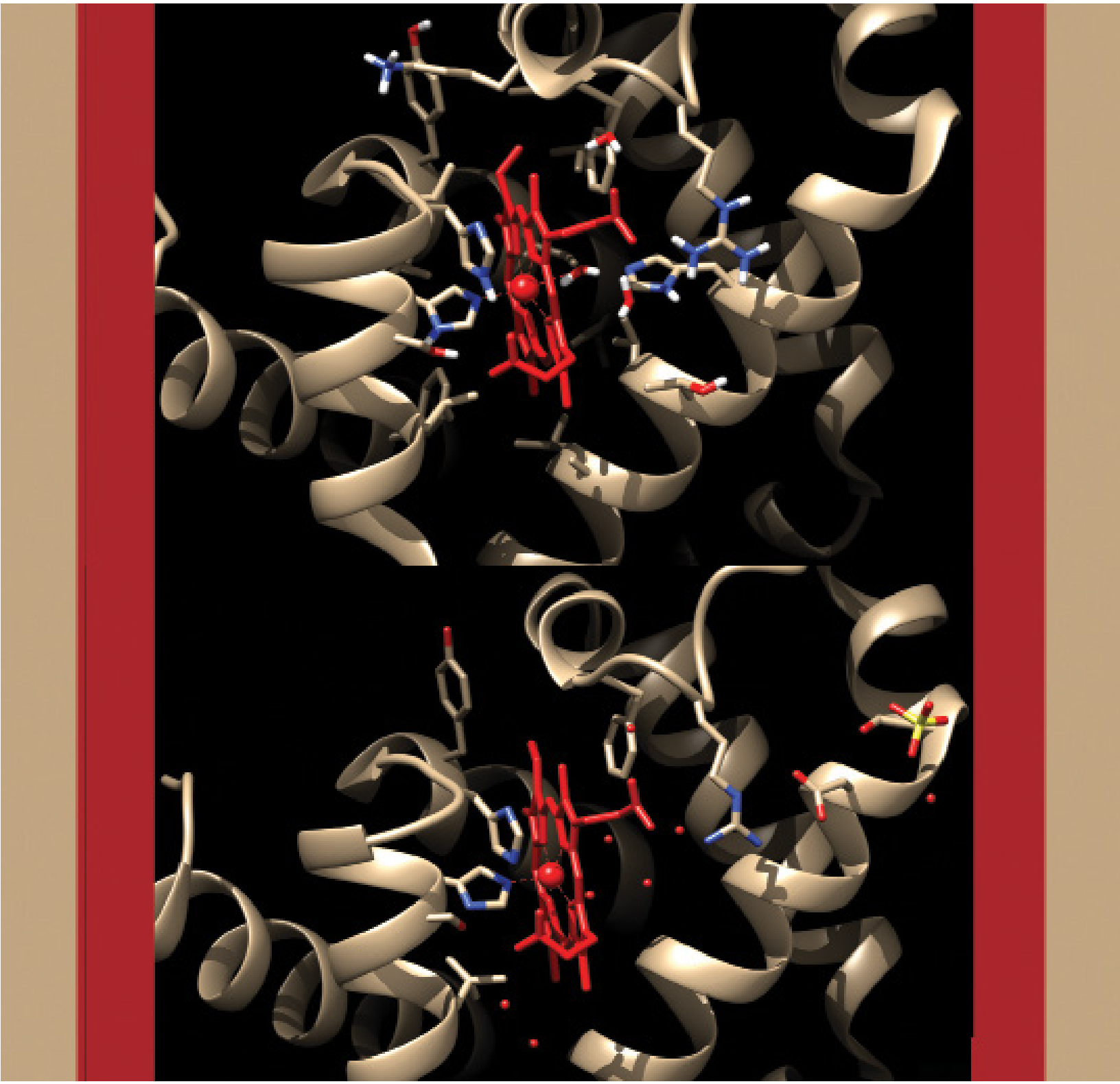
ACA RefleXions

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION
STRUCTURE MATTERS

Number 4

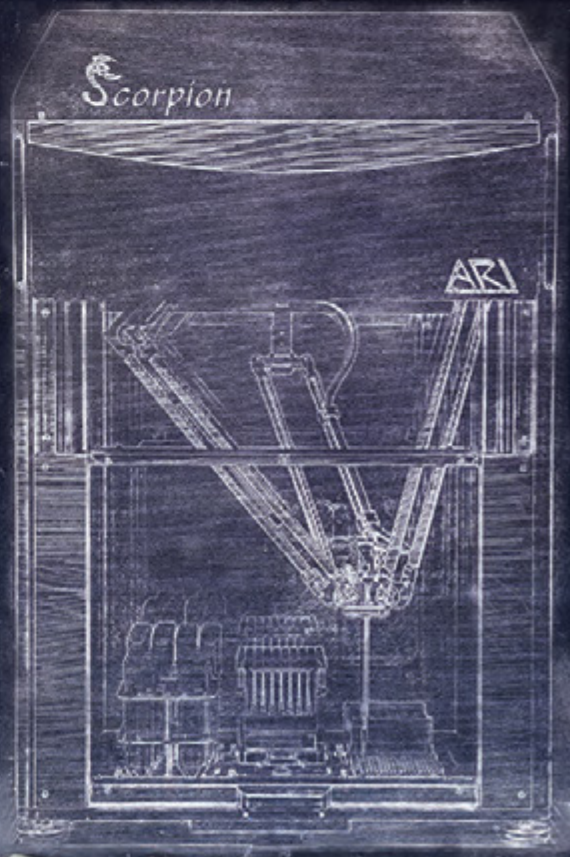
Winter 2016



2016 Bau Award at Denver ACA Meeting

TODAY'S LESSON:
WHAT CAN A SCORPION SCREEN BUILDER DO?

- ✓ Build screen blocks
- ✓ Optimize screen conditions
- ✓ Room for 96x 15 ml reagent tubes
- ✓ Access 1.5, 15 and 50 ml tubes
- ✓ Aliquot and normalize salt screens for LCP reactions
- ✓ Aspirate and dispense 1 ul to 1 ml
- ✓ Build multi-dimensional grids, pH, concentrations & titrate additives
- ✓ Set up 24-well plates, protein + screen
- ✓ Anything you can do with a handheld pipettor



Scorpion = Versatility

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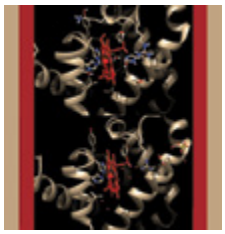

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Election Results

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Dear ACA Members and Colleagues,

The ACA Council and ACA Succession Committee have been working hard for the past year to plan for a strong ACA now and in the future. In this column I would like to give you an idea of what has been discussed and a summary of longer-term plans for the ACA.

Status of the American Crystallographic Association: We are a strong membership organization with over 1000 members devoted to structural science. We have a long-term record of running outstanding Annual Meetings, publishing the quarterly *RefleXions* magazine and the journal *Structural Dynamics*, and reaching out to the professional, student, and wider communities through our website, social media, the ACA History Portal, crystal growing competitions and support of student travel to the our Annual Meetings. Our Annual Meetings are attended by both members and non-members interested in atomic structure and provide an exceptional environment for presenting scientific results, networking, and keeping up with the latest science.

Challenges and opportunities for the ACA: There are several immediate challenges for the ACA. One is a working deficit in recent years of about $30,000 per year that may be as high as $80,000 for 2016. A second is the upcoming retirement of key personnel in the ACA Buffalo office. A third is a decade-long decline in overall membership and attendance at our Annual Meetings.

At the same time there are opportunities for the ACA. One is the opportunity of bringing in newly-expanding structural communities such as cryo-EM and NMR crystallography to the ACA. Another is the opportunity to enhance the partnerships between the ACA and the International Union of Crystallography, between the ACA and the American Institute of Physics, and between the ACA and the Hauptman-Woodward Institute in Buffalo where it is housed.

Strategic Planning: Our ACA Council and the ACA Succession Committee have been planning the near- and longer-term success of the ACA over the past year. Our overall goal is to continue its outstanding operations focusing on the Annual Meeting, *RefleXions*, *Structural Dynamics* and outreach.

A key strategy for accomplishing this goal is to reduce the operating deficit to near zero while maintaining current operations through cost savings obtained by hiring of new staff at early career stages and through the modest increase in dues approved by the membership at the 2016 ACA Membership meeting. A second key strategy for an outstanding ACA will be working with ACA partners to achieve efficiencies in operations and to maximize the ACA benefits to members and positive impact on society.

ACA 2017 Transition: Our long-term Director of Administrative Services (Marcia Colquhoun) is planning to work part-time through 2017 and serve as a consultant in 2018. We are now beginning a search for a new Director of Administrative Services, to be hired at a relatively junior level during early 2017. With this change in staffing, the personnel costs for the ACA Buffalo office are expected to be substantially lower than at present. Along with the small increase in income anticipated from increased dues and from donations to the ACA, this is expected to lead to a balanced budget for the ACA going forward.

ACA Long-term Plans: A key element of the our long-term plan is to provide maximal benefits for current members and to increase membership by broadening the scope of the ACA to include newly-emerging areas of structural science.

The immediate approach to increasing membership will be to encourage members of the cryo-EM and NMR crystallography fields to come to the 2017 ACA meeting where there will be sessions devoted to these fields, to join the ACA, and to become active in planning future meetings that will be of even more interest to them.

We plan to take advantage of several important new opportunities. One is working more closely with the IUCr. The ACA is a Regional Associate of the IUCr. The IUCr and the ACA benefit each other in many ways such as their joint missions of promoting structural science around the world, and the IUCr has helped the ACA for years through student travel awards for attending the ACA Annual Meeting. The IUCr is working with the ACA to help even more through support for archiving ACA Annual Meeting abstracts and possibly on meeting software.

In addition to its close relationship to the IUCr, the ACA is a member of the AIP. This membership in AIP gives our members free access to *Physics Today*, publishes the ACA journal *Structural Dynamics*, and enables the ACA to take advantage of the AIP's expertise in public relations, and supports the AIP's mission to promote science to the general public. We plan to continue this close relationship and to use our role in the AIP to encourage the AIP to even further enhance its outreach to the general public on the importance and benefits of science.

We have an opportunity to further develop ACA's relationship with the Hauptman-Woodward Institute as well. The HWI is a scientific organization heavily invested in structural science that has substantial overlap with the ACA in vision and goals. The HWI has administrative and management services that could potentially benefit the ACA and lead to further cost savings.

Prospects: The ACA Council and Succession Committee have developed a clear and thoughtful plan for maintaining the outstanding benefits of the ACA to our members and to the public while transitioning to new staffing in the ACA Buffalo Office, increasing membership, and building closer relationships to its partners including the IUCr, the AIP and the Hauptman-Woodward Institute.

Tom Terwilliger

Dispatch from an AIP Fellow December 2016

I am delighted to pen a few final remarks regarding my 2015-2016 year as the American Institute of Physics State Department Science Fellow. In case you are just tuning in, let me encourage you to dig up the Spring and Summer 2016 issues of *RefleXions* for a bit of the back story as to how I engaged with the Bureau of International Security and Nonproliferation's Office of Weapons of Mass Destruction - Terrorism's Nuclear Forensics Team. Now, post sabbatical, I have safely re-entered academia at the George Washington University (GW) for the fall 2016 semester enlightened with an exceptional set of experiences.

As I began to prepare some remarks for this column, I envisioned reporting on a theme of re-entering the classroom and my research lab with the newfound knowledge of how the federal government works, how the intersection of science and policy is such fertile ground for intellectual inquiry and how it may impact one's research directions. I thought I would comment on how I now have a bit of celebrity status at GW as 'the guy that was at State last year,' and how my policy graduate students are all now asking me how to get a job there. I might have also commented on how the phone is ringing off the hook with requests for panel participation and to speak to student groups and the like about 'alternative careers.' [Side note - I hate that phrase. We should all commit to 'career alternatives' as it sounds less like one has 'settled' for something other than what was originally desired.] I also might have commented on how it felt wonderful to be serving one's country in a capacity never before imagined. And finally, I also might have commented on how I got used to wearing a suit to work each day. That habit followed me (sans tie) back to GW as it's actually quite liberating to wear the same thing every day, and you feel that much more comfortable on the days you do wear jeans and a T-shirt.

It turns out however, that a different, more personal theme emerged that is perhaps more valuable to readers looking for either entertainment (ha ha) or guidance on pursuing non-bench top or leadership trajectories. The past year turned on an attraction in me for the complexity of the scientific enterprise as a whole. I developed a real appreciation for the diversity of participants who either push our science forward, or use our work products on a daily basis. Over the past year, I engaged with national lab personnel, congressional staffers, FBI and CIA agents, Homeland Security, military scientists, Foreign Service Officers, Ambassadors and representatives of scientific societies with missions I did not know existed. The breadth of the exposure was mind boggling to put it mildly. If one is in a single position for some extended period of time, like I've been with GW for 16 years, one can develop a bit of myopia that one does not even know they have. I feel like the last year was a perfect storm of professional development opportunities. Beyond the AIP Fellowship (which actually *is* designated as professional development), my service on ACA Council and participation in the Council of Scientific Society Presidents semi-annual meetings has allowed me to develop a capacity to recognize the perspectives of a diverse range of stakeholders and communities. Moreover, exposure to the *cultures* of different communities has been enlightening in terms of learning how other scientists or policy folks get things done. I hope to bring some best practices from these experiences into not only my role at GW, but also to my continued advisory role at ACA as well as whatever other opportunities are on the horizon. I feel empowered as a mentor, enlightened as a citizen and perhaps a bit more effective with respect to leadership. As such, I would encourage everyone to get out of their comfort zone for a bit and see what else you are capable of and what sparks your curiosity. Perhaps diving into the government is not appealing, yet I argue there are numerous opportunities for new experiences simply by engaging with communities a bit further afield than usual. Even looking locally, the ACA is rich with opportunities to serve - whether it's a SIG, standing committee, session chair or Council member. Thanks for reading and please consider me a resource on this and related fellowship opportunities.

Chris Cahill

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Report from the Canadian Representative

Towards the end of my article in the fall issue of *RefleXions*, I mentioned the passing of Stanley C. Nyburg, formerly of the Chemistry Department of the U of Toronto. A more complete obituary for Stan can be found elsewhere in this issue of *RefleXions (pp 37-39)*. Stan wrote an autobiography for the Canadian National Committee for Crystallography in 2009. It has been archived by Virginia Pett and can be found at: ***www.amercrystalassn.org/h-stanley-nyburg***. Stan's early years spent during the Second World War makes for very interesting reading.

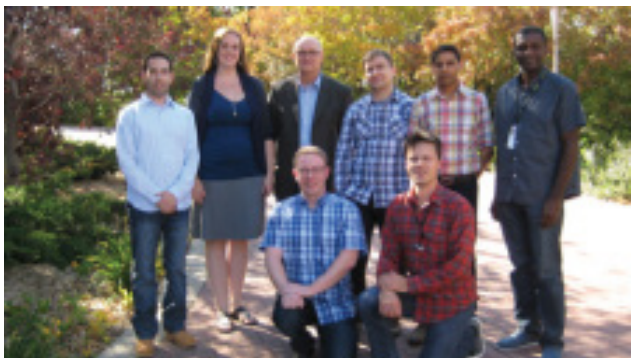
The Canadian Institute for Neutron Scattering (CINS) held its annual meeting at McMaster U in Hamilton, Ontario on October 14 and 15, 2016. This is a critical time for Canadian neutron scientists as the reactor at the Canadian Nuclear Laboratories (the NRU at the CNL) in Chalk River, Ontario is due to be shut down in 2018. One of the first items of business at this meeting was to elect a new board of directors of the CINS. The following people were elected: Thad Harroun (President, Department of Physics, Brock U, Ontario); Chris Wiebe, (Past President of CINS, Department of Chemistry, U of Winnipeg, Manitoba); Chris Heysel (Director of Nuclear Operations and Facilities at the McMaster Nuclear Reactor, McMaster U, Hamilton, Ontario); Dean Chapman (Science Director at the Canadian Light Source, Saskatoon, Saskatchewan) and Dominic Ryan (Department of Physics, McGill U, Montreal, Quebec). At this meeting the CINS also elected a new Science Council whose responsibilities are to oversee the promotion and best practices of neutron scattering in Canada. More details can be found at: ***cins.ca/who-we-are/science-council/.***

The main discussion at this meeting was on the future of the neutron scattering community in Canada. Planning for the Chalk River Reactor shutdown has already started, and the future plans for materials science research using neutrons iare of major importance. Several international representatives of other neutron scattering sources were invited to the meeting to present plans for how Europe and the United States are forging ahead and to present ideas on how Canadian scientists may be involved in their facilities. Andreas Schreyer (Director for Science at the European Spallation Source (ESS)) and Kim Leffman (lecturer for x-ray and neutron science, the Niels Bohr Institute, Copenhagen), each gave presentations on the current state of the ESS project. The ESS is a multidisciplinary research facility based on what will be the world's most intense neutron source, under construction in Lund, Sweden. Dan Neumann (head of the Neutron Condensed Matter Science Group at the NIST Centre for Neutron Research (NCNR)) gave an update on activity at that laboratory and how a Canadian partnership on neutron research might fit within the NCNR organizational framework. Ken Herring (Oak Ridge National Laboratory) presented an update on the activity ongoing at the Spallation Neutron Source Second Target Station at Oak Ridge, Tennessee and how Canadian needs might fit in there. Following these presentations, Bruce Gaulin, (Director, Brockhouse Institute for Materials Research at McMaster U), led a discussion that centered around which of the foreign sources would best fit the current and future needs of the CINS community in Canada. The CINS has been involved for some time now on what will happen upon the NRU closure in 2018. These plans as they currently are formulated can be read at ***cins.ca/2016/04/01/long-range-plan-for-neutron-scattering-in-canada/.***

In an upbeat announcement at the meeting, it was noted that a major experimental verification of the predicted "Haldane gap" named after one of the three winners of the 2016 Nobel Prize in Physics (shared by D. J. Thouless, F.D.M. Haldane and J.M. Kosterlitz) was first confirmed in 1985 by Bill Buyers, Rose Morra, Robin Armstrong, Mike Hogan and Peter Gerlach at the NRU reactor at Chalk River, Ontario ***(cins.ca/2016/10/06/2016-nobel-prize/.)***

Canadian Macromolecular Crystallography Facility (CMCF): It is a pleasure to congratulate CMCF on their 10 years of service to Canadian and international users. The first CMCF beamline (08ID-1) came online in 2006 and the first paper to be published from data collected there appeared in the same year. A second beamline that uses a bending magnet (08B1-1) to generate the x-rays came on line in 2009. From the inception of CMCF more that 425 peer-reviewed papers have been published and over 800 structures have been deposited in the PDB. Pawel Grochulski and his CMCF team are doing a great job in providing this service to structural biologists in Canada.

Canadian Light Source (CLS): The CLS was featured prominently in an article in *Chemistry and Engineering News*



This photo was taken in the midst of the Fall colors in Saskatoon, Saskatchewan. Front row: James Gorin and Cuylar Conly. Back row: Shaun Labiuk, Kathryn Janzen, Pawel Grochulski, Denis Spasyuk, Kiran Mandboth and Michel Fodje.

(August 8, 2016) extolling the virtues and capabilities of synchrotron radiation for studies in materials science. The author of the article, Mitch Jacoby, interviewed Alexander Moewes, a high-energy physicist (U of Saskatchewan and CLS in Saskatoon) regarding his role at CLS, ***cen.acs.org/articles/94/i32/Revealing-materialssecrets-synchrotron-light-html.***

The 10th Canadian Powder Diffraction Workshop will take place on June 2-4, 2017 as a satellite event prior to the 54th Annual Clay Minerals Society Conference (***www.cms2017.com***). Patrick Mercier (National Research Council, Ottawa and current Chair of the CNCC), is organizing the Workshop that will be held at the Northern Alberta Institute of Technology's (NAIT) facilities in Edmonton, Alberta where powder diffraction instrumentation and software will be made available to Workshop participants. The Workshop is targeted towards students, postdocs and practitioners

who would benefit from an improved understanding of the basic theory and practice of powder diffraction for analyzing materials. Short demonstrations and presentations will be spread out over the three days in order for participants to appreciate some of the theory and practice behind the process. Examples of some simple and some more difficult powder diffraction analyses and Rietveld refinements will be presented, as well as hints on preparing data for publication. Those who do not have access to a powder diffractometer can arrange to collect data in advance of the Workshop. Several practice data sets will be supplied. A website with the details of the Workshop and the program is currently being organized by Patrick. ***www.cms2017.com/10thcpdw***.

David Bryce from the U of Ottawa will be one of the keynote speakers for the IUCr Congress to be held in Hyderabad, India in August, 2017. David's research field is solid state NMR crystallography.

Saskatoon has been chosen as the site to host a major X-ray Microscopy (XRM) conference in August 2018. Stephen Urquart (Department of Chemistry, U of Saskatchewan) is the chair of the 2018 XRM organizing committee. This year's XRM conference is being held in Oxford in the UK. More details can be found at: ***globalnews.ca/news/2916273/Saskatoon-to-host-major-international-science-conference/.***

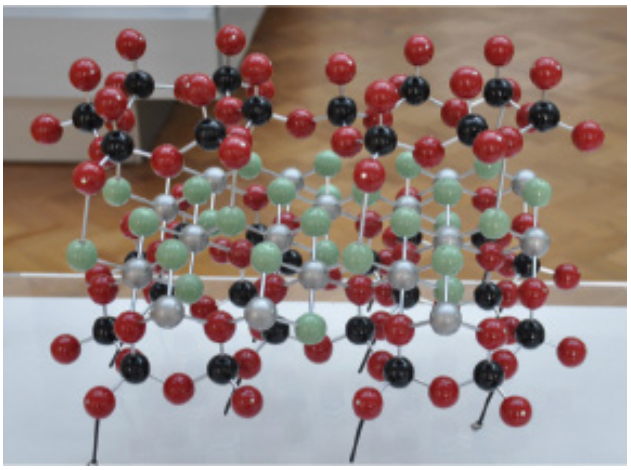
Buffalo-Hamilton-Toronto (BHT) Meeting: Just a reminder that the meeting was held in Hamilton at McMaster U on November 4, 2016. The meeting was organized by Alba Guarne and hosted by Sick Children's Hospital in Toronto. This year was particularly exciting with the keynote address given by Isabel Uson (Institut de Biologia Molecular in Barcelona, Spain). She spoke on: *Small Fragment Search for High Resolution Phasing in High Throughput Crystallography*. More details can be found at: ***bht.research.sickkids.ca***.

