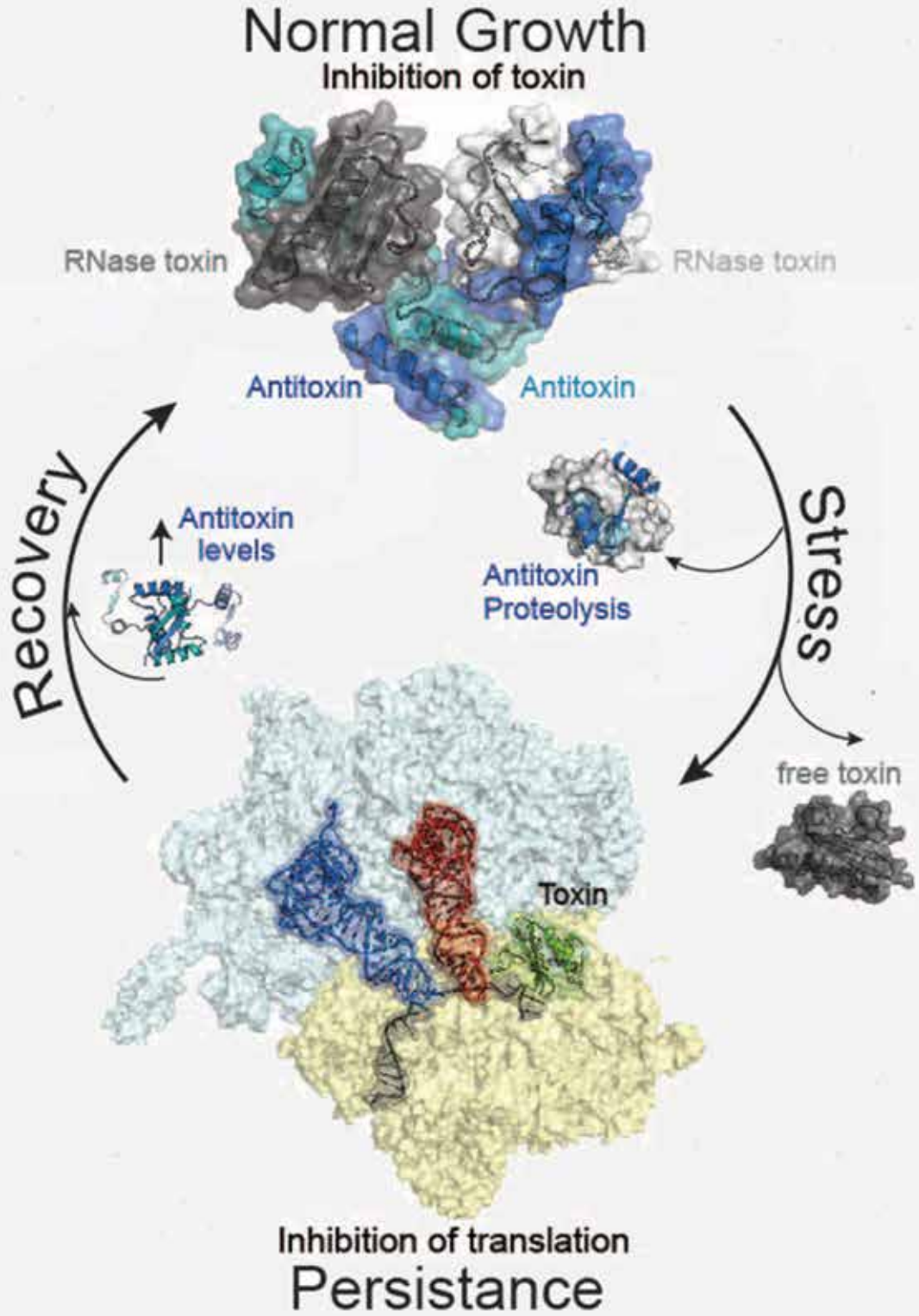
ACA RefleXions

American Crystallographic Association
Structure Matters

Number 1

Spring 2017



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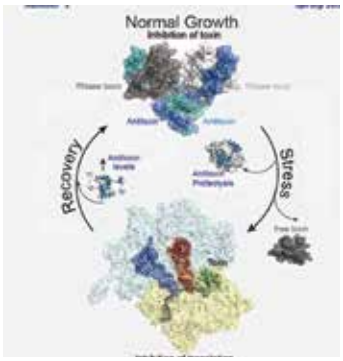

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President's Column

Amy Sarjeant

As I write this missive, the first month of 2017 is drawing to a close. Already the New Year has started off with a bang at the ACA. We're well into planning of all sorts – both for the annual meeting in New Orleans (more on that in a minute) and for finding a new employee for Buffalo HQ. As many of you know, our long-time friend and colleague Marcia Colquhoun has transitioned to a part-time position this year and will be fully retired as of 2018. Kristina Vitale has moved to a full-time position in Buffalo, and we're looking to bring on another member to the ACA team to spearhead meeting planning and membership services. In addition to changes in staffing in Buffalo, ACA Council is also exploring improvements to the website, ways to attract new members, and more advanced program planning for our annual meetings.

Speaking of meetings, our 2017 Program Chairs, Ilia Guzei and Yulia Sevryugina, have been doing an outstanding job organizing our annual conference to be held this May in New Orleans. We have an exciting program in store including an opening reception featuring 2016 Nobel Laureate Sir Fraser Stoddart. Our *Transactions Symposium* will focus on the burgeoning field of cryo electron microscopy, and we're pleased to welcome this new discipline to our regular line-up of topics. The full program is available on the ACA website, so be sure to visit the site and see what you can learn in NOLA this spring. Last year's banquet entertainment got rave reviews, and we've decided to continue the tradition. The 2017 Wood Awardee, James O'Brien, will be our guest speaker, and we'll have live jazz afterwards. The banquet is included in your registration fee, so there's nothing stopping you from attending!

We've been working on improving our conference planning activities, starting with the 2018 meeting in Toronto. Program Chairs for that meeting, Gerald Audette and Tiffany Kinnibrugh, are already hard at work soliciting session proposals from SIGs. These proposals will be vetted during the SIG meetings held in New Orleans, and from them we'll create a comprehensive and robust program featuring the highest quality science, cutting-edge techniques, and brilliant educational content for all ACA members. If you have a session in mind for 2018, get in touch with your SIG officers and they can help you submit your proposal.

Ilia, Yulia, Gerald and Tiffany are only a few of the volunteers who step up every day and help out with various ACA activities. From planning meetings, to organizing outreach activities, to writing content for our website and *RefleXions*, to sending out a Tweet about some scientific curiosity, our members do a lot to keep the ACA a vibrant society. I can't think of many other scientific communities where it's this easy to get involved on such a deep level with the activities of the association. We're always looking for enthusiastic members to serve as SIG officers, on standing committees, or as program or session chairs, and if you've been looking to become more involved in ACA activities, I encourage you to pitch in.

Finally, if you're looking for ways to support the ACA, but don't have a whole lot of time, I'd like to draw your attention to a few fund-raising campaigns we are running. If you are a frequent Amazon shopper, you can shop through Amazon's Smile program and set the ACA as your preferred charity. This way, Amazon will donate a small percentage of the cost of your order to the ACA – at no cost to you! It's a great way to get your shopping done and support the ACA at the same time. Check out the link on the ACA homepage for more information. Hopefully by now you've purchased an ACA New Orleans T-shirt. Our Program Chairs designed the shirt to commemorate the 2017 meeting, and proceeds from the sale will support general operations at the ACA. We hope to make this T-shirt fundraiser an annual event with new designs every year. And of course, the ACA will still accept donations through the website at any time – not just when you renew your membership. Just click the "Donate Now" tab on the ACA homepage.

The year ahead will be challenging as we restructure the Buffalo office and seek to attract new members and meeting attendees. But it will also be exciting, as we continue to expand the focus of our meetings to include dynamic new fields and seek out more ways to promote crystallography. Do what you can to be involved with the ACA, whether presenting your research at a meeting, writing an article for *RefleXions*, or donating your time to serve on a committee. The ACA is one of the best scientific communities I know, and I can't wait to see what we can do together.

Amy Sarjeant

Editor's Note: For more on ACA's transition plans and other society news, see ACA Secretary Diana Tomchick's report on highlights from the 2016 fall Council meeting on pp. 31-32.

RefleXions from Canada

Tomislav Friščić

This is my first column in *ACA RefleXions* on Canadian activities and to start off I would like to offer my sincere gratitude to Michael James, whose big shoes I am trying to fill. I am hopeful that I will manage to keep up the level of dynamic reporting and detailed updates, and also keep you interested. So, thank you very much Mike, and I hope we will be able to get you back on board here occasionally!

In this postcard from Canada I would like to highlight two outstanding contributors to chemical crystallography and crystal engineering, **Daniel Leznoff** and **Stephen Loeb**, who have been doing a remarkable job in combining synthesis and crystallography to generate new materials. I would consider them movers and shakers of crystal engineering.

The group of Danny Leznoff (see Fig. 1 facing at the top of p. 3) has been making strides in utilizing coordination-driven assembly to design crystal structures with targeted optical properties – accomplished, as he puts it, with the help of his excellent graduate students who, "live and breathe X-ray crystallography."

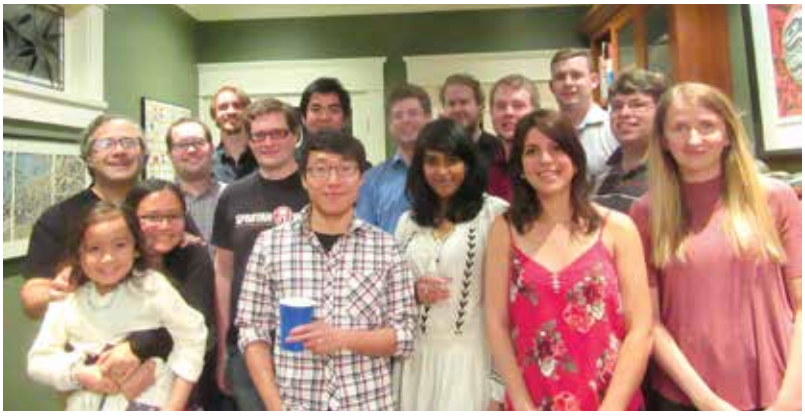

Fig. 1: The Leznoff group, who live and breathe X-ray crystallography to create new optical materials.

This truly unique research focuses on designing and preparing birefringent coordination polymer crystalline materials, and developing a detailed understanding of how the phenomenon of birefringence is controlled by the solid-state crystal structure, the molecular packing, and the crystal morphology and faces. Coordination polymers are metal-containing materials in which a metal cation and a bridging ligand are linked *via* metal-ligand coordinate bonds to form infinite network materials. One of the great strengths of coordination polymer synthetic methodology is its modular nature, *i.e.*, the ability to readily change metal cations and/or bridging ligands to design and target a particular structure and property. Danny's group is one of the first in the world to target birefringent coordination polymers. But what is birefringence? The property of optical birefringence (Δn), often neglected by crystal engineers, occurs when a material exhibits different refractive indices in different directions. It is exploited in optical elements such as circular polarizers and non-linear optical (NLO) materials, and birefringent materials are critical for microscopy, telecommunications and other applications involving optical components. The commercial birefringence standard is calcite, with Δn=0.17. However Danny's group designed target molecules that show excellent properties for high birefringence, and they have made a large series of coordination polymers using these targets as ligands to bridge metal ions. Their introduction of bis(benzimidazole)pyridine was a landmark contribution that led to some of the most highly birefringent crystalline materials in the world, with Δn values around 0.65, and utilized X-ray single-crystal diffraction to outline the first design criteria for preparing such materials (see Fig. 2 below). However, it does not end there – when I was talking with Danny recently he revealed that his group might be close to achieving the "holy grail" of birefringence design with materials whose Δn is approaching 1. Check out some of this really nice work: *Chem. Eur. J.* **2013**, *19*, 16572; *J. Am. Chem. Soc.* **2009**, *131*, 18435.

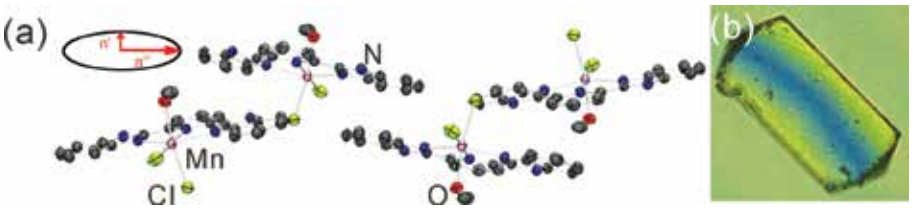

Fig. 2: (a) Fragment of a manganese-based coordination polymer exhibiting the remarkable Δn=0.69; and (b) the corresponding birefringent crystal.

Danny Leznoff completed his B.Sc. at York University (1992) and also studied Japanese language and literature. He spent a year at Meiji University in Tokyo where he had the chance to study chemistry exclusively in Japanese, winning several provincial and national Japanese language speech competitions. Today we're all very grateful for this, as it makes him one of the central figures in organizing the Canada-Japan Joint Symposia on Coordination Chemistry. Danny obtained the *NSERC 1967 Science and Engineering Scholarship* during his doctoral studies with Michael Fryzuk at the University of British Columbia, working on organometallics with unpaired electrons. His interest in magnetic materials led him as an NSERC Postdoctoral Fellow to work with Olivier Kahn (1997-1999), who was one of the fathers of the field of *molecular magnetism* at the Bordeaux Institute for Condensed Matter Chemistry in France. In 1999, Danny joined Simon Fraser University and was promoted to Professor in 2009. His interests include cyanometallate coordination polymers (especially with metallophilic interactions), paramagnetic organometallics and phthalocyanines. He was the Chair of the Canadian Society of Chemistry (CSC) Inorganic Division (2010-2012), was elected a Fellow of the Chemical Institute of Canada in 2015, and was the Scientific Program Chair for CSC2014, the Canadian national chemistry conference. He currently serves on the Editorial Boards of the *Canadian Journal of Chemistry* and *Gold Bulletin*, and in 2010 he received the CSC Strem Chemicals Award for Pure or Applied Inorganic Chemistry.

The group of Steve Loeb (see Fig. 3 at the top of p. 4) at the University of Windsor are pioneers in creating dynamic metal-organic frameworks (MOFs) by combining this hot and challenging area of materials science with the concept of rotaxanes – a type of mechanically interlocked molecules (MIMs), which have recently been made additionally famous by the 2016 Nobel Prize (Stoddart, Sauvage, Feringa).

Steve Loeb is the Canada Research Chair in *Supramolecular Chemistry and Functional Materials* in the Department of Chemistry and Biochemistry at the University of Windsor. He completed his Ph.D. at the University of Western Ontario, working with Christopher Willis, after which he took on a postdoctoral fellow position with Martin Cowie at the University of Alberta. In 1997 Steve was elected a Fellow of the Chemical Institute of Canada; he became a Fellow of the Royal Society for Chemistry in 2007, and in 2012 received the CSC's Rio Tinto Alcan Award for outstanding achievement in Inorganic Chemistry. In 2016 he was an Erskine Fellow at the University of Canterbury, New Zealand. Steve is most widely known for his pioneering work on the incorporation of MIMs into MOFs. To be more specific, Steve's group has introduced an ingenious design that utilizes the MOF linker organic ligands as rails for the motion of mechanically attached molecular shuttles. In technical terms this

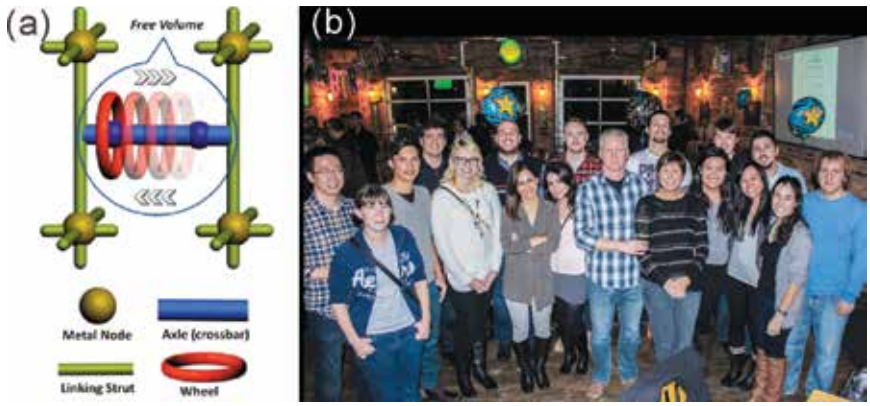

Fig. 3: (a) A schematic representation of the Loeb group's design for incorporating molecular shuttles in open crystalline structures of MOFs; and (b) the group having a good time.

means utilizing organic synthesis and self-assembly to develop new supramolecular templating motifs for the formation of interpenetrated host-guest species, called pseudorotaxanes, and their conversion into permanently interlocked molecules such as *rotaxanes* and *catenanes*. However the ultimate goal of this work is to create completely novel, organized solid-state materials that incorporate these artificial molecular switches and machines as dynamic elements. This higher level of molecular organization is being achieved in Steve's group by placing the dynamic molecular components of a MIM (*e.g.*, rotation or translation) into either the pores of a MOF or the core structure of a mesomorphic liquid-crystalline material.

This is a challenging goal, and the major breakthrough in this research came recently as outlined in the 2015 paper, "*A molecular shuttle that operates inside a metal-organic framework*" (*Nature Chem.* **2015**, *7*, 514), which describes a "molecular shuttle" – an interlocked molecular assembly in which a macrocyclic ring is able to move back and forth between two recognition sites, operating as an inherent part of a MOF architecture. The large amplitude translational motion associated with molecular shuttles of this type was first characterized in solution in 1991 and, since then, many MIMs have been designed, synthesized and shown to mimic the complex functions of macroscopic switches and machines. Steve's group was the first to show that this fundamental concept – the translational motion of a molecular shuttle – can be organized, initiated and made to operate inside a crystalline solid-state material. Specifically, a MOF designated **UWDM-4** was prepared containing a rigid linker that is a molecular shuttle. Whereas the formation of a rotaxane-based MOF was demonstrated through a feat of single-crystal X-ray diffraction, pinning down the dynamic "shuttling" behavior required a different kind of probe. Characteristic of Steve's group, this was achieved by complementing X-ray crystallography with solid-state nuclear magnetic resonance (ssNMR) spectroscopy. By conducting variable-temperature ^{1}H-^{13}C CP/MAS and ^{13}C 2D EXSY ssNMR measurements on a ^{13}C-enriched sample, they demonstrated that the macrocyclic ring undergoes rapid shuttling along the rigid axle built between struts of the MOF.

