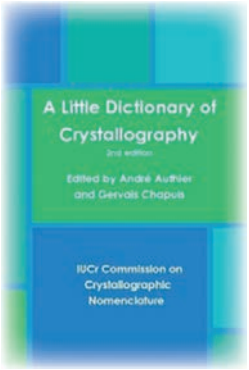
I came across this book in paperback format browsing the "stacks" at Amazon. The author is the Richard Snell Professor of Physics at Arizona State University, a fellow of both the Royal Society and the ACA. The first edition was originally published in 1980. The fourth edition was published in 2013 as a hard cover and in 2017 as a paperback. There are some references dated between 2013 and 2017, inclusive, that suggest the book is bit more current than the copyright page indicates.

This is a text book. The author goes into each area of electron microscopy in great mathematical detail with the exception of the first chapter, which covers some basics and history. The next three chapters (2-4) cover the subjects of electron optics, wave optics, and coherence and Fourier optics. The next two chapters (5-6) cover the types of experiments one can perform

with electron microscopy: transmission electron microscopy of thin crystals and imaging molecules including the hot topic of CryoEM.

The next six chapters (7-12) cover the practical aspects of the instrumentation: image processing, super-resolution and diffractive imaging, scanning transmission electron microscopy, source and detectors, electron-optical parameters, stability and experimental methods. The last chapter examines ancillary techniques.

Overall, Spence offers over four decades of expertise and refinement in one source. If you are looking for a book that will provide a detailed reference for electron microscopy, this is the book for you.



A Little Dictionary of Crystallography, 2nd Edition, by Andre Authier and Gervais Chapuis, Editors, 2017, International Union of Crystallography, 300 pages.

To call this book a dictionary is a bit of a misnomer. About the only entry that fits this definition is the entry for crystallography itself. There are over 300 terms defined and expounded upon in the book. In addition to a definition of a specific term that might cover a page or more, you may find French, German, Italian, Spanish and even Japanese (日本語) translations, examples, historical notes, references and cross-references within ALDOC. Given all this, I might call this a handbook. ALDOC covers a wide range of terms with the majority related to the fundamentals of the science of crystallography. In addition, there are entries related to chemical and macromolecular crystallography as well as entries relevant to X-ray spectroscopic methods (EXAFS, IXS, XAFS, etc.). There are more than 20 entries on the subject of twinning, providing clear explanations of all the nomenclature. Is every crystallography term included? No, but you will find most here and in sufficient detail to settle any argument, or conversely start an argument.

This book is not available on Amazon because it is a nonstandard size. However, it is currently available on a print-on-demand basis from Lulu (https://tinyurl.com/aldoc-2e). It is printed in a size smaller than a conventional IUCr text but larger than a paperback. It is also quite inexpensive and well worth the cost.

Joseph D. Ferrara

Puzzle Corner

For this issue, we have new DISORDERED and Crystal Connections puzzles, the solutions to the previous DISORDERED puzzle and to Guest Puzzler **Joe Ferrara's** crossword puzzle and also mention of those who provided solutions to previous puzzles.

DISORDERED

Distill these smashed words down into sober ones

MITIVIPER	◯ ◯ ◯
COINRATH	◯◯◯◯
WRECS	◯ ◯◯
LAXIBIA	◯ ◯ ◯

Two space groups walked into a bar
$P2_1$ couldn't get a drink because

Answer:

DISORDERED

Translate these words into standard setting

SCABENE	A B S E N C E
SAVARIB	B R A V A I S
CALTITE	L A T T I C E
SMIGINS	M I S S I N G
MESSYT	S Y S T E M

By examining all the h+k odd reflections, he could

Answer:

" S E E " C E N T E R I N G

1 C	2 R	3 A	4 B	■	5 S	6 A	7 G	8 E	■	9 F	10 U	11 S	12 E	13 S
14 O	U	S	E	■	15 P	L	O	W	■	16 A	N	O	D	E
17 A	H	E	M	■	18 R	O	L	E	■	19 T	I	L	D	E
20 X	R	A	Y	21 D	I	F	F	R	22 A	C	T	I	O	N
■	■	■	23 G	E	N	T	■	■	24 M	A	Y	■	■	■
25 J	26 E	27 S	U	I	T	■	28 K	29 N	O	T	■	30 P	31 U	32 S
33 O	G	L	E	S	■	34 G	O	O	N	■	35 M	I	S	T
36 C	R	Y	S	T	37 A	L	L	O	G	38 R	A	P	H	Y
39 K	E	L	T	■	40 B	E	A	K	■	41 O	R	I	E	L
42 S	T	Y	■	43 S	H	E	S	■	44 B	I	S	T	R	E
■	■	■	45 D	U	O	■	■	46 L	U	L	U	■	■	■
47 R	48 E	49 C	I	P	R	50 O	51 C	A	L	S	P	52 A	53 C	54 E
55 U	S	U	R	P	■	56 P	U	R	L	■	57 I	C	O	N
58 S	A	R	G	E	■	59 U	R	G	E	■	60 A	R	C	O
61 T	U	B	E	R	■	62 S	L	O	T	■	63 L	E	A	L

Crystal Connections #14

1) The Caltech _____ baseball team won a game in 2013 after 228 straight losses.

2) _____ Mooney-Slater was the first female X-ray crystallographer in the USA.

3) "In the middle of our walk of life, I found myself within a _____ dark, for the straightforward pathway had been lost." – Dante, The Devine Comedy.

4) "The Picture of Dorian _____" by Oscar Wilde.

5) "Ambition should be made of _____er stuff." Julius Caesar, Act 3, Scene 2.

6) Xylology is the study of the structure of _____.

7) Average of particle size in fluid dynamics: _____ Mean Diameter.

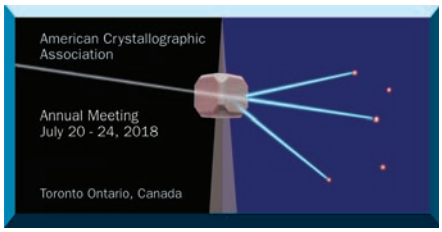
8) The part of Capt. Jean-Luc Picard was played by _____ Stewart.

Ilia Guzei (Dept. of Chemistry, U. Wisconsin-Madison) provided the solution to the previous DISORDERED puzzle and but nobody submitted a solution to Joe's crossword puzzle.

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

Frank Fronczek – ffroncz@lsu.edu

JULY 2018



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

24-28 **ACNS-2018**. American Conference on Neutron Scattering
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

SEPTEMBER 2018

23-27 **Hot Topics in Contemporary Crystallography 3. Bol, Croatia**
http://htcc2018.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

JANUARY 2019

28-2 Feb **PCCr-2. 2nd Pan African Conference on Crystallography**
Accra, Ghana
http://www.pccrafrica.org

JULY 2019

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

28-2 Aug **19th International Conference on Crystal Growth and Epitaxy**
Keystone, Colorado
http://www.crystalgrowth.org

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