Who's Who in Canadian Crystallography: I am very pleased to present to the readers of *Reflexions* two very talented and productive Canadian Mineralogists. Patrick Mercier (Senior Research Officer at the National Research Council (NRC) in Ottawa, Ontario) and Frank Hawthorne (Distinguished Professor in Geological Sciences at the U of Manitoba, Winnipeg, Manitoba). Both of these scientists have made major advances in the understanding of the structures and chemical bonding in complex minerals.

Patrick H.J. Mercier attended the Royal Military College in Kingston, Ontario and graduated with a BS in Engineering Physics. From there he went to the U of Ottawa, Ottawa, Ontario and did an MSc in Physics on an ^{57} Fe Mossbauer spectroscopic study of the Fe^{+2} and Fe^{+3} in synthetic annite micas. He stayed on with his MSc supervisor, D.G. Rancourt, for his PhD degree on the crystal chemistry of natural and synthetic trioctahedral micas. After receiving his PhD, Patrick did a postdoctoral fellowship in the NRC labs in Ottawa where he worked closely with Yvon Le Page on several challenging research problems.

The Athabasca Oil Sands constitute a huge deposit of heavy crude or bituminous oil, located in Northern Alberta. Oil sands consist of a mixture of a semi-solid form of sand, crude oil (bitumen), clay minerals and water. The Athabasca deposit is the largest reservoir of bitumen in the world. Because the oil sands lie buried under boreal forest and muskeg, it is extremely costly to recover the crude bitumen. The general methods that are used are: *in situ* extraction and *open-pit* mining. The open pit method leaves behind large toxic tailing ponds. Scientists at the NRC have long been studying the relationship of the extraction of the bitumen from the oil sands and the clay minerals that in part make up the oil sand composite.

Mercier published a series of four papers on which he is first author, describing a number of predicted structures of polytypes of kaolin. Kaolin is a group of alumino-silicate clay minerals with the chemical composition $Al_2Si_2O_5(OH)_4$. These are hydrogen-bonded layered minerals with SiO_4 tetrahedral layers linked through oxygen atoms to alumina AlO_6 octahedral layers . Kaolin has many uses; it is the main material of fine china porcelain; it is used in cosmetics and in a variety of paper products.



A model of the structure of the mineral Kaolinite. Si atoms are black; Al atoms are silver; oxygen atoms are red and the hydroxide ions are light green.

There are three naturally occurring kaolin minerals, kaolinite, dickite and nacrite. Patrick Mercier and Yvon le Page developed a method, based on *ab initio* density function theory (DFT) and computations using the Vienna *ab initio* simulation package (VASP), of predicting new polytypes of the kaolin minerals. These predictions arose from the theoretical derivations of geometrically vs. energetically distinguishable stacking polytypes in the kaolin system. Their method allowed for the clarification of the phase of stability of the three natural polymorphs of kaolin as well as for the prediction of several new polymorphs that developed at moderately higher pressures.

Pressures in the range of 10 GPa revealed two stacking translations, $-a/3$ and $(a+b)/3$, that lead to a five-fold coordination of the Si atoms in kaolinite. In addition, two new polytypes of kaolinite (kaolinite II and kaolinite III) were predicted at these moderate pressures. Shortly after the appearance of Mercier & Le

Page's paper (*Acta Cryst B64*, 131-143, (2008)) an experimental verification of their prediction was published by Welch and Crichton (*Amer. Mineralogist* 95, 651-654 (2010)). Other predicted moderate pressure polytypes, dickite III and nacrite II have yet to be characterized experimentally. A high-pressure polytype (at ~57GPa) of kaolinite IV has also yet to be observed experimentally. It is very satisfying that the *ab initio* methods of polytype prediction developed by Mercier and Le Page have led to the production of dickite II, and kaolinite II and III under moderate pressures of the naturally occurring minerals and that these polytypes have been characterized by x-ray diffraction and by infrared and Raman spectroscopy.

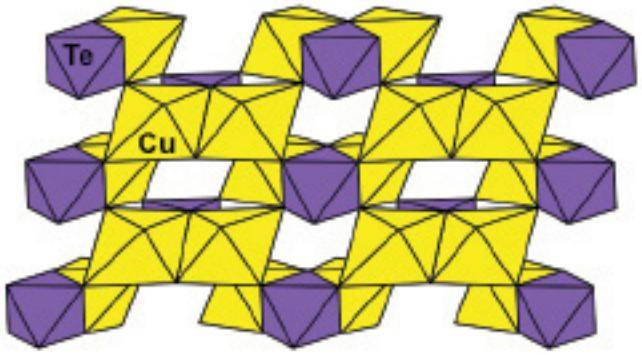
Just how to employ this new methodology for dealing with experimentally difficult systems like the extraction of bitumen from the Oil Sands has yet to be realized. However, it is now clear that relatively inexpensive and fast quantum mechanical computations can lead to predictions that can be experimentally verified or disproven. There are a vast number of hydrogen-bonded layered systems that have been determined from single crystal x-ray studies where systematic DFT *ab initio* modeling could accelerate progress in the geological or technological applications involving such minerals.

The determination of crystal structures from single crystal x-ray diffraction data most often leaves little doubt about the precision and accuracy of atomic coordinates. However, for those materials that cannot be studied by single crystal methods, one has to resort to the powder diffraction technique to determine the atomic coordinates from very small crystallites. The main drawback of this method is that the diffraction peaks are grossly overlapped often preventing the determination of the structures. In the late 1960's, Hugo Rietveld developed a method for the virtual separation of these overlapped peaks, thereby allowing for an accurate determination of the atomic coordinates from the powder diffraction data.

In a paper published in *J. of Appl. Cryst.*, **39:** 369-375, (2006), Mercier and colleagues developed a method for crystal-chemical Rietveld refinement using the program TOPAS, the pattern analysis software developed by Bruker. The diffraction data used was that from the powder diffraction pattern of fluorapatite ($Ca_{10}(PO_4)_6F_2$) in space group $P6_3/m$. This method provides least squares standard uncertainty values that are nearly an order of magnitude lower than those obtained indirectly from standard Rietveld refinement. The method funnels the precision and accuracy into the crystal-chemical distance parameters rather than into the unit cell parameters. The atomic parameters refined by the method proposed by Mercier et al. are as reliable as those derived from analysis by single crystal refinements. This method thereby results in a greater accuracy of the interatomic bond distances and angles over those obtained by standard Rietveld refinement.

Frank C. Hawthorne was born in Bristol, England. He obtained an associate degree at the Royal School of Mines in London and then a BSc in Geology from Imperial College, London. Frank came to Canada for his PhD in Geology at McMaster U in Hamilton, Ontario. The title of his PhD thesis is: *The Crystal Chemistry of the Amphiboles*. Frank traveled to Winnipeg to take up a postdoctoral fellowship in the Department of Earth Sciences at the U of Manitoba. As it turns out Frank stayed on in Winnipeg after his Ph.D. and is still there. He has worked hard in building up the study of minerals as is attested by his prodigious publication record of more than 700 peer-reviewed articles, books and book chapters. Frank has solved and refined the structures of many mineral samples collected from all over the world.

Among the many honors bestowed upon Frank is a mineral that has been named after him. Frankhawthorneite is a rare mineral discovered first in the Centennial Eureka Mine, Jaub County, Utah, US. It is a Cu-bearing tellurate with the chemical formula: $Ca^{2+}{}_2Te^{6+}O_4(OH)_2$. The x-ray structure was solved and refined by Joel Grice and Andrew Roberts and was published in the *Canadian Mineralogist* **33**, 649-653 (1995). The atomic arrangements of the Cu^{2+} octahedra and the Te^{6+} octahedra are shown here.



. The space group is monoclinic, $P2_1/n$ with unit cell dimensions of a=9.107Å, b=5.213Å and c=4.605Å and β=98.74°. There are 2 formula units per unit cell with the Te^{6+} ions at the origin and the Cu^{2+} ions at 0.178, 0.635 and -0.0002. The final R factor for the anisotropic refinement was 4.6%. Now you may wonder why I am giving you this trivia regarding the structure of Frankhawthorneite.

Well, it is nostalgia on my part; I earned an MSc in the Department of Earth Sciences at the U of Manitoba under the guidance of Bob Ferguson just before Frank joined the U of

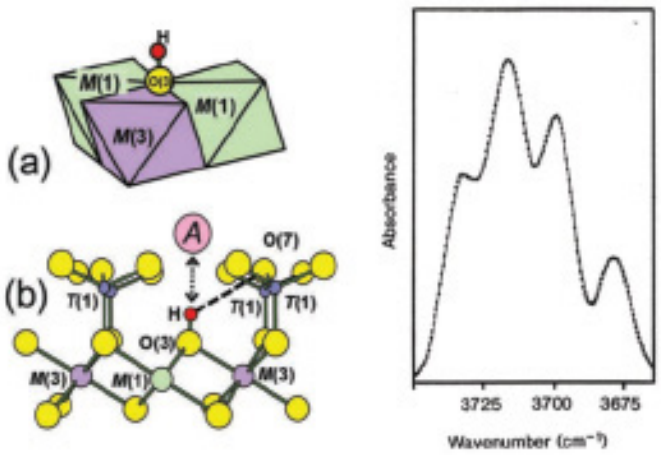
Manitoba. I worked on the structure of sillimanite. Reading the paper on the structure of Frankhawthorneite reminded me of my studies of the structure of sillimanite, Al_2SiO_5.

So what are Frank Hawthorne's main interests? He has many and varied interests but they boil down to: (1) understanding chemical bond topology in minerals; (2) understanding and deriving from theoretical principles the energetics of inorganic structures, Frank is also interested in combining the results of crystal structure refinement of minerals with spectroscopic studies of those minerals (spectroscopic results from infrared (IR) Raman, and magic angle spinning (MAS) NMR studies). We are all aware that mineral structures are very complicated. Much of the complexity arises from crystallization from aqueous solutions where the relative proportions of the cations can vary over a wide range. It is this process that brings on the wide variation in mineral structures that Frank is also seeking to enhance our understanding.

I can only touch on some of Frank's wide-ranging interests. In 2013 Frank was awarded the Roebling Medal from the Mineralogical Society of America. The title of the paper that he wrote for that occasion is *Toward theoretical mineralogy: A bond-topological approach*, *Am. Min.* **100**, 696-713 (2015). In this paper Frank reviews the current established theoretical methods such as crystal chemistry, thermodynamics and the computational mineralogy used to understand the properties of minerals. He points out the drawbacks of the present methods and introduces new concepts such as graph theory, bond-valence theory and the moments approach to the electronic-energy density-of-states of solids to understand and interpret the topological aspects of mineral structures. As indicated by the title of his Roebling Medal Paper, Frank is introducing these concepts to theoretical mineralogy; he urges mineralogists and students of mineralogy to continue on with the development of these topics in the future.

In a paper presented at the 8th European Conference on Mineralogy and Spectroscopy, September, 2015; Frank discusses the short-range interactions in the amphiboles, tourmaline and pyroxene mineral subgroups (*European Journal of Mineralogy* **28**; 513-536 (2016)). Frank's long-standing interests in the amphiboles goes back to his PhD studies at McMaster U. Amphiboles are minerals derived from either igneous or metamorphic origins. They were originally named by René Just Haüy and included tremolite, actinolite, tourmaline and hornblende. Four of the minerals of the amphibole subgroup are commonly referred to as asbestos: actinolite/tremolite, cummingtonite/grunerite, riebeckite and anthophylite. Understanding the properties of these minerals is clearly very important due to their role in human health.

Infared spectroscopy in mineral studies has an approximate 5 decade history. The O-H stretching region of the amphiboles has been particularly informative. The groups of cations in the chemical formulae of the amphiboles can be represented as follows $AB_2C_5T_8O_{22}W_2$. For example, the simple chemical formula of tremolite is $Ca_2Mg_5Si_8O_{22}(OH)_2$. The x-ray and neutron radiation crystal structures of a naturally occurring monoclinic C2/m tremolite crystal (chemical composition $(Na_{0.38}\,K_{0.12}\,Ca_{1.8})(Mg_5)(Al_{0.23}\,Si_{7.77})O_{22}((OH)_{1.33}\,F_{0.65}\,Cl_{0.01})$ clearly showed the position of the hydrogen atom on the O(3) atom linking the M(1) and M(3) octahedra (Hawthorne, F.C. & Grundy, H.D., *Can Min.* **14**, 334-345 (1976)) as shown in a and b in the figure below).

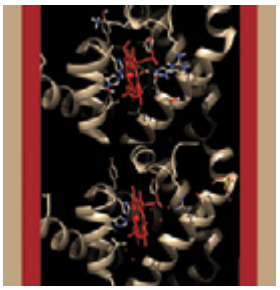


(a) The environment of oxygen atom O(3) with the hydrogen atom. The three octahedra M(1)M(1)M(3) are the nearest neighbor clusters. (b) A view of the structure down the crystallographic b axis showing the H….O(7) hydrogen bond. Oxygen atoms are colored yellow; the cations in M(1)M(1)M(3) are all Mg^{2+}; the cation in site A is Na; the sites T(1) are Si atoms. The right side of the images shows the Infrared vibrational spectrum in the region of the O-H stretching frequency for $K(CaNa)(Mg_3Co_2)\,Si_8O_{22}\,(OH)_2$.

The site O(3) is coordinated by two M(1) octahedra and one M(3) octahedron; in this case all three cations are Mg^{2+}. The *A* site in the figures above is occupied by a Na^+ ion. The principal O-H stretching frequency is sensitive to the nature of the cations that are coordinating the O(3) site. (in the right side of the figure above) shows the IR vibrational spectrum (absorbance) in the region of the principal OH stretching frequency for a synthetic amphibole: $K(CaNa)(Mg_3Co_2)\,Si_8O_{22}\,(OH)_2$. There are 4 bands in decreasing wavenumbers that may be assigned to the local arrangements and hence the short-range coordination of O(3); M(1)M(1)M(3) = MgMgMg, MgMgCo, MgCoCo, and CoCoCo. Using these IR spectral results in conjunction with the crystal structure results provides highly detailed views of short-range atomic arrangements in minerals that cannot be derived from Bragg diffraction data alone. Frank Hawthorne has made many significant contributions to the structural characterization of minerals using infrared, Raman, magic-angle-spinning nuclear magnetic resonance, Mossbauer and x-ray photoelectron spectroscopies.

Acknowledgements: I would like to thank Patrick and Frank for their help in writing their brief vignettes. Thad Harroun was a big help in putting the CINS meeting notes together.

Michael James



The ***Bau Neutron Diffraction Award*** recognizes exceptional research achievement in neutron diffraction. It was named in memory of Robert Bau who made major contributions to the development of single crystal neutron diffraction. The 2016 Award was presented to **Benno Schoenborn** in Denver for his pioneering work on neutron crystallography and its' application to biology.

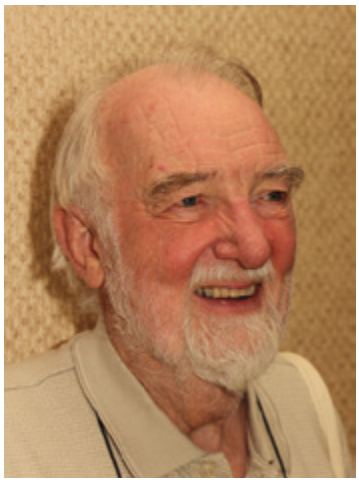
Benno in his lab at LANL (photo from LANL website)

Benno has applied neutron scattering to a large variety of biologically relevant molecules, including the 30S subunit of the bacterial ribosome, Na-KATPase, gramicidin A, thermolysin, hemoglobin, and the acetylcholine receptor. He has more than 140 publications on the subject, and has mentored, trained and inspired numerous students, post-docs and early-career scientists, expanding the reach of neutron crystallography to a larger community and setting the grounds for its further development. Now retired, Schoenborn was a Senior Fellow in the **L**os **A**lamos **N**ational **L**aboratory where he designed and developed the neutron crystallography beamline (Protein Crystallography Station) at the Los Alamos Neutron Scattering Center (LANSCE) and has been called the 'father of neutron protein crystallography'. Schoenborn's award lecture was entitled ***Neutron Protein Crystallography - History of My Research since 1962.***

Myoglobin was the first protein structure determined by neutron crystallography (Schoenborn, Bennno P, *Nature* **224** (5215), 143-146, 1969) and it remained a central theme throughout his distinguished career. The front cover image shows the heme group in myoglobin which plays a key role in the transport and storage of oxygen. The Native protontated structure, for which data was collected in the very early days (Phillips, Simon EV, Schoenborn, Benno P, *Nature* **292**, 81-82, 1981). is shown on the top. The fully deuterated myoglobin, for which data was collected some years later when the technique was reaching maturity, is shown on the bottom (Shu, F, Ramakrishnan, V, Schoenborn, B P, , *Proc Natl Acad Sci USA* **97**, 3872-3877, 2000),

Details of the heme group in native protonated (top), and fully deuterated myoglobin (botttom) show the iron atom coordinated by four porphyrin nitrogen atoms, NΣof the invariant 'proximal' histidine (F8), and molecular oxygen. The porphyrin and iron are shown in red and relevant parts of the structure are shown attached to the main chain ribbon. The oxygen molecule lies in a tight pocket, bounded by two hydrophobic groups (Phe CD1 Val E11) and the side chain of the 'distal' histidine (E7).

The cover was designed by Connie Rajnak. Robert Knott (ANSTO Lucas Heights, Australia), who collaborated with Schoenborn for more than 30 years, produced the images from Benno's published work using the UCSF Chimera package.



I. David Brown was educated at the University of London and then emigrated to Canada where he was a professor at McMaster University until his retirement in 1996. He specialized in inorganic crystallography, and with R.D. Shannon he developed the bond valence method in coordination chemistry. He was instrumental in establishing the Inorganic Crystal Structure Database.

At the age of ten I had a chemistry set and puzzled over the meaning of the chemical formulae. My grandfather was the director of a large industrial research laboratory, and served as my role model, and while we both enjoyed science I inherited neither his energy nor his administrative abilities. Unfortunately he died when I was only 16. It was around this time that I was given a Periodic Table which included the quantum numbers of the different atoms. The family had many physicist friends who did their best to explain quantum mechanics to me but to no avail. At King's College, London I studied physics and chemistry. The publication of Coulson's book *Valence*, which was required reading for chemists at the time, coincided with Coulson's move from King's College to Oxford, and the start of my university studies. In the Mathematics Department Hermann Bondi was working on the van der Waals radii of atoms and in the Biophysics Unit Rosalind Franklin was taking x-ray diffraction photos of DNA, but as a freshman undergraduate I was unaware of most of these people. Instead, I belonged to a group of students that included Peter Higgs and Mike Fisher. I struggled to understand the theory of chemical bonding. Orbitals were newly in fashion, but I could never understand how a carbon atom decided whether to adopt sp^2 or sp^3 hybridization. Did it wake up in the morning and say "I feel very sp^2 today, I will go and look for three atoms to bond to"? In my second year Watson and Crick published the structure of DNA and the Physics Department was on cloud nine, unaware that they had been scooped by their own measurements.

For graduate work I moved to the Royal Institution, where Lawrence Bragg was the director, and my graduate supervisor was Jack Dunitz. John Kendrew came from Cambridge bringing the first low resolution charge density map of myoglobin to show Bragg. We all gathered around, craning our necks and imaginations to convince ourselves that we could see the first experimental observation of an alpha helix. In the days before computers, solving a crystal structure was no trivial matter: few small cell structures were determined, refined and published in less than twelve months. When Jack told me "We will train you to solve crystal structures" I replied "OK, but I hope I can also contribute to the theory of chemical bonding" to which Jack replied "You don't want to go there". I read Coulson on valence and helped Jack proofread the paper in which he and Leslie Orgel introduced the Jahn-Teller theorem into solid state chemistry. At the International Coordination Chemistry meeting in 1959 in London Linus Pauling entertained us with the skill of a television chef, using his hands to mix *d* and *p* orbitals into a bowlful of flavourful hybrids.

In my second graduate year Jack moved to the ETH in Zurich leaving me in the hands of David Phillips who, while always generous, was a physicist who lacked the chemical background that my project needed. In addition, my many extracurricular interests were starting to squeeze out my science. I regularly scanned the titles of the papers in each new issue of the *Journal of Chemical Physics*, but only now admitted to myself that I had no idea what they meant. David recommended that I cut loose from my hobbies and join Jack at the ETH where I could focus on completing my thesis under proper supervision. The timing was propitious as my funding agency was encouraging graduate students to gain experience abroad. As my thesis took shape I asked Jack where I should go for postdoctoral experience. He said "Bring me a globe, where would you like to go?" At this time the whole world was open and most new PhDs crossed the Atlantic. We had many transatlantic visitors in Zurich. Ray Pepinsky from Penn State University was spending a sabbatical in the Mineralogy Department. He would hire anyone who was prepared to sign an employment contract that kept control firmly in his hands. Gay and José Donnay gave a talk on neutron diffraction which seemed an area with a future, so when McMaster University advertised for a crystallographer to help set up neutron diffraction at its newly opened swimming pool reactor, I applied and was offered a three year fellowship.

At this time McMaster was a small Baptist university in Hamilton, Ontario with an enrollment of less than two thousand students, but it was spreading its wings under a scientific leadership ready and qualified to take full advantage of the coming university expansion. It was already well known for high resolution mass spectrometry measurements of nuclear binding energies and its future was promising. It also met the criteria for the place where I would like to settle: I could avoid the hour and a half daily commute in London, McMaster was setting high standards for scientific research, and it encouraged interdisciplinary collaboration which suited my catholic interests that extended well beyond science. I was welcomed into the faculty, where my colleagues included Bert Brockhouse, who later won a Nobel prize for his pioneering work on neutron spectroscopy, Ron Gillespie, whose VSEPR

model of lone pair bonding is now taught in schools around the world, and Richard Bader whose QTAIM interpretation of charge density is familiar to all chemists. Together with my late colleague, Chris Calvo, there was an opportunity to establish a centre for both X-ray and neutron diffraction. What better place to work on the problem of chemical bonding? With luck I might find the answer to the carbon atom's dilemma.

The path behind is always clearer than the path ahead. My colleagues all seemed to know where their research was going but I was struggling to find the way. Perhaps there was no path. Even if there was a path where did it start? Our group published some neutron diffraction papers, but when I failed to solve the structures of several borates I started to question my own scientific ability. I finally solved the structure of lithium hydrazinium sulfate though I missed being scooped by a matter of only days. Two of Pepinsky's students had solved the structure some years earlier but delayed publishing for fear of breaking their contract. When they finally decided to submit their paper, it arrived on the same editor's desk shortly after mine! The two papers were eventually published back to back in *Acta Crystallographica*.