Upcoming Events

Complementing X-ray diffraction through ssNMR is a topic of great interest to me, so this may be a good moment to start highlighting some of the exciting conferences and workshops organized in Canada or by Canadian researchers. So, please keep an eye out for the *NMR Crystallography* topic of Symposium 2.1.4 at the upcoming **ACA Annual Meeting** in New Orleans. This, to the best of my knowledge, might be the first of such symposia held at an ACA meeting, chaired by Manish Mehta and myself. So, please hang around on Sunday, May 28 for some NMR crystallography. This is a good place to mention also that Michael James is co-organizing a symposium in New Orleans dedicated to *Conformational Dynamics of Ligand Binding*; this Symposium 4.1.3 will take place on May 30. Here is the link to the ACA Annual Meeting program:

http://www.amercrystalassn.org/2017-scientific-program

Unfortunately it is unlikely that there will be a strong Canadian participation in New Orleans, due to an overlap with the annual meeting of the CSC. This year's meeting in Toronto is special, as it falls on the CSC's 100th Anniversary.

• Just before the CSC100, however, Louise Dawe (who was highlighted in the spring 2016 issue of *RefleXions*) and Kenneth Maly are co-organizing the fourth consecutive **Crystal Engineering and Emerging Materials Workshop of Ontario and Quebec (CEMWOQ-4)** at Wilfrid Laurier University, in Waterloo, Ontario, from May 26-28, 2017. Four previous meetings have taken place (at McGill University, the University of Guelph, and the University of Windsor) with attendance increasing each year. This year Christer Aakeröy, Marc Fourmigue and Vladimir Fedin are attending as invited speakers. Last year at Windsor (see Fig. 4 below) we had a crowd of almost 70 people, and this is certainly becoming the place to go for crystallographers to mingle with crystal engineers and materials scientists. And the best part of it is there no registration fee!

Fig. 4: Group picture from last year's CEMWOQ-3 with invited speakers in the front row, L-R: Amy Sarjeant (CCDC), Jagadese Vittal (National University of Singapore) and Omar Farha (Northwestern University).

Information on this most recent CEMWOQ meeting, and links to previous meetings, can be viewed at the following website:

http://cemwoq.cs.uwindsor.ca/Contact/About/index.html

• Jim Britten is organizing the **8th Canadian Chemical Crystallography Workshop (CCCW17)** this year in Hamilton, Ontario. The Workshop will be taking place May 22-26, so there will be enough time to attend it, pay a visit to Wilfrid Laurier for CEMWOQ-4, and then move on to the 100th CSC. CCCW17 is targeted towards chemistry graduate students and postdocs who would benefit

from an improved understanding of the basic theory and practice of structure determination using single-crystal X-ray diffraction methods:

http://xtallography.ca/index.php/xtal/meetings/cccw17/

• In addition to the events leading up to the 100th CSC in Toronto, a lot of things are happening there as well. Most notably Dmitriy Soldatov and Kathryn Preuss from the University of Guelph are organizing a symposium on *Crystalline and Semi-crystalline Molecule-based Materials*, which will run for two full days (May 30-31, 2017). Looking at the list of confirmed speakers, it promises to be a rich program of Canadian and international speakers! Check out the CSC program at:

www.csc2017.ca

• Following the CSC, in June, Patrick Mercier is organizing the **10th Canadian Powder Diffraction Workshop** in Edmonton, Alberta. The workshop will be held June 2-4, as a satellite meeting ahead of the 54th Annual Clay Minerals Society Conference. Participation in the Workshop will be limited to approximately 30 registrants. This will ensure plenty of facetime for all participants, lecturers and instructors to interact – but it also means you should watch out to register as soon as possible in order not to lose your place! The webpage for the workshop is here:

http://www.cms2017.com/10thcpdw/

• In August this year we are all looking forward to the **24th Congress & General Assembly of the IUCr** in Hyderabad, India. Some of the activities of Canadian crystallographers there will include David Bryce (University of Ottawa) giving a keynote lecture on *Structure and properties of materials by solid-state nuclear magnetic resonance (SSNMR) observables*, Patrick Mercier (National Research Council Canada) co-chairing the microsymposium *Minerals/gems in Industrial Applications*, Natalie Strynadka (University of British Columbia) co-chairing the microsymposium *Mechanisms of Bacterial Resistance*, and Louise Dawe (Wilfrid Laurier University) co-chairing the microsymposium *New Approaches in Crystallographic Teaching*. Louise and I are also invited speakers in different microsymposia. Importantly, Louise is chairing the Canadian delegation and would like to hear from all Canadians who are attending the Congress (***ldawe@wlu.ca***).

• Very importantly, our Canadian National Committee for Crystallography, chaired by Patrick Mercier, now has a brand new, exciting webpage, courtesy of Louise Dawe:

http://xtallography.ca/

The webpage is a work in progress, but we'd love to hear suggestions from visitors!

Well, I guess this kind of wraps it up for these latest updates from Canada. I'm sure that there is more stuff, but it did not reach my INBOX yet – I will try to make up for it next time. In the meantime, do contact me if you have events you want to highlight, or reports from past meetings organized or involving our Canadian colleagues (***tomislav.friscic@mcgill.ca***).

Thanks again to Michael James for running this column so brilliantly, and hopefully I did not mess it up too much already!

So long for now – cheers from rainy Montreal in March!

Tomislav Friščić

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CristAL – Crystallography News from Latin America

Graciela Díaz de Delgado

Several crystallography-related activities took place in Latin America in 2016. The IUCr-UNESCO Bruker OpenLab Uruguay 2, "Resolución de Estructuras Cristalinas por Difracción de Rayos X de Monocristal" (Montevideo, Uruguay, February 23–29, 2016), "Crystallography for Space Sciences" (April 17-29, 2016 at Instituto de Astrofísica, Óptica y Electrónica (INAOE) and Benemérita Universidad de Puebla, Puebla, México) and the Crystal Growing Competition in Argentina (which will be reported later) are among the highlights. A number of ACA members took part in these activities. In this issue, we report on two very important events during 2016 in our region.

The **IUCr-UNESCO Rigaku OpenLab** at Facultad de Ciencias Puras y Naturales of Universidad Mayor de San Andrés (UMSA) in La Paz, Bolivia, September 12-16, 2016. At the General Assembly of the Latin American Crystallographic Association (LACA) meeting, formally the first meeting of LACA, which took place in São Paulo, Brazil, in September 2015, Wilma and Julián Ticona Chambi, two very enthusiastic young scientists from UMSA, La Paz, advanced the idea of organizing a crystallography event in Bolivia. They mentioned there had never been an event in crystallography in their country and that they will be very happy to work in the organization of such an event. The LACA General Assembly supported the proposal, in the collaborative spirit that permeates the LACA organization and fulfilling its mission to promote and expand crystallography in our region. Given the success of the IUCr-UNESCO OpenLabs program, it was considered appropriate to organize an OpenLab at UMSA, taking advantage of the instrumentation available. They have a Rigaku powder diffractometer (an old equipment but still in excellent working condition) and a new PANalytical XPERT diffractometer. Rigaku Latin America co-sponsored the OpenLab along with the Institut de Recherche pour le Développement (IRD) and the International Centre for Diffraction Data (ICDD). Several companies including Benton, Save SRL, ESLC SRL and Oberon SRL provided additional support.

The OpenLab was attended by about 100 young scientists and students from La Paz, Potosí, and Cochabamba (Bolivia) and from Chile, El Salvador, México, Nicaragua and Perú.

Prof. Santiago García-Granda (U. Oviedo, Spain / IUCr Executive Committee), Dr. Michele Zema (U. Pavia, Italy / IUCr), Prof. Diego Lamas (U. San Martín, Argentina / Vice-President LACA), Prof. Miguel Delgado (U. de Los Andes, Venezuela / ICDD Regional Co-Chair) and Dr. Akihiko Iwata (Rigaku Latin America) constituted the International Advisory Committee. They worked closely with the Local Organizing Committee composed of Dra. María Eugenia García (Vice-Dean of Facultad de Ciencias Puras y Naturales), M.Sc. Luis Morales Escobar (Director of the Chemistry Program), Dra. Giovanna Almanza Vega, Ing. Victor Ismael Ramírez, Ing. Mario Blanco Cazas, Dr. Rigoberto Choque A., and Dr. Oswaldo Ramos (Chair). The wonderful and enthusiastic team of young scientists and students needs to be recognized for their hard work: Lics. Wilma Ticona Chambi and Naviana Leiva, Julián Ticona Chambi, Macguiver Pilco, Grace Villanueva, Leydi Salinas, Carolina Trigero, Neddy Alejo, Alison Parisaca and Samuel Lonza.

Participants of the IUCr-UNESCO OpenLab, La Paz, Bolivia, September 12-16, 2016.

To provide additional help to the students with little crystallography background, a two-day mini course was held on September 8-9, taught by Miguel Delgado, Diego Lamas and Graciela Díaz de Delgado. For the OpenLab, Prof. José Antonio Henao (UIS, Colombia) and Dr. Akilesh Tripathy (Rigaku Americas) also participated as instructors. Santiago García-Granda could not participate as an instructor due to many commitments as part of his inauguration as Rector of Universidad de Oviedo in Spain (Congratulations, Santiago!). Ing. Mario Blanco Cazas, Head of Instituto de Investigaciones Geológicas y del Medio Ambiente, and Ing. Ariana Zeballos were in charge of the practical sessions showing the students sample mounting and powder data collection. Inasmuch as Bolivia is a country with an extraordinary mineral diversity and a vibrant mining activity, the OpenLab was centered on powder diffraction. However several lectures dealt with single-crystal X-ray diffraction, and an event dedicated to structure determination and refinement from single-crystal data is being planned for 2017 to celebrate the 50th anniversary of the Chemistry Program at UMSA. Several formal and informal meetings were held during the week to start and strengthen collaborations between the institutions involved in this OpenLab.

On a personal note, all the instructors agree that this was one of the most memorable events in which we have ever participated. The warm reception with the attention provided by University officials and faculty members of the Facultad de Ciencias Puras y Naturales, the enthusiastic participation of all the attendees, and the help provided by the local students created a superb academic

environment. At the closing ceremony, M.Sc. Luis Morales Escobar (Director of Chemistry Studies), M.Sc. Franz Cuevas Quiroz (Dean of Facultad de Ciencias Puras y Naturales) and Dr. Waldo Albarracin Sánchez (Rector of UMSA) highlighted the importance of the OpenLab and opened the doors of the institution to continue and strengthen collaborations, particularly in crystallography. We felt so welcome, and we hope to return to Bolivia soon for another academic (or other!) activity.

Second Meeting of the Latin American Crystallographic Association (LACA), Mérida, Yucatán, México, October 22-27, 2016. A new meeting of LACA took place in Mérida, Yucatán, México, in October 2016. This was LACA's second meeting after the organization was accepted as a Regional Associate of the International Union of Crystallography by the General Assembly of the 23rd IUCr Congress celebrated in Montreal, Canada, in 2014. The II-LACA meeting was organized by Sociedad Mexicana de Cristalografía (SMCr) as part of the VI Mexican Synchrotron Light Users Meeting and the VIII National Congress of Crystallography of the Mexican Crystallographic Society.

The LACA organization was created at a meeting attended by representatives from Argentina, Brazil, México, Chile, Colombia, Cuba, Perú, Uruguay, and Venezuela, held during the IX annual meeting of the Argentinean Crystallographic Association (AACr) in 2013, at Universidad Nacional de Córdoba (UNC), in Córdoba, Argentina. The first formal meeting of LACA was held in São Paulo, Brazil, at the Institute of Physics of the Universidade de São Paulo, in September 2015, in conjunction with the XII meeting of the Brazilian Crystallographic Association (ABCr).

The scientific program of II-LACA included five plenary lectures, 20 invited lectures and close to 100 poster presentations by participants from Argentina, Bolivia, Brazil, Chile, Colombia, Costa Rica, México, Uruguay, Venezuela and from the U.S., Spain and Belgium. Professor Miguel José Yacamán from the Physics Department of University of Texas at San Antonio delivered the first plenary lecture.

Other invited speakers included Marvin Hackert (U. Texas at Austin, President of the IUCr and Past President of the ACA), Santiago García Granda (U. Oviedo, Spain, member of the Executive Committee of the IUCr), Amy Sarjeant (CCDC, USA, Current President of the ACA), Gabriela Aurelio (CAB-CNEA, Argentina), Aldo Craievich (U. São Paulo, Brazil), Miguel Delgado and Graciela Delgado (U. Los Andes, Venezuela), Márcia Fantini (U. São Paulo, Brazil), Diego Lamas (U. San Martín, Argentina), Stavros Nicolopoulos (Nanomegas, Belgium), Bruce Noll (Bruker, USA), Oscar Piro (U. La Plata, Argentina) and Iris Torriani (U. Campinas, Brazil). Several distinguished Mexican scientists were also invited speakers, among them Otilio Acevedo Sandoval (UAEH, Hidalgo), Gerardo Aguirre (IT-Tijuana), Sylvain Bernés (IF-BUAP, Puebla), Luis Fuentes Cobas (CIMAV, Chihuahua), Mayra Cuéllar Cruz (U. de Guanajuato, León), Gonzalo González (IIM-UNAM, México City), Erick A. Juárez Arellano (U. del Papaloapan, Oaxaca), Rufino Lozano Santacruz (IG-UNAM, México City), Abel Moreno Cárcamo (IQ, UNAM, México City), María Elena Montero Cabrera (CIMAV, Chihuahua), Teresa Pi Puig (IG-UNAM, México City) and Guadalupe de la Rosa Alvarez (U. de Guanajuato, León).

Participants of the Second Meeting of the Latin American Crystallographic Association (LACA), Mérida, Yucatán, México, October 22-27, 2016.

In keeping with the tradition and format of the SMCr events, six workshops and courses on different crystallographic topics took place October 22-23 at the Mérida Unit of CINVESTAV. They were: "Crystallography Databases: I. Introduction to CSD-Enterprise and II. The ICDD's Powder Diffraction File," a workshop led by Amy Sarjeant and Paul Sanschagrin (CCDC), Thomas Blanton (ICDD), Graciela Díaz de Delgado and Miguel Delgado (ULA); "Synchrotron Crystallography," coordinated by Abel Moreno Cárcamo (IQ, UNAM, México City); "Physical Properties of Crystals," taught by Jacques Soullard Saintrais (IF-UNAM, México City); a "Crystal Growth" course run by Héctor Riveros Rotge, (IF-UNAM, México City); and "Basic Crystallography" and "Roentgen-Crystallography" courses, for which the instructors were Alfredo Gómez Rodríguez (IF-UNAM, México City) and Rubén Alfredo Toscano (IQ-UNAM, México City), respectively. Graduate students and young scientists participated in these courses.

Three poster sessions were held in the exhibition hall along with an equipment and software display from manufacturers including Bruker (Bruker Mexicana, S.A.), Micra-Nanotecnología/Nanomegas, PANalytical (PANalytical México), Rigaku (Martek, S.A.), Stoe-Inel (Spectramex, S.A.), Thermo Scientific (Falcón/División Analítica), Alta Tecnología de Laboratorios, S.A., and the International Centre for Diffraction Data (ICDD). In each poster session, the two best posters presented by students were selected. A certificate and a piece of Mexican artisanry were presented to each winner at the farewell dinner. The IUCr and ICDD provided funds to cover the travel and accommodation expenses for about 20 students.

Professors Patricia Quintana Owen (CINVESTAV-Unidad Mérida, IPN) and Rudy Almicar Trejo Tzab (U. Autónoma de Yucatán) for the Local Committee, the National Committee headed by Professors José Reyes Gasga (IF-UNAM), Lauro Bucio Galindo (IF-UNAM), Jesús Ángel Arenas Alatorre (IF-UNAM) and Gustavo

Tavizón Alvarado (FQ-UNAM), and the support team headed by Ms. Gabriela García Rosales, Secretary of SMCr, did a superb job in the organization of all the aspects of these events.

The General Assembly of LACA met during the event to discuss the status and progress of the organization and to elect a new Executive Board. The members elected are Diego Lamas (President, Argentina), José Reyes-Gasga (Vice-President, México), Graciela Díaz de Delgado (Secretary, Venezuela), and Iris Torriani (Treasurer, Brazil). An Adjunct Secretary of the board (José Vega Baudrit, Costa Rica) was elected after consulting the national crystallographic organizations.

Since the 24th Congress and General Assembly of the IUCr will take place in Hyderabad, India, in 2017, the next meeting of LACA is scheduled for 2018 in Valparaíso, Chile, organized by Prof. Mauricio Fuentealba of Pontificia Universidad Católica de Valparaíso, Chile. The venue for the 2019 LACA is under consideration. Colombia is a strong candidate, with Prof. José Antonio Henao as the organizer.

Graciela Díaz de Delgado

YSIG Activities in New Orleans

Vicky Doan-Ngyen

With the ACA New Orleans conference just three months away at this writing, the members of YSIG are gearing up for an exciting meeting. YSIG has continued to work to build opportunities for young scientists of ACA to be involved in a multitude of roles. YSIG members are co-chairing scientific sessions throughout the conference. Marty Donakowski (YSIG chair 2016-2017) will be chairing a career development workshop, sponsored in part by Crystallographic Resources, Inc. This session will include an introduction to honing professional presentation skills to best highlight one's skills for a range of audiences. The availability of experts for one-on-one CV critiques provides for a valuable opportunity that can't be missed! YSIG looks forward to the three poster sessions, which will be a fantastic opportunity for young scientists to highlight their work. The poster sessions will also allow for recognition of young scientists with eight poster prizes. The day after the opening ceremony celebrating the lifetime achievement of Sir J. Fraser Stoddart, we turn to two sessions involving undergraduate research. In conjunction with the AIP Society of Physics Students (SPS), undergraduate research will be showcased at the *Undergraduate Research Symposium*. During this session, SPS Director Brad Conrad will lead a stimulating session on career pathways and resources for undergraduate attendees and their mentors. Joe Tanski and Rachel Powers will co-chair a session to "engage undergraduates with crystallographic research." This session is particularly timely, as this topic has also recently received attention in a September 2016 issue of *Chemical and Engineering News*. YSIG is excited to hear how advances in crystallographic tools and analysis software can make crystallography more accessible to young scientists at an earlier stage in their research career. Outside of the scientific and career development sessions, YSIG will be hosting the *Networking Mixer*, which is sponsored in part by Bruker. This will be a chance for all conference attendees to connect with fellow scientists in a fun, relaxed atmosphere. Registered students and postdoctoral fellows receive free admissions. We look forward to seeing everyone in New Orleans!

Vicky Doan-Nguyen

From the Editor's Desk

In addition to society news, and information on our exciting annual meeting to be held in New Orleans at the end of May, this issue of *ACA RefleXions* includes an inspiring *Living History* from Manuel Soriano-Garcia; an update on ACA's flagship journal *Structural Dynamics* published jointly with AIP Publishing; and remembrances of Dick Marsh, a beloved former President of the ACA who passed away in January; along with all of our regular *RefleXions* features.

We're extremely pleased to annouce that Kay Onan has joined the *RefleXions* staff and is handling our *News & Awards* feature. Welcome aboard, Kay!

