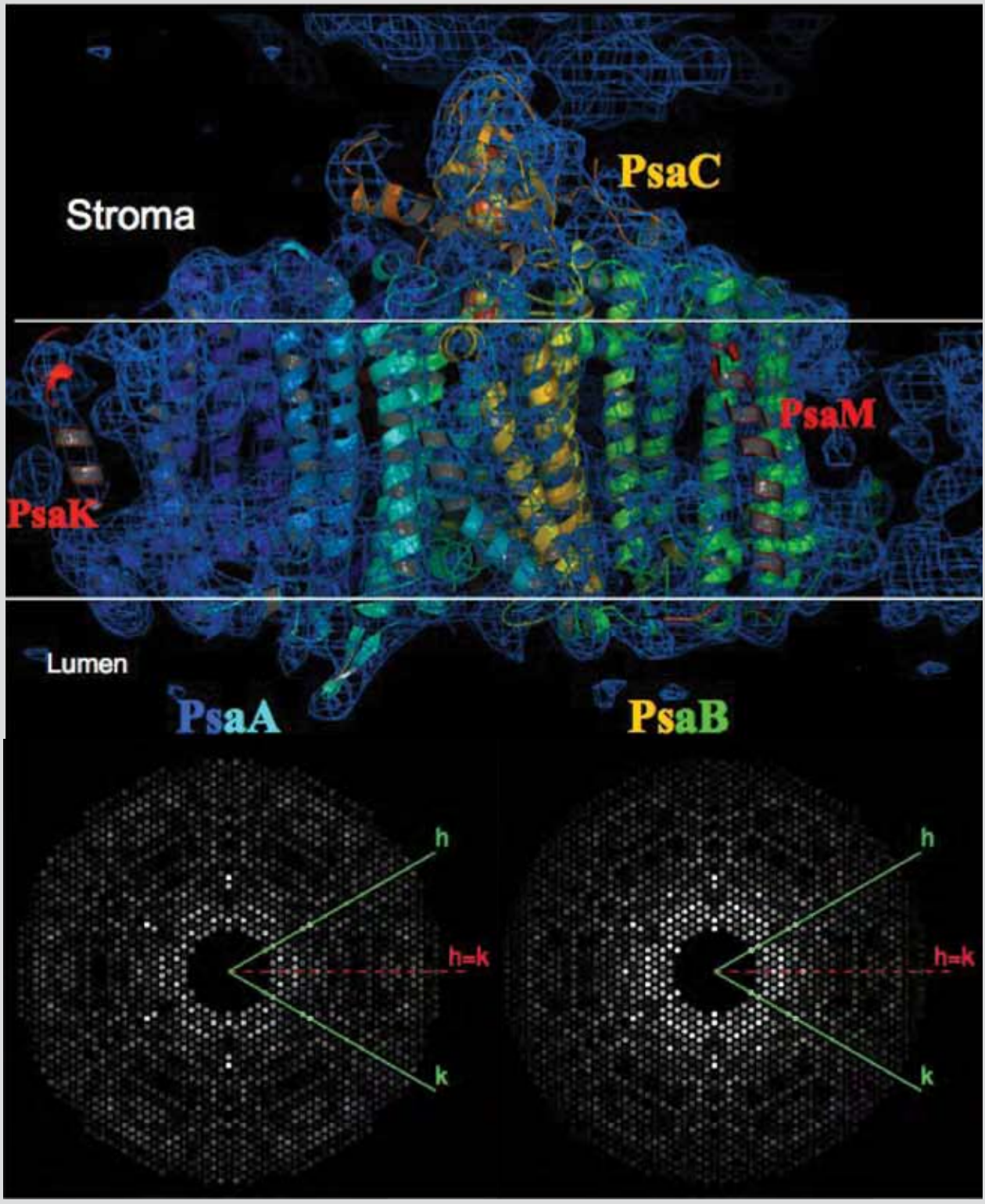
ACA RefleXions

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION

Number 2 Summer 2012



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American Crystallographic Association

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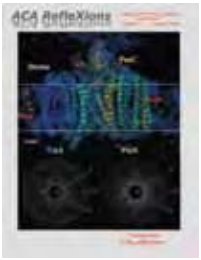

What's on the Cover - page 40

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Presidents Column

Well, here's another update on what happening with the ACA. First of all, I hope you are looking forward as much as I am to the upcoming meeting in Boston July 28-August 1. The organizers have got a real show set up for you, and the mood is set to celebrate the century of progress since Max von Laue and the father-son Bragg team founded the field of x-ray crystallography. Plus, Beantown is great place to be in the summer. The 2013 meeting is set for Honolulu, which was very well attended when we last had a meeting there, so get your grass skirts and longboards ready.