At King's College and at the Royal Institution there was pressure to move into molecular biology. It was a field with a great future, but the competition was intense and I am not competitive. I prefer to paddle gently in some neglected backwater of science where I can make progress at my own speed without the fear of being scooped. In the 1960s transition metal complexes were in fashion but few people were working on the structures of real inorganic crystals, those untainted by C-H bonds, but solving the structures of other people's crystals was leading me nowhere. Perhaps the path really did lie in molecular biology. To find out I spent a sabbatical with David Phillips, who was now running a large macromolecular group in Oxford. My job was to design a multi-film rotation camera for rapid measurement of protein diffraction patterns, but the lure of Oxford's Bodleian Library proved too strong and my interest again wandered back to history. The rotation camera was never built, but I published a book on the finds of British coin hoards.

David and Mariana with daughter Elizabeth at the 1986 ACA Meeting at McMaster University.

At one time I thought of a career as a librarian. I rejected this because I wanted to explore science, not merely catalogue it, but my talent for cataloguing found an outlet as an associate editor of *Structure Reports*, a publication that in the days before databases provided a critical compilation of the crystal structures published each year. By the late sixties it was struggling to keep up with the rapid growth in the number of crystal structures being published and it was many years out of date. My wife, Mariana, and I produced BIDICS, a Bond Index to the Determination of Inorganic Crystal Structures, which allowed recent structure determinations to be located by searching on the bonds they contained. It was simple to prepare on punch cards and quick to publish. It acted as an up-to-date stop gap, but I realized that such an index would become unmanageable after about ten years, just enough time, I hoped though hardly believed, to establish a computer database of inorganic crystal structures.

Shortly after my return from Oxford in1970, Bob Shannon appeared at McMaster to spend a year's leave of absence from the DuPont research laboratories. We met each other after lunch on his first day and spent the afternoon standing in the corridor talking about the bond strengths that Gay Donnay and Rudolf Allmann were using to track down elusive hydrogen atoms in crystal structures. Suddenly I saw the path opening up before me. I knew that something big was about to happen, though at that stage I had no idea that it would lead me to the physical theory underlying the chemical bond. Bob and I spent the next two weeks developing the ideas and the rest of the year writing the paper that showed all the things that one could do with Pauling's concept of bond strength (later called bond valence), though as happens with powerful new ideas, it took a long time before anyone else noticed. When we look at new ideas we are tempted to say "that's interesting, but I think I will stick with what I know." Converts have to discover for themselves what works, and they are only willing to try something new after everything else has failed. It took the discovery of high temperature superconductors in the 1980s for the world to discover my little backwater. Suddenly solid state inorganic chemistry was in vogue, but I was now ahead of the game and could help lead the way.

In 1975 the International Union of Crystallography Congress was held in Amsterdam in the middle of a heat wave, but in spite of the heat I needed to talk about the bond valence model to anyone who would listen. At the reception in the Rijksmuseum I met Gunter Bergerhoff and under the gaze of *The Night Watch* we laid plans to produce an Inorganic Crystal Structure Database. We collaborated for a number of years, and the project was finally adopted by Germany with its long tradition of compiling scientific compendia. This suited me well as I had no interest in compiling the database, I only wanted to use it. I was glad to find someone else to undertake the librarian's role of assembly and management.

Unlike many universities, McMaster encourages interactions between disciplines and this was reflected in the design of our building which housed three departments with an interest in condensed matter, Geology, Chemistry and the solid state part of Physics. We all shared a single lounge. Here every morning I would meet for coffee with members of my group: graduate

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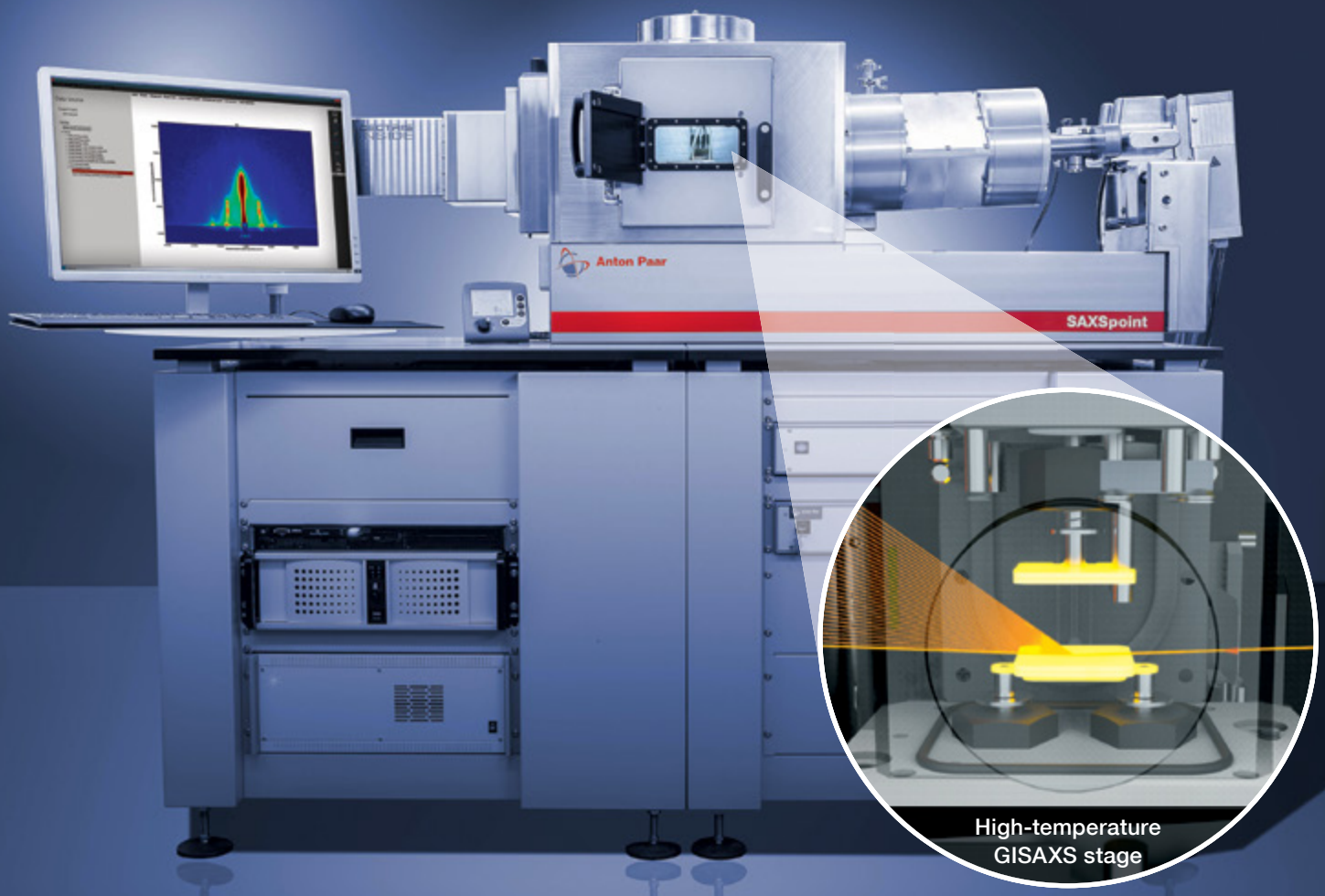

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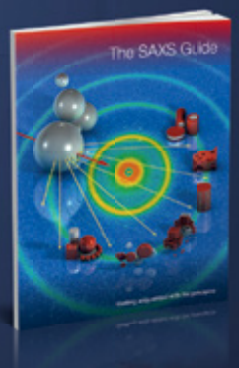

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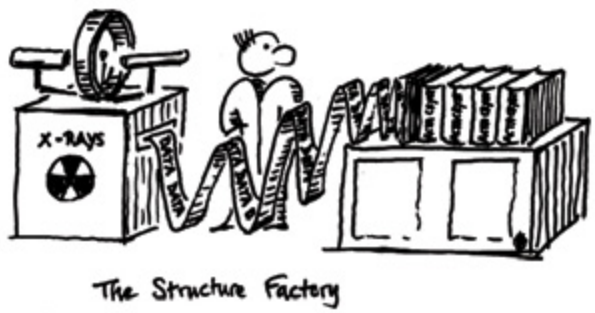
students, post doctoral fellows, undergraduate students in the summer, and anyone else who wanted to join us. We discussed many subjects including the projects we were working on. Sometimes we explored what we could do with bond valences and I would point out why a particular speculation could not possibly work, only to realize later that it was a winner and the source of another publication.

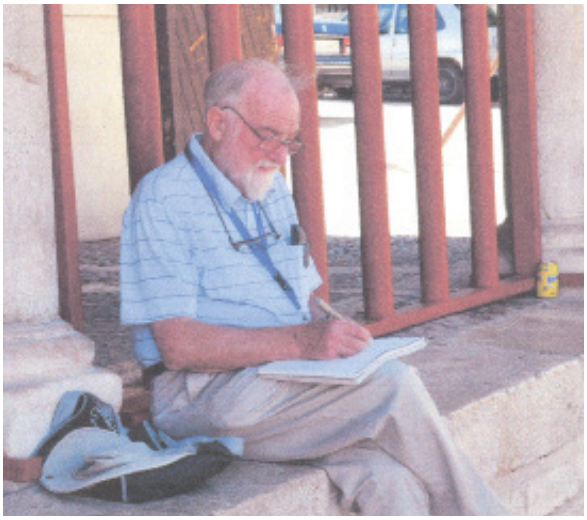
Any model that describes chemical structure as successfully as the bond valence model, must have some basis in physics. I looked forward to the day when Richard Bader and I would publish a paper reconciling our two very different approaches though alas this was not to be. One might have thought that chemical bonding would be the topic of many a lively discussion at McMaster, but Ron Gillespie, Richard Bader and I had three very different ideas about the meaning of the term 'chemical bond', and as we were each convinced that our own definition was without question the only true definition, dialogue was virtually impossible. I learned much from Richard, though the exchange of ideas was not reciprocal. On occasions when he had stumbled across my latest paper, he would phone me at 11 o'clock at night in a state of disbelief and say "David, what the *hell* is going on?" On one occasion we were discussing some scientific problem which we could not resolve, and pointing to up to the sky I said "One day when we are up there we will be able to ask Himself", to which Richard replied "Yes, but will we understand the answer?"

For several years during the nineties a group of graduate students from Trömel's laboratory in Frankfurt would spend a month in the summer with me. With Trömel's support, one of them, Christof Preiser, wrote a thesis which demonstrated that in the ionic model the bond valence was the same as the electrostatic flux that links the cations to the anions. This started as one of those coffee-morning ideas that I initially dismissed out of hand before realizing that this was the holy grail I had been looking for. Pauling and Bragg had hinted at this connection before I was even born but no one had pursued it as a quantitative theory. Bond valence and flux not only had the same values, they shared another important property: neither depended on how the charge density was distributed, explaining why a century of quantum mechanical studies had failed to reveal the secrets of the traditional chemical bond. Identifying the chemical bond with the flux allows the rules of the ionic, covalent and VSEPR models all to be derived using the theorems of classical electrostatics, resulting in a simple but robust physical theory of chemical bonding that does not depend on, but yet is completely compatible with, quantum mechanics.



The crystallographer's dream, circa 1978.

Since my systematic studies of structure and bonding involved recalculating the geometry of many crystal structures, I became convinced that life would be much simpler if everyone used the same file format for recording their crystal structures. It would make moving crystallographic information between programs easier, and it would simplify the submission of crystal structure publications to the journals and databases without the need to rekeyboard all the tables of coordinates. After a couple of false starts in the 1970s, we launched CIF, where my librarian talents were again put to good use in creating CIF dictionaries. This was surprisingly hard work, but the reward was a much better understanding of the concepts of crystallography.



David sketching on a break from the IUCr Congress in Madrid, 2013.

After several of my early papers were rightly rejected, I realized that the only way to convince the referees was to make sure that the evidence that supported my ideas was well documented. Crystal structure information can be downloaded from the databases, but I avoided blindly analysing them with statistics. The results of statistical studies are usually only meaningful if they are already visible in the input measurements. More importantly the quality of any result can never be higher than the quality of the information from which it is derived. I prefer to hand pick the numbers that I use as input. The input to a statistical study is like a family. Each item has its own personality and all must be individually understood and lovingly cherished. A close curating of the input can remove bias as well as incorrect or questionable observations. One gets to know each item within its own context. Without this involvement it is easy to miss the occasional structure that by not fitting the pattern points the way to the next big step forward.

I have now discovered the answer to the carbon atom's dilemma. It is the size of the atoms, not the hybridization of orbitals, that determines the coordination number. Unless one of the ligands is hydrogen, the highest coordination number of carbon is three, as in graphite and the carbonate ion. The myth of the tetrahedral carbon found in the metastable high-pressure diamond structure arises from the fortuitous similarity of this metastable coordination number with the number of spherical harmonics (sometimes called orbitals) used as the basis set in

quantum calculations. There is no physical connection between the two. The light elements are known with all the coordination numbers between two and eight according to their size. There is nothing special about four.

After my grandfather's death my grandmother became my mentor and provided me with some useful scientific connections. She had been a nurse in the days of Florence Nightingale and told me stories of her grandfather, an architect who had apprenticed as a shipwright at the time of the Napoleonic wars. I listened with interest to the tale of her terror in having to phone her husband's boss as the first call she made on the newly invented telephone, and of how my grandfather as a young scientist explained in simple words the workings of Kelvin's tide machine (an early mechanical computer) to an elderly visitor whom he later discovered to be Lord Kelvin himself. As a teenager I was conscious of how each generation passes its wisdom on to the next; of the ever repeating cycle of life. Even at that age I could see that my path would have its beginning and its end. When I was young it was never my ambition to be a famous sports star. It was the wisdom of my elders that I admired. My ambition was one day to be old and wise like them, to be able to look back on the adventures I encountered along the path in the company of my life partner. Mariana has left me with three daughters and many grandchildren, each of whom will, in their own way, leave their mark on the world. I love them all, even though none of them has the slightest interest in chemical bonds.

Crystallography in the Americas: ACA History Site Update

Another new section was recently added to the ACA History pages online: Crystallography in the Americas, with 18 new articles. The new section will focus on advances in structural science in the US and Canada, as well as highlighting scientific outreach activities of prominent US/Canadian researchers to Latin America.

As you probably know, the ACA represents both Canada and the US to the International Union of Crystallography. For this reason we thought it especially appropriate to initiate the new section with a series of articles on Canadian crystallographers reprinted from the Canadian National Committee for Crystallography newsletter. In addition there is an article by Bill Duax, "Crystallography in North America", which emphasizes the contributions of US and Canadian structural scientists.

The Latin American structural scientists are independent from the ACA. In 2014 the **Latin American Crystallographic Association (LACA)** became a Regional Associate of the IUCr. Several Latin American countries have a national crystallographic organization including Mexico ***www.smcr.fisica.unam.mx*** and Brazil ***www.abcristalografia.org.br***. These organizations have posted online information about the history of crystallography in their region on their web pages.

Complementing the new online section that highlights Canadian structural scientists, I. David Brown's "Living History" in this issue of *ACA RefleXions* magazine tells the story of his contributions, notably the bond valence method in coordination chemistry.

Also new on the ACA History pages online is information about David Harker, "a founding father of modern crystallography" according to the online obituary by Bill Duax. In addition, David Haas condensed the biographical memoir of Harker by Herbert Hauptman, and provided an interesting newsletter article about his former PhD advisor.

Virginia Pett

From the history portal: ACA History || ACA Beginnings

"Scientists from other societies who attend our meetings often comment on the friendliness and mutual helpfulness of crystallographers. This good spirit became a tradition in the earlier days when the Society was small, and it is hoped that it will be continued. Practical jokes were not ruled out. For example, the supplement to the program and abstracts of the 1953 meeting at the University of Michigan contained many puzzling papers. Careful study showed the author, Regreub Nitram to be the mirror image of one Martin Buerger and the 'emptiness function' in crystal structure analysis to be nothing more than one of the simple mathematical theorems of G. Willikers."

Elizabeth Wood and William Parrish, History of the American Crystallographic Association.

The Rigaku Symposium on X-ray Diffraction (Yale May 19-20, 2016)

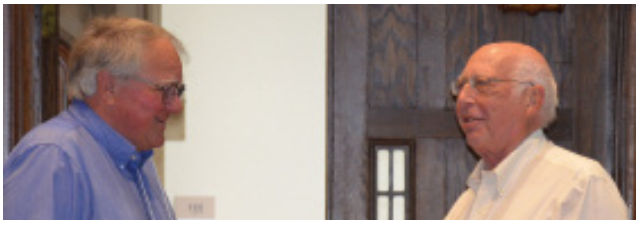
The two-day event featured a diverse array of workshops, lectures, and research presentations. On Thursday, attendees participated in hands-on demonstrations and tutorials; they chose from three separate short courses that focused on either macromolecular, materials, or small-molecule analysis and techniques. These courses were taught at Yale West Campus's new Materials Characterization Core with top-flight instrumentation. The suite of newly installed tools for materials characterization includes a Rigaku SmartLab X-ray diffractometer and a Rigaku Primus II X-ray fluorescence spectrometer. These systems, managed by Min Li (Yale), enabled participants to gain practical knowledge and learn fundamental concepts as taught by experts in the field. Many members of both Yale University and Rigaku Corporation collaborated to host a successful event. Christopher Incarvito (Yale, Director of Research Operations and Technology) shared his thoughts on inaugurating the Materials Characterization Core with its first conference: "The Rigaku Symposium is a great opportunity to showcase the kind of high-value instrumentation and expertise we provide across Yale. I am proud to support this effort, and look forward to hosting future events with Rigaku and with collaborators across Yale."

Workshop participants having a productive breakfast at Yale West Campus's Materials Characterization Core.

Joe Ferrara (Rigaku) demonstrated how to mount and collect data with an XtalLabMini, a bench top diffractometer on loan from Rigaku for the purpose of enhancing attendees' experience with hands-on access to a live, single-crystal instrument. Eric Reinheimer (Rigaku) instructed participants on how to use CrysAlis^{Pro} to integrate and solve twinned crystal data collected on the XtalLab Mini. Brandon Mercado (Yale) held an introductory tutorial on how to use Olex2 and SHELXL to solve and refine disordered data. Tom McNulty's (Rigaku) lecture on high speed x-ray tomography of soft materials at the nanoscale expanded the scope of the workshop beyond x-ray diffraction. In a similar effort to discuss the versatility of x-rays, Jeff Borgeson (Rigaku) used the newly installed Primus II to demonstrate how to identify the atom contained in trace amounts of pharmaceuticals by x-ray fluorescence. Aya Takase (Rigaku) held multiple small group sessions and elaborated on how multi-dimensional detectors will advance the field of powder and thin-flim diffraction with Rigaku's SmartLab. Simon Bates (Triclinic Labs) and Joe Ferrara (Rigkau) shared an exceptional commitment to the symposium; they both taught courses and contributed formal presentations during Friday's symposium. Simon instructed workshop attendees on how to analyze inorganic and organic, crystalline material with pair distribution functions. Thursday's events concluded with a reception in the heart of the Material Characterization Core, where all instructors were available to answer additional questions and spend one-on-one time with attendees in front of the x-ray equipment.

Aya Takase leading her workshop session titled, "Future of X-ray diffraction; use of multi-dimensional detectors".

Friday was devoted to academic presentations. Attendees of the Rigaku Symposium reconvened at Yale University in the Sterling Chemistry Laboratory to hear Simon Bates give an intriguing talk on non-crystalline metastable materials and how x-rays can be used to probe their structures. Ankit Disa (Yale) presented how to control the atomic and electronic structure of near-perfect complex oxides. The focus of late morning talks shifted to macromolecular diffraction with Michael Robertson's (Yale) presentation on structure-based drug design related to the macrophage migration inhibitory factor. His talk complemented by the following lecture from Kathryn Ferguson (Yale) on extracellular control of receptor tyrosine kinases. The symposium's attendees then adjourned to the courtyard of the Class of 1954 Chemical Research Building for lunch and an opportunity to discuss the morning's events. The talks concluded with organometallic flare. Liam Sharninghausen (Yale) presented a series of catalytically active iridium dimers, while James Mayer (Yale) focused on cerium oxide nanoparticles. Both talks possessed the common theme of how to improve water oxidation catalysis. Linda Doerrer (Boston University) and Alan Blach (University of California, Davis) also shared a common subject: metallophilic interactions in extended 1D materials. All attendees found a common interest in Joe Ferrara's presentation on the innovative, new products offered by Rigaku.



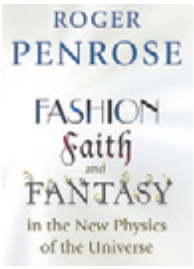
Alan Balch (University of California, Davis) speaking with Jack Faller (Yale) during a break.

Brandon Mercado (Yale) presenting Yekaterina Rokhlenko (Yale) with her prize.

Friday's events concluded with a poster session and reception where Yekaterina Rokhlenko (Yale) took home the top prize. Rigaku generously sponsored a travel award for Yekaterina's attendance at an upcoming national conference on x-ray diffraction where she will present her work, *Using Small-angle X-ray Scattering to Study the Alignment of Coil-Coil Block Copolymers with Magnetic Fields*. Kelli Rutledge (University of Connecticut) received an honorable mention for her work, *Substitution at allylic stereogenic centers of a [13]-macrodilactone: effects on macrocyclization efficiency and topology.*

Brandon Mercado

Fashion, Faith and Fantasy in the New Physics of the Universe, Roger Penrose, Princeton University Press, Princeton, 2016, 520 pages, ISBN: 978-0-691-11979-3.



This book is the result of a series of lectures Roger Penrose gave at Princeton in the early 2000s. I heard about this book on *Science Friday* so I bought a copy. Be forewarned: this is not light reading. This is not a text book, but the concepts might have been better related had this been presented as a textbook.

The first three chapters cover the fields of *String Theory (Fashion), Quantum Field Theory (Faith) and the Big Bang Theory with Inflation (Fantasy)*. The titles of the chapters are meant to let the reader know how Penrose feels about the particular subject.

The chapters on *String Theory* and the *Big Bang Theory* both receive treatments that suggest there are fundamental flaws with both theories: many more than four dimensions for the former and inflation after the Big Bang for the latter. He makes a good point that both theories are virtually impossible to prove and physics should focus on that which can be proven. The chapter on *Quantum Field Theory* concludes with the paradigm that the current theory works well enough "for all practical purposes".