Errata: The photo that appeared in the obituary for Ahmed Zewail on p. 7 of our fall 2016 issue is actually that of Phil Plait. We regret this unfortunate error. In our winter 2016 issue, under *News and Awards*, the articles on Alex Wlodawer and Charles F. Majkrzak on pp. 20-21 have been commingled resulting in incorrect placement of the figure displaying the *Postępy Biochemii* Wlodawer issue cover. Corrected versions of the Wlodawer and Majkrzak articles will appear in the online archive of *ACA RefleXions*. Also in our winter issue, in the header on p. 41, David Davies's birth year (1927) was incorrectly printed as 19XX. Finally, in the listing of 2016 contributors to ACA funds on p. 46 of our winter issue, we erroneously flagged as deceased two of our active members, *Pavel Karen* (donor to the Pauling Award fund) and *Pavol Juhas* (donor to the Outreach fund). Our apologies to Pavel and Pavol!

Tom Koetzle

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

JULY 22-26, 2016 | DENVER, CO

This Special Topic issue features papers presented during the 2016 meeting, which highlighted structural dynamics across the disciplines represented by the ACA. The collection focuses on the rapidly growing areas of structural dynamics of both chemical and biological systems, as well as solid materials. The papers showcase exciting recent work on both equilibrium and non-equilibrium dynamics involving time-scales from seconds to femtoseconds. The special issue also includes case studies and cutting-edge advances in methodology that are critical for advancing the science of molecules and materials in motion. ***All articles are gold open access and are freely available without a subscription.***

Guest Editors
Jason Benedict - Department of Chemistry, University 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
Structural Dynamics 4, 032201 (2017); http://doi.org/10.1063/1.4974172

Combining multi-mutant and modular thermodynamic cycles to measure energetic coupling networks in enzyme catalysis Charles W. Carter, Jr., Srinivas Niranj Chandrasekaran, Violetta Weinreb, Li Li, and Tishan Williams
Structural Dynamics 4, 032101 (2017); http://doi.org/10.1063/1.4974218

Augmenting the anisotropic network model with torsional potentials improves the performance of PATH Srinivas Niranj Chandrasekaran and Charles W. Carter, Jr. *Structural Dynamics 4, 032102 (2017); http://doi.org/10.1063/1.496142*

Insights into the mechansim of membrane pyrophosphatases by combining experiment and computer simulation Nita R. Shah, Craig Wilkinson, Steven P. D. Harborne, Ainoleena Turki, Kun-Mou Li, Yuh-Ju Sun, Sarah Harris, and Adrian Goldman

Partial-occupancy binders identified by the Pan-Dataset Density Analysis method offer new chemical opportunities and reveal cryptic binding sites Nicholas M. Pearce, Anthony R. Bradley, Tobias Krojet, Brian D. Marsden, Charlotte M. Deane, and Frank von Delft *Structural Dynamics 4, 032104 (2017); http://doi.org/10.1063/1.4974176*

Microfluidic addressing the challenges of serial time-resolved crystallography Shuo Sui, and Sarah L. Perry

The dramatic development of x-ray photocrystallography over the past six decades Philip Coppens
Structural Dynamics 4, 032102 (2017); http://doi.org/10.1063/1.4975301

Structural Dynamics
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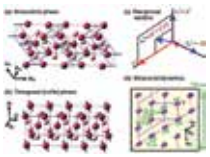
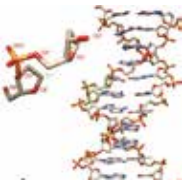
2015 IMPACT FACTOR: 3.667

Most read articles from 2016

The articles listed below are a selection of the most read articles published in 2016 from *Structural Dynamics*. As an open access journal, articles in *Structural Dynamics* are always freely available to read, download, and share without a subscription. The number of downloads are given in parentheses.

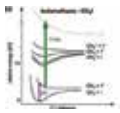


Ultrafast electron crystallography of the cooperative reaction path in vanadium dioxide Ding-Shyue Yang, Peter Baum, Ahmed H. Zewail *(2294)* ***SD* 3**, 034304 (2016); dx.doi.org/10.1063/1.4953370



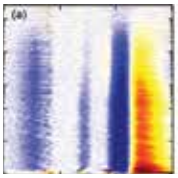
Ultrafast vibrational dynamics of the DNA backbone at different hydration levels mapped by two-dimensional infrared spectroscopy Biswajit Guchhait, Yingliang Liu, Torsten Siebert, Thomas Elsaesser *(2177)* ***SD* 3**, 043202 (2016); dx.doi.org/10.1063/1.4936567

Femtosecond X-ray solution scattering reveals that bond formation mechanism of a gold trimer complex is independent of excitation wavelength Kyung Hwan Kim, Jong Goo Kim, Key Young Oang, Tae Wu Kim, *et al. (1135)* ***SD* 3**, 043209 (2016); dx.doi.org/10.1063/1.4948516

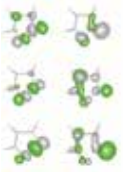


Charge transfer in dissociating iodomethane and fluoromethane molecules ionized by intense femtosecond X-ray pulses Rebecca Boll, Benjamin Erk, Ryan Coffee, Sebastian Trippel, *et al.(1084)* ***SD* 3**, 043207 (2016); dx.doi.org/10.1063/1.4944344

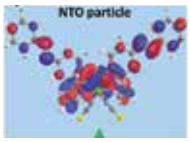
Harmonium: A pulse preserving source of monochromatic extreme ultraviolet (30-110 eV) radiation for ultrafast photoelectron spectroscopy of liquids J. Ojeda, C. A. Arrell, J. Grilj, F. Frassetto, *et al. (916)* ***SD* 3**, 023602 (2016); dx.doi.org/10.1063/1.4933008



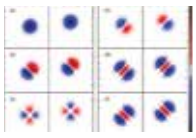
Excited-state intramolecular proton transfer of 2-acetylindan-1,3-dione studied by ultrafast absorption and fluorescence spectroscopy Pramod Kumar Verma, Andreas Steinbacher, Alexander Schmiedel, Patrick Nuernberger, *et al. (902)* ***SD* 3**, 023606 (2016); dx.doi.org/10.106D/1.4937363



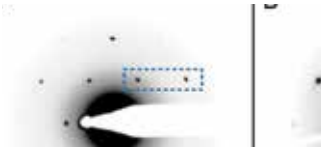
Monitoring conical intersections in the ring opening of furan by attosecond stimulated X-ray Raman spectroscopy Weijie Hua, Sven Oesterling, Jason D. Biggs, Yu Zhang, *et al. (796)* ***SD* 3**, 023601 (2016); dx.doi.org/10.1063/1.4933007



Activation of coherent lattice phonon following ultrafast molecular spin-state photo-switching: A molecule-to-lattice energy transfer A. Marino, M. Cammarata, S. F. Matar, J.-F. Létard, *et al. (747)* ***SD* 3**, 023605 (2016); dx.doi.org/10.1063/1.4936290



Exciton dynamics in perturbed vibronic molecular aggregates C. Brüning, J. Wehner, J. Hausner, M. Wenzel, *et al. (742)* **SD 3**, 043201 (2016); dx.doi.org/10.1063/1.4936127



Ultrafast electron diffraction optimized for studying structural dynamics in thin films and monolayers D. S. Badali, R. Y. N. Gengler, R. J. D. Miller *(740)* **SD 3**, 034302 (2016); dx.doi.org/10.1063/1.4949538

Meeting logo designed by Kandis Elliott

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Friday, May 26 – Tuesday, May 30, 2017

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We are pleased to present the 67th meeting of the ACA in Fabulous NOLA!

2017 ACA Awards

Christine Dunham
Etter Early Career Award

Zbigniew Dauter
Patterson Award

Helen Berman
Rognlie Award

James O'Brien
Wood Science Writing Award

for meeting sponsor information, abstracts, on-line registration, and details including room sharing feature see:
http://www.amercrystalassn.org/2017-meeting-homepage

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Special Opening Plenary Lecture

Sir James Fraser Stoddart
2016 Nobel Laureate in Chemistry (photo by Jim Prisching)

Educational and YSIG Events

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

Sessions

Transactions Symposium – Cryo Electron Microscopy
NMR Crystallography
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Advanced Surface and Interface Scattering and Applications
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Christine Dunham, Asst. Professor of Biochemistry at the Emory University School of Medicine, is the **2017 Etter Early Career Award** winner. Christine earned her B.A. in Biochemistry from Barnard College, Columbia University, and her Ph.D. in the laboratory of William Scott at the University of California at Santa Cruz. She was an American Cancer Society Postdoctoral fellow in Venki Ramakrishnan's laboratory at the MRC Laboratory of Molecular Biology in Cambridge, England where she focused on solving X-ray crystal structures of functional states of the bacterial ribosome. At Emory, Christine was named a Pew Biomedical Scholar in 2011, received an NSF Faculty Early Career Development (CAREER) award from 2010-2015, and was named a 2016 Burroughs Wellcome Fund Investigator in the Pathogenesis of Infectious Diseases.

Christine in her lab at Emory University

The Dunham laboratory continues to study the regulation of protein synthesis using structural biology and biochemical approaches. One particular area of focus is in the study of bacterial toxin-antitoxin complexes that inhibit protein synthesis during stress (Cover figure). During nutrient-rich growth, toxin-antitoxin pairs function as transcriptional repressors to limit their own expression. Stress results in the proteolysis of antitoxins while the released toxin inhibits protein synthesis to halt growth. Research in the Dunham laboratory has focused on understanding the structural basis of inhibition of toxin by their cognate antitoxins (top) and the molecular basis for toxin specificity for mRNAs bound to the bacterial 70S ribosome (bottom).

The **Margaret C. Etter Early Career Award** recognizes outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career. The award was established to honor the memory of Professor Margaret C. Etter (1943-1992), who was a major contributor to the field of organic solid-state chemistry.

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Nominations for 2018

ACA Awards: Nominations for the 2018 **B. Warren, M. J. Buerger,** and **Margaret C. Etter Early Career** awards were due by April 1, 2017. **Nominations** for **ACA Fellows** were also due by April 1.

ACA Offices and Committees: In fall 2017 we will elect an ACA Vice President, Council Secretary, and one person to each of the ACA Standing Committees (Continuing Education, Communications, and Data, Standards & Computing). To suggest a candidate for one of the above positions, please contact a member of the Nominating Committee: **Louise Dawe: ldawe@wlu.ca**, **Chris Cahill: cahill@gwu.edu**, and **David Rose: drose@uwaterloo.ca**. Full details describing the criteria for all ACA awards and offices can be found on the ACA website.

2017 Dues are Due: Please renew promptly and remember to support your favorite ACA Award Funds.

NOTE: It is now possible to renew online.

ACA website: www.AmerCrystalAssn.org

Send all award nominations to: marcia@hwi.buffalo.edu

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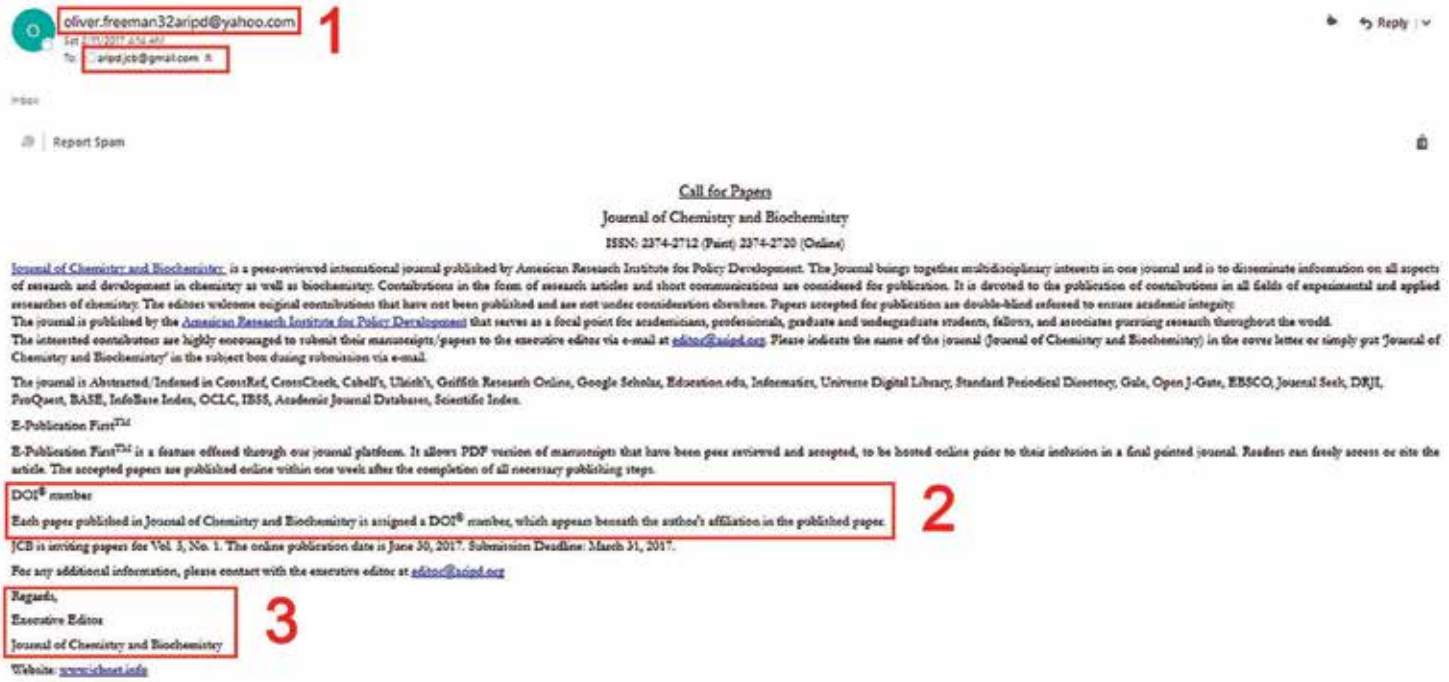
Anastasiya Vinokur

Net RefleXions

As a young scientist, I often hear a mantra in academia: "publish or perish." The increase in this pressure to reach an arbitrary number of publications per year (presumably to be deemed sufficiently successful) appears to have accelerated with the rising popularity and availability of open access journals. Yet not all open access journals are created equal. One must be careful not to fall prey to a subset of less than trustworthy publishers that cut corners and exploit scientists by charging fees without providing the necessary editorial and publishing services that one has come to expect of legitimate publishers, such as peer review, digital preservation, and proper indexation.

One popular list of "predatory" publishers was compiled by Jeffrey Beall, an Associate Professor at University of Colorado Denver, on his blog "Scholarly Open Access." In January 2017 this list disappeared from the blog, in the process generating a flurry of conspiracy theories surrounding the sudden mysterious vanishing. Luckily, nothing really disappears from the Internet, and the list along with (most importantly) the criteria against which the publishers were judged has been safely archived. I found them, after a little digging, on the site web.archive.org (***https://web.archive.org/web/20170112125427/https://scholarlyoa.com/publishers/*** and ***https://web.archive.org/web/20170105195017/https://scholarlyoa.files.wordpress.com/2015/01/criteria-2015.pdf***).

Since the list is no longer publicly updated, I decided to be my own detective and apply the published criteria to a call for papers that I received recently for *Journal of Chemistry and Biochemistry* published by American Research Institute for Policy Development. As you can see in the screenshot below, the request roughly follows a general format one might come to expect of scientific journals. But on closer inspection, a few problems arise. One: the request was sent from yahoo.com and gmail.com addresses. Two: the executive editor is lacking a name. Three: the call boasts that published papers will receive a DOI number (a standard practice for scholarly publications). According to Beall's criteria, all of these are red flags.



I decided to do a little bit more digging and went to the publisher's website. The criteria suggest taking a look at other journals published by the same publisher; the more diverse and unrelated the topics, the more suspect the publisher becomes. How broad is the selection in the case of the American Research Institute for Policy Development? From the complete list, I gathered that one could publish not only in a *Review of History and Political Science*, but also in the *International Journal of Art and Art History* as well as *Strategic Management Quarterly*, in addition to a smattering of physical science and technology publications ranging from a journal covering mathematics and statistics to one covering nursing. The websites for most of the journals have roughly the same formatting, which the criteria list warns as being another red flag.

On the positive side, the website for *Journal of Chemistry and Biochemistry* does list an editorial board consisting of five international researchers. But, when I googled one of them, Prof. Dr. Thresa O. Corcoro, only other journal websites belonging to American Research Institute for Policy Development came up. No research page. No staff directory.

My conclusion: too many red flags for me to comfortably spend my money and submit a manuscript to *Journal of Chemistry*

and Biochemistry. Checking my conclusion against the compiled list, American Research Institute for Policy Development was flagged as one of the problematic publishers. Following the criteria list worked!

So, next time, dear reader, you consider publishing in an unfamiliar journal, take the time to check out the publisher using the archived criteria. It could save you from a scam.

Anastasiya Vinokur

News & Awards

2017 Ludo Frevel Scholarships Announced

The ICDD **Ludo Frevel Scholarship Awards** are given annually to support the education and research programs of promising graduate students in crystallography-related fields. These competitive awards are given to cultivate aspiring crystallographers and are accompanied by a check for $2,500. This year 10 recipients were chosen from 43 commendable applications. One of the scholarship winners is an ACA member, **Ivana Brekalo** from Georgetown University. Ivana's award was given for *Solid State Synthesis and Templation of Metal Organic Frameworks*.

ICDD Announces New Executive Director, Tom Blanton

Tom Blanton

The International Centre for Diffraction Data has named **Tom Blanton** as its new Executive Director. Tom has been a long-time ICDD member, an ICDD Distinguished Fellow, and past Director and Chairman of the ICDD Board of Directors. He has been on staff at ICDD since 2013 when he became Publication Manager. After a year he was promoted to Principal Scientist and Database Manager. Tom spent over 31 years at Eastman Kodak in Rochester, New York, where he served in a dual role as Analytical Scientist and Materials Characterization Scientist, rising to the position of Senior Principal Scientist. He assumed a leadership role where he supervised an X-ray Spectroscopy laboratory and invented, developed and commercialized materials, resulting in his being the co-inventor of dozens of patents.

Symposium Honors Donald Caspar for his Work in Structural Biology

Donald Casper

Florida State University at Tallahassee hosted a symposium January 7-8, 2017, to honor Professor Emeritus of Biological Science **Donald Caspar** on the occasion of his 90th birthday for his contributions to the world of structural biology, a term he coined. Caspar earned his Ph.D. in biophysics from Yale in 1955. His thesis was entitled *The Radial Structure of Tobacco Mosaic Virus*. He worked in Max Delbruck's laboratory at California Institute of Technology and, while at Caltech, met James D. Watson, a man with whom he had close professional ties throughout his career. Having been awarded a fellowship at King's College London under Rosalind Franklin, he moved to England. She and he worked together from 1955-1956 at Birkbeck College London on the structure of tobacco mosaic virus. This work culminated in their publishing complementary papers in *Nature* demonstrating new aspects of the virus's structure. They maintained a close friendship through the rest of her life. Another of his collaborators at Birkbeck College was Aaron Klug, with whom he developed the concept of quasi-equivalence to account for the arrangement of proteins on the surface of icosahedral virus particles.