There have been some other interesting developments that I also want to share with you. First of all, the first steps have been taken to establish a Latin American Division of the ACA, to go along with the Canadian Division. This would allow formal participation in the ACA of all crystallographers in the western hemisphere. We expect to have an interim Latin American Division Council member appointed soon and are hoping to have one of our ACA scientific meetings somewhere in Latin America in the next few years. Send your ideas in to us about potential locations. ¡Es bueno! C'est bien! It's good!

On another front, the ACA Council has agreed to begin a strategic planning process. No one can remember if this has been done since the original founding. This will give all the ACA stakeholders a chance to review everything from our mission statement to operations procedures, and to both set and steer a course that serves our membership well into the future. Members will have ample opportunities to get involved in the process and there will be vote(s) by the members to formalize the plan when the time comes.

On the financial front, I can report that we are on track toward our goal of having reserve funds approximately equal to one year's worth of operating expenses. However, we are also well aware that one bad year could put us in serious trouble so please do your part as a member by keeping your dues current and getting involved. One good way to get involved is by helping us grow the membership. One other piece of financial news is that we now have a Donate Now button on the website (found under the awards button on the top menu bar). It would be great to be able to raise the honorarium connected to our major awards and, if you have been enjoying the living history articles in *RefleXions* you might consider supporting the new 'History Fund' that will be used to help record our heritage, including recording of special lectures and making more historical documents available on our web site.

Let's all find some way to contribute to the special festive celebrations of a hundred years of x-ray crystallography. The view from the shoulders of our own giants is indeed spectacular.

George Phillips

At the spring council meeting. Back row: Canadian representative - David Rose, CEO - Bill Duax, Past-president - Tom Koetzle, Secretary - Patrick Loll, YSSIG representative - Jamaine Davis. Front row: Administrative manager - Marcia Colquhoun, CFO - S. N. Rao, Vice-president - Cheryl Klein Stevens, President - George Phillips. Inset lower right: IUCr representative - Marvin Hackert.

News from Canada

This was a special anniversary for the regional BHT meeting, the 20th Annual Meeting. BHT (Buffalo-Hamilton-Toronto) now extends far beyond its original locations, including participants from Rochester, London, Guelph, Kingston and Waterloo. Apart from the first 3 years or so, the meeting has been held at McMaster University in Hamilton, due to its central location (and excellent hosts).

Each year the meeting has featured morning technical sessions from an international expert. Early speakers included the late Herb Hauptman at the second meeting in Buffalo. As befits a special anniversary meeting, this year's visiting speaker was one of the founding fathers of macromolecular crystallography, Michael Rossmann. Michael's contributions to our field are almost too numerous to list. For the BHT, he gave a wonderful overview of the history and background of Molecular Replacement (complete with a physical demonstration of crystallographic *versus* non-crystallographic symmetry). For us old-timers it was a terrific walk down memory lane, while for the younger members, it was a stimulating exposure to one of the great pioneers of our field.

Speaking of inspiring, the afternoon session featured superb talks from trainees and new investigators in the region. Twenty years ago, most of these talks consisted of progress reports on failed expression or crystallization trials. This year, it was structure after beautiful structure, a testament to how much structural biology has progressed in the region. Particularly noteworthy was that two of the new faculty members at the meeting were graduates of the region (Howell lab in this case); there were so many new investigators that only 3 could speak this year, with another 2 or more postponed until next year's meeting.

The slate of featured trainee speakers included Carter Mitchell (Gulick lab, Buffalo), John Whitney (Howell lab, Toronto), Yu Seon Chung (Guarné lab, Hamilton), Tianjun Sun (Davies lab, Kingston), Caroline Delorme (Allingham lab, Kinsgton), Sara Andres (Junop lab, Hamilton). New faculty speaking this year were Jeff Lee, Oliver Earnst and Jason Maynes (all from Toronto).