I interpret the first three chapters as a diatribe against the aforementioned theories which allows Penrose to segue into the final chapter. Here he makes the case for his own pet theory, *Twistor Theory* (A New Physics for the Universe). The chapter ends with a discussion on *conformal cyclic cosmology*. *CCC* suggests that we are simply in a never ending cycle of big bang (minimum entropy) to black hole death (maximum entropy) and ultimately a sea of massless particles resulting in another big bang, over a time period on the order of 10^{100} years for each cycle.

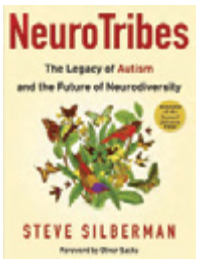
There is a quote at the end that seems relevant today. One could remove "scientific" from the paragraph and describe a broader problem with information glut:

Let me end by making a few final comments about the role of fashion in its frequent grip on scientific ideas. I very much admire and benefit from the way that modern technology, mainly by way of the internet, allows immediate access to so much of the broadening body of scientific knowledge. Yet I fear that this very breadth may itself lead to a tightening of the grip of fashion. There is so much out there which is now so accessible that it is extremely difficult to know which things among that multitude contain new ideas to which attention should be paid. How does one make judgments as to what may be important and what owes its prominence merely to its popularity?

There is a detailed mathematical appendix that covers some of the concepts in the main text including iterated exponents, fields and topology.

You will need your thinking cap for this book, and be prepared to expand your horizons.

NeuroTribes: The Legacy of Autism and the Future of Neurodiversity by Steve Silberman, Penguin Random House, New York, 2015, 543 pages, ISBN: 978-1-58333-467-6.



My daughter, Jeanette, gave this book to me when I last visited her in May thinking I would enjoy it. She was right – *NeuroTtribes* is fascinating. The author sets out to provide a comprehensive view of autism as we understand it today and does it well. Silberman begins with his introduction to the title subject through a Geek Cruise he sailed in 2000. The personalities of the hundred or so developers he interacted with on the cruise led him to research and write this book.

Silberman provides a short biography of the discoverer of hydrogen, Henry Cavendish, who showed all the symptoms of an autistic person: inattention to other people, regimented routine and singular focus on a problem, to name a few. Paul Dirac, who predicted the existence of the positron, is offered as another example of a historical figure with what we consider the modern markers of autism. I learned he was on the autistic spectrum when I reviewed Graham Farmelo's biography a few years back. Silberman fast-forwards into the modern era with a case study of a boy named Leo Rosa. Leo's parents worked endlessly to try to help him through diet and therapy to find these only alleviated symptoms caused by the autistic behavior, not autism itself.

Then, Silberman rewinds to the early 20th century to look at the work of Hans Asperger at the Heilpädagogik Station in Vienna. Asperger had worked out many of the details we understand about autism today, but this information was lost in the Anschluss and subsequent purge of Viennese medicine. Asperger stayed in Vienna during WWII, but his work was suspect after the war ended because of the Nazi influence in Austria.

After the war, Leo Kanner, a psychotherapist in the United States, developed the model of autism that became the standard for many years. He proposed that autism was the result of toxic parenting. Silberman then takes a moment and clarifies what behaviors are associated with autism, citing radio hobbyists as a group that embraced technical prowess with real human contact. A similar situation occurred when computers became available and the same personalities that handled the radio so well came to work with this new technology.

Silberman's history of autism and its role in fostering the idea of neurodiversity is perhaps best summarized by this quote from Temple Grandin in the book:

"*Aware adults with autism and their parents are often angry about autism. They may ask why nature or God created such horrible conditions as autism, manic depression and schizophrenia. However, if the genes that caused these conditions were eliminated there might be a terrible price to pay. It is possible that persons with bits of these traits are more creative, or possibly even geniuses. If science eliminated these genes, maybe the whole world would be taken over by accountants*."

Dark Matter by Blake Crouch, Penguin Random House, New York, 2016, 352 pages, ISBN: 978-1101904220.

I listened to an interview with the author, Blake Crouch, on *Science Friday*. Then, when I saw copies of the book all over the place, I picked one up for myself. The author spent 10 years writing this book because he spent considerable time with scientists in order to make the idea of traversing the multiverse plausible. The premise is that the antagonist has developed a human version of Schrödinger's Cat and uses the device to traverse space, but not time. This a fun summer read but don't think too hard or the ideas of the multiverse and quantum coherence/decoherence are likely to give you a headache.

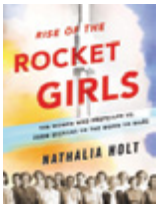
This month's theme on *Science Friday* is women in science. While listening I came across *Unlocking the Clubhouse* and *Rise of the Rocket Girls*. I highly recommend fathers of young girls read both books as they give insight into overcoming the "but you're a girl" mentality of many people.

Unlocking the Clubhouse: Women in Computing by Jane Margolis and Allan Fisher, 2002, MIT Press, Cambridge, 182 pages, ISBN: 978-0262632690.

This is a report on how computer science has become male dominated over the last 30 years. The authors' analysis suggests this started in the 1980's with the first widespread distribution of home computers like the TRS-80, Commodore 64 and Apple II. The authors suggest further these computers wound up in the hands of boys, mostly, since the machines provided a release for less social boys that more social girls did not need. The authors followed several cohorts through the computer science program at Carnegie Mellon University and found that the women tended to lose confidence more quickly than male counterparts. The loss of confidence and failure to become part of the male culture caused a large dropout rate. Finally, the authors looked at how CMU reversed these trends by first teaching practical applications of computer science, providing a more gender neutral environment and improving teaching. The result is much higher retention and matriculation rates for women in the computer science program at CMU.

My takeaway lesson from this book is that fathers need to work with their daughters in the same way they work boys in terms of teaching the basics: how to use them, program them and take them apart and put them back together.

The Rise of the Rocket Girls: The Women Who Propelled Us, From Missiles to the Moon to Mars Nathalia Holt, 2016, Little, Brown and Co., New York, 352 pages, ISBN: 978-0316338929.



This book is a history of the women at the Jet Propulsion Laboratory. I have often asked myself why the JPL is called the JPL: the only thing JPL had to do with jet propulsion was the design of rocket motors to launch heavy bombers off of aircraft carriers during WWII. The reason the word "jet" is used and not "rocket" has to do with the wider defense community's belief that rockets were a bad idea at the time of JPL's birth late 1930s. Everything JPL has ***Book Reviews continued from page 16***

done since has involved getting objects into space and monitoring them once there.

Before electronic computers became commonplace, human "Computers" were the machines that generated the algorithms and performed the calculations needed to predict the motions of the planets, construct buildings, etc. Macie Roberts, the manager of Computers at JPL, created a team of engineers that was made up entirely of talented young women. They were engineers and scientists, some with degrees and some without. These pioneering women calculated the yields of rocket propellants and trajectories for the original Corporal and Sargent rockets for the Army to the first American satellite, Explorer, for Mercury, Gemini, Apollo manned programs, and the host of subsequent satellites from Mariner and Viking to Voyager and beyond. First they used slide rules and tables, then Friden calculators. When the electronic computers came into the picture they became the first coders, first in assembly and then FORTRAN.

The author shows how the same principles that allowed women to succeed as scientists that were outlined in *Unlocking the Clubhouse* could actually work, long before the studies reported there were done in *Unlocking the Clubhouse*.

All book reviews by Joe Ferrera

Keeping Aloft with Science on Twitter

The exponential increase in scientific literature published over the years is both the boon and bane of scientists. While this trend is generally positive for the communication of ideas, it is difficult to keep up-to-date with current literature. Keeping tabs with developments has historically (and powerfully) been addressed with *(i)* communication among peers at conferences, *(ii)* scientific journalism such as trade journals and magazines, *(iii)* summaries in abstract services, and *(iv)* journal clubs. A powerful form of media that combines these for the modern era is social media platforms (such as Twitter).

The Young Scientists' Interest Group has addressed *(i)-(iv)* with management of the ACA twitter account ***twitter.com/ACAxtal***. While *(i)-(iv)* are indispensable for the scientific discipline (collaboration still requires in-person meetings), social media can compliment traditional communications. For example, for those not present at the 2016 ACA meeting in Denver, portions of the conference were sent out with descriptions of talks and more extensive press releases coordinated by the ACA communications committee. The @ACAxtal account was noticed by the banquet speaker Phil Plait (whose talk was subsequently 'live tweeted' with quotes and pictures of his presentation).

The account @ACAxtal has highlighted specific crystallographic articles of interest to the broader community. The publication of tweets on crystallographic news and 'hot topics' is difficult as the crystallographic community has such broad interests. For this reason, YSIG welcomes suggestions and would like more crystallographers to get twitter accounts! In regards to abstract services *(iii)*, academic journals have begun their own twitter feeds to capture readers' interest with a TOC image and 2-3 sentence descriptions. This boils the abstract down from a traditional 300-500 word abstract even further. While this is frustrating, it is also powerful as people are more apt to understand a shorter description that is heavily edited. Indeed, while managing the @ACAXtal account, we frequently find it difficult to distill the essence of an article into 140 characters!

A most interesting topic is the *discussion* among scientists (and the general public). For example, on Dec 1 2016, the House of Representatives Science Committee tweeted something that cited an article from *Breitbart News*.

This was met with fast admonishment from scientific experts and immediate peer review. A staff scientist at Mount Desert Island Biological Laboratory, Karen James, replied and provided a long form response on Facebook ***(bit.ly/2hl2oSW/)***, another valuble social media tool for emerging scientific literature discovery and discussion.

The responses to the *Breitbart News* article continue to add up which can provide a fast check of scientific media by prominent scientists.

Of course, as scientists we are aware that not all posts are equal and some may not be fact based, or not even representative of the majority of current opinion based on solid academic research.

The bottom line is that social media is important and can be fun! But we are already falling prey to our succes with a the huge number of tweets (we are back to the original problem of an-all-too-prolific scientific community). This can be accommodated by focusing on specific Twitter users (such as @ACAXtal!) rather than casting a large net and following many sources at once.

Marty Donakowski

Editor's note: For those of you out there like me that need a roadmap to interpert the bottom line of the tweet - the backwards arrow represents 'followers', the nested arrows represent 'retweets' and the little heart tells us how many others 'like' the tweet. The numbers listed here are as of December 9, 2016 and they will surely be much higher by the time we go to print..

CrystalCon 2016

Logo design: Kirsten Knecht
Photo credit: Sarah Smaga

CrystalCon 2016 was a great success! The program was designed to be a half-day program for high school students focused solely on x-ray crystallography. The day was divided into three parts: 1) a seminar to provide a foundational knowledge of x-ray crystallography, 2) hands-on activity tables for the students to interact with different concepts in crystallography, and 3) a career panel to showcase different jobs related to crystallography.

Pre-event: We focused on two major goals prior to CrystalCon: recruiting volunteers and advertising to students. To recruit volunteers, we personally emailed the graduate students in structural biology labs across campus, which resulted in volunteers from many departments, including chemistry, geology, molecular biophysics and biochemistry, and pharmacology. Each graduate student was responsible for their own activity table that would highlight a different aspect of crystallography. Overall, we had twenty graduate student volunteers, two volunteers from the local museum with a *Rocks of Connecticut* exhibit, and four career panelists.

One of our primary concerns was attracting students to an event where they probably were unaware of the subject matter. We partnered with the Yale chapter of *ManyMentors*, a group of graduate students that mentor high school students interested in STEM. Through *ManyMentors*, we met with the Office of New Haven State and Public Affairs (ONHSA), which has an office dedicated solely to STEM outreach to New Haven students. We advertised our event through this office, as well as the Yale Calendar of Events, and received approximately 120 pre-event registrations. One of our most successful advertising strategies was to set up one of our activity tables and hand out fliers at another science outreach program hosted through Yale. Ultimately, 64 students checked in, most of whom brought family members, which brought our total to over 120 people. We originally advertised to high school students, but because we encouraged this as a family event, we actually had a diverse spread of attendees ranging from elementary school to seniors in high school, as well as parents.

CrystalCon 2016: CrystalCon was held in Yale's geology building, which has a beautiful display area for crystalline rocks. The event was divided into a thirty-minute seminar, an hour of activities, and thirty minutes to talk to the career panel. The money provided by the ACA Small Outreach Grant was used to purchase materials for the activity tables, as well as T-shirts for volunteers and snacks for the participants. This was augmented by $100 provided by the McDougal Graduate Student Center at Yale.

The lecture, designed as a basic introduction to crystallography and its importance in research was given by one of our graduate student volunteers. We also took care to highlight women scientists such as Rosalind Franklin. The students enjoyed the lecture, rating it 4.5 out of 5 in the post-event evaluation form.

The next section of the event was the activity tables. We have included all of the activity tables and their protocols in the *For Educators* tab on our website ***crystalcon.wordpress.com*** so that others can use and improve upon our activities. The activity tables were the favorite part of most of our participants, with many commneting that they would like to see more next year. Overall, they received an average rating of 4.6 out of 5.

Finally, the career panel was designed to showcase different careers that involve crystallography. We had a graduate student in a computational biology lab that did crystallography in his undergraduate institution, a graduate student who uses x-ray crystallography in his geology lab, a research scientist in pharmacology, and an MD/PhD practicing dermatologist who leads an x-ray crystallography research lab. The career panel received an average rating of 4.2 out of 5.

Overall, our event successfully increased each participants' awareness of and excitement for x-ray Crystallography. When asked how interested in x-ray crystallography they were before and after CrystalCon, students reported a much higher interest after the event. When asked whether they would attend CrystalCon again next year, 65% of students replied yes, 3% no, and 33% said it depended on their schedule or whether we added new content. We are excited for next year!

Future Goals: After the event, we collected suggestions from our volunteers for improving CrystalCon for next year. All of our volunteers expressed interest in participating again next year. With regards to the lecture, it was very protein crystallography heavy. One parent recommended that we introduce crystallography using inorganic molecules, which might be simpler for students to understand. We also have many ideas to improve the career panel for next year. One would be to separate the younger children from the high school students, for whom the career panel was designed. The younger children had some interesting questions for our panelists, but they were not focused on the career aspect. Furthermore, we will include at least one undergraduate student on the panel because most questions asked by the high school students were about undergraduate applications and college life. Lastly, we will be more conscious of our panelist diversity for next year. Some parents commented that there was only one woman on the panel.

Thank you for this opportunity to introduce x-ray crystallography to students throughout New Haven! We believe that we have succeeded in generating enthusiasm for crystallography and providing relevance of crystallography to students in grades K-12 (as well as some very enthusiastic parents!).

Kirsten Knecht
Samantha Ziegler

ACA 2017 Wood Award to James O'Brien

James F. O'Brien attended Villanova University, receiving a BS in Chemistry yet finding time to be the co-captain of the 1962-63 varsity basketball team. He obtained his PhD at the University of Minnesota and married his wife Barbara who had a career as a psychiatric nurse, both in a hospital setting and an academic one. After graduate school O'Brien spent a post-doctoral year at Los Alamos National Laboratory working with Mohammed Alei (yes really, but not related to the more famous near-eponymous fighter.)

O'Brien began his academic career as a physical chemist at Missouri State University (then Southwest Missouri State College) in 1969. He was a highly respected faculty member as noted by both his peers and his students, winning three teaching awards during his career including the Governor of Missouri's Award for Teaching Excellence in 2001, and earning two terms as a distinguished scholar between 1991 and 2001. In 2002 he was granted the status of Distinguished Professor – the highest status awarded to faculty at Missouri State University. During his academic career he published 31 papers in peer-reviewed journals, presented 84 times at chemistry conferences and earned three research awards from Missouri State University.

O'Brien's writing for the general public has focused on Sherlock Holmes. His book *The Scientific Sherlock Holmes* won an Edgar Award from the Mystery Writers of America as the best book of 2013 in the critical/biographical category. O'Brien has written three articles that have appeared in the *Baker Street Journal* and an invited piece for the *Encyclopedia Britannica* (***www.britannica.com/topic/Sherlock-Holmes-Pioneer-in-Forensic-Science-1976713***). Other Holmes articles by O'Brien were featured on the cover of the June 1993 issue of *Chemistry and Industry* and in the *Huffington Post* (***www.huffingtonpost.com/jim-obrien/sherlock-holmes-ascience_b_2549834.html***). A chapter on Holmes by O'Brien was included in the book *Chemistry and Science Fiction* (1998). O'Brien's latest work, a chapter entitled *Sherlock Holmes: Forensic Science Pioneer*, has been accepted for a forthcoming book (2016).

Early in his career O'Brien began presenting general lectures as part of the American Chemical Society speaker series. He has given an astonishing two hundred ninety-three invited talks at seminars, banquets, and meetings including 135 Sherlock Holmes lectures and 136 *Famous Mad Hatter* talks. The *Famous Mad Hatter* talks are about mercury poisoning. In 2010 O'Brien was elected to the Missouri State University Wall of Fame which recognizes and honors employees who have excelled at Missouri State and significantly contributed to the success and positive collegiate experience of students.

In retirement since 2003, O'Brien has spent time playing golf and competitive bridge. He and Barbara have done several European river cruises, as well as travel in the US. They have been in all 50 states. He recently completed 13 years as a volunteer on the Institutional Review Board of a Springfield hospital. O'Brien is a New Orleans aficionado who looks forward to attending the ACA banquet in May.

Tamera Jahnke
Tom Terwilliger

Issue of Advances in Biochemisty dedicated to Alex Wlodawer

In celebration of Alex Wlodawer's 70th Birthday and to emphasize his achievements, the Polish Biochemical Society has dedicated one issue of *Advances in Biochemistry* (*Postepy Biochemii* in Polish) to structural biology. All articles in this issue (Volume 62, Number 3, 2016), written by distinguished scientists,friends and collaborators of Alex's, are in English (***www.postepybiochemii.pl/***). Alex, a long time member of the ACA was elected as an ACA Fellow in 2013. We congratulate him on this timely honor.

Charles F. Majkrzak Wins Clifford G. Shull Prize

Char;es Majkrzak (NIST) is the recipient of the 2016 Clifford G. Shull Prize of the Neutron Scattering Society of America (NSSA) with the citation "*For leadership in the development, application and establishment of neutron reflectometry as an essential measurement tool for nanoscale materials*".

NSSA established the Clifford G. Shull Prize in Neutron Science in 2002 to recognize outstanding research in neutron science and leadership promoting the North American neutron scattering community. The prize is named in honor of Clifford G. Shull, who received the Nobel Prize in 1994 with Bertram Brockhouse for seminal developments in the field of neutron science.

Majkrzak is recognized for his creativity in the development of neutron optical and polarizing devices, for the design of sophisticated instrumentation for neutron reflectometry, and for his significant contributions to the complex formalism for interpreting

scattering from surfaces and interfaces. He has applied these methodologies to emerging materials of fundamental and technological importance including magnetic nanostructures, block co-polymer films, and biological membranes. In addition, his generous advice and outreach to the scientific community have greatly advanced the effective use of reflectometry methods.

He has made significant contributions to the investigations of ternary rare earth alloys, paramagnetic nickel, amorphous ferromagnetic alloys, and magnetic nanostructures. In the mid 1980's he led a seminal study on

reliability · versatility · performance

liquid handlers for protein crystallography

create with mosquito

- sitting/hanging drop
- lipidic cubic phase
- microbatch and more...

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Gd/Y superlattices that revealed unexpected oscillatory exchange coupling across non-magnetic layers. This research provided a context for interpreting giant magnetoresistance (GMR) in transition-metal multilayers, a phenomenon that revolutionized magnetic recording.

Majkrzak has also advanced reflectometry applications in soft matter. Soon after building the first NIST reflectometer, he and his associates performed classic experiments on the surface-induced ordering of block copolymers and pioneered the use of neutron reflectivity to characterize the interactions between proteins and biological membranes. Realizing that the inherent phase ambiguity in any scattering experiment can lead to erroneous results with standard refinement techniques, Majkrzak led an effort that resulted in a straightforward method to directly invert reflectivity data into real space structure. The resulting protocol has proven to be of immense importance to neutron reflectivity studies of unknown structures.

Majkrzak's efforts to advance reflectometry measurement technology continue to this day with his development of a new multi-wavelength reflectometer, CANDOR. This instrument will be unique in the world and promises to boost data collection rates for specular reflectivity possibly by an order of magnitude over current reflectometers at the NCNR. This concept can be readily adapted to other instrument classes and has the potential to revolutionize neutron measurements at steady state sources.

. He received the Department of Commerce Silver Medal in 1993 and 2004, and the Gold Medal in 1999. He was appointed a NIST Fellow in 2007, and received NIST's highest honor for measurement science, the 2013 Allen V. Astin Award, for his "*leadership in the development and application of neutron reflectometry methods*." The ACA recognized his accomplishments with the Bertram E. Warren Diffraction Physics Award in 2006, which is given for important contributions to the physics of solids or liquids using x-ray, neutron, or electron diffraction techniques.

Robert J. Cava Selected as the 2016 Materials Research Society Medalist

The MRS Medal, endowed by Toh-Ming Lu and Gwo-Ching Wang, is awarded for a specific outstanding recent discovery or advancement that has a major impact on the progress of a materials-related field. Robert J. Cava (Princeton) is being honored "*for pioneering contributions in the discovery of new classes of 3D Topological Insulators.*" He was recognized during the Award Ceremony at the 2016 MRS Fall Meeting in Boston.

His research emphasizes the relationships between chemistry, crystal structure, and electronic and magnetic properties of non-molecular solids; synthesis, structure, and physical property characterization of new transition-metal oxides, chalcogenides, intermetallics, and pnictides; and the study of the properties and materials chemistry of superconductors, magnetic materials, transparent electronic conductors, dielectrics, thermoelectrics, topological insulators, geometrically frustrated magnets, and correlated electron systems.

Cava has worked in combining physics and chemistry to create accessible materials that can be widely studied through a process of understanding the physics and how to incorporate the materials. Although topological surface states were first found on the edges of thin buried layers of HgTe in quantum wells fabricated by molecular beam epitaxy, their discovery soon thereafter on the surfaces of bulk crystals of Sb-doped Bi grown by Cava caused a rise of interest and activity in the field.

Cava has continued to make contributions to address questions about the physics of topological surface states by translating those questions into materials terms, and then finding new compounds or altering known compounds. Cava has collaborated extensively with physicists to understand the physics they are trying to probe in topological insulators, and through physics-materials feedback, develop model compounds in single-crystal form

His recognitions include the Linus Pauling Award (ACS), Stephanie Kwolek Award in Materials Chemistry (RSC), James C. McGroddy Prize in New Materials (APS), and the Humboldt Research Award. He is a Fellow of the Neutron Scattering Society of America, The American Ceramic Society, and the American Physical Society. He is a member of the U.S. National Academy of Sciences and a foreign member of The Royal Society (London).