Donald Caspar is a Fellow of the American Academy of Arts & Sciences and an elected member of the Biophysics and Computational Biology section of the National Academy of Sciences. Fifteen members of the National Academy of Sciences spoke at his symposium, and it was said that this symposium brought more National Academy members to Tallahassee than had ever been gathered there before.

2017 CCDC Chemical Crystallography Prize for Younger Scientists to Lauren Hatcher

Lauren Hatcher

The CCDC Chemical Crystallography Prize for Younger Scientists is a prize that aims to encourage the next generation of structural scientists. This year's prize goes to **Lauren Hatcher**, a Research Associate at the University of Bath, U.K., where she is currently working in the Metastable Materials Group. The Metastable Materials Group is a collaborative project across the Department of Chemistry at Bath, aiming to develop new classes of functional materials in which long-lived metastable states are the key to introducing useful switchable functionalities that are desirable in a variety of real-world device media. Lauren's education has taken place at Bath, where her Ph.D. was focused on the study of photo-active linkage isomer systems using non-ambient crystallographic techniques. Her main research interests lie in the field of photocrystallography, which involves the study of photochemical processes in the solid state using X-ray methods.

ACA Members Named as 2016 Society Fellows

Two ACA members were among the 57 chemists elected to the 2016 class of **ACS Fellows**. **Gregory Ferrence**, Professor of Chemistry at Illinois State University, was honored for having served the ACS community both locally and by his leadership on the national Committee on Ethics. He was honored also because of his contribution to structural science. The ACS honored him as,

Gregory Ferrence, bottom row center, surrounded by students.

"a world expert in chemical education using crystallographic data." In 2009 Ferrence was named Carnegie Foundation for the Advancement of Teaching and CASE Illinois Professor of the Year.

Hong-Cai "Joe" Zhou

Hong-Cai "Joe" Zhou, Robert A. Welch Chair in Chemistry at Texas A&M University, was named an **ACS Fellow** recognized for his novel synthetic routes to prepare metal-organic frameworks and porous polymer networks that demonstrate unique catalytic activities or exhibit desirable properties for clean-energy-related applications. He was honored for his editorial service to the ACS and his distinguished service as an "ACS Ambassador" giving keynotes around the world.

Zhou was also named a 2016 **AAAS Fellow**, an honor bestowed on scientists, "whose efforts on behalf of the advancement of science or its applications in service to society have distinguished them."

Bryan Chakoumakos

Bryan Chakoumakos, Senior Research Scientist and leader of the Structure of Matter Group in the Quantum Condensed Matter Division at the Department of Energy's Oak Ridge National Laboratory, was named a 2016 **AAAS Fellow**. He is also the scientific director of the National School on Neutron and X-Ray Scattering, which is an educational program for graduate student researchers. In 2016, Chakoumakos was also elected as a Fellow of the ACA.

Howard Flack (1943 – 2017)

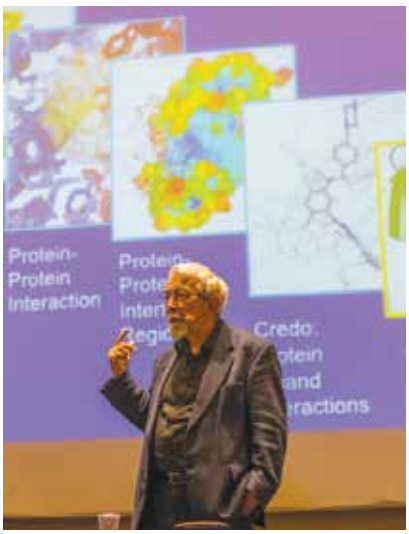
It is with sadness that we note the death of **Howard Flack** on February 2, 2017. As Professor in the Department of Inorganic, Analytical and Applied Chemistry at the University of Geneva, Switzerland, Flack was well-known in the crystallographic community. He was deeply involved with the International Union of Crystallography serving on a broad variety of its committees, from the Commission on Computing to the Committee on Electronic Publishing to the Commission on Mathematical and Theoretical Crystallography. A full obituary is being prepared for *IUCr News*.

Kay Onan

Tom Blundell Awarded the 2017 Ewald Prize

Tom Blundell has been awarded the **2017 Ewald Prize**, recognizing his very broad contributions to the field of crystallography. Tom will receive the award at the IUCr triennial congress in Hyderabad, India, on August 21 and will give a lecture following the award presentation.

Professor Sir Tom Blundell has been one of the worldwide leaders in crystallographic innovation, especially at the interface



Tom Blundell, Director of the Erice International School of Crystallography, describing advances in his laboratory's program in drug discovery at the 2014 School on Crystallography in Structure-Based Drug Design. Photo by Jeff Blaney.

with life sciences, starting with his work on determining the structure of insulin with Dorothy Hodgkin. Tom has determined an exceptionally broad array of medically critical human-protein structures, has championed methods enabling drug design and discovery through structural optimization, crystallographic fragment screening, and computational modeling, and has been a leader in advanced crystallography education on the international scale.

Tom began his brilliant career in macromolecular crystallography as a postdoctoral associate with the 1964 Nobel prize winner Professor Dorothy Crowfoot Hodgkin at Oxford University, and was a member of the team that obtained the structure solution of insulin, the first three-dimensional structure of a protein hormone. Tom has established the molecular structures and mechanisms of a remarkable array of medically significant human proteins, including polypeptide hormones (insulin, glucagon, pancreatic polypeptide and oxytocin), growth factors (NGF, FGF, HGF/SF), DNA repair factors (RAD51/BRCA, DNA-PKcs, PAXX), lens crystallins proteins, and aspartic proteases (renins, HIV protease), among many others, often in complex with receptors or small-molecule ligands. His group's highly creative work on building advanced computational tools for structural bioinformatics (such as Composer, Modeller, Fugue, SDM and mCSM) and chemoinformatics (CREDO, CHOPIN) has enabled structure-informed design of small-molecule drugs and engineered macromolecules. He has pioneered the use of crystallography in fragment-based drug discovery, both in academia and through the co-founding of Astex, moving many candidate drugs into clinical trials.

Tom has been heavily involved in education, first teaching in Brasenose and Linacre Colleges in Oxford University until 1973, before moving to Sussex briefly to work in Biological Sciences, and then between 1976 and 1996 as Bernal Professor of Crystallography at Birkbeck where he developed a major multidisciplinary crystallographic team researching on a range of themes, from materials to macromolecules, with extensive teaching programs. In 1996 Tom moved to the Sir William Dunn Chair of Biochemistry in Cambridge, where crystallography remains a central experimental theme in understanding complex multicomponent cell regulatory systems. Tom has been the Director of the International School of Crystallography at Erice since 1980 when Dorothy Hodgkin stepped down as the director

L-R: Tom Blundell, Samar Hasnain and Louise Johnson at the 2011 Dedication of the Barkla X-ray Laboratory of Biophysics at the University of Liverpool.

after a four years' stint. Tom's commitment to crystallographic education is demonstrated by his uninterrupted engagement as the Erice School director for nearly 40 years, contributing to the education of thousands of crystallographers through the yearly courses on advanced topics in crystallography. *Protein Crystallography*, a book that he co-authored in 1976 with the late Professor Dame Louise Johnson, remains the best treatment of the subject on many fronts.

Tom has also managed to find time to be an elected Labour Councillor in charge of city planning in Oxford, an advisor to Prime Minister Margaret Thatcher, a Chief Executive of UK research councils, including founding CEO and Chair of the Biotechnology and Biological Sciences Research Council, Chairman for six years of the Royal Commission on the Environment, and President of UK Science Council. Tom's scientific achievements and service to science have been recognized through many awards and prizes including Fellowship of the Royal Society (1984), FEBS Krebs Medal (1987), Royal Society's Bernal Medal (1998) and Knighthood in 1997. His international stature is evidenced by the many high honors he has received including honorary doctorates from 16 universities. Tom's son Ricky, a computer scientist, and his wife Raffy have produced two wonderful grandchildren, Giorgio and Leandro. Tom and his wife and long-time co-worker Lynn, originally from Zimbabwe, have two beautiful daughters, Kelesi, now a lawyer, and Lisa, a medical doctor, who share their parents' passion for world travel.

Eddy Arnold and Samar Hasnain

Remembering Dick Marsh

Richard Marsh, senior research associate in chemistry, *emeritus*, at Caltech, passed away on January 3, 2017, at the age of 94. Doug Rees, the Roscoe Gilkey Dickinson Professor of Chemistry and faculty director of the Molecular Observatory for Macromolecular Crystallography at Caltech, said, "Dick was a legendary one-of-a-kind crystallographer who was recognized for his mastery of the field and his rigorous standards. He trained generations of students and postdocs and was widely respected as representing the heart and soul of crystallography." Following are the remembrances of several of our community who knew Dick well.

Harry Gray: I met Dick Marsh briefly when I first visited Caltech in 1964. But I got to know him well on a second visit in the spring of 1965. We both had deep interests in the structures of inorganic compounds, and we hit it off right away. I well recall the discussions we had on trigonal prismatic dithiolene complexes that were being investigated in my lab at Columbia. When I moved from Columbia to Caltech in 1966, I began collaborations with Dick that lasted until he left us late last year.

Dick and I did science and played tennis together for many years. The tennis game at his home on Saturday mornings was a highlight of my week during the 80s and 90s. He was a natural athlete, and he gave me fits when I played against him. I always tried to get him on my side, so I would not have to face his sneaky shots. But even when he tortured me with drop shots and wild top spin lobs, it was fun!

Doing science with Dick was special. His standards were off the charts. In doing structures of my inorganic compounds, I did not want to be 'Marshed.' So, on very challenging structures, I worked closely with him. One of our first joint papers, published in 1969, reported the structure of the first binuclear complex containing molecular nitrogen. That work caused quite a stir in the inorganic chemistry community. Other papers with me and members of my group were on the structures of linear chain platinum compounds. These structures were very challenging, and we could not have solved them without his help.

Dick and I talked almost every day, most especially when the X-ray gang had coffee on the 4th floor of the Beckman Institute, just down the hall from my office. More often than not, I would drop in the coffee room and ask Dick about a structure that I was confused about. Dick would always set me straight!

It is not the same on the 4th floor now. Dick was a great scientist and a treasured friend. I miss him every day.

Jenny Glusker: I am saddened by the news that Dick Marsh is no longer with us. He was in the lab at Caltech when I came in 1955 as a postdoctoral student to work with Bob Corey. At that time Caltech was somewhat like a monastery, and I had come from England having just obtained a doctoral degree there. How lucky I was to have Dick there in the lab! He was so generous with his time, helping anyone who needed assistance with machine usage, structure determination and publication. What he did was stress what a wonderful science subject – X-ray crystallography – we had chosen for study, and how important the results of our work were. But he also emphasized firmly that such crystallographic investigations had to be done correctly, with no short cuts and with close attention to any problems that we might detect on the way. Dick and I actually worked together on the crystal structure of a tripeptide, glycylphenylalanylglycine. Since then, through the years, we have often communicated and he helped me when I first acquired a laboratory to run and whenever I received interesting papers that needed strict review so that they could not be refused as 'Marshed.' I shall miss his exuberant laugh and the joy he showed whenever a difficult problem was correctly solved by any member of the crystallographic community.

David Duchamp: Dick Marsh was a great thesis advisor, mentor and friend to me. The four years, 1961 through 1965, that I spent as Dick's graduate student were among the most productive and

Dick Marsh at work in the Caltech X-ray lab in the 1970s.

the most enjoyable of my life. I arrived at Caltech in the fall of 1961 with a bachelor's degree in chemistry and mathematics, having spent the summer working with John Burns at Oak Ridge National Laboratory. While at Oak Ridge, I learned about crystallography, and I met some of the top crystallographers at the time, including Bill Busing, Henri Levy, and George Brown, among others. When they found out I was going to Caltech, they strongly recommended that I try to work for Dick Marsh. I followed their advice, and Dick took me on as a new graduate student. This was one of the best decisions I ever made.

One of Dick's policies was that before a student could use a computer program to calculate Fourier maps, the student had to calculate a Fourier section by hand using Beevers-Lipson strips – this was to ensure that the student understood how Fourier calculations worked. I understood how the strips worked, but I couldn't see myself summing up all those numbers and getting the right answer – boring! So I had a discussion with Dick, and we decided that if I would write a computer program to calculate a general plane Fourier section (any orientation and any size), it would serve the same purpose and would provide a program that was useful to the group. I devised an efficient algorithm and wrote the program in machine language for the Burroughs 220 computer. Thereby I began a very worthwhile collaboration with Dick on crystallographic computer programs.

Sloppy crystallographic work was not well tolerated by Dick. He was an editor of *Acta Crystallographica*, and he meticulously checked all papers that came to his desk. Early on, I learned from other members of Dick's group, Ned Webb, B. D. Sharma, and Noel Jones, to watch for Dick's reaction when he found mistakes in crystallographic work. One member of the group would watch Dick's mailbox when a new issue of *Acta Crystallographica* was due. When Dick brought his mail to his office, we had been alerted and speculated on how long it would take Dick to find something wrong. When he did, we all knew instantly from the loud reaction coming from his office. Dick's insistence on doing the best job possible with the data available rubbed off on me and on other students of his.

One day when I was in search of a suitable crystal structure to work on, Harden McConnell came to Dick asking if someone could determine the structure of trimesic acid, benzene-1,3,5-tricarboxylic acid. McConnell's group was interested in studying the excitons of crystalline trimesic acid. Dick turned the task over to me. I quickly determined that there were six independent trimesic acid molecules in the asymmetric unit of the crystal structure. This knowledge resulted in McConnell's group abandoning their project. However, Dick and I both thought that trimesic acid must have a very interesting crystal structure. We both understood the magnitude of the task of determining its crystal structure – 90 independent carbon and oxygen atoms in the asymmetric unit, no heavy atoms, and about 12,000 independent reflections. (This was before automatic diffractometers and before direct methods.) I was eager to try to determine this complex structure, and Dick encouraged me to give it a try. Always concerned for his students, Dick promised that if it didn't work out, he would find me a different structure to work on for my thesis.

Dick did not micromanage his students, but he kept up with what was going on and didn't hesitate to offer advice when he felt it was needed. One day I remember he found me studying precession photographs trying to understand what the diffraction pattern of trimesic acid would look like in various orientations. Dick told me about a large optical diffraction machine in the basement that Holmes Sturdivant had constructed. He suggested that I might use this instrument to better understand the diffraction pattern of trimesic acid. As with other advice he offered, Dick's suggestion was right on the money. Sturdivant was happy for me to use his optical diffractometer. The insight I gained from optical diffraction helped with the solution of the trimesic acid structure.

When Dick learned that Caltech was going to get an IBM 7094 computer to replace the aging Burroughs machine that we were then using, he got a group of us together to work on crystallographic software for the new computer. Dick thought it was wasteful for a crystallographer to have to run separate programs for each type of calculation – the way crystallographic computing was done at that time. He challenged us to come up with an integrated system where the user could move effortlessly from one calculation to the next. We divided up the work, with each of us working in areas that would benefit his current crystallographic project. Ned Webb worked on high-symmetry least-squares software, Carlo Gramaccioli (then a new postdoc in the group) worked on low-symmetry least-squares software, and I had the data reduction component, Fourier calculation software, and overall responsibility for integrating the system. George Reeke and Ivar Ambats also contributed software to the project. Early on we named our new system CRYRM, in light of the fact that when we hit a problem, we cried for help from Richard Marsh. Under Dick's guidance we produced the first truly integrated crystallographic computing system.

After I completed my Ph.D. at Caltech, and moved on to work in the pharmaceutical industry at Upjohn, Dick and I continued our collaboration on crystallographic software. I rewrote the CRYRM system in Fortran in collaboration with Dick and his people at Caltech. (Of necessity to handle large problems, like trimesic acid, CRYRM was written in assembler language because the IBM 7094 had limited random access memory.) We changed the name of the Fortran version to CRYM to differentiate it from its predecessor. Dick's group implemented CRYM on VAX machines, and I made it work on the IBM 360 – Upjohn's

research computer.

In summary, Dick Marsh had a tremendous positive influence on me. While I was a graduate student, and since, we had many discussions that were both educational and inspirational. He molded me into the scientist I became, and in the process I adopted many of Dick's traits, such as, intolerance for sloppy scientific work, and not to be afraid to tackle tough problems.

Ton Spek: Early papers by Dick Marsh made me aware of the issue of missed higher symmetry in published papers and of the danger of 'being Marshed.' Over the years, Dick reported on over 1,000 such cases. Not everyone was amused when appearing in his "Some More Space Group Corrections" papers. Several other authors joined in the effort to correct the literature.

My response to the problem was the development of software, based on an excellent algorithm published by Yvon LePage, to routinely and automatically address the missed symmetry issue. With that software, I was able to find and correct one of my early structures before Dick might have found out.

Dick did most of this corrective work by hand and by visual inspection of ORTEP illustrations. One of his papers made me send him an automatically-prepared list of structures deposited in the Cambridge Crystallographic Database that might be candidates for a space group correction. He immediately started to work on that list. The result was a joint paper with more corrections along with the message that there is software available to detect and address the problem before publication. Interestingly, Dick found out that one of the structures he had corrected previously needed again an update to an even higher symmetry. According to 'hear-say,' Dick enjoyed very much to have been 'Marshed' as well.

The permanent impact of his work in this context is that structure analysts and referees are now well aware of the missed symmetry issue, and if not, warned with an ALERT as part of the now standard IUCr checkCIF procedures. Dick also advocated the archiving of the observed reflection data along with the published structure report. The latter is now also becoming the standard. Suggestions for space group corrections without access to the primary reflection data might be invalid. It was an interesting experience to learn from and work together on one paper with Dick.

Howard Einspahr: I was a postdoc with Dick Marsh from September 1970 to August 1972. It was a wonderful experience in every respect. He was an excellent mentor, tolerating my naive efforts at drafting papers, guiding me to improvements in incomplete projects, and importantly, finding me new and exciting projects to develop. He was an open-access advisor, that is, his door was always open … literally, when he was in, his door was open. In discussing my work, it was always a two-way conversation that he guided carefully by asking questions until I understood. I have said before in another context that as a mentor, it was not just what he said, it was often what he didn't say.

Dick's lab was continuously filled with interesting grad students, undergrads, postdocs, sabbatical scientists, and visitors, including prior students. I shared lab space with Jim 'Lou' Sherfinski and Tom Kistenmacher, and Frank Fronczek was a contemporary and friend, but there were upwards of 25 people who came through the lab and stayed for varying periods of time. Lou, Tom, Frank and I are still in frequent contact.