As always, the meeting was sponsored by a number of loyal vendors, who do so much to support the crystallographic community: Art Robbins, Bruker, Formulatrix, FortéBio, Hampton Research, Molecular Dimensions, Norton and Rigaku, as well as the Canadian Light Source. Before braving the rush-hour traffic, we enjoyed a wine&cheese reception sponsored by Rigaku and Art Robbins. We can only imagine what the next 20 years will bring!

Finally, I'd like to welcome Gerald Audette as the new Canadian Division Secretary, joining Michael Murphy in steering that Division. Thanks to Pawel Grochulski for his contributions, and to John Allingham for standing for election – I'm sure you will be called on next time! It is pleasing to see the Division taking an active role in the ACA annual meeting session planning, and I hope more Canadians will be inspired to join us at the meetings.

David Rose

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION, INC.
BALANCE SHEET - December 31, 2011 and 2010

	CURRENT FUNDS (2011)		TOTAL	
	Unrestricted	Restricted*	All Funds	
			2011	2010
ASSETS				
Current Assets:				
Cash	263,599		263,599	208,659
Investments	359,385	433,214	792,599	709,288
Inventory	5,923		5,923	2,225
Accounts Receivable	6,701		6,701	10,500
Total Current Assets	635,608	433,214	1,068,822	930,672
Fixed Assets:				
Computers and Printers	0		0	4,598
Office Equipment	0		0	1,300
Accumulated Depreciation	0		0	0
Total Fixed Assets	0		0	5,898
TOTAL ASSETS	635,608	433,214	1,068,822	936,570
Liabilities:				
Unearned Revenues	49,164		49,164	30,752
Credit Card Liabilities	477		477	(134)
Total Liabilities	49,641		49,641	30,618
Fund Balance:				
Unrestricted	585,967		585,967	498,269
Restricted		433,214	433,214	407,683
Total Fund Balance	585,967	433,214	1,019,181	905,952
TOTAL LIABILITIES & FUND BALANCE	635,608	433,214	1,068,822	936,570

*** Current Balances in individual restricted funds - as of December 31, 2011**

Bau Neutron Award	35,211
Buerger Award	37,202
Etter Award	64,596
Fankuchen Award	68,899
History Fund	749
Latin American Initiativee	3,043
Patterson Award	44,145
Pauling Award	34,835
Supper Award	12,013
Student Travel Fund	13,389
Trueblood Award	36,496
Warren Award	29,918
Wood Science Writing Award	52,718

A more detailed report on the ACA finances may be obtained by sending a written request to the ACA office in Buffalo, PO Box 96, Ellicott Station, Buffalo, NY 14205-0906.

From the Editor's Desk

On page 4 of this issue you will find the report from our CFO, SN Rao, providing the audited budget report on ACA finances at the end of 2011. Since that time additional donations have come in and the new fund totals are given here. These donations have come in as part of the membership renewal process that, until now, has been the only way to donate to your favorite funds. This is certainly an easy way to do it and I would encourage anyone who has not yet renewed to go ahead and renew your membership and consider making a donation at the same time.

Fund Name	12/31/11	3/31/2012
Bau Neutron Diffraction	35,211	35,396
Buerger	37,202	37,513
Etter / SIG	64,596	65,497
Fankuchen	68,899	69,389
Patterson	44,145	44,870
Pauling	34,835	35,560
Supper	12,013	12,088
Trueblood	36,496	37,392
Warren	29,918	30,128
Wood	52,718	53,029
Latin American Initiative	3,043	3,243
Student Travel	13,389	15,274
History Fund	749	3,009
Summer School		456
Total	433,214	442,844

For those of you who have already renewed but would like to add a bit to one of our funds you can now do it any time the mood hits using the new Donate Now button on the ACA website (***www.amercrystalassn.org/donate-page***). You can donate online or download a form that can be faxed or sent by snail mail. Not that I (the acknowledged queen of nag) would ever try to influence you but you might want to consider supporting the history fund, student travel and summer school funds. That way you can ensure that we preserve both our heritage and our future. Virginia Pett is doing a fantastic job as the ACA Historian. We have had great positive feedback on the living history articles published in *RefleXions*. In some cases we have not been able to publish the entire biography but the full article has been archived with the AIP and when we have enough money in the History Fund (unabashed plug) we will be able to make them available online through the ACA. Virginia is also working on standardizing the procedures for recording (video as well as audio) our award lectures.