Matteo Leoni and Paolo Scardi selected to receive 2016 ICCD Hanawalt Award

The International Centre for Diffraction Data (ICDD) J.D. Hanawalt Award is named for J. Donald Hanawalt, whose pioneering work in the 1930s led to the development of the PDF database structure and search/match procedures still in use today. The award is presented every three years for an important, recent contribution to the field of powder diffraction. The 2016 recipients are Matteo Leoni and Paolo Scardi (University of Trento, Italy).

Matteo Leoni is currently working on the development, validation and application of novel methods for the quantitative analysis of structure and microstructure evolution of real materials (i.e. materials with defects) using powder diffraction and combined techniques. Of particular interest are those systems lacking 3D periodicity (e.g. nano, 2D, layered, intercalated materials and, in general, materials with stacking defects).

Paolo Scardi's main scientific interest has been Line Profile Analysis. Early ideas on the whole powder pattern modelling approach date back to his first years as an assistant professor, along with the collaboration of several students, among them, Matteo Leoni, co-winner of the award. Scardi's current research interests span across several themes of materials science and technology, including nanostructured materials, thin films and coatings, residual stress, texture and plastic deformation of materials,

with special attention to understand the role of microstructure in developing and modifying material properties and behavior. His work includes measurement studies at synchrotron radiation facilities, dating back to the early 1990s. Recent work focuses increasingly on atomistic modeling, e.g. by molecular dynamics, to support the interpretation of x-ray spectroscopy results, and use of the Debye Scattering Equation to analyze nanostructured systems.

Majed Chergui - Elected APS Fellow

The APS has elected Majed Chergui, Professor of Physics and Chemistry at EPFL, as a Fellow. This is a distinct honor considering that Fellows make up a mere 0.5% of the Society's membership. According to its criteria, fellowship is awarded for "exceptional contributions to the physics enterprise; e.g., outstanding physics research, important applications of physics, leadership in or service to physics, or significant contributions to physics education.

At EPFL, Chergui pursues a variety of ultrafast UV and x-ray spectroscopic studies on chemical and biological systems. Since 2013, he has been Editor-in-Chief of Structural Dynamics, ACA's flagship journal published jointly with the American Institute of Physics.

With the Fellowship, the APS recognizes Majed Chergui for, "pioneering ultrafast x-ray spectroscopy, developing novel ultrafast optical spectroscopic methods that were used to answer scientific questions on molecular and biomolecular dynamics in solutions and on the charge carrier dynamics in nanoparticles."

Spotlight on Stamps: In Memoriam: Hugo Rietveld (1932-2016)

Hugo Rietveld, a distinguished Dutch crystallographer, passed away at the age of 84 on 16 July 2016. He is best known for the invention of the refinement method widely used to characterize crystalline materials based on powder diffraction data, a procedure that now bears his name.

Rietveld obtained his PhD from the University of Western Australia in 1964 and then returned to his homeland to join the neutron diffraction research group at the *Reactor Centrum Nederland* in the small coastal town of Petten. Since there were no single crystals available of the inorganic materials under investigation at the RCN, he started developing a procedure to analyze and refine powder diffraction data. Two years later, Rietveld disclosed his method for the first time at the 7th Congress of the International Union of Crystallography (IUCr), held in Moscow from 12 to 19 July 1966. The postage stamp illustrated in this note was issued in Russia to commemorate the event and is still today the only one ever released honoring an IUCr congress.

Remarkably, Rietveld's report at the IUCr congress was almost completely ignored, perhaps because much more attention was being paid at the time to single-crystal X-ray diffraction, particularly for the structural elucidation of complex biomolecules. Indeed, protein crystallography was "hot" in the wake of the Nobel Prizes in Chemistry awarded to Max Perutz and John Kendrew in 1962, "for their studies of the structures of globular proteins," and to Dorothy Crowfoot Hodgkin in 1964 "for her determinations by X-ray techniques of the structures of important biochemical substances."

In any event, Rietveld's refinement method started getting some traction in 1969 with the publication of a full paper in the *Journal of Applied Crystallography*. Enhancements to the software, the applicability of the method to both neutron and X-ray data, and the availability of better and faster computers led in the ensuing years to the widespread adoption of the method, which is now applied in fields as diverse as metallurgy, forensics, archeology, and the pharmaceutical industry. Significantly, a recent search of the *Web of Science* citation database revealed that Rietveld's aforementioned paper has been cited almost 10,000 times to date! Somewhere up there Hugo Rietveld is smiling…

Daniel Rabinovich

Structural Dynamics

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Special Topic:
Transactions of the 66th Annual Meeting of the American Crystallographic Association

JULY 22-26, 2016 | DENVER, CO

This Special Topic will feature papers presented at the 2016 meeting which highlighted Structural Dynamics across the disciplines represented by the ACA. The collection will focus on the rapidly growing areas of structural dynamics of both chemical and biological systems, as well as solid materials. The papers will showcase exciting recent work on both equilibrium and non-equilibrium dynamics involving time-scales from seconds to femtoseconds. The special issue will also include case studies and cutting edge advances in methodology that are critical for advancing the science of molecules and materials in motion.

Structural Dynamics is an open access journal, all articles are freely available without a subscription

Guest Editors
Jason Benedict - Department of Chemistry, State University of New York at Buffalo, Buffalo, NY
Arwen Pearson - The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany

A short history of structure based research on the photocycle of photoactive yellow protein Marius Schmidt

Combining multi-mutant and modular thermodynamic cycles to measure energetic coupling networks in enzyme catalysis Charles Carter Jr., Srinivas Niranj Chandrasekaran, Violetta Weinreb, Li Li, and Tishan Williams

Augmenting the Anisotropic Network Model with torsional potentials improves the performance of PATH Srinivas Niranj Chandrasekaran and Charles W. Carter Jr

Molecular dynamics simulations support a loop-closing mechanism in membrane pyrophosphatases Nita R. Shah, Craig Wilkinson, Steven P. D. Harborne, Kun-Mou Li, Yuh-Ju Sun, Sarah Harris, and Adrian Goldman

Rigorous analysis of crystallographic fragment screening data reveals new chemical opportunities and a cryptic site for targeting KDM4D Nicholas M Pearce, Anthony R Bradley, Brian D Marsden, Charlotte M Deane, and Frank von Delft

Microfluidic Platforms for the Crystallographic Analysis of Protein Structural Dynamics Shuo Sui, and Sarah L. Perry

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The CSD Python API: A Foundation for Innovation

This summer marked the first anniversary of the initial launch of the CSD Python API – version 0.7 was released back in July 2015 – and we thought this was an ideal time to hold our first introductory workshop on the system at a major crystallography conference.

The Cambridge Crystallographic Data Centre (CCDC) is a not-for-profit organization whose primary goal is the advancement of chemistry and crystallography by making crystallographic data and knowledge derived therefrom as accessible as possible to the general public. While we have a broad spectrum of software to access the CSD, we have often been asked about doing so programmatically to help automate analyses, integrate with other platforms, and produce custom research applications. As a result, we have been focusing on developing an application programming interface (API) for our users, to provide flexibility and functionality within the Cambridge Structural Database (CSD) in whatever way they can imagine!

More and more scientists are turning to scripting to help with their research. Python is at the forefront of this movement due to its ease of learning and the wide range of existing scientific libraries available (such as SciPy, NumPy, BioPython and MatPlotLib). In fact, Python is currently the most popular introductory coding language for teaching computer science courses.

Peter Wood explaining why the CCDC chose to use Python as the basis of an application programming interface (API) to the CSD.

The workshop was a half-day of hands-on tutorials held at the 66th Annual Meeting of the American Crystallographic Association (ACA) meeting in Denver. It walked participants through using the CSD Python API, in an increasingly feature-rich fashion, from simple to advanced examples. The format was geared towards users exploring functionality at their own pace, with experts readily providing support. This went over very well, and users covered a lot of ground.

We opened the workshop with a brief talk by Pete Wood, to provide background and a high level overview of the API. The attendees were guided through a simple example that illustrated some Python commands and showed how scripts can be run from within Mercury, the well-known crystal structure visualization and analysis program.

The next two sections of the workshop built up the scientific and programming concepts. This covered the automated generation of a report based on a single crystal structure, and then how to write a script that combines detailed CSD search and analysis all at once. Finally, the attendees were encouraged to tackle one of a set of four scientific challenges using the CSD Python API, with a few hints about the best approach to take. These challenges provided a stretching target for the attendees, and most started one of these projects. Quite a few actually put together a Python script in the workshop which answered the scientific question posed. Well done everyone!

The CSD Python API workshop in full swing.

The workshop was well attended, with 33 participants on the day. All the attendees were provided with a printed set of workshop notes, as well as an electronic package after the event containing example Python scripts for every challenge in the workshop along with the course notes.

We were extremely pleased to see the level of interest and enthusiasm from the ACA community towards getting involved with the CSD Python API. We're very excited about the expanding user base as the API continues to develop and the CCDC user community continues to discover the tremendous potential of using the API!

Peter A. Wood & Paul C. Sanschagrin

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Application of SANS/SAXS to Structural Biology

William Heller (Oak Ridge National Laboratories) reported on the application small-angle neutron scattering (SANS) to the study of cellular membranes, which includes proteins, lipids and other molecules. This is an area that continues to challenge structural biologists because of issues such as membrane protein solubility and the complex phase behavior of lipids. Using the examples of the Sinbidis Virus, Light Harversting Complex II, Bacterial Photosystem I, and antimicrobial peptides, it was illustrated how contrast variation methods using isotopic exchange and experimental neutrons made it possible to gain unique structural insights not accessible by other approaches.

Sangita Sinham (North Dakota State University) presented her group's research on the structure and function of BECN1, a key component of the autophagy nucleation complex. This complex is involved in the degradation and recycling of unwanted, damaged, or harmful cytoplasmic components. An integrative approach to the study of this protein was presented, including bioinformatics, x-ray crystallography, small-angle x-ray scattering (SAXS), circular dichroism (CD), and molecular dynamics (MD). Together, these results revealed key insights into the structure and dynamics of the protein, revealing the presence of transient structural changes to an ordered structure upon binding to partner.

Left to right Adam Round, William Heller, Jill Trewhella, Nikolina Seculic, Joseph Curtis, Susan Krueger, Sangita Sinha

This talk was followed by ***Nikolina Sekulic*** (The Perelman School of Medicine at the University of Pennsylvania), who reported on contrast variation studies of centromeric mononucleosomes. Centromeres are vital to the proper segregation of chromosomes, and are defined by a variant histone protein called CENP-A and slightly A-T rich repetitive DNA sequences. Using analytical ultracentrifugation and SANS contrast variation, a more extended conformation of CENP-A derived nucleosomes in solution was determined relative to the canonical form. These results reveal the role of DNA in the physical basis of how the CENP-A histone distinguishes centromeres from the rest of chromatin.

In the next talk, ***Jill Trewhella*** (The University of Sydney) demonstrated the utility of small-angle scattering to the study of macromolecular structure in the presentation of work done by her group on proteins from HIV, including matrix (MA) and its interaction with calmodulin, and HIV reverse transcriptase. In both cases, it was illustrated how the marriage of the complementary information from solution scattering with available crystallographic information, hydrogen-exchange mass spectrometry, fluorescence, and other approaches together could provide unique insights into the structure and dynamics of these proteins.

Adam Round (BM29 at ESRF) reported on innovations at this synchrotron SAXS beam line, including SEC-SAXS, streamlined data management and analysis with the ISPyB database, and microfluidic devices. To make data acquisition more efficient, droplet microfluidics were implemented and their utility illustrated with regards to adjustable additive concentrations, radiation damage, and background scattering. As a proof-of-principle, *in situ* crystallization of glucose isomerase performed to show that crystals could be grown and transported within the droplets, allowing for the study of nucleation in different additive conditions.

Susan Krueger (NIST Center for Neutron Research (NCNR)) reported on the application of SANS and contrast variation to the study of disordered proteins in the context of two-subunit complexes, using the example of Skp OmpW bound to Skp OmpA. Using the program SASSIE, Monte Carlo sampling of backbone dihedral angles within protein models was used to generate ensembles of energetically relevant conformations for the disordered regions of the complex, using structural models that satisfy the contrast variation data obtained.

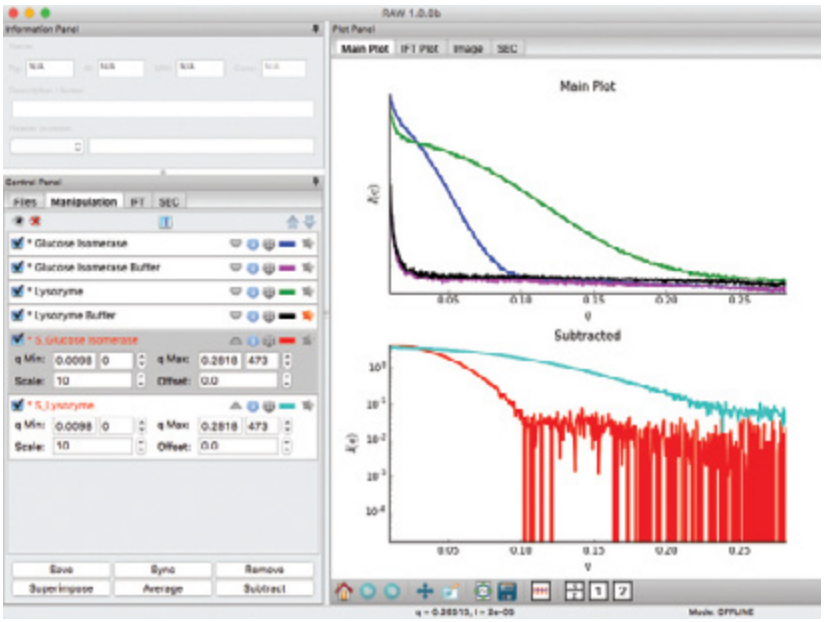
Her colleague ***Joseph Curtis*** (NCNR) closed the session by providing a report on the progress of the CCP-SAS initiative, an NSF-funded joint UK/USA collaboration. The goal of this effort is to produce a new generation of open-source software which facilitates the atomistic modeling of macromolecules using SANS/SAXS data. These web-based applications include the SASSIE/SCT and the modeling of analytical ultracentrifugation data using US-SOMO. The software will be open-source, easy to use, and stable. Research examples using these new tools were provided.

Kushol Gupta
Alvin Acerbo

Processing SAXS Data with RAW: An Overview and Hands-On Tutorial

L-R: Tutorial organizers Richard Gillilan, Jesse Hopkins, Søren Skou. Photo courtesy of Richard Gillilan.

As Small Angle X-ray Solution scattering (SAXS) has become a must-have component of many structural biology studies, there is an increasing need for easy-to-use software that can take the user from detector images, through quality-control checks, to final processed data. Originally part of the BioXTAS project, the RAW software package came to Cornell's High Energy Synchrotron Source (CHESS) via Søren Skou (Nielsen) in 2010 and has been continuously developed and improved in response to beamline user feedback since that time. As a multi-platform, free, open source package that can run efficiently on a personal laptop and is capable of handling a wide variety of detector images and beamline configurations, RAW is gaining popularity worldwide. In the spirit of the BioSAXS Essentials training courses offered annually at CHESS each spring, we offered a free, abbreviated, Saturday noon-time tutorial session to interested attendees of the annual ACA meeting this year in Denver.



RAW, an open-source program for processing SAXS data: http://bit.ly/saxsraw.

We were fortunate to have ***Søren Skou*** (SAXSLAB, Copenhagen, Denmark), the original author of the code, present to give an introduction and overview of the current version. RAW now reads some 27 different image formats, including Pilatus tiff and CBF type, and has sophisticated masking and beamstop normalization capabilities. Beyond the requisite standard plots and Guinier analysis, RAW provides four different types of molecular weight estimates, including built-in absolute scale. Two different indirect Fourier transform methods are implemented (GNOM and BIFT), and the user interface is seamlessly integrated with the most widely-used components of the popular ATSAS suite including GNOM, DAMMIF, and the new AMBIMETER program for determining shape ambiguity.

Jesse Hopkins (MacCHESS, Cornell U), conducted a step-by-step tutorial for students emphasizing good standard practice and introducing some of the many new functions he has implemented in RAW. The software is now customized for inline Size Exclusion Chromatography (SEC-SAXS), a new technique widely requested at beamlines that requires efficient processing of large numbers of detector images automatically. RAW runs on Windows, Mac, and Linux computers and is freely available on Sourceforge, where you can find source code, installable packages, a complete printable manual, and the tutorials and data used in this session, as well as links to YouTube videos for beginners: ***sourceforge.net/projects/bioxtasraw***.

Thanks to Jesper Nygaard, Kurt Andersen, Alvin Acerbo, and the many BioSAXS users whose feedback has contributed greatly to RAW. Thanks also to SAXSLAB (***www.saxlab.com***) for helping make this tutorial possible.

Richard Gillilan
Jesse Hopkins

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The following notes were written by the 2016 recipients of travel grants and /or the young researchers selected for the SIG Etter Award Lectures. They were asked to comment on their personal experiences at the meeting: the venue, the events for young scientists, the overall program and their own presentations and whether or not they are (and plan to continue to be) ACA members. Many would not have been able to come to the meeting without the financial support provided by ACA members when they generously contribute to the travel award funds.

Darpandeep Aulakh: The meeting provided an opportunity to showcase my research and also get valuable input from some of the best crystallographers in the country. I was fortunate to be able to exchange my research ideas with them and gain insights from their opinions.

In addition, I also learned about the research currently trending in the field of crystallography, which definitely showed me various directions into which I can expand my research. So much is going on in the field of crystallography and it is almost impossible to keep oneself updated, so this was an opportune moment to get apprised of the current scenario.

The YSG meeting was yet another great platform to get acquainted with my peers in this field and at the same time explore future collaborations for future. The meeting on the whole was a great platform to learn and meet researchers in this field. The only thing that was little upsetting was that some of the sessions were being run at the same time. I realize that there is not enough time to hold only one session at a time for such a huge event and it cannot be changed, however if you can somehow figure out that times for similar talks don't clash, that would be the icing on the cake.

I am a member of ACA and definitely plan to continue my membership.

Amber Larson: I was very honored to participate in the *Magnetic Entanglement and Complex Magnetic Materials* session, chaired by Branton Campbell and Anna Llobet. I really appreciated the discussion and constructive feedback that I received after my talk. For me, the highlight of the Denver meeting was getting to meet new people and discuss their science and careers. The interdisciplinary setup of the poster sessions and the diversity of talks presented allowed me to branch out of my own area of research and learn more about other exciting areas of crystallography. It was a very welcoming environment, and there seems to be a lot of support for young scientists within the ACA!

One change that I think would improve the meeting would be to incorporate the workshops into the daily programming. Having those events scheduled before the bulk of the meeting can make it difficult for some interested members to attend. I would also like to see more sessions for neutron scattering in the future.

I am currently a member of ACA, and the Neutron Scattering Society of America, and plan on continuing my membership in both of these organizations.

Elizabeth Koch: This was my second trip to an ACA conference, the first in which I was awarded a travel grant, and I could not be more complimentary of the organization and content of the meeting. The schedule was very well organized so that all talks were relevant within the individual sessions. I really enjoyed the *Cool Structures* session especially since I was able to give a talk. The work presented by others was incredibly motivating for my own research. I also really enjoyed the various talks about modulated structures and how different crystallographers throughout the community are dealing with this complex issue. I am excited to see what New Orleans has to offer in 2017!

Nara Guimaraes: Denver was my first ACA meeting, and I was very anxious and excited to be able to join this great event with many important professionals and researchers. Getting the travel grant made my attendance possible, without it I wouldn't have been able to personally join the event. Even before it happened, I was very well assisted and oriented by Kristina Vitale and Marcia Colquhoun; they helped me kindly and very patiently, making my pre-meeting preparation much easier. Since day one of the meeting I had a wonderful time, learned at lot about techniques, equipment and analysis, and last but not least, I met amazing and lovely people.

I would like to start by congratulating the whole team that put this event together. The workshops were amazing, the lectures and awards were outstanding and very well deserved, the winners are absolutely worthy of the prizes, and the city and hotel chosen were more than adequate. The program covered a wide variety of subjects giving all the attendees options to choose the sessions fitted best with their interests.

The opening reception was very special, not only for the delicious food and drinks, but also for the cozy environment that was created providing an opportunity to start friendships, establish connections and partnerships. The exhibitors were very friendly, and I learned a lot from their explanations, brochures and demonstrations. I was able to bring lots of material back to Brazil and share the information with my lab colleagues, because unfortunately I was the only graduate student from Brazil and Latin America attending the meeting. I would suggest a wider disclosure in South America, there are many research groups that would definitely join the meeting if they were more aware of it.

About the sessions and talks, the ones I attended were all very catchy. I thought that all award lectures were amazing: the awardees not only showed a little bit of their work, but also how passionate and self satisfied they are doing what they do. I was very inspired by their research, giving me many ideas for future projects.

Among the sessions I was monitoring, I really liked the poster preview, because that five-minute summary of their work made me want to visit their posters and get more information about them. All talks in the *Etter Early Career Session* stood out for me, because it brought young scientists, like myself, to talk about their contributions so far. It was great to get in touch with them.

About my poster presentation, from the judges, I was congratulated for my work, although they thought it was very hard to understand because I combined modeling and simulation with

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my x-ray analysis, but that was also what caught their attention because I had shown interesting results. Those who stopped at my poster gave very positive feedback, they commented on the fact that I was one of the very few people there who worked with ceramics, and it was very interesting to compare my work with the ones that studied molecules or had a biological focus.

The event couldn't haven ended better, with the fabulous banquet that summarized with pictures and speeches how incredible those five days were. I hope to be attending the 2017 ACA meeting in New Orleans.

Akilah Murray: The ACA meeting exposed me to many crystallographic techniques that I was previously unaware of. I really appreciated meeting experts in the field, however, I do wish there were more undergraduate and first-year graduate students present. I am a member of the American Society for Biochemistry and Molecular Biology (ASBMB), which draws a larger crowd due to the wider variety of topics. However, there are very few crystallographers at ASBMB, which is why I plan to continue my membership in ACA. Overall, I enjoyed my time in Denver and at the meeting and I look forward to New Orleans in 2017.