I said Dick's door was always open. You knew this because you would hear him frequently. His powers of concentration were unrivaled, but Dick periodically broke that concentration to clear his mind and start afresh. Two times of the day were particularly important for breaks, mid-morning coffee and lunch. Coffee involved a two-block walk to the cafeteria where we would meet crystallographers of all stripes, notably those of the Schaefer, Samson, and Dickerson labs, but actually anyone who wanted to join us that day. Time for coffee for us would usually be signaled by a hearty, "Who, she cried," from Dick's office that echoed throughout the basement (or 'bowels') of Noyes. At that signal, we would pause, stop, bookmark whatever we were doing, to meet in the hall and walk over. Dick also had a fine sense of when coffee break was over, and after about 30 minutes, when there was an appropriate break, he would strike the table with his forefingers in a tattoo, a sort of shave-and-a-haircut thing, or a ba-doom-siss, and folks began to drift back to their labs.

Lunches were a different matter altogether. These were off-campus in one or another nearby restaurant, were typically in Dick's yellow convertible Mustang, and the destination was chosen always by consensus. However, when the destination was likely to be Mijare's, the group expanded to include a wider circle, and guacamole would be on the table waiting for us. I will never forget the Mijare's enchilada ranchera, which became my only order. Mijare's is still in business, now in two convenient locations, by the way.

After I left, I visited the lab a couple of times, always rewarding, and saw Dick at many ACA meetings. I realize now I always thought of Dick Marsh as immortal. I wish I'd had more time with him.

Frank Fronczek: When I was beginning to learn crystallography at Caltech in about 1970, an older graduate student referred to Dick Marsh as, "*The Guardian of Goodness and Purity in Crystallography*." How prophetic those words turned out to be, for Dick had a profound influence on the quality of crystallography practiced by everyone who ever spent time at Caltech, but also on an untold number of scientists worldwide. Some years later, Dick and I were touring a botanical garden together at an ACA meeting, and we noted that a new word had been coined; he had been *Verbed*. He recognized that some who used the term 'Marshed' did so in a pejorative sense, but those who care about *Goodness and Purity in Crystallography* have always used it with great admiration. For his intent was only to help others get it right, and he always afforded authors kindness and respect when he pointed out their errors. Once as a student, I proudly announced that I had solved a structure with $Z'=2$ in Cc. Dick gently suggested that I go look for an inversion center, and of course it was there. Later, when I did publish a P-1 structure in $P1$ (oops), he contacted me to allow me to publish a correction myself. This was always his approach, always with kindness, never with malice.

Caltech was a wonderful place to be in the early 1970s. Not only were we younger folks in the presence of such legendary crystallographers as J. Holmes Sturdivant, Edward W. Hughes,

Jürg Waser and others, but Linus Pauling also made an occasional visit, and best of all, my lab was next door to Dick Marsh's office in the 'bowels of Noyes' (the basement). Dick had a quick wit and a wonderful sense of humor, which led to his unmistakable booming laughter echoing down the hall several times a day. Once, I was trying to solve the structure of a cobalt peroxo dimer with $Z'>1$ and quite a few potassium ions. The Patterson map was fairly complex for a student of my limited experience. I had traced the contours onto plexiglass sheets with a grease pencil and stacked them up, the 3D graphics of the day. I spent probably a week staring at the map and occasionally running off to try out what I thought might be a solution, but to no avail. One day, Dick walked in and looked over my shoulder at my graphics masterpiece. I heard, "Hmmm." Then a minute or two later, "Oh…" then "HAHAHAHAHA," that laugh, as he walked out of the room. *He had it!* And in just a couple of minutes. But he wasn't going to deprive me of the joy of figuring it out for myself. A day or so later, he suggested that I try direct methods. There were a few programs available on punch cards for doing the rote operations like assigning *E* values and finding *Sigma2* relations, but much of it had to be done manually. I learned a lot, solved the structure, and still take pride in the result. After the fact, he and I talked about why the Patterson looked so confusing, given what the structure turned out to be. This story speaks of both his brilliance and his teaching methods. Thank you Dick Marsh.

An important part of the workday then was Coffeetime. Dick would announce it to everyone in earshot, we would take a short walk across campus, and then spend some time drinking coffee, talking about people's research problems, bug fixes in the CRYM software, and other things, even working puzzles. It will come as no surprise to anyone, given his life's work, that Dick loved puzzles, and he was very good at solving them. For awhile, he used JUMBLE puzzles from the newspaper as a way to help a non-native English speaking visiting scientist improve her English. I still cannot work a JUMBLE (or write one) without thinking of Dick Marsh.

Dick was legendary for having memorized tables of sines and cosines. In the days before computers, when a slide rule and a pencil were the only available means of doing laborious crystallographic computations, he found it easier to memorize the trig functions than to spend time looking them up. A few years ago at an ACA meeting (Cincinnati?) a session was organized to allow some seasoned crystallographers to speak on how things were done back in the pencil and slide rule days. After Dick's talk, the first question from the audience was, "Dick, what's the cosine of 26.5 degrees?" asked as I recall by Wally Cordes. His answer: "Let's see now, 0.89 4, uh…, 8?, no, nine!" Correct. Amazing.

We have lost one of our giants, *The Guardian*. Despite his advanced age, Dick Marsh's vitality and keen mind made it seem that he would be with us forever. And in a sense he will, in the memories of those who had the great honor of knowing him, and in the quality of the structural results we produce because of his steadying influence.

Bernie Santarsiero: I moved to Caltech in 1980 to join Dick as a postdoctoral research fellow. I recall showing up on campus on a Monday morning, and hunting around for his office in the basement of Noyes Lab. It must have been around 9:30 am since he was leaving Noyes and heading east towards "the Greasy Spoon," more conventionally known as Chandler, the campus cafeteria. His ritual was to have morning coffee with the crystallographers, where typically Dick Dickerson would join us; lunch at the Continental Burger; and afternoon coffee with the programmers, including Jean Westphal, his main programmer. Conversations were always casual, cordial, and entertaining. Dick was interested and knowledgeable in everything.

Unlike a conventional postdoc, where you are given a number of options to pursue, Dick encouraged me to design my own project, and I researched his past interests as well as learned more about the organometallic chemistry research going on. I often pitched ideas to him about interesting studies, only to find out that he had the same ideas decades before. The X-ray laboratory at Caltech was a teaching lab, and once a student or postdoc was trained, they had access to everything. There were more than eight cameras available to screen crystals (and powders) at different wavelengths, and two diffractometers, soon to be three, that could collect data from 20K to room temperature. The computing system was home-grown, CRYM, and if an error was suspected, Dick was asked to check the crystallographic equations while Jean would check the code. Later on, when we converted from an IBM to Digital/VAX computer, his daughter Kirby also helped with programming. The lab offered an opportunity to work with great chemists and train them in crystallography while fine-tuning my own understanding.

Dick was an amazing crystallographer. I recall working with a graduate student who had crystallized a Pt complex with a Pt–Pt bond and 4-fold symmetry. I guided the student into taking a series of photographs to determine the space group and unit-cell parameters. After a few days, we reported on our interpretation of the Weissenberg photographs, choice of tetragonal space group, and collected a complete data set on one of the diffractometers. Dick had asked us to show him the Weissenberg photographs. Following that, we generated the Patterson map, determined the coordinates of the two Pt atoms, and then completed and refined the structure. Upon reporting back to him, he asked for the coordinates of the Pt atoms. He retrieved a note on his desk, and had the coordinates of the two Pt atoms written out to three places, from the interpretation of the photographs, and they matched! He had noticed the modulation in the intensities down the *c*-axis yielding the Pt–Pt distance, and worked out the rest of the coordinates as a special position. This kind of insight led to his uncanny ability to look at hundreds of structures and recognize from the figures and coordinates that the space groups were assigned to 'unnecessarily low symmetry.' I had the office next door, and often I would hear his characteristic hoop and holler at finding another suspicious structure. Many were the result of an unrecognized inversion center, but others were far more complicated and required changing from one crystal system to another. I vividly recall one conversation with him where we were discussing a crystallographic problem, and he shouted out, "Oh good!" I asked what he meant, and he replied that he thought I was going to take the opposite side, and that would have been more difficult to argue against. He was unflappable,

and he was brilliant.

Dick was an avid tennis player and golfer. He was always in good cheer. It was uncommon for him to get a '4' on a hole, but when he did, he would roar with laughter. When I visited him and his wife Helen last summer, he was, as always, working on crossword and jigsaw puzzles, sippin' on a Manhattan, and asking me, "What's new?" He never lost his passion for crystallography, or life.

Larry Henling: One day in 1990, Dick walked into the X-ray lab when we were collecting data on our Enraf-Nonius CAD4. He looked briefly at the reflection listing on the line printer and, without knowing anything about the compound, said, "You have a heavy atom at (*x, y, z*)." After the structure was refined, I ran a Patterson map for comparison. Dick's mentally calculated numbers were actually closer to the final refined coordinates than those obtained from the Patterson map. So the published paper states, "Ta atomic coordinates found by visual inspection of diffractometer intensity listing." [CheckCIF would not approve.] But more remarkable than Dick's mastery of crystallography and computation was his generosity in sharing his knowledge. His office door was always open and he was always willing to stop and answer questions, even if he had answered the same question a few weeks or months ago. You could give him a problem structure; within a day or two you would find on your chair a typewritten sheet of paper with one or two paragraphs explaining the proper approach. Despite all the assistance he gave us, Dick seemed a bit apologetic about troubling us whenever he asked for help, usually for just a minor computer issue.

Dick was of course known for correcting erroneous space-group assignments. In fact, in December the last structure he was working on was ... well, perhaps we can let that slide. While Dick felt strongly that crystallography ought to be done correctly, he also viewed these as puzzles to be solved. And Dick enjoyed puzzles and word play of all sorts, including cryptic/diagramless crosswords. He was always amused that, "unit-cell constants were determined to be." One newspaper headline taped to his wall was about a high-school basketball player who had "scored 69,126 points in two games."

Coffee time was a fixture in Dick's life. It was a time to discuss crystallography, science, or anything with local and visiting scientists. As a new research fellow at Caltech in the mid-1950's, Dick would sometimes have morning meetings with Robert Corey. But if they were not finished at coffee time, Dick would just get up and walk out. In recent years, without Verner Schomaker and Bill Schaefer, the scientific rigor of coffee time decreased markedly. But we did do the Daily Jumble puzzle, which is unscrambling five- or six-letter words. Dick would do these instantaneously; if not, the wrong letters were written on the board. He could also come up with the words if you just read him all but one of the letters. The only way we could slow him down was to have someone write some of the letters in Macedonian.

Dick was known at his favorite restaurants, where he usually ate the same thing. When we went to lunch at Primo's, a local sandwich shop, he was greeted with, "Mr. Meatball-ie," and without ordering would be served his meatball sandwich and iced tea.

Dick did not give much attention to things he didn't care about. When he had to get a new car (the old one caught fire in his driveway), we asked him what he bought. "A red car," was his reply. After a few years of teasing, he did eventually learn what it was. But after leaving one evening, he returned to the office to call his wife Helen as he had locked his keys in his car. This was odd since he usually left the car unlocked with the key under the floor mat. I went out and retrieved his key from his car. The locked vehicle parked next to his, however, was a car and it was red.

Dick said that in college he majored in tennis and golf (he was also a good third baseman on the Caltech team). He enjoyed playing and watching both sports.

Dick's description of Lindo Patterson applies equally well to himself: "[his] high standing among crystallographers, particularly in America, goes far beyond his published scientific work. It derives to a very great extent from his character and personality, for he possessed the rare combination of a keen mind, a lively humor, and a gentle disposition."

Editor's Note: The Winter 2012 issue of *ACA RefleXions* contains a *Living History* of Dick Marsh that incorporates a memoir and comments from B.C. Wang and John Rose.

Highlights from 2016 Fall ACA Council Meeting

The 2016 Fall Council Meeting was held at Hauptman-Woodward Institute (HWI) in Buffalo, NY on October 17-18. This was an unusual meeting in that it spanned two days, which was deemed necessary in order to address the challenge of establishing a fiscally prudent succession plan for the ACA Headquarters as well as the regular business of running the organization.

The ACA Headquarters currently resides in Buffalo and is staffed by Chief Executive Officer William Duax and Director of Administrative Services Marcia Colquhoun, with Membership Secretary Kristina Vitale. Chief Financial Officer S.N. Rao, in addition to Duax and Colquhoun, have announced plans to transition out of these positions within the next 2-4 years, and have provided succession proposals to the Council. Council approved the formation of a Transition Committee, headed by former ACA President Chris Cahill and composed of non-Council members, to work out details of these transitions and to make recommendations on the Succession Plans.

Much of the discussion regarding the Succession Plans centered around how to seamlessly continue to deliver the core benefits (and ideally, increase benefits and membership) of the ACA to the members for the lowest financial burden to the organization, both in the short and long term. Numerous plans were presented that incorporated hiring external providers to plan and organize the annual meeting, provide accounting and bookkeeping services, office space, website services, and general membership services. External providers considered included the IUCr, the HWI, Meeting Expectations (an event management company) and the American Institute of Physics. After hours of discussion, Council settled on a strategic plan that includes the hiring in 2017 of a full-time Administrative Services Director (ideally with event management experience) to replace Marcia Colquhoun, who will transition to part-time in 2017. The ACA Headquarters will remain in Buffalo, and efforts will be made (in a financially prudent manner) to outsource selected services to partner agencies. For example, the 2017 ACA meeting abstracts will be archived by the IUCr for a competitive fee. Many details of this strategic plan will require future negotiations and action on the part of the ACA Council; however significant cost savings are predicted to result from savings in salary by hiring an early-career professional and through negotiation of more favorable expenses for future meetings (by planning for fewer attendees).

Vice President Amy Sarjeant provided updated ACA annual meeting Program Chair Guidelines that have also been sent to the Program Chairs (Ilia Guzei and Yulia Sevryugina) for the 2017 meeting in New Orleans. Amy also reported on the First Pan African Conference on Crystallography in Cameroon in October, 2016, and there was much Council discussion on how to support the African crystallographic community in terms of data collection and also travel funds to the U.S. for both students and senior scientists to attend meetings and to spend time in a crystallographic facility for practical experience.

Michael James, the Canadian Representative, highlighted several upcoming Canadian meetings, including the 2016 Annual General Meeting of the Canadian Institute for Neutron Scattering to be held at McMaster University, October 14-15; The Canadian Powder Diffraction Workshop to be held at the Northern Alberta Institute of Technology, June 2-4, 2017; an X-ray microscopy conference at the University of Saskatchewan in August, 2018; and the Buffalo-Hamilton-Toronto meeting at McMaster University, November 4, 2016.

Hanna Dabkowska, the IUCr Representative to the Council, presented highlights of IUCr activities, including the upcoming 24th IUCr Congress & General Assembly to be held in Hyderabad, India (from August 21-28, 2017), and the selection of Prague, Czech Republic, for the 25th IUCr Congress in 2020; the launch of a new open-access data publication, IUCrData (***http://iucrdata.iucr.org/x/***); the support for 80 international meetings and schools since January 2015; the creation of the IYCr2014 Legacy Fund to support various activities started during the IYCr; and the successful joint organization with COSPAR of the "Crystallography in Space" Workshop in Puebla, Mexico.

Highlights of the report from Martin Donakowski, the Young Scientists Interest Group (YSIG) representative, included a recap of the YSIG sponsored "Diversity and Inclusion" session at the 2016 Denver ACA meeting, which was deemed to be so successful that the session chair has volunteered to repeat the session for the 2017 meeting. Marty discussed the YSIG plan to apply to the National Science Foundation for student travel funds to the 2017 ACA meeting [Note: this grant proposal was submitted in early January]. A request was made to have the YSIG chair and the YSIG representative to the ACA Council be declared separate positions, as the workload for both positions is felt to be too demanding for one person. The Council deemed this a decision to be made internally by the YSIG.

Sue Byram, the ACA Treasurer, highlighted the financial issues faced by the ACA, namely the need to increase revenue and to lower expenses. During the ACA Business Meeting at the Denver 2016 meeting, dues were increased, but other sources of revenue (*i.e.*, meeting registrations, newsletter advertisements) are decreasing. Sue presented several potential methods to increase ACA revenue including increasing the attractiveness of the organization and the annual meeting, by reaching out to a wider scientific interest group, which could attract additional meeting exhibitors and potentially higher ad revenue. Council is also in favor of acquiring information on how to attract potential donors to the society, for example *via* estate planning.

Despite a slow decrease in total membership, the ACA is financially sound, but this is primarily due to diligent cost-cutting measures by the ACA Headquarters staff in Buffalo. This includes changing the starting day of the annual meeting to Friday, as this results in a significant savings in charges from the event hotel, as well as on-site cost-saving measures during the meeting. Chief Financial Officer S.N. Rao asked Council members to present ideas to cut the budget by 10%, and several items (web site redesign, educational outreach activities, and support for the Pan African crystallographic community) were not included in the resulting budget.

The annual meeting is a core benefit of membership in the

ACA, and this was reflected in the results from the surveys of members (173 responses) and of exhibitors (14 responses) conducted at the 2016 Denver meeting. The take-away from the member survey is that people really do value the science presented at the meeting, but that many people now have limited travel funds. Constructive criticisms included a sense that there should be a greater emphasis on professional development and value for younger scientists, plus a plethora of suggestions for how to organize the ACA meeting during IUCr Congress years. With that in mind, four workshops will be provided at the 2017 meeting in New Orleans. Council approved the ACA meeting selection committee recommendation of Covington, KY as the 2019 ACA Annual meeting site [Note: Covington is directly south of the Ohio River from Cincinnati, OH]. While most of the exhibitors felt that the ACA Exhibition was successful for their organization, many responded that the hours required to man the exhibitor booths at the meeting were too long.

At the 2017 annual meeting the ACA will present the Patterson, Rognlie, Etter Early Career and Elizabeth Wood Science Writing Awards. New this year is the David G. Rognlie Award, to recognize an exceptional discovery or technical development of particularly high impact in any area of structural science, to be awarded every third year.

Last but not least, considerable thanks for their services are due to the outgoing ACA officers and representatives: Tom Terwilliger as President, Chris Cahill as Past President, Michael James as Canadian Representative and Martin Donakowski as YSIG Representative.

Diana Tomchick

ACA Council 2016; L-R: Martin Donakowski, Michael James (at rear), S.N. Rao, William Duax (at rear), Marcia Colquhoun, Sue Byram, Diana Tomchick, Chris Cahill (at rear), Hanna Dabkowska, Tom Terwilliger (at rear), Amy Sarjeant. Photo by Kristina Vitale.

Small Grants for Outreach

The ACA Outreach Task Force is awarding several small grants (average $300; maximum ~$1,200) to ACA members for demonstration outreach projects that can be replicated by other members. The intent is to enable each member to articulate essential features of crystallography in non-technical language, generate enthusiasm for crystallography, and engage K-12, local communities, organizations or politicians in exciting activities (*e.g.* growing crystals) and in understanding relevance (applications) of crystallography today. Long-range goals are attracting young students to crystallography, combating anti-science attitudes, and raising the status of crystallography in the academic community.