Speaking of the ACA website (***www.amercrystalassn.org***) you should be checking in regularly to see what's new. You will find news that comes in between editions of *RefleXions* including notices of upcoming events and meetings and updated deadlines. In keeping with the times you can now "Friend" us on Facebook where you will find photos and interesting posts and you can stay in touch with your crystallographic colleagues by "Getting Connected" through LinkedIn.

Judy Flippen-Anderson

IUCr Partners with AIP and its UniPHY Scientific Networking Site

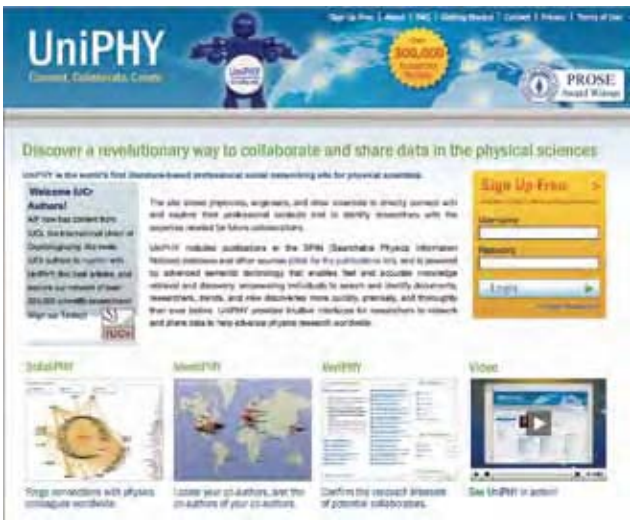
The International Union of Crystallography (IUCr) has partnered with the American Institute of Physics (AIP) to provide bibliographic data from its publications to UniPHY (***www.aipuniphy.org***). UniPHY is AIP's scientific social and professional networking site designed to enhance and accelerate collaboration among physical science researchers.

The IUCr has submitted data to UniPHY from all its journals from 1948 to the present day. Physicists who publish in IUCr Journals will now be able to access abstracts and author information and expand their network with this additional data, helping them to advance their research and raise their profiles within their community.

UniPHY's "six-degrees"-style mapping allows users to discover the research conducted by more than 300,000 of their colleagues and follow a web of connections showing the co-authors that have worked with these colleagues. Other features include discussion groups, recommend an article, congratulate an author, job postings and upcoming industry events.

Researchers who have published at least three physics articles in IUCr publications may already have a profile on UniPHY. If not, they can simply sign up (***www.aipuniphy.org/Portal/Registration.aspx***)and then use UniPHY's Publication Wizard to create their profile by adding their articles individually. As more scientists and research articles are added to UniPHY, it will become a more robust resource for the entire scientific community.

Andrea Sharpe



Errata: In the spring 2012 issue of *RefleXions* we listed Camille Jones as Camille Young on the USNCCr members page. As of this writing Camille's contact info has not changed from what was published in the spring. Our apologies and thanks to Camille for bringing it to our attention.

The 7th Meeting of the Argentinian Crystallography Association (AACr, San Carlos de Bariloche, Argentina, November 2 – 4, 2011.

Approximately 100 participants from different provinces of Argentina were in attendance, giving the meeting a true national relevance. Other countries represented included: Brazil, Uruguay, Venezuela, Spain and France. The meeting included 4 plenary talks (Gabriel Cuello, Oscar Piro, Griselda Polla and Juan Manuel García Ruiz), one special talk given as Instituto Balseiro Colloquium (Juan Rodríguez-Carvajal), 10 oral presentations, 90 posters and a panel discussion on large facilities for crystallography research. In addition, a special session was held in memory of Andrés Goeta, an outstanding Argentinian crystallographer working at Durham University (UK), who passed away in July of 2010.