Victoria Hall: Something I really enjoyed at my first ACA meeting was being able to meet and network with the scientists that I read about through their published work. I felt the atmosphere really promoted this interaction through the poster sessions and in particular the discussion and questions that followed my talk. I also appreciated the student lectures being mixed in with those of well-respected PhDs, which allowed a more serious tone to be brought to the student talks. I am grateful to have received a travel grant, as well as receiving the Etter Student Lecture Award for the Small Molecule SIG. I am planning on renewing my ACA membership and look forward to the next conference in New Orleans.

Raúl Castañeda: I loved different moments during the ACA meeting at Denver. Since I moved on from New Mexico Highlands University to do a PhD at the University of Ottawa, meeting my past colleagues was very special to me. I had the opportunity to meet my former advisor, Tatiana Timofeeva, and past students from Highlands. Upon invitation of Tatiana a group of her past students came together, and it was really great. I was very pleased that Sofia Antal, one of my high-school students when I was at Highlands, won a poster prize as an undergraduate. On top of that I learned about a field of crystallography that was new to me: protein crystallography. Protein crystallography had always been confusing to me, but in Denver I had the opportunity to ask different questions and learn something about it. To me the best way to improve ACA meetings would be to involve more undergraduates and maybe even students from local high schools. I had the impression that very few undergraduates attended this meeting. I am currently not a member from ACA, but I will surely apply for it soon, since I love crystallography and I would like to keep coming to the ACA meetings. I am very grateful for the travel award, which made my attendance in Denver possible.

Lauren Hatcher: Denver was my third ACA meeting, having previously travelled as a PhD student to New Orleans in 2011 and Hawaii in 2013. This year I was lucky enough to attend the meeting to give an invited contribution to the *Structure-Property Relationships* session. I always enjoy coming to the ACA and this year was no exception, thanks to a great location in the busy, vibrant center of downtown Denver and an exciting and varied scientific program.

In addition to *Structure-Property Relationships*, I found topics in the *Transactions* symposium very informative and I particularly enjoyed *Cool Structures* on Monday morning. As always at ACA meetings, the poster sessions were really interesting and well attended, and I particularly enjoyed Bruker's "Rodeo"-themed evening!

If I could suggest something to improve it would perhaps be an earlier publication of the talk abstracts, even in a preliminary form, which would make it easier to plan a personal meeting program and ensure that attendees can make the most of future meetings.

Being based in the UK I am an active member of the British Crystallographic Association, in addition to being an associate member of the Royal Society of Chemistry. I am a current ACA member and would plan to continue my ACA membership in future.

Gracia El-Ayle: I am extremely grateful for the support I received to attend the ACA meeting in Denver. As a first-time attendee and presenter, I was looking forward to meeting scientists specializing in crystallography with whom I could discuss my research and get feedback relevant to my work. The conference was well organized and offered a wide breadth of topics and crystallographic techniques. It was a great opportunity to learn from distinguished speakers who are passionate and driven about their research. All the talks and sessions I attended were interesting and extremely informative.

I gave a talk in the *Advances in Supramolecular Chemistry* session and got very insightful feedback from the discussions that followed. The chairs were very friendly and welcoming. I really appreciated them proposing to the speakers to go to dinner after the session. It was a great opportunity to talk to students and professors in a casual atmosphere and get to know them on a personal level. The conference overall was rewarding, and I definitely plan on attending the future meetings.

Daniel Taylor: This was my first time attending an ACA meeting, and it was a truly great experience. As my research is focused on using advanced diffraction techniques to study structure-property relationships in transmission metal oxides, my favorite part of the meeting was learning about the different analysis techniques people employ in their own research – even on Mars. I also enjoyed that this was a smaller meeting as it can be easy to get lost at larger conferences such as ACS or ECS.

In the future I would like to see more of a presence covering new advanced powder diffraction techniques, such as *ab initio* structural solutions. I also think that workshops are a great way to pick up skills, however, it would be nice if they were offered throughout the week instead of all being on the first day.

I am currently a member of the ACA, American Chemical Society (ACS), and Electrochemical Society (ECS) and I intend to remain a member in these organizations.

Claudia Wandtke: It was a great pleasure to come to the 2016 ACA meeting in Denver. I enjoyed numerous good opportunities to broaden my horizon to different fields of crystallography and meet possible future employers. Especially interesting and fruitful were discussions with fellow crystallographers working in similar and different research areas. The positive responseto my talk was very encouraging. Receiving an Etter Student Lecturer Award was the perfect icing on the cake for an overall great conference. Thank you Service SIG.

If I could suggest an improvement to the meeting, it would be two small things. First, to ask for an AV technician to be available at all times to supply batteries for headsets and help connecting computers if necessary. One person for all rooms together would be fine if the location is communicated to the session chairs before. Second, to actually give notice of the Etter Student Lecturer Award to the awardees, before talking about the fine print of their award. Then It would really be clear to the awardees that they indeed will be awarded something. It was pretty confusing to me, until I got to the meeting. Although I am grateful anyway.

Additionally, I would like to say that it was not obvious to me, that by attending the conference I would become a member of the ACA for one year. If this is the case, as some emails suggest, then it would be nice to know more about this. Maybe it was in some fine print, but neither my colleagues nor I knew about it.

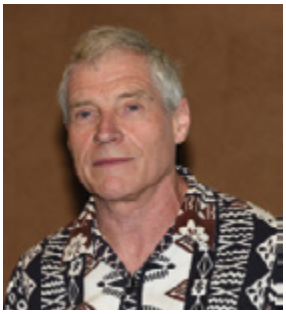
So to my knowledge, I am currently not a member of any scientific society, because it is possible that I will leave the field of crystallography after finishing my PhD and I do not see an advantage of becoming a member to a society for less than two years. However, I would consider joining the according European association if appropriate once I have a new job. The ECA would be my first choice, since I am not from America and just enjoy the cross Atlantic exchange about science from time to time.

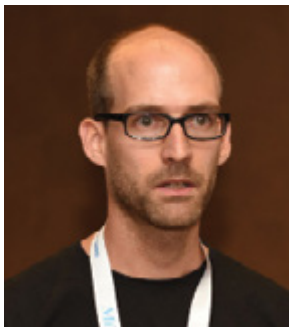
Jose Luis Olmos: When I attend conferences, I generally approach attendees with questions about their research, especially if they have just given a talk. After giving my student lecture at ACA on time-resolved crystallography, I was delighted to be approached by various attendees, with questions, encouraging comments, and very helpful suggestions. The one-on-one interactions were valuable to me and also nucleated a collaboration with a conference attendee who also works on time-resolved crystallography.

I also greatly appreciated the numerous breaks between sessions where attendees were able to interact freely. I was able to not only visit with crystallographers from my undergraduate student days, but also to interact with crystallographers whom I had not previously met. In general, what I most liked about the conference was the ability to engage other scientists.

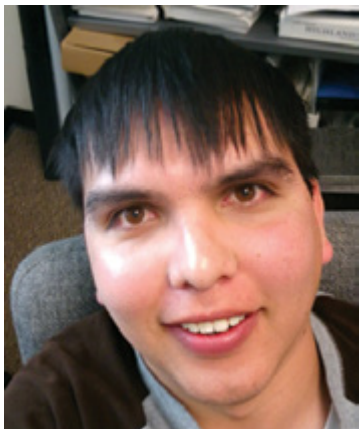
One way I would like to see the ACA evolve is to include sesions on rapidly developing fields at the time of the meeting. For example, many methods are currently being developed to take more dynamic approaches to structural biology using X-ray Free Electron Lasers (XFELs). I could easily see an interest group being developed for this subset of experiments. In fact, my Etter Student Lecturer Award was for my project on time-resolved experiments at an XFEL. Further, CryoEM has recently made large advancements in both the resolution achievable for single molecules and the imaging of progressively smaller molecules. As CryoEM and crystallography could easily complement each other, it would also be a good idea to implement a section on this technique as well.

I am currently an ACA member, and I plan to continue my membership in ACA. I am also considering becoming a member of the Biophysical Society, due to its wide range of biophysical research, including crystallography and CryoEM.

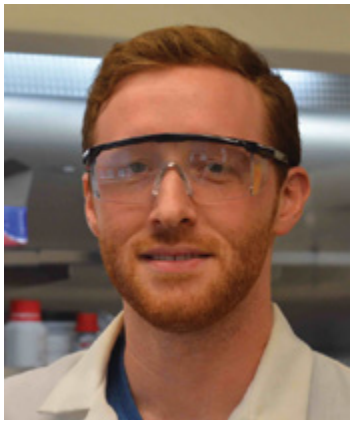




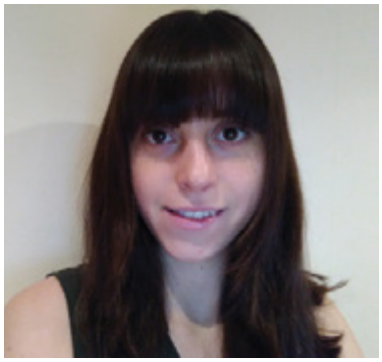

ACA Denver 2016 - SHELXL Workshop: Top: Bill Clegg and Claudia Wandtke, Middle: Daniel Kratzert and Xiaoping Wang, Bottom: Ton Spek and George Sheldrick. Speaker photos by Peter Müller. George's photo is from the ACA archives.







Row 1 - left to right: Akilah Murray, Raúl Castañeda, Darpandeep Aulakh. Row 2 - left to right: Jose Olmos, Claudia Wandtke, Dan Taylor. Row 3 - left to right: Amber Larson, Victoria Hall, Gracia El-Ayia. Row 4 - left to right: Elizabeth Koch, Lauren Hatcher.

Remembering Stanley C. Nyburg, an Inspiring Mentor

Stanley Nyburg had many students, post-docs, and associates while he was a faculty member in the Chemistry Department of the University of Toronto. The following are reminiscences from some of those who worked with him.

Susan K. Byram : Stan Nyburg was my entry to the world of x-ray crystallography. If he had not newly arrived at the University of Toronto when I entered as a freshman in mathematics, physics and chemistry, I would not have had the career I have much enjoyed in x-ray crystallography. He was an inspirational teacher of undergraduate chemistry and introduced many of us to x-ray crystallography at a much earlier level than was usual. He created an excellent group of graduate students and post-doctoral researchers who coached me as I pursued my master's degree with the Nyburg group. It was an exciting event when his first card-controlled single crystal diffractometer arrived in Toronto.

After he retired and moved back to London, England (along with the original diffractometer), he remained an inspiration as he continued to pursue his life-long research and with his own hands, kept his diffractometer functional. We met from time to time, principally at European Crystallographic Meetings and IUCr meetings, and also at the 2001 Pittsburgh Diffraction Conference where he gave a tribute to one of his mentors, George Jeffrey. There was a wonderful reunion of the Nyburg group at University of Toronto in 2010, organized by Vlad Kocman, which Stan and his wife Jo made a special effort to attend. It reminded all of us of the great times in Toronto learning novel techniques, pursuing sometimes difficult research, and enjoying friendships fostered by the Nyburg group social gatherings.

Nyburg group reunion, University of Toronto 2010.

Klaus Dichmann: Stan Nyburg was my thesis supervisor for my MSc and PhD degrees at the University of Toronto from 1966 through 1972. I have many fond memories from my time in his lab from mounting crystals for the x-ray cameras to my time on the Picker "green giants" at UT and the Ontario Science Centre. I still do not understand why a Picker unit was purchased for the Science Centre but I was grateful for the time that I was allowed to use it. I remember taking off to go home with a goniometer head on the roof of my car and the sound it made falling off the roof and hitting the trunk. With the help of a friendly police officer we found it on the side of the road broken into two pieces. Stan took it with a sense of humor and the machine shop was able to repair it. I still remember Stan's support during my PhD orals. One of the examiners was asking silly inappropriate questions and Stan came to my defense. Stan was extremely supportive of his students. I spent one year at the University of Quebec as a post doc and when I was looking for another position Stan offered me a position at the lab in Toronto, a very gracious gesture from a kind and gentle man. I found a teaching position in the community college (CEGEP) system in Montreal and retired after 35 years. I will always have good memories from my time as a graduate student under Stan Nyburg.

Vlad Kocman: I joined the x-ray crystallography group of Stanley Nyburg at the University of Toronto in August 1968, just a few days before the Soviet occupation of then Czechoslovakia. We were freshly married and my wife Eva was waiting in Brno for exit visa to join me. Stan showed me the lab and introduced me to all the post-graduate students and post-docs. It was a very friendly team, who accepted me as a first Czech very warmly. The lab was amazingly well equipped with a 4-circle Picker diffractometer, a bunch of Weissenberg and Precession cameras, plus low temperature equipment. Intensity data were collected on punched tape, which was converted in the Physics Department to IBM cards. The computer in 1968 was an IBM 7094 with drum memory, occupying the space of a two-bedroom apartment on the 11th floor of the Physics Bldg. The programming language was Fortran-II. Later we used an IBM 360/50 mainframe in the Engineering Bldg.

To relieve the fatigue of the day, Stan often invited us to his office at 5 p.m. for high tea and the world news by BBC radio. My wife Eva joined me at the end of September and later helped us financially through her employment. Together, we were invited usually twice a year to Stan and Jo's residence in Rosedale for parties for the whole group. Jo and her daughters served us some goodies, sherry and wine. Stan entertained us on his Steinway piano, playing Rachmaninov, Chopin and Mozart. These were good times in Canada as the US was nearing the peak of its industrial expansion.

As an Englishman, Stan was also a good tennis player, who often asked me about strategy on the court. One day, several years later, he came to me in a park and said: "Terrible, I can't learn the slice serve". I said: "Stan, you have to visualize the ball as a clock. For slice you hit it at 3 o'clock, for a twist or kicker you hit it at one o'clock". We both laughed at this when we met in Wimbledon 40 years later. We met again in May, 2009 by a sheer luck in Wimbledon, where Stan retired. I remember vividly his straight and slim figure at 85 and a brisk walk on the street. "I want to take you to the Mecca of tennis", Stan said and we

walked over the fields to Wimbledon Tennis Club only a mile away. Stopped at the gate by a typical British policeman in a helmet, who said: "You cannot enter as there is no tournament this week". Stan said: "You cannot be serious, this chap came a long way from Canada". Finally, we were admitted. I kissed the grass and Stan smiled. We met a few times again and in Toronto, at the 2010 Reunion of the group, after 40 years.

I am indebted to Stan for my professional career in Canada and would always remember him as a perfect gentleman.

Stan with Vlad and Vlad's wife Eva.

Stan's group photo in 1969.

John Rylaarsdam: After earning a BSc in chemistry from MIT in 1967, I worked briefly for the late George Wolf, whom I met during my final year. When I moved to Canada in 1968, a reference from Wolf led to an interview with Theo Hofmann and Stanley Nyburg at the University of Toronto, who were beginning a collaboration on a protein-structure project. They hired me to measure precession photographs for that project, and I began increasing my understanding of crystallography.

Once I'd gathered a sufficient initial set of measurements, I had to do some data processing, which was something completely new to me. Initially I simply punched my data onto cards, put them behind a program deck, fed them to an IBM 7094, and collected the printed results for analysis. Intrigued by this computer magic, I started learning Fortran IV. The University had expanded its computer facility with two IBM 360-series machines. I volunteered to take on the task of migrating all of the programs in use in the laboratory to run on the new machines, and modify them all to use standardized data formats. Eventually I also moved most program and data storage to magnetic disks and tapes. I also learned PDP-8 assembly language, in order to automate data collection from the Picker 4-circle diffractometer. Once we acquired an automatic drum densitometer for scanning the films, my days as a laboratory technician were over, and my career as a computer scientist was launched.

That turned out well, because the funding for my salary ran out in 1973. (Either that or I had made myself redundant.) Luckily what I had learned during the five years in Stan Nyburg's laboratory helped me become the first computer support person in the Department of Geology, and entry into a part-time program to earn a master's degree in Computer Science. I spent twelve more years at the University, seven at the Toronto Stock Exchange, and the remainder of my computer science career in corporate Canada.

The last time I saw Stan Nyburg was at a reunion of his Toronto group in 2010. When he saw me, I got what I remember as his characteristic smile and, after we exchanged hellos, I discovered how well he remembered me when the first thing that he said was "We found a bug in the code for the Picker, but only a tiny one."

Winnie Wong-Ng: I spent 6 memorable and fun years with Stan first as a post-doc, then as a research associate (and part-time lecturer). I learned a great deal from Stan, not only the knowledge of crystallography, the importance of modeling to complement experimental findings, and even the "secrets" of how to identify new projects, but most importantly how to live life to its fullest.

Stan helped me a great deal in areas outside of science. We took music lessons at the Toronto Conservatory of Music. Stan was an excellent piano player and I miss his piano playing. My daughter Connie was born in Toronto. In the baby's first six months, I took her to work, and Stan even helped out with baby-sitting.

Stan's passion for tennis was legendary. I recall that his home in Toronto was in the neighborhood of a tennis court. Many times during breaks at work, his almost one-way discussion with me about how to perfect one's tennis skill took place in front of the blackboard in his office. He had many lively demonstrations of the physics and body movements about tennis playing. Apparently all that "virtual training" from Stan was stored in my brain unknowingly because earlier this year, for the first time, when I picked up a tennis racket and played with my husband (who is a tennis fanatic), he couldn't believe that was my first time ever playing tennis. Stan, thank you!

I miss Stan and will always remember him fondly. His magnetic personality, great sense of humor, distinctive laughter, positive outlook in life, and his in-depth knowledge of crystallography have had a great impact in my life.

Stan and his Picker Diffractometer.

John Wood: I commenced doing crystallography research with Stan Nyburg in early 1959. Together with fellow Englishman, John Mills, I was one of the first two graduate students working under Stan's direction to carry out doctoral work, and received my PhD degree from the University of Manchester in 1962.

(At that time, Keele, being a University College, did not have its own graduate school, so both John and I were registered at Manchester University, where we had secondary research mentors, in addition to Stan.) Later in 1962, after "seeing us safely on our way", Stan took a sabbatical leave with George Jeffrey at the University of Pittsburgh and then eventually moved to the University of Toronto, where, of course, he spent most of his teaching and research career.

Those early days at Keele were a continuous mix of excitement and frustration. I have many fond memories of my time there and of the guidance and encouragement that Stan offered to both John and to me. In many respects, we were pioneers, for we worked with a rather primitive 'home-built' x-ray machine, having a continuously evacuated tube powered by an H.T. transformer, which was a 'cast-off' from a local hospital! Needless to say, this was not a particularly stable source, frequently breaking down in the middle of the long periods of data collections, which were made on our sole Weissenberg camera. However, despite these experimental tribulations, Stan's sense of humor and encouragement kept us going, when we often felt it was time to look for another project! Likewise, our computational facilities were very sparse, but Stan managed to negotiate with the English Electric Co. for us to use their punched-card operated DEUCE computer overnight to carry out our calculations. In those early days, it took 4-5 hours to compute a 3-D electron density map!

The research projects that John Mills and I were engaged with demonstrated the diversity of Stan's interests in various structural problems and structure solving techniques. In addition to solving the structure of a complex natural product by standard heavy-atom methods, John also determined the structures of some photo- and thermochromic organic compounds using optical transform methods. My own research was concerned with the structures and electronic properties of some coordination compounds of nickel. A triclinic form of one of these turned out to contain three different structural arrangements around the nickel atom in the same unit cell - a rather unusual arrangement - and giving a total of 73 atoms in the asymmetric unit – a large problem to solve at that time. When I announced to Stan that I had three molecules in a triclinic cell, he smiled, laughed in his characteristic fashion and said "I think you had better re-measure the crystal density, my boy!"

I found Stan's mentorship and the space that he gave me to develop my knowledge of crystallography to be particularly especially appropriate when I went on to become a post-doc in Al Cotton's group at MIT and had the job of mentoring several of his graduate students when they were learning the rudiments of structure solving. In summary, I am indebted to Stan for his guidance and encouragement during those early years and for pointing me in the direction of my subsequent teaching and research career.

David Davies (1927-2016)

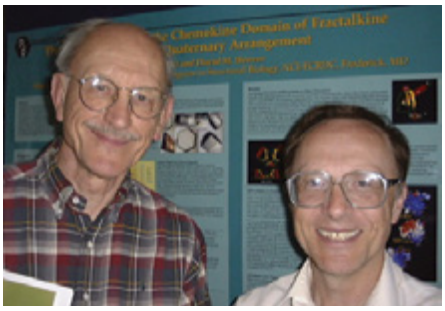
David Davies had a long and illustrious career covering multiple aspects of structural science. Here he is remembered by two of his long-standing colleaugues.

Alex Wlodawer: I met David for the first time almost exactly 40 years ago. I was introduced to him during a Gordon Conference by Hal Wyckoff, who recommended me as a candidate for an open position in macromolecular neutron crystallography at the National Bureau of Standards. At that time I knew that David was well-known for his work on the structure of antibodies, but his relationship to the neutron project was a bit puzzling to me. Only later, when I got the job, which ultimately involved working both at NBS and NIH, did I realize that David was a truly remarkable and generous person: although he took a keen interest in the field of application of neutrons to protein crystallography and funded the project from his own laboratory resources, he never interfered with it. During the eight years I spent at NIH in Bethesda he left the conduct of the project entirely to me and he never put his name on any of the resulting publications. After a while he also provided me with a postdoctoral fellow position (nominally his), but again without taking any credits for his (and later her) accomplishments. On the other hand, he was always there when I needed scientific or any other advice; his knowledge of crystallography was simply incredible. Such a level of generosity in the interest of science is very rare, and this is one of the reasons why those of us who had the privilege of knowing him and interacting with him will miss David so much.

David spent some time in Cambridge (UK) during the incredibly exciting period when the first protein structures were being determined. In that way he became one of the pioneers of the field and contributed to its development in a very significant way. Who could predict that the structure of rhisopuspepsin that was determined in his laboratory in the mid-1970s would become crucial a decade later for the clarification of the structure and function of HIV protease, the first structure-based target for the design of drugs against AIDS? David himself became directly involved in the HIV-related projects by solving the first structure of the catalytic domain of HIV integrase, another key drug design target. Other important projects, some carried out until

quite recently, involved very challenging studies of tryptophan synthase, Tol-like receptors, and TGF-beta, to mention just a few. The latter structure was very important to me personally, since a few months prior to its publication Tom Blundell published the structure of nerve growth factor, a result of a long collaboration between his and my laboratories. We proposed in that paper that NGF contains a cystine knot, an unusual topological feature never observed before, but we were rather concerned about the correctness of our structure in view of the limited quality of the available diffraction data. However, the topology of TGF turned out to be the same as that of NGF and we were much relieved.