The successful proposal should:

1. Impact a large number of people, especially young scientists, in appreciating/choosing crystallography;

2. Include matching funds equal to the award from outside sources by the deadline if over $300 is requested;

3. Specify follow-up and evaluation of the event impact;

4. Delineate a plan for replication by other ACA members.

Proposals should be sent by **May 15, 2017** *via* e-mail to ***martha.teeter@gmail.com*** with the subject header, "Small Grants for Outreach." Proposals are limited to three pages, including the budget. Awards will be made in June. Projects should be completed in calendar year 2017 and a report submitted in early January 2018. Presentations of the projects will be made at the 2018 ACA meeting in Toronto.

ACA Outreach Task Force
Martha Teeter, Cora Lind-Kovacs, and Ilia Guzei

X-Ray Cameras and Equipment for Donation

Five X-ray cameras (three precession cameras, two Weissenberg cameras) are available for the cost of shipping: Huber precession/rotation camera (Huber 205) with telescope and internal light source for observing reflections from crystal faces (uses conventional film or Polaroid cassette); two Weissenberg cameras (Supper); two Buerger precession cameras (Supper). Cameras include all original equipment: film holders, screens, collimators. Other equipment such as goniometer heads, Donnay optical analyzer, circular film-measuring instrument, and crystallization equipment are also available. Contact Virginia Pett for more information, ***pett@wooster.edu***.

Contributors to this Issue

Eddy Arnold, Jason Benedict, Vicky Doan-Ngyen, Graciela Díaz de Delgado, David Duchamp, Howard Einspahr, Jeanette Ferrara, Joseph Ferrara, Ana Ferreras, Tomislav Friščić, Frank Fronczek, Jenny Glusker, Chuck Goodman, Harry Gray, Ilia Guzei, Samar Hasnain, Larry Henlung, Cora Lind-Kovacs, Kay Onan, Virginia Pett, Daniel Rabinovich, Connie Rajnak, Allison Rein, Bernie Santarsiero, Amy Sarjeant, Manuel Soriano-García, Ton Spek, Martha Teeter, Diana Tomchick, Anastasiya Vinokur, Christine Zardecki

ACA History Project News

Manuel Soriano-García's Living History on pp. 40-45 of this issue of *ACA RefleXions* magazine describes his graduate work at SUNY Buffalo under the direction of R. Parthasarathy as well as his experiences with David Harker, whose courses he took. After receiving his Ph.D. degree, Soriano-García pioneered small-molecule and protein crystallography in Mexico. This Living History is a most fitting addition to the recently added online section *Crystallography in the Americas*.

Webmaster Vanessa Reitz reports that ACA History online now includes information for over 70 structural scientists. Also, in the last few weeks she has added obituaries for Herbert Hauptman and Jerome Karle, winners of the Nobel Prize in 1985 for their discovery of direct methods to solve the phase problem in crystallography. See also the recent obituary for Ahmed Zewail, 1999 recipient of the Nobel Prize for his research in ultrafast electron crystallography and electron microscopy. Our goal is to provide a comprehensive historical perspective on structural science.

More items have been added to the *Impact of Structural Science* section of ACA History online, notably a link to an informative set of timelines produced for 2014's IYCr. Up to five timelines can be displayed simultaneously on topics such as Nobel Prizes, Chemical Crystallography, Crystallographic Information, and Crystallography and Stamps. See also the link to the YouTube video "From Molecules to Medicine: How Structure Helps Cure Disease" (Greg Petsko, moderated by Martha Teeter) and the link to "The Protein Data Bank archive as an open data resource" (Helen Berman *et al.*). If you have suggestions for additional articles and videos that illustrate the historical importance of structural science, please send them to me.

Have you ever wondered how X-ray security machines at airports were developed? In David J. Haas's online Living History we learn about the history of these devices and Haas's part in developing the technology and educating airport workers in their use. During his career he worked with some of the most distinguished names in crystallographic history: David Harker, Jerome and Isabella Karle, David Phillips, Michael Rossmann. After his postdoctoral work he migrated from academia to industry. Later David and his wife Sandra founded Temtec, Inc. to sell self-expiring visitor badges that he designed.

Haas's memoir gives an enlightening perspective on how scientific discoveries are made and recognized. He set out to test whether crosslinking a protein might stabilize its crystals and ended up discovering that freezing the crystals vastly extends their lifetime in the X-ray beam. The value of this observation was not appreciated until much later, when freezing crystals at synchrotron sources became necessary. As is frequently the case with these Living Histories, there wasn't space to publish Haas's complete memoir in *RefleXions* magazine; the full document with additional photographs is published online.

Virginia Pett
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Wisconsin Crystal Growing Contest Announces Space Crystal Prize for International Space Station

The University of Wisconsin – Madison Chemistry Department Molecular Structure Laboratory is proud to announce a collaborative project with the **Center for the Advancement of Science in Space (CASIS)**, the manager of the International Space Station U. S. National Laboratory.

Students selected as overall and best quality crystal winners of the 2017 **University of Wisconsin Crystal Growing Contest** will be awarded an opportunity for their crystals to grow aboard the International Space Station U. S. National Lab through a partnership with the **CASIS** and their **Space Station Explorers (SSE)** education program. The two winners of the contest-inspired art contest will be chosen to design the "space crystal mission logo" that will be flown to the ISS.

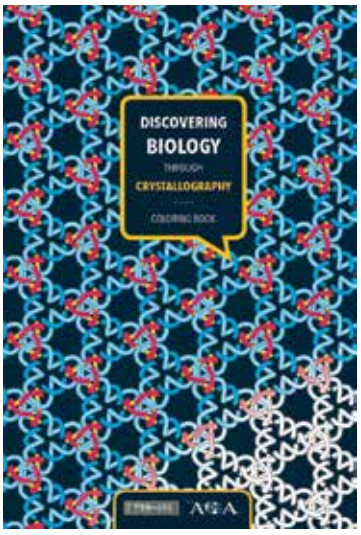
Students will work with the UW – Madison Molecular Structure Laboratory and the CASIS SSE team to translate their optimum growth conditions into an experiment to be conducted on the ISS National Lab. The students will be challenged to adapt their growth conditions to the flight hardware, prepare their experiment for launch, and compare the resulting microgravity-grown crystals with crystals grown on Earth! In addition to the technical work, the Space Crystal Prize winners will be required to communicate their experiences through a blog, social media, and possible media opportunities in preparation for launch at Kennedy Space Center in Florida! Activities will be

Continued on p. 34

highlighted on the SSE website as well. Finally, after results are collected, the Space Crystal Prize winners will publish a short report in the CASIS *Upward* quarterly magazine.

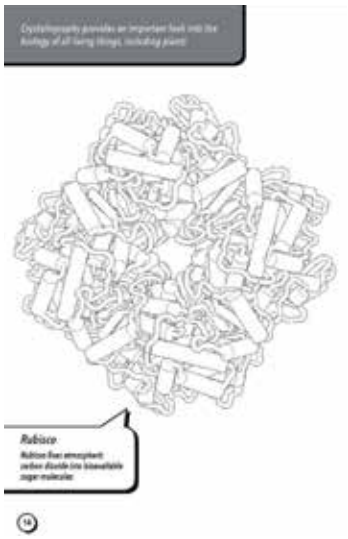
For more information visit ***http://wicgc.chem.wisc.edu/index.php/crystals-in-space/***.

Ilia Guzei, University of Wisconsin Crystal Growing Contest Lead, ***iguzei@chem.wisc.edu***
Diane Matthews, Space Crystal Lead Educator, ***dmatthews@iss-casis.org***
Ilia Guzei



Download the PDF or request bulk copies for use in outreach and education from http://pdb101.rcsb.org/color.

This coloring book illustrates the crystallographic pipeline.



Structures from the CSD and PDB are highlighted.

Promoting Crystallography Through Coloring

In 2015, 12 million coloring books were sold in the United States.[1] These coloring books are used by an extremely varied audience, from school children to adults as a means of relaxation and meditation (as documented by *Forbes*,[2] *The Atlantic*,[3] *The New York Times*,[4] and others[5]).

Thanks to a **Small Grant for Outreach** from the ACA, RCSB PDB developed a coloring book, *Discovering Biology through Crystallography* that leverages this trend with the beauty inherent in molecular structures to create a new venue for scientific education and outreach. The coloring book uses illustrations of three scientists to highlight the crystallographic pipeline; provides examples of molecules contained in the Cambridge Structural Database (CSD) and Protein Data Bank (PDB); and displays a drawing of a full cellular scene.

Discovering Biology through Crystallography is distributed freely online at ***http://pdb101.rcsb.org/color*** as complete PDFs and as individual images. Since publication at the end of October 2016, it has been accessed online more than 7,600 times. A limited edition of printed copies was produced, and these are being distributed by the RCSB PDB at Rutgers. So far, approximately 2,100 copies have been requested for education and outreach throughout North America at local ACS ChemExpos, science teacher conventions, high schools, universities, middle schools, kindergartens, and a Science Café event.

We thank the ACA for providing us with the means to pursue this unique outreach and education opportunity.

Christine Zardecki

[1]Alexandra Alter, We're Buying Paperbacks, Audiobooks and Coloring Books — but Not E-Books, May 26, 2016 ***http://www.nytimes.com/2016/05/27/books/were-buying-paperbacks-audiobooks-and-coloring-books-but-not-e-books.html***

[2]Kate Harrison, The Adult Coloring Craze Continues and There Is No End In Sight, February 2, 2016, ***http://www.forbes.com/sites/kateharrison/2016/02/02/the-adult-coloring-craze-continues-and-there-is-no-end-in-sight/***

[3]Julie Beck, The Zen of Adult Coloring Books, November 4, 2015, ***http://www.theatlantic.com/health/archive/2015/11/sorry-benedict-cumberbatch-your-head-is-fine/414010/***

[4]Caroline Tell, Coloring Books for Adults Seeking Playtime, April 20, 2016 ***http://www.nytimes.com/2016/04/21/fashion/adult-coloring-books-relaxation.html***

[5]Kelly Fitzpatrick, Why Adult Coloring Books Are Good for You, January 6, 2016 ***http://www.cnn.com/2016/01/06/health/adult-coloring-books-popularity-mental-health/***; Jordan Gaines Lewis, A Neuroscientist Patiently Explains the Allure of the Adult Coloring Book, January 10, 2016 ***http://nymag.com/scienceofus/2016/01/neuroscientist-explains-adult-coloring-books.html***

2016 U. S. Crystal Growing Competition

Jason Benedict displays the Best Teacher crystal grown by Jessica Weedon from Bronx High School of Science. Photo by Douglas Levere.

"Thanks again for putting on such a great contest and making it easier to keep my students interested in science. Many of them made special arrangements to stay after school just for this project." – Excerpt from thank you note from educator David Adamson of the CREC Montessori Magnet School in Hartford, CT. Adamson's student, Matteo Dolzadelli won first place overall for grades K-8.

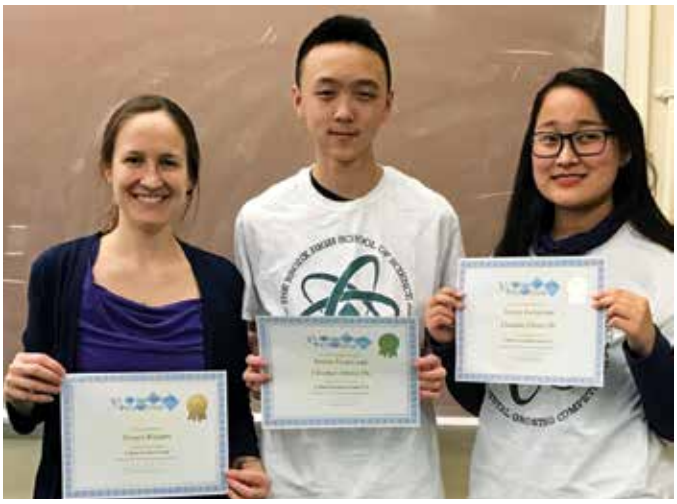
The contest, which began during National Chemistry Week in mid-October and concluded in early December, was judged by a number of veteran judges that included UB Professors from Chemistry and Physics: Timothy Cook, Ekin Atilla-Gokcumen and Luis Velarde (Chemistry), and Andrea Markelz (Physics). We welcomed a new judge as well: Travis Nelson, a geologist and graduate instructional support technician.

The 2016 U.S. Crystal Growing Competition (USCGC, ***http://www.uscrystalgrowingcompetition.org/***) concluded with an exciting blend of 83 participating schools and households in 26 states. The third running of this nationwide competition, based

Isabella and Sophia Elge, homeschoolers from Bellevue, NE, proudly display the alum seed crystals they used for the 2016 USCGC. Photo by Shanael Elge.

upon a similar contest developed in Canada, challenged America's youth in grades K-12 to grow the largest, highest quality crystal of potassium aluminum sulfate possible over a five-week period. Sponsored in part by ACA, the USCGC brings the science of crystals into America's classrooms. And guess what? The crystal growing is getting really, really good!

The Bronx High School of Science in Bronx, New York is becoming a crystal growing powerhouse! For the second year in a row, Jessica Weedon took home the "Best Teacher Crystal" and a check for $100. Her students, Tenzin Tsetan and Hans Hu, won 1st place Overall grades 9-12 and will split $200. Rounding out the Overall category were 2nd place finishers Dawn Kelley's students from Lyme-Old Lyme High School (Old Lyme, CT)



Winners of the Best Teacher Crystal, Jessica Weedon (left), and first place Overall grades 9-12, Hans Hu (Center) and Tenzin Tsetan (right), all from Bronx High School of Science.

and in 3rd place Torrey Black's students from Lockport High School (Lockport, NY).

For grades K-8, 1st place Overall (along with a check for $200) went to a student of David Adamson at CREC Montessori Magnet School (Hartford, CT), as I've noted at the top. Students of Eric Walstrom at Monte Vista Elementary (Albuquerque, NM) won 2nd place Overall. A homeschool entry from Heather Costner (Springville, NY) took 3rd place Overall.

The contest used social media to advertise and provide contest updates! The winners were announced via the contest Twitter account, ***@USCrystalComp***. Many participants sent in pictures of their progress, which were also shared with the world via social media. Want to see the action? Check out ***#2016USCGC*** on Twitter!

The USCGC gratefully acknowledges the Benedict Research Group graduate students, and the support of our sponsors: ACA, National Science Foundation, Ward's Scientific/VWR, Bruker AXS, Krackeler Scientific, Cambridge Crystallographic Data Centre, the Western New York section of the American Chemical Society, and the UB Department of Chemistry. Please consider helping with the 2017 contest. For more information, please visit the USCGC website or e-mail Jason Benedict at ***jbb6@buffalo.edu***.

Jason Benedict

Judges for the contest can be seen gearing up to score the numerous crystals sent in from across the country. Photo by Douglas Levere.

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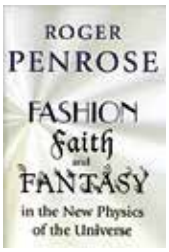
Book Reviews



Fashion, Faith and Fantasy in the New Physics of the Universe: Roger Penrose, Princeton University Press, Princeton, 2016, 520 pp., ISBN-13: 978-0691119793.

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 NPR's *Science Friday* so I bought a copy. Be forewarned: this is not light reading. This is not a textbook, 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 that allows Penrose to segue into the fourth and 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 led 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.

Joseph Ferrara

A Survival Guide to the Misinformation Age: Scientific Habits of Mind: David J. Helfand, Columbia University Press, New York, 2016, 344 pp., ISBN-13: 978-0231168724

Longtime Columbia University astronomy professor David Helfand's *Survival Guide* seems even more pertinent now, in the wake of the recent presidential election and the fake news epidemic, than it was almost a year ago at the time of its first publication. Helfand's book certainly isn't a "how to determine if the news you are reading is fake" guide, but many of the principles of scientific discovery he explores could certainly be applied to the aforementioned dilemma.

Two of the most useful parts of the book didn't fall under the auspices of the thirteen numbered chapters, but within two "Interludes." The first, on numbers, gave a good introduction to numbers, in the sense that many, many people – even well-educated people – are what you might call "innumerate" (that is, the number equivalent of illiterate). As such, when given certain kinds of number-based information, some people cannot immediately recognize when the math is off. It's always important when dealing with number-related information to do simple "sanity checks" to ensure that the information is accurate and not off by a factor of 10 (or even 10,000 or 10,000,000). For example, if you read a report that 20 billion illegal immigrants came to the United States in 2016, you should pause before you believe it. After all, there are only ~7 billion people on the planet as a whole, so the numbers really just don't make sense. That's an extreme example, but you can see the point he is trying to make.

The second interlude, on logic and language, was also particularly helpful, though it would be hard to top the everyday usefulness of that on numbers.

Interludes aside, the chapters were incredibly useful as well. Two of the most pertinent chapters, one on statistics and the other on the relationship (or lack thereof) between correlation and causation, address some of the most critical issues involving data interpretation facing our world today. The fact is, information is power, and data is information in its purest, rawest form. Being able to understand and interpret data accurately and efficiently can be a daunting task, but it is an important one. The sheer quantity of fake news that stems from inaccurate data analysis likening correlation to causation is astounding.

Helfand's prose certainly isn't aimed at a particularly broad audience, but it serves as a helpful reminder, especially for scientists and the like who ought to know better, to always check the source before believing any information.

Jeanette Ferrara

Join Us in Fabulous NOLA in May!

Algorithms to Live By: The Computer Science of Human Decisions: Brian Christian and Tom Griffiths, Henry Holt and Co., New York, 2016, 368 pp., ISBN-13: 978-1627790369

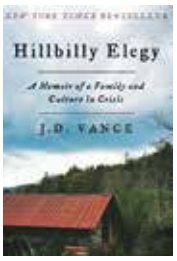
I came across this title in the list of books Amazon thought I might like. I bought it, and it sat in my "to read" pile for a couple of months. I finally read it over the holidays, and it is the most fun self-help book I have read in quite a while.

The authors, Brian Christian and Tom Griffiths, are both experts in cognitive science. Christian has published articles in *The Wall Street Journal*, *The Atlantic*, *Gizmodo*, and *Cognitive Science*, to name a few places. Griffiths is the director of the Computational Cognitive Science Lab at UC Berkeley.

The authors follow the pattern of describing a problem in computer science, explaining the solution as it pertains to the computer, then expounding upon how that solution can be used to simplify your life. The underlying theme is to reduce your effort on a number of problems from n^2 to $n\ log(n)$ or ideally n steps.