A satellite event, the 3rd School of Crystallography which focused on x-ray and neutron diffraction in polycrystalline materials, was held from November 7th to the 18th and was partially supported by the IUCr. It was attended by 41 students, mostly from Argentina, but also some from Brazil, Uruguay and Colombia. This School was divided into two modules. The first module, led by Juan Rodríguez-Carvajal and Gabriel Cuello, consisted of a compact version of the well-established "FullProf School" held annually at the Institut Laue-Langevin in Grenoble. The second module, led by Raúl Bolmaro, Javier Santisteban, Miguel Vicente-Álvarez, Aldo Craievich and Eduardo Granado, focused on scientific and technological applications in polycrystals, such as internal stresses and strains, texture and size effects, and synchrotron radiation techniques. Lectures and special topics given by invited speakers were held in the morning sessions with the afternoons dedicated to several supplementary demonstrations and practical sessions during which the students worked on real problems.

As usual, the ordinary AACr Annual Assembly was held during the meeting, where new authorities of the association were elected and it was confirmed that the 8th Meeting will be held in Santa Fe from October 31 to November 2, 2012. The 4th School of Crystallography will focus on fundamentals and applications of x-ray powder diffraction, and will include a workshop on synchrotron light techniques for materials characterization. It was also decided that the 9th Meeting will be held in 2013 at Córdoba and crystallographers of other Latin American countries will be invited to organize this event as the First Latin American Congress on Crystallography.

Diego G. Lamas Gabriela Aurelio

Contributors to this issue: Gabriela Aurelio, Chuck Campana, Graciela Delgado, Jeanette Ferrara, Joe Ferrara, Frank Fronczek, Jenny Glusker, James Kaduk, Janos Kirz, Diego Lamas, Eaton Lattman, Aline McNaull, Virginia Pett, George Phillips, S.N. Rao , David Rose, Nick Salvaggi, Carl Schwalbe, Andrea Sharpe, Richard Staples, Martha Teeter, Tom Terwilliger, and Kraig Wheeler Photo from the LA ACA meeting provided by Bill Duax.

Cover: Images provided by John Spence.

Cartoons: Pages 8 and 36, courtesy of Randall Munro (***xkcd.com).***

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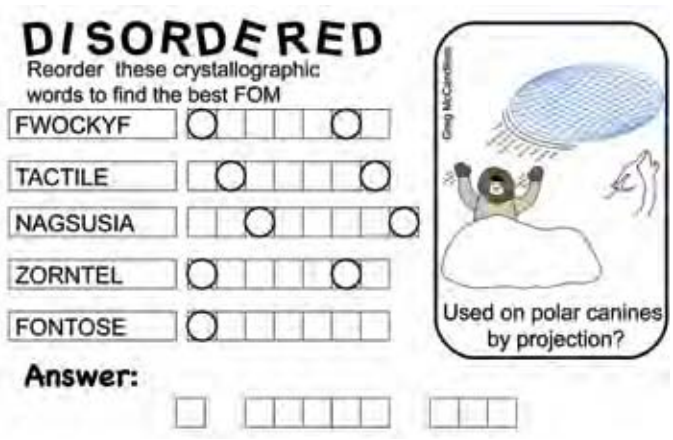
***Answer to the puzzle in the spring ACA RefleXions*:**

"So we must be sure that our product is the result of care and thought, not expediency. I believe that it is better to do a thorough job than a hasty one, to work carefully on a limited number of projects rather than to rush after a larger number of less considered results." ***Dick Marsh, ACA President, 1993.***

A. Turns light just right?	**D**EXTROROTATORY
B. Fish people	**I**CHTHYOLOGISTS
C.How Pauling often solved problems; he	**C**ONJECTURED (***Dick worked with Pauling on amino acids***)
D. Kind of vacuum	**K**IRBY ***(Dick has a daughter named Kirby)***
E. Threatened soap use	**M**OUTHWASH
F. Curing phthisis	**A**NTITUBERCULAR
G. Smashed Iceland spar fragments	**R**HOMBOHEDRA
H. Theophrastus wrote on them	**S**TONES
I. State capital in Lewis and Clark county	**H**ELENA ***(Dick's wife is named Helen)***
J. Passages at the end of a book	**A**FTERWORDS
K. AB - BA if A, B are operators; slip ring wired to act as rotary switch	**C**OMMUTATOR
L. The molecule _____ a conformation ... *Acta Cryst*. B**29** 1611	**A**DOPTS ***(authors: H Einspahr, JB Robert, RE Marsh & JD Roberts)***
M. What scholarship isn't in JACS	**P**UBLISHABLE ***(Dick had a paper of corrections rejected, since JACS doesn't publish "works of scholarship")***
N. Restores to youthfulness	**R**EJUVENATES
O. A good place to reach 72 (two words)	**E**IGHTEENTH HOLE ***(In college, Dick majored in golf)***
P. Set of atoms in a unit cell having a simpler pattern than the whole	**S**UBSTRUCTURE
Q. The filling in of intermediate values	**I**NTERPOLATION
R. Those unlikely to succeed at clue 'O'	**D**UFFERS ***(definitely NOT Dick)***
S. Fete use of crawfish or shrimp dishes served over rice	**E**TOUFFEES ***(Helen Marsh is from New Orleans, and Dick spent time there in the Navy)***
T. Air broken? This will fix most of it naturally	**N**ITROGENASE
U. [Type of] forms occur[ing] when we have a union of one-fourth of all the similar possible planes ... of any crystallographic system (Marshman Edward Wadsworth)	**T**ETARTOHEDRAL