Although I moved out of the attic of NIH Bldg. 2 in the mid-1980s, I never lost touch with David. His stature as the most accomplished structural biologist at NIH helped convince the leaders of that institution to fund the inter-institute project that has provided access to synchrotron beamlines, first at Brookhaven and now at Argonne. Most importantly, it was my fortune and true privilege to be able to learn from David. Although we wrote only one paper together (a 1995 review of cytokines and their receptors), I benefitted enormously from knowing this remarkable scientist.



His passing closes an important chapter in the development of macromolecular crystallography as a tool and as a discipline concerned with the most important molecules of life.

Bob Stroud: David Davies is for me, one of the finest examples of positive cooperativity in science and in life. I met David for the first time in 1969 when he visited Caltech. I was a newly arrived postdoctoral, from J.D. Bernal's group in London, where I had worked on direct methods solutions to nucleoside antibiotics. David was already an established lab head at the NIDDK. I was thrilled to have joined Richard Dickerson's laboratory. Dick had been key to the myoglobin structure from John Kendrew's laboratory, and I was to determine the structure of bovine trypsin with Dick. David had also worked extensively on nucleotide pairings and was determining the structure of gamma-chymotrypsin, named because it crystallized in the 'active' pH range in space group $P4_22_12$. David was so genuinely enthusiastic and supportive of our efforts with closely related trypsin; he was so encouraging and calmly excited as to what would be a fascinating comparison. All these early proteins came from natural sources; usually cows, whales, or horses! And he was so completely excited by the potential of structural biology for the future. From our first meeting he became one of the most formative influences in my scientific life; someone who was always interested in the answers and looked forward to other's successes with anticipation. He was instantly the kind of person who, if you hit a good point against him at tennis, far from being dismayed would say, and mean, well done!

Parts of our parallel heritage, frame-shifted in time, we shared on many occasions; David grew up in the coal mining area of South Wales, and I 200 miles north near the coal mining areas of Lancashire England. He had gone to Oxford and I to Cambridge. We both had to learn new accents! David had been at Caltech at a very exciting period in structural biology. He was there with Linus Pauling and Bob Corey soon after they proposed the alpha helix and the beta sheet in 1951. David was at the historic Caltech meeting when in 1953 Perutz and Ingram, working in Cambridge on horse hemoglobin, reported the mercury position in two dimensions, first showing that protein structures could be determined! Crick showed that twisted helices could account for the peaks seen at 5.1Å rather than the 5.4Å expected from the pitch of the Pauling model. 1952 was also a landmark year for direct methods: the Sayre equation, Karle and Hauptman, Cochran, and Zachariasen. David was a true pioneer of discovery building on these discoveries from the birth of protein structural crystallography until today.

David's heritage lives with us today at UCSF. When David went to the NIDDK/NIH along with Gordon Tomkins, Gary Felsenfeld, Bruce Ames and Harvey Itano, they had decided with Gordon as their lab head, to have joint meetings such that they all shared their insights and vision. Gordon later joined Bill Rutter in founding the current version of the Department of Biochemistry and Biophysics here at UCSF. This tradition was imported by Gordon and Bill to UCSF and is still the essence of our institution. Now the room is packed with 80 faculty members, but the principles that David Davies, Gordon Tomkins and Bill Rutter *et al*. started are at the core of UCSF today.

David loved science and was a key figure in structural biology from his early undergraduate days at Oxford as a crystallographer with 'Tiny' Powell, and next door to Dorothy Hodgkin's lab, to publications with John Kendrew, and Richard Dickerson on myoglobin in 1960 that led to the Nobel Prize for Kendrew and Perutz for the first structure of myoglobin and its evolutionary cousin hemoglobin, to today.

And he loved life in balance: reflected in his love for family, the garden and the mountains, for sailing and the sea, and for tennis. I visited his home in Bethesda in the 1970s. He walked me through his lovely garden on a cold spring afternoon, and pointed out one small struggling medicinal plant that he seemed very pleased with! One of David's favorite stories involved his love of the garden. I had moved from Caltech to UCSF in San Francisco in 1977 with children tearing around. We had found a place to live, with, as it happened, three conjoined greenhouses in the back corner of the garden. The previous owner had won numerous prizes for his amazing orchid collection that had long since been transported to the San Francisco Arboretum. David came to stay at our new house. He pondered the garden. Gardens are somewhat a source of pride in England and Wales though I had never caught on in this area, but I was pleased that David asked to walk around the garden. We walked around, I somewhat pleased to see his interest, and his incredible knowledge of these leafy species. It was a leafy glade with, lo and behold, exotic plants and trees imported from far off countries by the previous Scottish horticulturalist. I had no idea! He asked what was inside the greenhouses. I had barely looked inside, but I knew that the next-door neighbor's 13 year old had asked my wife if he could

use the greenhouses to grow his marigolds. His father, a local lawyer, described him as the 'Marigold King' and my wife had agreed, so I vaguely knew that there might be some marigolds. I mentioned the 'Marigold King' to David and when I pried open the door, we were greeted with over a hundred plastic containers in a phalanx array, each with a perfect leafy marijuana plant. 100 very healthy clones growing in sync! David was amused beyond belief - he enjoyed the thrill ever since! So much better than the plant he showed me in his own garden struggling through the Bethesda winter!.. Those were less tolerant days than today. My young neighbor went on to a great career in agriculture, and his lawyer father never knew…. But David never failed to remind me of the Marigold King!

David is also well known for his vast impact on immunology over several decades. He determined landmark structures of antibody Fab fragments complexed to lysozyme, and 'cryoglobulins': whole antibodies from myeloma patients. In 2008 his interests in innate immunity led to his 'Structural basis of Toll receptor signaling'. It was a major recent breakthrough!

Our scientific interests overlapped again in the structures of HIV integrase where David, Bob Craigie and Fred Dyda obtained a structure of the catalytic core dimer in 1994, followed by bound inhibitors and mechanistic roles for the metal ions in 1998/1999. We had been working for many years with Harold Varmus in vain trying to prepare and crystallize complexes of the multi-domain integrase and complexes with DNA. This was not for the faint of heart! David and I would often resonate on the problems, and eventually with Andy Leavitt we added other mutants to Craigie's 'solubility' mutant and obtained the first structure of two of the three domains, the dimer of core and C-terminal DNA binding domain in 2000.

David remained an incredibly warm and inspirational figure who was a key driving intellect from the beginnings of the x-ray crystallography of proteins. He traced his experiences in a very personal and enlightening recollection *A Quiet Life with Proteins*, published in the *Annual Reviews of Biophysics and Biomolecular Structure* 2005 **34** 1-20 that is available at ***bit.ly/2bGuTs8.*** Above all David Davies consistently augmented the sum of the parts to be so much more. He brought humor and enthusiasm to science and an amazing balance to life at the forefront of discovery. He made profound discoveries in the fundamentals of protease mechanisms, the fundamentals of antibodies in the immune system, HIV integrase, innate immunity and more. For me personally he is a reminder of the thrill of a life in science surrounded by those we love and admire, where every day is newly defined by discovery, and where the possibilities are limited only by our imagination.

Douglas (Doug) Dorset (1942-2016)

We are sad to announce that Douglas Dorset passed away on 8 December 2016. Son of the late David and Mary (Steele) Dorset, Douglas is survived by his beloved wife of 49 years, Bonnie (Border) Dorset; his son, Erik Lloyd Dorset and his wife, Dörthe, of Leipzig, Germany; his brother, Ted Dorset; his sister, Cheryl, and his two grandchildren, Hannah and Rebecca.

Douglas L. Dorset was born in southeastern Pennsylvania on August 29, 1942. He attended Juniata College majoring in Chemistry and received his PhD degree in Biophysics from the University of Maryland in 1971 with Albert Hybl. He joined Donald Parson's electron crystallography laboratory at Roswell Park Cancer Institute that year and in 1973 moved to the Medical Foundation of Buffalo-now the Hauptman Woodward Medical Research Institute-where he headed the Electron Diffraction Department and did the fundamental work for which he is best known. Douglas worked on challenging, electron beam-sensitive materials that required strong experimental skills to record representative patterns, and specialized sample preparation methods (e.g. epitaxial growth from multiphase systems).

Douglas moved to ExxonMobil Research and Engineering Company in 2000, investigating the structure of wax crystals and how these change in the presence of modifiers. His research encompassed new methods (e.g. use of maximum entropy techniques with Chris Gilmore and Precession Electron Diffraction) and an array of crystallographic studies on zeolites, polyolefins and other materials. While at ExxonMobil, Douglas quickly assumed a leadership role in the helping to establish a new materials discovery capability. This included many new

catalytic materials that showed promise in separations and catalysis applications, and led to many patents in the area.

In the face of those who said that electron diffraction data could not yield quantitative results, he argued long and hard that the problem of dynamical scattering could be overcome and that electron diffraction data could yield *ab initio* structure determinations. He was responsible for bringing the work on electron crystallography of Vainshtein and Zvyagin in Moscow to the attention of a larger western audience. He developed techniques to overcome the problems of the missing cone of data, dynamical scattering, radiation damage and sample problems. His breadth of applications included polymers, waxes, zeolites, fibers, cholesterol derivatives, fullerenes, phthalocyanines, solid solutions of paraffins and proteins at low resolution. It was typical of his thorough approach that the structural work on long chain compounds was combined with thermal studies to correlate the thermodynamic measurements of phase changes with chain packing. He was the first to carry out an *ab initio* solution of a membrane protein structure using electron diffraction data at 6 Å resolution. He also published on model validation using least-squares methods.

In 1995 he published *Structural Electron Crystallography*, the first definitive text on the subject and still an invaluable resource. This book, together with his pioneering work in electron crystallography, laid the foundation for an explosion of the field in the 21st century. Many of his methods are the basis for powerful methods of solving the structure of crystals which are not readily amenable to study using x-ray diffraction methods, employing techniques such as Precession Electron Diffraction, Automated Diffraction Tomography and methods for solving surface structures.

Douglas received the ACA's A.L. Patterson Award in 2002. He was within the top 1% of most-cited authors in the chemical literature, world-wide, 1981-1997 (compilation of David A. Pendlebury, Institute for Scientific Information). He was a member of the IUCr Commission on Electron Diffraction (now Electron Crystallography) 1993 -2002 (Chair 1999-2003), and a Co-Editor of *Acta Crystallographica A* 1999-2011. He was on the Editorial Board of the *Journal of Electron Microscopy Technique*, 1988-2010 and Associate Editor, *Microscopy Society of America Bulletin*, 1992-1994.

Douglas was involved in organizing several of the IUCr international schools of crystallography in Erice, Sicily as well as many other schools on crystallography around the world and numerous sessions at major national and international meetings. He was a good teacher and co-supervised research students in several countries, an enthusiastic supporter of many young researchers - who are now active electron crystallographers. Douglas always had time to discuss the finer points of an analysis, or to mentor others in need of some inspiration. He encouraged many of us in our work during the early years of electron crystallography, when its power was not fully embraced by the global crystallography community. His impressive knowledge of all aspects of crystallography will be remembered by all who met him.

Apart from his interest in science, he was also very interested in politics, culture, history and languages. It was impossible to walk away from a conversation with Douglas without learning something new and acquiring a handful of new inspirations. Discussions with Douglas would start out on a scientific note, then end up encompassing music, languages, typefaces, geography, and a multitude of other fascinating subjects. Music was important in his life, not the least because his son Erik is a professional violinist. He was also an avid collector of old books, and would visit antique bookstores in every city that he visited. It was the typography of old books which was his hobby. He taught himself Dutch to better understand the medieval printing techniques, and despite his illness over several years had nearly completed a book on the Dutch printing methods.

His wife Bonnie was at his side always and they nearly made it to their 50th wedding anniversary in 2017. Bonnie was also a dear friend for many of us who met her at numerous crystallography meetings, and a generous host for those who had come from various parts of the world to work with Douglas.

We will miss a dear friend, but will always remember his scientific integrity, knowledge and humor.

Lisa Baugh, Mark Disko, Bill Duax, John Fryer, Sven Hovmöller, William Lamberti, Laurie Marks, Stavros Nicolopoulos, Karl Strohmaier and Xiaodong Zou.

ACA History

Stanley Nyburg's memoir is online at the ACA History website, part of the new section titled Crystallography in the Americas. You can find his autobiography from the People listing or from the Crystallography in the Americas page. Autobiographies by those authors who have contributed "Living History" memoirs to this magazine are also on the website. If we have permission, we can post autobiographies published elsewhere, such as the recently added one by Philip Coppens, "The Old and the New: My Participation in the Development of Chemical Crystallography during 50+ years".

Part of the rich history of crystallography resides in the obituaries of individuals who played a major role in the development of structural science. You can find obituaries for Martin Buerger, Gabrielle Donnay, Joseph Donnay, David Harker, Edgar Meyer, David Sayre, Clara Shoemaker, James Stewart, Muttaiya Sundaralingam, Elizabeth Wood, and Ahmed Zewail on the ACA History website by looking for their names in the People listing.

ACA Election Results

Council Officers

Vice President
Lisa Keefe

Canadian Representative
Thomislav Friscic

Standing Committees

Communications
Brian Patrick

Education
Charlotte Stern

Data and Standards
Nicholas Sauter

SIGS

Biological Macromolecules
Chair-elect: Elizabeth Goldsmith

General Interest
Chair-elect: Mike Takase

Industrial
Chair-elect:Anna Gardberg
Secretary: Richard Staples

Light Sources
Chair-elect: Ray Sierra

Materials Science
Chair-elect: Karena Chapman

Neutron Scattering
Chair-elect: Brent Melot

Powder Diffraction
Chair-elect: Daniel Shoemaker

Service Crystallography
Chair-elect: Jeff Bacon

Small Angle Scattering
Chair-elect: Thomas Weiss

Small Molecules
Chair-elect: Graciela Diaz de Delgado

Young Scientist's Group
Chair-elect: Chelsey Chesterman
Secretary: Anastasiya Vinokur

Lisa J Keefe
Vice-President

Director of (IMCA-CAT), Vice-President of Center for Advancing Therapeutics, Hauptman-Woodward Medical Research Institute @ APS Argonne

Statement: The ACA is a rich and vital part of our scientific mission. While providing core services including hosting enriching annual meetings, recognizing the groundbreaking research of our members, and publishing our journal *Structural Dynamics* and *ACA RefleXions*, the ACA also serves to advocate for structure-based science, educate future generations of researchers, and provide professional guidance and development. We connect with each other as crystallographers and that connection transcends our varied scientific interests that are becoming increasingly diverse, driven by technological advances and expanding research frontiers. Our scientific disciplines are dynamic and thus our scholarly approaches are constantly shifting. The ACA is continually challenged to keep pace with these changes and respond to the evolving needs of crystallographers across the spectrum of SIGs as well as academia, government, and industrial research environments. As our science grows and becomes more global and more collaborative, we rely on the ACA to provide the intellectual space for us to share knowledge, discoveries, and ideas.

I was introduced to crystallography during my senior year of college and attended my first ACA meeting a few years later. The exciting science and supportive community of crystallographers shaped my course of graduate study and guided my career. As our science has advanced and our community has grown, the ACA has proven responsive to our expanding needs. Early in my postdoctoral appointment, I and several fellow postdocs had a vision for promoting young scientists and we collaborated on a proposal to ACA for establishing a new special interest group targeted to students, postdocs, and early-career scientists. The ACA was overwhelmingly supportive and, in 1994, the Young Scientist's Group was launched. Over the years, it has been gratifying to observe the growth of the YSG and witness the positive impact it has had in propelling the career of so many young crystallographers.

My scientific career began in small molecule crystallography before migrating to macromolecular crystallography. Currently, I work with industry, at a government laboratory, and under the umbrella of an academic research institute. Regardless of the perspective, the ACA has demonstrated flexibility by listening to its members, drafting new strategies, and implementing change while traversing boundaries. The ACA Council leads this process. Reflecting on my experience serving as ACA Secretary for six years I know that the Committees, the Canadian National Division, and SIGs are integral components of the ACA. Collaboration between these components is essential as the ACA confronts significant challenges in today's limited funding climate, namely increasing the engagement of the crystallographic community, providing relevant benefit to individual scientists across the full spectrum of special interest groups, and ensuring sustainability for future generations. These challenges may seem enormous, but the opportunities are abundant.

As a member of Council, I will focus resources on strengthening and growing ACA's core services to members, advocating for structure-based science, educating future generations of crystallographers, and providing the value expected from membership. Great benefit can be realized by bridging the crystallography disciplines and connecting with academia, government, and industry researchers. There is no substitute for the annual ACA meeting where we have the opportunity to strengthen our research through face-to-face discussions and

advance our careers through networking. As the climate for research funding becomes ever-more limiting and negatively impacts attendance, the ACA can creatively adapt by implementing mechanisms for increasing participation in a way that enhances professional value. While we rely on the ACA to connect with our peers to discuss and debate our research and advance our careers, the ACA relies on us to contribute our time and expertise to advocate, educate, and advance crystallography. As a member of Council, I will guide the ACA on a course for sustainability that will be inclusive across the spectrum of special interests, collaborative between the diverse research environments, and valuable at all career levels.

Thomislav Friscic
Canadian Representative

Assist Professor, Dept of Chemistry, McGill U, Montreal, Quebec, Canada

Statement. The greatest asset I can provide to the ACA and its Canadian members is a dedicated, dynamic attitude, directed towards promoting crystallography and its ability to solve wonderfully different problems. I offer diverse research and international experience, and a broad perspective of how crystallography fits into the colorful fabric of science. I joined the crystallographic community >20 years ago (while in high-school). Working with. Branko Kaitner at University of Zagreb, I received my first formal training in x-ray diffraction and crystallography – and still remember those fun and chilly winter mornings in the lab, figuring out unit cells and space groups, while the buzzer on a Picker machine announced peaks! This is really when my connection to Canadian crystallography started, as Branko got us all running NRCVAX, reminiscing over his visits to the Ferguson lab at Guelph. My first scientific collaboration: George Ferguson and Alan Lough helped us with a disorder problem, resulting in a joint *Acta C* paper. Since then I have been jumping in and out of different labs (in Croatia, USA, UK, Canada) and different research areas, making me realize how crystallography can be a key element of seemingly diverse activities, from structural determination via x-ray powder diffraction and crystal engineering, to reaction mechanisms monitoring and organic synthesis! I have been a member and supporter of a number of crystallographic communities around the world and currently serve as Vice-Chair of the Canadian NationalCommittee for Crystallography. I want to broadly present crystallography as a powerful and all-pervasive effort, as seen from my activities as the Social Media Editor of *Crystal Growth & Design*, Editorial Board member of *CrystEngComm* and Associate Editor of *Molecular Crystals & Liquid Crystals*.

At the level of ACA, the first and foremost important question that I want to address is the membership of the Canadian crystallography community. I would like to know how can we contribute more and encourage more Canadian crystallographers and solid-state and materials scientists to join the ACA. And I don't mean only membership numbers, I mean events, workshops and summer schools. I also mean publishing in our journal S*tructural Dynamics*. I am not the only one thinking along these lines. The fantastic *IYCr 2014* meeting in Montréal organized by Mirek Cygler and Albert Berghuis demonstrated the interest and dedication of the crystallographers in Canada. And now strictly talking to Canadian crystallographers: how we increase our numbers and broaden our scope? How do we engage researchers in x-ray crystallography, crystal engineering, solid-state NMR spectroscopy or crystal structure prediction and modelling to participate? How do we engage Canadian researchers living abroad to join scientific events in Canada? This may sound very broad – true - but I strongly believe in crystallography as a dynamic, inclusive and continuously growing discipline.

I like to think that I have a good presence within the ACA community. I have never refused an invitation to participate at an ACA event until this year when, alas, scheduled beamtime at DESY overlapped with the fantastic symposium spearheaded by Jason Benedict. I have organized two Crystal Engineering Symposia at ACA meetings which, I believe, reflect my view of crystallography as a broad and diverse discipline. I also enthusiastically participate in the Canadian crystallography community. Starting from a modest workshop supported by NSERC and FRQNT we have spun off a new tradition in Canada: the *Crystal Engineering and Emerging Materials Workshop* (CEMWOQ), taking place this year in Windsor with 70 participants. As a guest Editor,I have encouraged the participation of Canadian researchers in special issues of *CrystEngComm* dedicated to the *IYCr* (2014), and *New Talents in Crystal Engineering* (2016).

Since arriving to Canada and joining McGill University in 2011 I have been wonderfully welcomed and supported by colleagues across Canada. I would like to return this support by serving as a dedicated and dynamic representative of Canada's great crystallography community at the ACA Council, and will strive to the utmost of my abilities to grow the importance and activity of Canadian crystallography in this association.

Nicholas Sauter
Data, Standards & Computing

Computer Staff Scientist, Lawrence Berkeley National Lab, Berkeley, CA

Statement: My election to this committee is fortuitous because "Big Data" challenges are foremost in mind for me and other developers of primary data processing software for biosciences. I am heartened that creators of all major macromolecular processing programs, plus beamline scientists, gathered at three community meetings in the summer of 2016 to look for common approaches for handling the expected deluge of data. One future issue to

consider is whether beamlines can partner with national supercomputer facilities to provide real-time processing coverage for the expected burst in data rates.

I'm very supportive of the widely accepted practice of archiving structure factors to the PDB, in addition to the atomic models, for this assures that structure solution and refinement can be repeated in the future as algorithms improve. However, this reasoning also extends to unmerged data from multi-crystal experiments that are gaining popularity generally, not just at XFEL sources. With multi-crystal processing algorithms still a matter of active research, there is great potential benefit in the future from reanalyzing subtle measurements from unmerged data that are not usually considered, such as the polarization anisotropy of anomalous scattering. The ACA should actively encourage standard approaches, such as the inclusion of enough metadata to accurately describe experimental conditions.

Likewise, it is encouraging to see growing community interest in archiving the raw diffraction images for successful structure solutions. While the details of data reduction may often be treated as a black box, improvements in detectors and light sources also mean that algorithms are in constant flux, so for example we may shortly see better profile fitting of Bragg spots leading to greater detail in the electron density. Also, there has been recent interest in drawing structural conclusions from diffuse scattering. Unless the complete diffraction pattern is archived, this information from photons outside the Bragg spots might otherwise be discarded when disks are cleared after publication. While archiving data takes effort and is not cost-free, there is a benefit to having post-publication public access, as readers can double check conclusions and form alternate hypotheses.