One early example is sorting. The authors describe how various sorting algorithms, like the bubble, merge and insertion sort, work and how to apply those algorithms to everyday life. A good example is what to do with the stack of e-mail that greets you every morning. Do you do multiple passes on your inbox and prioritize? Do you sort e-mail? If you sort, how do you sort e-mail? The authors' solution to dealing with e-mail is: go through it once or it becomes a nonlinear problem adding unnecessary work. The subject of sorting segues into search and ultimately the recommendation to not sort e-mail messages for archival use at all but to let search algorithms find them for you when you need them. I've been doing this for a few years now, and it is a huge time saver. The lesson is search when you can and sort only when you must do so, and if you do sort, sort efficiently.

Many topics are covered in addition to sorting and searching: Optimal Stopping, Explore/Exploit, Caching, Scheduling, Bayes's Rule, Overfitting, Relaxation, Randomness, Networking, and Game Theory. Each topic is approached with examples of practical applications for real life.



Hillbilly Elegy: A Memoir of a Family and a Culture in Crisis: J.D. Vance, HarperCollins, New York, 2016, 272 pp., ISBN-13: 978-0062300546

I wish I had read this book before the election. Had I done so, I might not have been so dazed when I got out of bed on the morning of 11/9. Between the lines of this book are some of the reasons the President is Donald Trump and not Hillary Clinton.

The group of people described herein moved from Appalachia into the manufacturing towns in the North after World War II. When manufacturing was central to the economies of the Midwest everyone did well. When manufacturing left, most did not. Now many people are unemployed or underemployed and feel the government is responsible. It is clear that there is plenty of blame to go around as some people no longer want to work, but stay on welfare. Those who want to work see the government as responsible for the jobs leaving the area and providing the entitlements for those who don't want to work. Those receiving entitlements don't want government interfering in their lives. Hence, the perceived need for change.

An elegy is an epic poem. But there is no poetry in here, just well-written prose. The author joined the Marines and completed one tour of duty as a public relations officer. The discipline and self-respect instilled by the Corps provided the wherewithal for Vance to go to college and ultimately graduate from Yale Law School.

It is not too late to read this book and begin to understand the problems of Middle America.

Born to Run: Bruce Springsteen, Simon and Schuster, New York, 2016, 528 pp., ISBN-13: 978-1501141515

In 1979 I first heard the WMMS broadcast of Springsteen's 1978 concert at the Cleveland Agora. I knew that my life would never be the same.

Springsteen writes prose with the same rhythm he writes lyrics – with ferocity. This makes a lot of sense – he has been writing his autobiography in his music for decades. The author describes his childhood in the Italian-Irish town of Freehold, New Jersey in the shadow of the Catholic Church and an alcoholic father. He realized music would become his life when he first saw Elvis Presley on the *Ed Sullivan Show* in 1956. Springsteen describes in detail the arc of his career from his first band, The Merchants, to the stadium-filled concerts of the 80s and 90s with the E Street Band, the 2009 Super Bowl XLVIII halftime show, and all the other tours. We learn about the members of the band, especially Clarence Clemons. Springsteen delves deep into the psyche of the American middle class and exposes his own demons. His is the story of one man who succeeded in his American Dream.

By the way, the WMMS concert I mentioned was recorded on a 24-track tape recorder and can be listened to in all its glory at the Western Reserve Historical Society.

Joseph Ferrara

News Flash

It gives us great pleasure to welcome Kristin Stevens to the ACA. Kristin comes to us from the New York Chapter of the American Academy of Matrimonial Lawyers where she served as the Executive Director. Over the next few months she will be learning the ins-and-outs of ACA Headquarters operations from Marcia Colquhoun.

Born and raised in Buffalo, NY, Kristin obtained her Bachelor's Degree from Medaille College. For over fifteen years she has been providing administrative and executive support to local law firms. In that capacity she managed the day-to-day mechanisms of an office as well as planned meetings and events.

Kristin is excited to join us and get to know our scientific community. You'll have an opportunity to meet Kristin in person at the ACA Annual Meeting this May in New Orleans.

Amy Sarjeant

Reaching for the (X-Ray) Stars

Daniel Rabinovich

The Universe is full of X rays. Not the conventional ones we encounter in medical practices and crystallography labs but those emanating from astronomical objects that contain exceedingly hot gases with temperatures over a million kelvin. Even though massive amounts of soft X rays originating from neutron stars and supernova remnants constantly crisscross the galaxies, the small portion of X-ray radiation that reaches the Earth is readily absorbed by the atmosphere. Thus, the detection of extraterrestrial X-ray sources had to initially rely on the use of special equipment on board sounding rockets and high-altitude balloons.

In June 1962, a team led by Riccardo Giacconi, an Italian-born astrophysicist working at American Science & Engineering, a company in Massachusetts that developed scientific instruments for NASA, used a rocket-borne detector to observe X rays arising from the constellation of Scorpius, the first X-ray source discovered outside the solar system. Giaconni himself, a professor at Johns Hopkins University since 1982, was honored with half of the 2002 Nobel Prize in Physics "for pioneering contributions to astrophysics, which have led to the discovery of cosmic X-ray sources."

Starting in the 1970s, X-ray telescopes carried by artificial satellites orbiting the Earth provided a tremendous boost to the field of X-ray astronomy. For example, the Uhuru satellite identified 339 different sources of X rays by systematically scanning the skies in the 2-20 keV energy range. Subsequent missions, including NASA's Chandra X-ray Observatory launched in 1999, which is still in operation, have provided critical evidence for the existence of black holes and the distribution of dark matter in the Universe.

The German stamp illustrated in this note was issued on October 14, 1999 and features an image of the explosion cloud of a supernova in the Vela constellation, captured by the X-ray telescope carried by the Röntgen Satellite (ROSAT). The brighter regions in the X-ray emission image reflect areas where more dense and hotter gas clouds are present. It is quite amazing that the same form of electromagnetic radiation can play an important role in the exploration of phenomena in such vastly different scales: from the structure of atoms and molecules to the nature of galaxy clusters. Live long and prosper, X rays!

Daniel Rabinovich

ACA Living History – Manuel Soriano García

Manuel Soriano-García

I was born in Mexico City, on October 9, 1947. I was the third of four boys. My father was a railroad man and my mother was a housewife. Both of them had only three years of elementary school education because at that time the elementary school offered only up to the 3rd year, which was enough to read and write in Spanish. My father was more interested in my older brothers and he was very hard on them. So by the time I arrived he was tired and disappointed that my brothers were so bad in school. My two older brothers only finished elementary school and high school, respectively. For that reason, my father did not force me to study and I was left alone to go through school the best I could. In that way my parents did not know what grade I was in until I graduated from college. Then my father was surprised but not pleased that I had gotten so far without any help.

When I finished high school I had to decide which bachelors degree to take. I looked into different schools and was impressed by the title "Biochemical Engineer." I liked chemistry and engineering and I felt that this would fulfill my goals at that time. I enrolled in the biochemical engineering degree at the National School of Biological Sciences at the National Polytechnic Institute (IPN). At that time IPN was one of the only schools for students of low-income families.

I also had to enlist in the military service, which was mandatory. In just one year of military service I earned the degree of Second Lieutenant. I had the opportunity to continue my stay in the army but decided against it. I was already in the second year of the biochemical engineering school and I did not want to feel like I had wasted two years of my life. With that in mind I continued my studies.

During my college years I had a very busy schedule. I used to be a truck driver, a middle-school teacher and a college student, at the same time. My whole day started at three in the morning and finished at nine at night from Monday to Friday. Saturdays and Sundays I was either sleeping or studying.

During my third year of college, I joined Professors Manuel Castañeda and Luz Maria Del Castillo's research group. I worked in their laboratory for three years, and they encouraged me to enroll in the Biophysical Sciences Department at SUNY Buffalo to learn crystallography. My professors gave me some publications regarding crystallography, to get me interested. It seemed to be a very exciting field!

I did not know how to speak English and I only knew how to translate using a dictionary. I took the TOEFL and I passed. For me it was a very simple exam because it was based on multiple choices and I was very good at multiple choice tests.

Anyway, I arrived at Buffalo, on Labor Day in 1971. I got in contact with Prof. Robert Spangler, Department Head of the Biophysical Sciences Department, at SUNY Buffalo. I stayed with him for several days until I was able to rent a room with Mr. Richard Perugini. He had me speak to him in English every day in order to improve my vocabulary and pronunciation. He corrected my language and with his help I was able to learn enough English to pass the critical courses in biophysics. His help will be always appreciated.

Manuel Soriano-García was educated in Mexico and received his Ph.D. in biophysics under the direction of R. Parthasarathy at SUNY Buffalo. As Research Professor at the National Autonomous University of México he established small-molecule and protein crystallography in Mexico, receiving many national awards. He studied the proteins of the amaranth plant, the rubber plant, and the anti-inflammatory properties of organoselenium compounds.

Prof. Rengachary Parthasarathy, my mentor.

At the start of my second year, I spoke to Prof. Rengachary Parthasarathy about carrying out my research work on crystallography under his supervision and he accepted me. During this time I met S. Narasinga Rao, who was writing his Ph.D. thesis. Dr. Rao helped me to understand the basic crystallography principles, which would be essential to successfully carry out my research. Unfortunately, a few months later he left the laboratory and moved to Oklahoma. We are still good friends.

L-R: Manuel Soriano-García, S. Narasinga Rao, Cynthia Lesh and Mrs. Narasinga Rao, standing in front of the Pyramid of the Sun (1998).

During the summer of 1973, I did my summer research on the crystal structures of several metal alkaline derivatives of malonic acid in order to understand the effect of these metals on their intermolecular hydrogen bonds of malonic acid. My research was approved and I became a Ph.D. candidate.

In September 24, 1973, I was introduced to Miss Cynthia Lesh and immediately we got along very well. We were engaged a week later and by May 30, 1975 we got married at City Hall in downtown Buffalo, in a very simple ceremony. In November 1975 my son Simon Manuel was born at Children's Hospital in Buffalo. He is now a mechanical engineer.

I worked very hard and solved several crystal structures of some modified nucleosides of tRNA and several plant hormones, which at that time were very hot topics. In May of 1975, I concluded my Ph.D. research and I was ready to finish my Ph.D. degree. Prof. Parthasarathy asked me if I wanted to do some extra work on anomalous dispersion. I agreed and I did it.

I took all of Prof. David Harker's courses; he was Department Head of the Biophysics Department at Roswell Park Memorial Institute. At the end of each course he would give an exam to solve. I always received an INCOMPLETE. I had to give a talk and a written report every week that covered the course topics. This was a nightmare; I was the only student that had to do this. Because of that, I learned a great deal and in great detail the topics that were given.

During the 1970s and early 1980s many crystallographers were working on the subject of developing the direct methods procedures to solve the three-dimensional crystal structure of small molecules and proteins. These methods make use of relationships between the intensities of the various reflections that lead directly to a solution of the crystallographic phase problem. I was very lucky as a graduate student to experience the development of these procedures and received lectures from Professors Herbert Hauptman, Jerome Karle, Isabella Karle, Peter Main, Henk Schenk, George Sheldrick, and Carmelo Giacovazzo amongst others.

L-R: Herbert Hauptman, Jerome Karle and Manuel Soriano-García (1994).

L-R: Jerome Karle, Isabella Karle and Manuel Soriano-García (1994).

After I received my Ph.D. degree, David Harker explained why he gave me the incompletes. He said: "When you leave this laboratory and return to Mexico you will not find anyone to help you and you will have to solve the problems by yourself." Since I was the only crystallographer in Mexico, I really did not have anyone to run to when I needed help. So Prof. Harker was right!

The National Research Council of Mexico gave me four years to get my Ph.D. I was really rushed. I did it in three and a half years to the amazement of everyone.

I presented my Ph.D. exam on November 5, 1975. I was very lucky to have on my dissertation committee: Professors David Harker, Gopinath Kartha, Herbert Hauptman, Robert Rain and Rengachary Parthasarathy.

In December 1975 I left Buffalo with my Ph.D. degree in hand, a wife and a son all-in-one package. Upon returning to Mexico, my aim was to establish crystallography. Great hopes and no job! On January 26, 1977 my daughter Michelle Ann was born.

By mid-1977, I had been in the country now for more than a year and I had a difficult time. Nobody knew about crystallography and, since I came from a poor family, I did not get much help. Now if I were rich, or came from an influential family, then doors would have been opened faster.

One day I met an old classmate, Prof. Erasmo Flores-Valverde, and he was the one who helped me get a job at the Chemistry Department, Metropolitan Autonomous University-Iztapalapa Unit (UAM-I).

I worked at UAM-I for five years teaching general chemistry, physical chemistry and biochemistry courses. While at UAM-I, I was able to raise just enough funds to buy the first automated diffractometer but because of monetary exchange rates and devaluation I was not able to purchase the instrument.

While I was working at UAM-I, I used my summer vacations to work with Dr. Parthasarathy on some of his projects. He provided me with the financial support that I needed. During this time I collected data for some of my crystals that I had grown in Mexico.

In May 1982 the Chemistry Institute at National Autonomous University of Mexico (UNAM) purchased an automatic X-ray diffractometer. The interesting thing was that they had the machine but no one knew how to use it. That's where my luck changed! I was asked to come and train two technicians and, if I really needed it, I could ask for some time on the machine. I replied that if they gave me a permanent position, then I would teach them. They agreed and I was hired as a researcher at UNAM. I was finally a research scientist in Olympus. That is what the Chemistry Institute was called because it was so hard to get in. I was the first researcher to be admitted that came from the IPN.

During the following five years I solved many different crystal structures from natural products, intermediates of chemical synthesis, organometallics, and inorganic compounds, amongst others. I trained two technicians; they did all the data collection and solved the crystal structures under my guidance.

In June of 1985, I organized the "1st Seminar of X-ray Crystallography on Small Molecules in Mexico." The idea behind this was to promote the impact of small-molecule crystallography in the fields of chemistry, physics and biochemistry in Mexico.

In April of 1988, I organized the "X Congress of the Latin American Group of Crystallography" at the Chemistry Institute, UNAM. The purpose of this academic event was to welcome the Spanish community crystallographers to Mexico. People from Spain, Colombia, Venezuela, Brazil, Argentina, Chile, Uruguay and the United States attended and presented their work.

In 1990, I received the National Award in Chemistry in Mexico from the Mexican Chemical Society due to my contributions on the crystal structure determinations of small molecules. This work helped many Mexican scientists with their research goals. My first scientific goal was achieved: to establish small-molecule crystallography in Mexico.

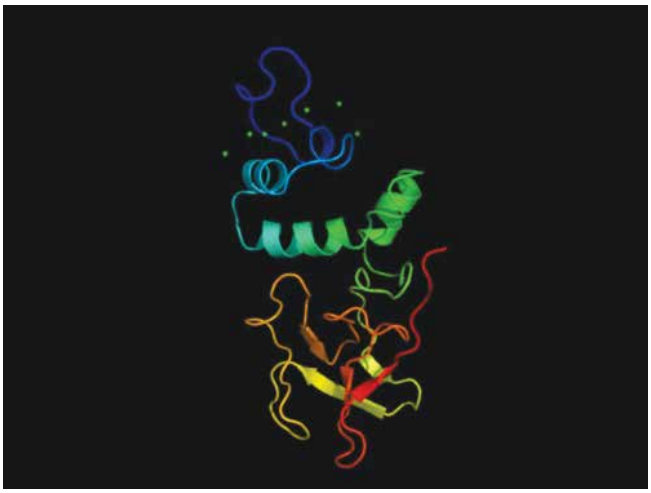
My next goal was to establish protein crystallography in Mexico. In May of 1985, we got the first protein crystals at our laboratory. We presented our results during the "First International Conference on Protein Crystal Growth," Stanford University (1985).

My very first problem was: I had protein crystals but the detector that I had was unsuitable for protein data collection. Fortunately during an ACA meeting I met Prof. Alexander Tulinsky and told him about my detector problem. He said that he had the same X-ray diffractometer with a long-arm detector for protein data collection and his group had developed the new software for protein data collection. I asked him if my group could have a copy of his software. He agreed to give me a copy, but suggested that I should visit his laboratory at Michigan State University to get hands-on experience using it. I spent three weeks at his laboratory and learned how to use this software, and went back to Mexico with a copy of the software. During this time I purchased the long-arm detector that was missing.

Colleagues at Michigan State University. In front, L-R: K. Padmanabham and T. P. Seshadri; standing and holding the baby, P. Padmanabham (1988).

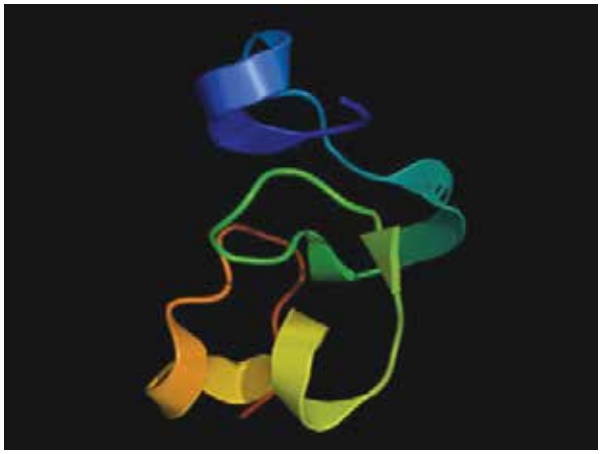
L-R: Michelle A. Soriano-Lesh, Manuel Soriano-García, Cynthia Lesh; and in front, Takao Matsusaki (Michigan State University, 1989).

In 1988, I spent my sabbatical leave with Prof. Tulinsky. I had a hard time in understanding the protein solution and refinement software, but fortunately K. G. Ravichandran, a graduate student of Prof. Tulinsky, helped me understand it. His help will be always appreciated. Prof. Tulinsky gave me a project to solve the structure of one of the blood coagulation cascade proteins. I was able to grow the crystals, collect data and solve the structure.



Structure of Ca(2+)-Prothrombin Fragment 1, a protein of the blood coagulation cascade (PDB 2PF2).

During my sabbatical leave, I was able to collect data on the Hevein (a protein isolated from the rubber tree latex) crystals that I had brought with me from Mexico. This helped me solve the first protein structure in Latin America, with the help of only one graduate student.



The structure of Hevein, a protein from the latex of Hevea brasiliensis (rubber tree); the first protein structure solved in Latin America.

In 1992, I received the national award to the Best Faculty Member at IPN. In 1994, I received the national award in science from the National Academy of Sciences of Cuba for my outstanding contribution to small-molecule crystallography.

Upon returning to Mexico, eight graduate students from Mexico and two postdocs from India contacted me. They wanted to work on the isolation, purification, and biochemical and spectroscopic characterization of plant proteins.

In 1993, it was the year to organize a series of conferences to introduce structural biology in Mexico. Well-known professors

from the United States were invited, including: David Davies, Johann Deisenhofer, James Hogle, Paul Sigler and Gerhard Wagner. The academic program was sponsored by the U.S. National Academy of Sciences.

Manuel Soriano-García (standing), William Duax (standing), Johann Deisenhofer (seated), and graduate students at the Chemistry Institute, UNAM (1994).