On a broader level, I'm always glad to see scientists question the computation, and feel that it is important to train beginning crystallographers to seek a deeper understanding. I see that the ACA could play a role here - perhaps the annual meeting's agenda could place an increased emphasis on methods workshops. I am looking forward to participating in this process as part of this committee.

Charlotte Stern
Education

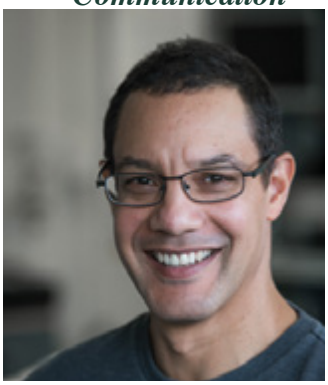
Staff Crystallographer, Dept of Chemistry, Northwestern U, Evanston Il

Statement: As it has become easier to obtain crystallographic data, the understanding of the fundamentals of x-ray diffraction has diminished. The ease of use and speed of the new instruments allows a the novice to use this technique without fully understanding its capabilities and limitations. It is my job as a crystallographer to ensure that the next generations of chemists have the tools and foundations of this technique. This technique cannot become a "black box" where problems are just swept under the rug.

At Northwestern I have had the opportunity to help develop courses in crystallography for both undergraduates and graduates. It is always exciting to see the undergraduates choose a crystallographic project for their independent research. It is just as exciting to see the graduate students learn to solve their own crystal structures. I have been very involved in coordinating ACA educational workshops designed to assist professional crystallographers in their tasks. I get excited working with individual students from around the world at the ACA Summer Course when a difficult concept is finally understood.

The duties of this committee provide a crucial service to the ACA and the crystallographic community. Committee members develop new workshops, provide professional development, and encourage student travel to the meetings. Many crystallographers are alone at their place of work. We need to be a center for them. Having an opportunity to go to a workshop to learn a new technique or look up a teaching manual from the ACA webpage to help understand a concept can make a big difference to them. These resources are indispensable to both novice and professional crystallographers. I will work to support these vital educational opportunities and try to facilitate others for the crystallographic community.

Brian Patrick
Communication



Dept. of Chemistry, University of British Columbia, Vancouver, BC, Canada.

Statement: As an ACA member for over 15 years, I owe it to the community to contribute to its continued success. One of the most satisfying things I've done this year was to visit my 7 year-old's 2nd grade class and spend half an hour telling them about what I do every day. It reminded me of how science can inspire, and also of how relatively invisible scientists are in general, and crystallographers are specifically. Teaching crystallography for the past 8 years has shown me that, even at the undergraduate and graduate levels, students are not fully aware of the role crystallography of one sort or another has played in the way science shapes our lives. The role of getting the word out, of making the public aware of the important work being done by ACA members falls, in part, to the Communications Committee and I look forward to helping the ACA in this part of its mission.

2017 Award Winners

Rognlie
Helen Berman

Patterson
Zbigniew Dauter

Wood Sceince
James O'Brien

Etter Early Career
Christine Dunham

AWARDS:

ETTER AWARD
Ueli Aebi
Gerald Ansell
Helen Berman
Carolyn Brock
*William Busing**
Horace Carrell
Charles Carter
Bryan Chakoumakos
Jon Clardy
Abraham Clearfield
Norma Duke
John Enemark
Janet Finer-Moore
Richard Gilardi
James Golen
Jane Griffin
Richard Harlow
Judith Ann Kelly
Mariusz Krawiec
Roger Lalancette
Marie Claire McKenna
William Ojala
James Phillips
Connie Rajnak
Bernhard Rupp
Timothy Rydel
Carl Schwalbe
George Sheldrick
Edward Snell
Dmitriy Soldatov
Vukica Srajer
William Stallings
Edwin Stevens
Robert Sweet
Raymond Trievel
Thomas Webb
Victor Young

PAULING
Richard Brennan
Horace Carrell
Charles Carter
Bryan Chakoumakos
Abraham Clearfield
David Cox
Lawrence Dahl
William Duax
David Duchamp
Frank Fronczek
Judith Gallucci
Richard Gilardi
Stephan Ginell
*Theodor Hahn**
Hakon Hope
Carol Huber
*Pavel Karen**
James Knox
Catherine Lawson
James Phillips
Connie Rajnak
Frank Rotella
Timothy Rydel
George Sheldrick
William Stallings
Edwin Stevens
Robert Sweet
Thomas Webb
Angus Wilkinson

WARREN
Andrew Allen
John Barnes
Michael Bedzyk
Bryan Chakoumakos
Abraham Clearfield
Henderson Cole
David Cox
Takeshi Egami
Howard Einspahr
Wilfred Fullagar
Richard Gilardi
James Golen
Robert Sweet
Dale Tronrud
Thomas Webb

PROGRAMS:

DEVELOPMENT
Donald Caspar
Bryan Chakoumakos
Abraham Clearfield
William Duax
Richard Gilardi
James Phillips
Robert Sweet

HISTORY
Richard Bromund
Charles Bugg
Susan Byram
Donald Caspar
Bryan Chakoumakos
Abraham Clearfield
J. Flippen-Anderson
C. M. Foris
Frank Fronczek
Wilfred Fullagar
Richard Gilardi
Anthony Glazer
James Golen
Judith Ann Kelly
Frank Milillo
William Ojala
Virginia Pett
Connie Rajnak
Timothy Rydel
Carl Schwalbe
William Stallings
Robert Sweet
Dale Tronrud
Winnie Wong-Ng

OUTREACH
Richard Brennan
Donald Caspar
Bryan Chakoumakos
Yang Chen
Abraham Clearfield
Joshua De Groot
William Duax
Richard Gilardi
James Golen
*Pavol Juhas**
Judith Ann Kelly
James Knox
Michael McGuire
Frode Mo
James Phillips
Connie Rajnak
Giovanna Scapin
Maria Mercedes Silvia
William Stallings
Robert Sweet
Doletha Szebenyi
Martha Teeter
Diana Tomchick
Thomas Webb

STUDENT TRAVEL
Krishnayan Basuroy
Charles Bugg
Roger Burnett
Donald Caspar
Bryan Chakoumakos
Abraham Clearfield
David Cox
William Duax
Drake Eggleston
Andrew Fisher
J. Flippen-Anderson
Judith Gallucci
Richard Gilardi
John Helliwell
Douglas Ho
Carol Huber
Pavol Juhas
Pavel Karen
Michael Jon Kelly
Judith Ann Kelly
Thomas Laube
Marilyn Olmstead
James Phillips
Connie Rajnak
Arthur Robbins
Gerold Rosenbaum
Frank Rotella
Timothy Rydel
Leroy Schroeder
George Sheldrick
Edward Snell
Vukica Srajer
William Stallings
Robyn Stanfield
Richard Staples
Robert Surbella
Robert Sweet
Dale Tronrud
Li Wan
Thomas Webb
Carrie Wilmot
Winnie Wong-Ng

SUMMER SCHOOL
Abubakar Abdullahi
Bryan Chakoumakos
Abraham Clearfield
David Duchamp
Frank Fronczek
Judith Gallucci
Richard Gilardi
Jenny Glusker
Jeanette Krause
Allen Oliver
Connie Rajnak
Timothy Rydel
Robert Scheidt
T. Somasundaram
William Stallings
Robert Surbella
Robert Sweet
Thomas Webb

** Deceased*

Puzzle Corner

Our ***Guest Puzzler***, ***Bill Ojala*** (Chemistry Department, University of St. Thomas, St. Paul, MN), designed the new Crystal Connections puzzle:

Crystal Connections #9

Fill in the missing words in the following song titles, for which artists and dates are given. What do the missing words have in common?

1) *Two*_____ *Have I* – Lou Christie, 1963
2) *Leader of the* _____ – The Shangri-Las, 1964; Twisted Sister, 1985
3) _____ – The Supremes, 1967
4) *The* _____ *Ship* – The Doors, 1967
5) _____ *Blue Persuasion* – Tommy James and the Shondells, 1968
6) _____ *of My Life* – The Marmalade, 1969
7) _____ Stevie Nicks & Lindsay Buckingham, 1973
8) *Music and the* _____ – From *A Chorus Line*, 1975
9) _____*field* – John Fogerty, 1985
10) *Man in the* _____ – Michael Jackson, 1988
11) _____ – Phish, 1992
12) *Perfect* _____ – Keane, 2008
13) *Poker* _____ – Lady Gaga, 2009

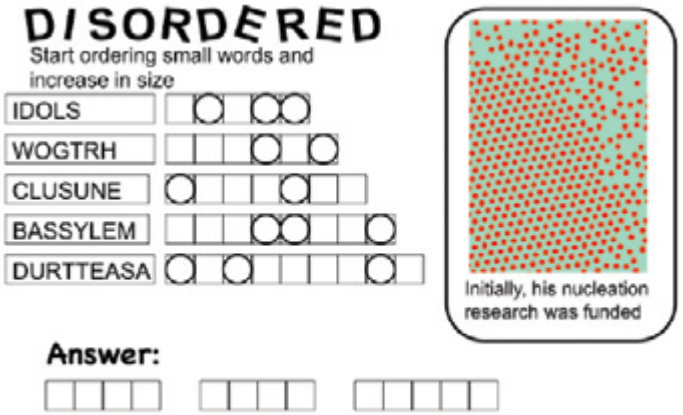
Previous Crystal Connections (#8) *Names of past presidents of the ACA:*

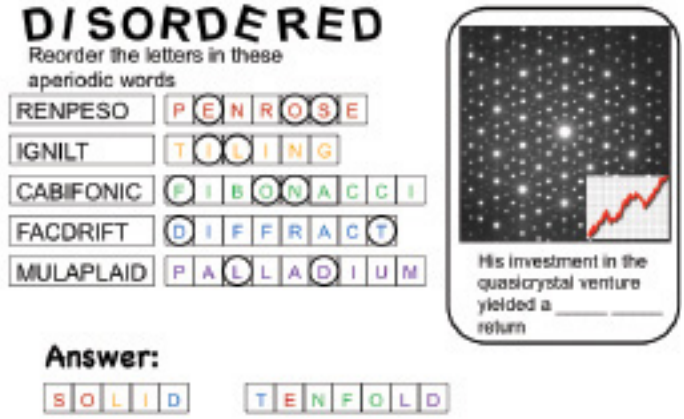
1) "Small", *auf Deutsch* - Cheryl Klein Stevens, 2013
2) Detective agency, founded 1850 - Alan Pinkerton, 2007
3) Wetland lacking trees - Dick Marsh, 1993
4) _____ Turks, Ottoman Empire, 1908 - R. A. Young, 1973
5) "Zapatero", *en Inglés* - David Shoemaker, 1970
6) Washington _____, John Philip Souza march - Ben Post, 1966
7) Structural material composed mostly of cellulose, hemicellulose and lignin - Elizabeth Wood, 1957

Somebody was first to provide the solution to the Crystal Connections puzzle, and ***Somebody else*** solved the DISORDERED 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 – ffronc@lsu.edu





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17. I certify that all information furnished on this form is true and complete.
(signed) Marcia Colquhoun for American Crystallographic Association, Inc.

ACA NEW ORLEANS

Friday, May 26 - Tuesday, May 30, 2017

Hyatt Regency New Orleans

Travel Grant Application Deadline: February 15, 2017
Abstract Deadline: February 15, 2017
Early Registration Deadline: March 31, 2017
Hotel Reservation Deadline: May 1, 2017

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

www.amercrystalassn.org

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

Meeting logo designed by Kandis Elliot

Program Chair - Yulia Sevryugina
y.sevryugina@tcu.edu

Program Chair - Ilia Guzei
iguzei@chem.wisc.edu

Posters Chair - Bruce Noll
bruce.noll@gmail.com

EDUCATIONAL SESSIONS & YSG EVENTS

Workshops
Lunch and Learn Sessions
YSSIG Orientation and Networking Mixer
Career Development Session
Undergraduate Research Symposium
Engaging Undergraduates with Crystallographic Research
Communicating Science to the Public
Diversity & Inclusion Session
Practicum on Macromolecular Crystallography
Standard Practices in Crystallography
How Do I Get My Data?

ACA AWARDS

Patterson Award honoring Zbigniew Dauter
David Rognlie Award honoring Helen Berman
Elizabeth Wood Science Writing Award honoring James O'Brien
Margaret C. Etter Early Career Award honoring Christine Dunham

SESSIONS

Transactions Symposium – Cryo Electron Microscopy
NMR Crystallography
Integrative Approaches to Structural Biology
Advanced Surface and Interface Scattering & Applications
In situ and Operando Methods
Crystal Structure and Property Prediction
Home-Built Software
Crystal Growth
Mineralogical Crystallography

Transactions Symposium – Cryo Electron Microscopy

Organizers: Stephen Burley (Rutgers University Center for Integrative Proteomics Research; sburley@proteomics.rutgers.edu)) and Michael Rossmann (Purdue) mr@purdue.edu

The theme of this year's Transactions Symposium is Cryo Electron Microscopy. Both the symposium and a new session this year on NMR crystallography are dedicated to covering topics of importance to scientists with a wide range of professional backgrounds and designed to emphasize our need for collaboration and cooperation.

Meeting participants working in protein crystallography and practitioners of cryo electron microscopy, tomography, and diffraction will have the opportunity to learn first-hand from internationally recognized experts contributing to the "Resolution Revolution." Recent advances in direct electron detection, automated cryogenic sample handling, phase plate technologies, and correlative cryo fluorescent light/electron microscopy hold considerable promise for protein crystallographers intent on studying larger, more complex, and often heterogeneous (conformational and compositional) assemblies of biological macromolecules that resist crystallization. At the close of the symposium, invited speakers will be asked to contribute to a round table discussion of the important roles that current and would-be cryo-EM/ET/ED practitioners can play in the future of the ACA.

General Meeting Information

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

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

Hotel Information: FREE WI-FI is included in the sleeping rooms, so bring your laptops and stay connected to home and office. The room rates at the Hyatt are competetitive with other properties in the vicinity. We are able to offer these rates by committing to fill a certain number of rooms. By staying in the conference hotel you will help us meet this commitment, which also brings with it free meeting space that helps keep registration fees affordable.

All of our contracts include a number of lower cost rooms available to students. Room sharing can make them even more reasonable – use the ***Room Sharing*** feature under accommodations on the meeting web site.

Financial Support: Travel support will be available for young scientists. Applications should be made by the abstract deadline – February 15, 2017.

Registration Fees

Early until March 31 - Late after March 31

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

EACH REGISTRATION FEE INCLUDES THE BANQUET ON TUESDAY, MAY 30 - but you must indicate participation when submitting registration

LOCAL* : a student registered at a college or university that is located within 150 miles of the city of New Orleans

Anyone registering as a student or postdoc must include documentation of status with the registration form.

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

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

WK.01 - CCDC- Commuication and Innovation

WK.02 CrysAlis^{Pro} and Olex2: From Raw Data to Publication

WK.03 Introduction to PHENIX for Beginning and Advanced Crystallographers

WK.04 Research Data Management

Register online or download forms to register by fax or mail.

www.amercrystalassn.org/2017-meeting-homepage
Questions: aca@hwi.buffalo.edu

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

Call for Nominations - 2018 Awards

2018 Warren Award: To recognize an important recent contribution to the physics of solids or liquids using X-ray, neutron, or electron diffraction techniques. Works published within a six-year period ending June 30 of the year preceding the Award may be nominated. A monetary award of $1,500, and up to $1,500 travel expenses to accept the award at the annual meeting, and a certificate are awarded every third year. Established in 1970 by students and friends of B.E. Warren on the occasion of his retirement from the Massachusetts Institute of Technology. (Selection committee: **L. Marks (Chair), Louise Dawe, Paul Langan and Brian Toby.)**

2018 Margaret C. Etter Early Career Award: To recognize outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career. The Award consists of a $1,000 honorarium and a plaque. The winner is also expected to present a lecture at the ACA annual meeting.

2018 M. J. Buerger Award: To recognize mature scientists who have made contributions of exceptional distinction in areas of interest to the ACA. There are no restrictions as to nationality, race, sex, religion, or membership in the ACA. Awarded triennially in memory of Martin J. Buerger, Institute Professor Emeritus of M.I.T. and University Professor Emeritus of the University of Connecticut, a mineralogist who made major contributions to many areas of crystallography. Established in 1983. The first award was made in 1985. A monetary award of $1,500, and up to $1,500 in travel expenses to accept award at the annual meeting (Selection committee: **Michael James (Chair), Lee Daniels, Greg Petsko, and Claudia Rawn.**)

The deadline for nominations for the 2018 ACA Awards is April 1, 2017.

2018 ACA Fellows: Serves to recognize a high level of excellence in scientific research, teaching, and professional duties, but also service, leadership, and personal engagement in the ACA and the broader world of crystallography and science. Our Fellows program celebrates the excellence of our own members from within the ACA, and promotes their recognition worldwide to constituencies outside of the ACA, such as their employers, other scientific societies, and the government. See ***www.amercrystalassn.org/aca-fellows*** for information on the nomination procedure. ***Nomination forms for 2018 ACA Fellows can be found at www.amercrystalassn.org/documents/ACAnomNEW.pdf and are due by February 28, 2017.***

2018 ACA Offices and Committees: In the fall of 2017 we will elect a new Vice-President, Secretary, and one person to each of the ACA Standing Committees (Continuing Education, Communications, and Data, Standards and Computing). Suggestions are due by February 15, 2017.

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

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

Communicating with Congress

The ability of a government agency to make or extend a research grant, fund a new instrument, or support a research program directly relates to legislation considered by Congress. On almost a daily basis, congressional action affects the efforts of scientists to contribute to the growth of knowledge and the well-being of the nation.

All too often, Congress makes decisions affecting the conduct of research in America with little participation by the physical sciences community. Few Members of Congress have direct knowledge about scientists and their work, and the impacts that congressional decisions have on research. The need for scientists to communicate with Congress has never been greater.

The AIP provides some excellent documentation on how to go about communicating with Congress at ***www.aip.org/policy/communicating-with-congress***

- Correspondence ***www.aip.org/policy/writing-to-congress***
- Personal visits ***www.aip.org/policy/visiting-congress***
- Contact information for the House of Representatives ***www.house.gov/***
- Contact information for the Senate ***www.senate.gov***

AIP also provides timely /ongoing updates on science policy issues being taken up by Congress. ***www.aip.org/fyi***

2017 Dues are Due

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

ACA Summer Course in Chemical Crystallography

www.acasummercourse.net

June 25th – July 2nd, 2017

Northwestern University

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

Important Dates:

Applications Open – January 2017

Acceptance Notifications – March 2017

Registration Deadline – May 1st 2017

NORTHWESTERN UNIVERSITY

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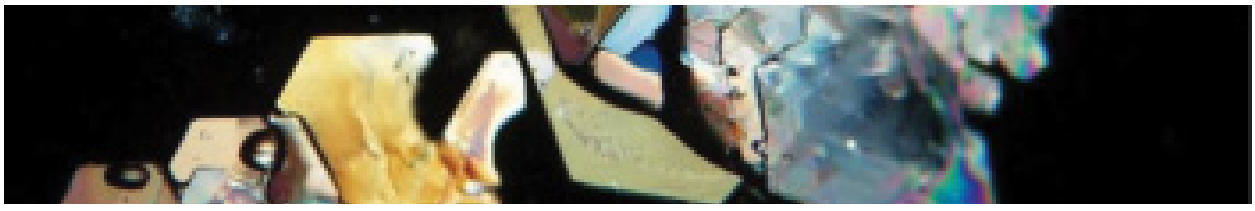


FEBRUARY 2017

11-15 **Biophysical Society. 61st Annual Meeting**. New Orleans, LA
www.biophysics.org/Meetings/AnnualMeeting

MARCH 2017

19-22 **XXIII West Coast Protein Crystallography Workshop, Asilomar, CA**
www.biochem.utah.edu/hill/wcpcw.html

APRIL 2017

10-13 **BCA Spring Meeting**. Lancaster University, U.K.
www.bcaspringmeetings.org.uk/home

17-21 **MRS Spring Meeting & Exhibit**. Phoenix, AZ
www.mrs.org/spring2017

MAY 2017

13-17 **Understanding Biology Through Structure, Santa Fe, NM**
conferences.newmexicoconsortium.org/conferences/ubts_17

26-30 **ACA 2017 Annual Meeting**. New Orleans, LA
www.AmerCrystalAssn.org

JUNE 2017

7-9 **Neutrons in Structural Biology**. Grenoble, France
indico.ill.fr/indico/event/58/

2-11 **50th Erice Course: Integrative Structural Biology**. Erice, Italy
www.crystalerice.org/2017/

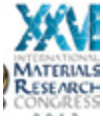
JULY 2017

9-13 **Int'l Conference on Neutron Scattering 2017,** Daejon, Republic of Korea
www.icns2017.org/

24-28 **Borate & Phosphate 2017.** St. Anne's College, Oxford, U.K.
www.borate-phosphate.sgt.org

AUGUST 2017

9-13 XXVI **International Materials Research Congress, Cancun, Mexico**
www.mrs.org/imrc-2017



21-28 **24th Congress and General Assembly of the IUCr**. Hyderabad, India
www.iucr2017.org

JULY 2018

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

JULY 2019

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

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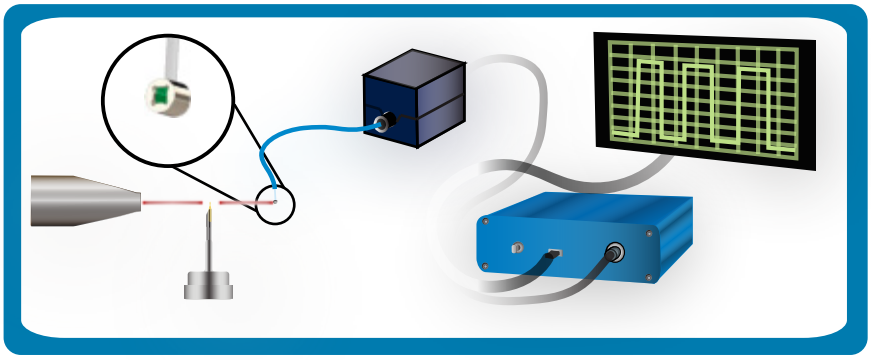

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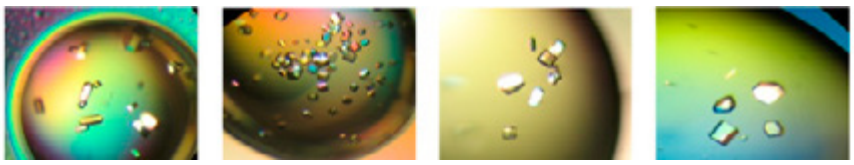

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