In 1994, I organized the "First School of Protein Crystallography in Mexico" at UNAM. This school was sponsored by the U.S. National Academy of Sciences and is offered annually as a course entitled, "X-ray Methods in Structural Biology," at the Cold Spring Harbor Laboratory, Cold Spring Harbor, NY. This time, the course was offered in my laboratory at UNAM. There were a total of twenty participants.

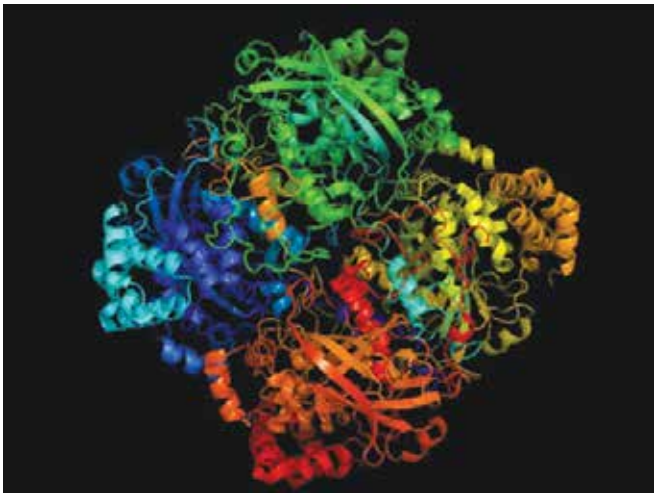
Because of this course, I received a grant and I was able to purchase an automatic X-ray diffractometer from Rigaku. It was equipped with an imaging plate that allowed me to create an experimental area for the isolation, purification and crystallization of plant proteins. That was really very good.

In 1997, not all is happiness! I had serious problems with the Director of the Chemistry Institute (UNAM) to the extent that all my research facilities were taken from me. After the Christmas vacation, upon returning to work, I found myself with no office and no lab. They were reassigned to another researcher, who had been my graduate student. At that time I felt that all of my work of 12 years was for nothing and as a result of this situation I went into a deep depression. This led me to diabetes.

One good bit of news was that my daughter received a bachelor degree in biomedical sciences from UNAM; she went on to receive a Ph.D. in immunology from Harvard Medical School and currently works for a pharmaceutical company in Paris, France.

In 1999, because of my work on the isolation, purification, biochemical characterization and preliminarily crystallization studies of Amaranth globulin proteins, I was awarded the National Award in Food Science and Technology from the National Council for Science and Technology (CONACyT) and the Mexican Coca-Cola Industry.

In 2000, I decide to visit my crystallographer friends and I spent five months (October 2000 to February 2001) working at the Consejo Superior de Investigaciones Cientificas (CSIC) of Spain in Barcelona. While I was there I helped to solve the structure of a Catalase isolated from *Pseudomonas syringue*, under the supervision of Prof. Ignacio Fita.



Structure of a Catalase isolated from Pseudomonas syringue (PDB 1M7S).

At that time, I realized how crystallography changes. Starting from small molecules, to large proteins, such as the Catalase, I realized that there is much more to learn.

Barcelona Crystallographic Group, L-R: Lourdes Campos, Juan Antonio Subirana, Cynthia Lesh, Ignacio Fita and Manuel Soriano-García (2000).

During my stay in Barcelona and Valencia, my wife and I made good friends with other crystallographers: Ignacio Fita, Juan Antonio Subirana, Lourdes Campos, Juan José Calvete and Libia Sanz. Our friendship continues to this day.

Manuel Soriano-García, Cynthia Lesh, Juan José Calvete and Libia Sanz (2000).

When I returned to Mexico in March 2001, things had not gotten any better at work. I had to share a laboratory with another researcher working under difficult conditions with no financial support and no equipment.

So I called upon an old friend from my days in Buffalo, Prof.

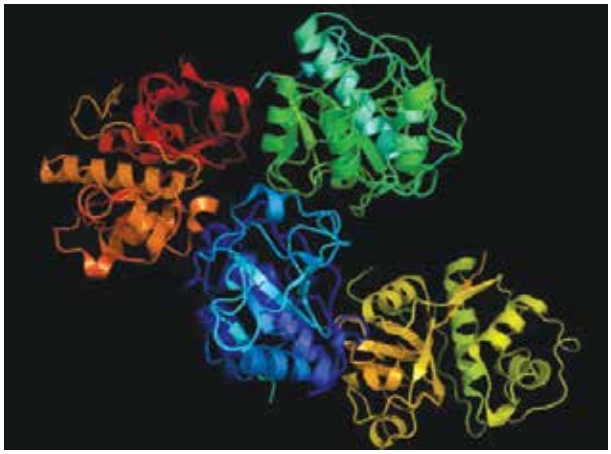
Takao Matsusaki. I asked him if he knew of any professor that could use my help. Prof. Matsusaki introduced me to Prof. Hideaki Moriyama, who invited me to work with him and I agreed. I spent four months (August to November, 2001) as an Invited Research Professor at the Japan Synchrotron Radiation Research Institute (JASRI/SPring-8) Japan.

The Japan Synchrotron Radiation Research Institute (JASRI/SPring-8) Japan. L-R: Manuel Soriano-García, Hideaki Moriyama and Cynthia Lesh (2001).

During my stay I helped crystallize some proteins that were of special interest to Prof. Moriyama. While I was there I was also able to obtain protein crystals of a globulin protein isolated from Amaranth seeds.

I was invited in February 2004 to give a lecture to a group of Amaranth farmers. I gave my talk as simply as possible. The farmers came and thanked me for the talk. One was quite frank, and in front of several people he said, "Doctor we did not understand your talk. You had beautiful slides with beautiful colors. The real questions are: What did it all mean? What can we, as Amaranth farmers, do with this information?" These questions made me realize that I could use my knowledge with proteins and crystallography to develop a product that would use the Amaranth seed. This product could have great potential.

In 2004, my graduate student crystallized an ancient proteolytic enzyme called Mexicain. During the Aztec Empire it was used it as a meat tenderizer. I solved the crystal structure and the action mechanism of this enzyme was elucidated using X-ray crystallography.



An ancient proteolytic enzyme called Mexicain. This enzyme was used as a meat tenderizer during the Aztec Empire in Mexico (PDB 2BDZ).

In 2004 I also started having terrible pains and swelling in the joints of two fingers in my right hand and the pain continued for several months. I decided to go to the doctor and he prescribed an analgesic. Not pleased with this prescription, I returned to my laboratory and decided to investigate this problem. I found that selenium and gold were used to alleviate pain and swelling in the joints. A few days later I received an invitation to write a review in the *Journal of Medicinal Chemistry*. I immediately replied to the editor and the title of the review was "Organoselenium compounds as potential therapeutic and chemopreventive agents: A review."

Several organoselenium compounds were prepared and the anti-inflammatory activity was tested on Wistar rats. The results were satisfactory. I made a cream with one of these compounds and put some of it on my affected joints. Lo and behold, the pain and swelling disappeared. I solved the problem of pain and swelling of the joints.

The more I use crystallography, the more applications I find. I believe so much in this that I asked my wife and son about starting a company together. I knew it would be hard but thought it was worth a try. We named the company Gastronomía Molecular S. A. (Molecular Gastronomy). This name came from gastronomía, which is related to nutrition, and molecular related to crystallography. I have so many ideas going on in my head all the time that this would be the best way to try them out. At the present time my son Simon is the CEO of this company.

Founders of Gastronomía Molecular S. A. L-R: Cynthia Lesh, Manuel Soriano-García and Simon M. Soriano-Lesh. April 24, 2014. National Awards in Productivity and Entrepreneur, 2014, presented by the National Institute of the Entrepreneur and Ministry of Economy of Mexico.

Because I did not have any backing, either from the university for my research or from private sources, I did not know what to do. That is where Dr. Alejandro Rodriguez from the Tecsiquim SA de CV came to my rescue. He helped me to produce my products at the industrial level. I wish to thank him for his generosity and friendship that has helped me through thick and thin.

For the last several years I have been invited to give many interviews on the radio, TV, magazines, and newspapers. I received four national awards for the work I have done. The first was the National City Award in Innovations "Heberto Castillo, Engineer," in 2012. The next were the National Award in Productivity and the National Entrepreneur Award both in 2014. These were given by the Economy Secretary in

Mexico. The last one was the National Award in Health 2014 given by Confederation of Employers of the Mexican Republic (COPARMEX). All these awards were given due to innovations, high quality and performance of my products.

National Awards in Productivity and Entrepreneur, 2014. L-R: Iidelfonso Guajardo, Economy Secretary; Manuel Soriano–García; Enrique Peña–Nieto, President of Mexico; Emilio Chuayffet, Education Secretary.

I continued working with several small proteins isolated from the Amaranth seeds called Non-specific Lipid Transfer Proteins (LTP) in plants and some other small proteins with great antibacterial and antifungal activities.

Now, do not forget I am doing all of this while I am still working at the Chemistry Institute during the day. During the afternoon and evening hours I work at our company.

I should mention that all my work has been done at UNAM, and I never left my working position in Mexico even under very difficult working conditions with limited funds and no support to attend any academic event. When I attended any academic event inside or outside of Mexico I had to pay for all my expenses such as registration, airplane tickets, hotel and food.

Since 1973 when I started working in the field of crystallography, my research productivity has been to publish 265 research papers in different national and international journals, to guide 10 undergraduate students, 16 with a Master in Science degree and 14 Ph.D. students, seven patents, and many presentation of my work at different academic events.

My solid academic background and extensive experience in the work of basic research, as well as my particular vocation, passion for science and endearing identity by the natural resources of Mexico, have allowed me to consolidate important technological developments for the benefit of a broad sector of the population in national priority emergency areas such as food and health.

Because I have always had such an active and inquisitive mind, crystallography has helped me to work in so many different fields from basic to applied science. I think my best work as a scientist was to work on the practical applications of crystallography to develop several innovative products that have helped thousands of people. I am very satisfied with my work.

I would to thank crystallography for magnifying my horizons.

Manuel Soriano-García

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Frank Fronczek

Puzzle Corner

We have new Crystal Connections and DISORDERED puzzles, solutions to the previous ones, and mention of those who provided solutions.

Crystal Connections #10
What do the answers to these clues have in common?

1) _____ springs eternal in the human breast. – *Pope*

2) That which we call a _____ by any other name would smell as sweet. – *Romeo and Juliet*, Act II, Scene II

3) Crater near the moon's southeastern limb; type of screwdriver

4) City in Kansas; county in South Dakota

5) Verb (*t*) – to correct a space group, particularly one of unnecessarily low symmetry

6) Originally Karfunkle

7) Name of his widely-used software is based on his own name

8) Acronym for Institute of Biological, Environmental and Rural Sciences, Wales

9) Das _____– First opera of *Der Ring des Nibelungen*, Richard Wagner

10) Color most commonly used by Rembrandt van Rijn, particularly in his later years.

Solution to Guest Puzzler, Bill Ojala's Crystal Connections (#9)
Words in song titles that are also used in crystallography

1) *Two Faces Have I* – Lou Christie, 1963

2) *Leader of the Pack* – The Shangri-Las, 1964; Twisted Sister, 1985

3) *Reflections* – The Supremes, 1967

4) *The Crystal Ship* – The Doors, 1967

5) *Crystal Blue Persuasion* – Tommy James and the Shondells, 1968

6) *Reflections of My Life* – The Marmalade, 1969

7) *Crystal* – Stevie Nicks & Lindsay Buckingham, 1973

8) *Music and the Mirror* – From *A Chorus Line*, 1975

9) *Centerfield* – John Fogerty, 1985

10) *Man in the Mirror* – Michael Jackson, 1988

11) *Glide* – Phish, 1992

12) *Perfect Symmetry* – Keane, 2008

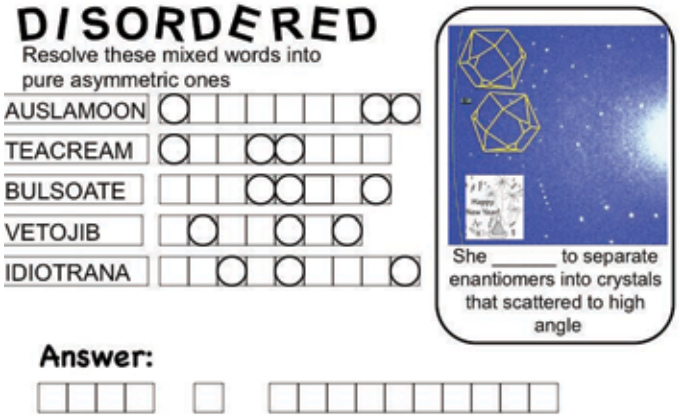
13) *Poker Face* – Lady Gaga, 2009

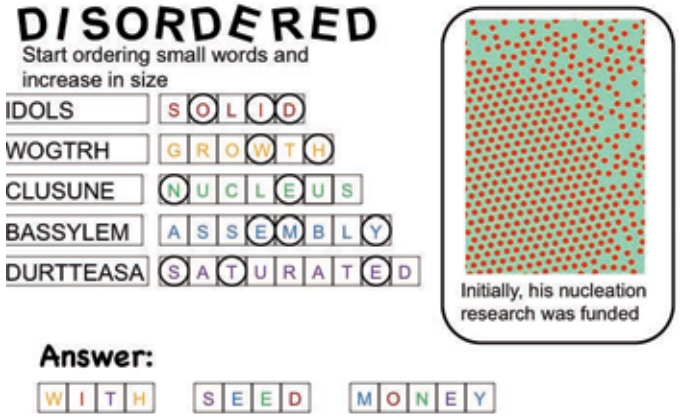
Note: By timely coincidence, *The Bad Astronomer* Phil Plait began his comments at the Denver ACA meeting banquet with mention of song #5 *Crystal Blue Persuasion*, but didn't get around to mentioning any of the other songs.

Frances Bernstein was first to provide the solution to the Crystal Connections puzzle #9, and **Christine Beavers** solved the DISORDERED puzzle. We inadvertently neglected to give the names of puzzle solvers in the winter issue. **Frances Bernstein** also solved Connections #8, and **Ilia Guzei** solved the quasicrystal 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
ffroncz@lsu.edu





MAY 2017

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

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

JUNE 2017

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

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

18-23 **Modern Methods in Rietveld Refinement for Structural Analysis**. Oak Ridge, TN
http://conference.sns.gov/mmrrsa

JULY 2017

2-7 **4th European Crystallographic School – ECS4**. Warsaw, Poland
http://ecs4.ecanews.org

9-13 **International Conference on Neutron Scattering**. 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

20-25 **XXVI International Materials Research Congress**. Cancun, Mexico
http://www.mrs.org/imrc-2017

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

OCTOBER 2017

16-31 **X-ray Methods in Structural Biology**. Cold Spring Harbor, NY
https://meetings.cshl.edu/courses

NOVEMBER 2017

13-23 **Macromolecular Crystallography School 2017**. Montevideo, Uruguay
http://pasteur.uy/mx2017

26-Dec 1 **MRS Fall Meeting & Exhibit**. Boston, MA
www.mrs.org/fall2017

JULY 2018

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

JULY 2019

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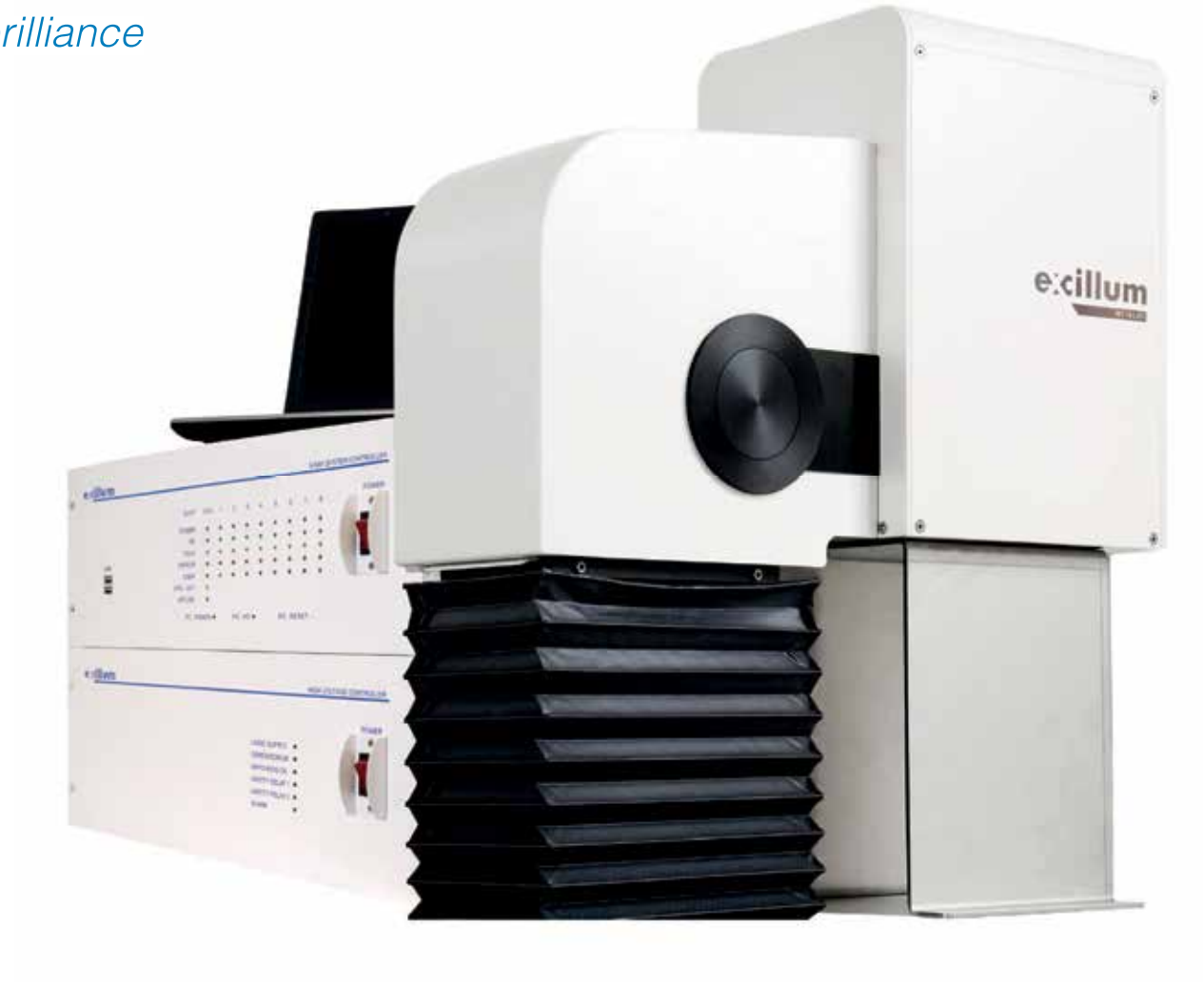

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