Notes: The puzzle was written by Charlene Tsay and Larry Henling to honor Dick Marsh on the occasion of his 90th birthday in March. It was attributed to "Charlene Lawrence", a pseudonym of the two authors. The quotation comes from "Corrigenda Publications of Richard E. Marsh 1953-1993" by Charles Simmons. Many of the clues contain allusions to Dick's career, family and past, given in ***blue*** in the answers. An additional clue for S was that "fete use of" is an anagram for the answer.



Crystal Engineering - A Textbook by G. R. Desiraju, J. J. Vittal and A. Ramanan , World Scientific Publishing Co. Pte. Ltd. 2011, ISBN: 978-981-4366-86-1

The authors claim that the book can be read in one sitting or in many. I chose the former (a 14 hour flight helps) but the latter is necessary for use as a textbook. The book is easy to read and very well written. It is divided into 7 chapters with wide margins to allow for ancillary information, elaborate on complex ideas or provide historical context. Each chapter closes with a summary, bibliography and problems. The book ends with an extensive glossary, a brief summary of space group data, a list of websites and further reading.

Chapter 1 is an introduction that provides historical context. Chapter 2 looks at how intermolecular interactions affect the solid state. Some basic information is provided about how interactions are observed and, with an emphasis on crystallography, the methods used to study interactions that yield crystals. Chapter 3 discusses synthesis and introduces the concept of a synthon - a moiety that provides a basis for creating a network. Chapter 4 takes an in-depth look at crystallization methods from thermodynamic and kinetic perspectives. Chapter 5 discusses polymorphism and its implications for industry, particularly the pharmaceutical industry. Chapter 6 reviews multi-component crystals, again with some emphasis on the pharmaceutical industry. The final chapter provides a current view of the state of coordination polymers, which is perhaps the largest part of the field of crystal engineering today. A number of applications are provided here and this finishes the book nicely.

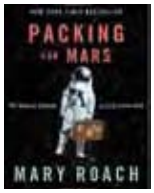
On China by Henry Kissinger, Penguin Press, 2011, ISBN-13: 978-1594202711

Who remembers the first person (at least as far back as I remember) for which the issue of changing the constitutional requirement of birth in the US for a president was seriously considered? It wasn't Arnold Schwarzenegger - it was Kissinger. This book will help you understand why. Kissinger starts off with a short history of China up to 1949 to give a basic understanding of how the Chinese came to be the way they are and how they think. He tells us that the strategy employed in the game *wei qi* is the paradigm of Chinese thinking. *Wei qi*, or "the Japanese," is a game of long-term strategy, as opposed to chess, which is a game of short-term strategy. I am told that *wei qi* has eluded computer modeling because the pieces that have not yet been played are unknown to the computer, which makes the game difficult to simulate.

Once Kissinger has provided the background necessary to understand China, he takes us through the first two decades of Mao Zedong's rule, including the revolution, the Korean War, the Great Leap Forward and the Cultural Revolution. While he makes this all quite interesting, I found most enlightening his own account of his secret meeting with Zhou Enlai that initiated the rapprochement that culminated with Nixon's visit in 1972. His narrative continues through the terms of Deng Xiaoping and Jiang Zemin with the ups and downs of the relationship between China and the US, and China and its neighbors. There are bits of history that I had totally forgotten, including the Third Vietnam War. He ends with some wisdom about the importance of sustaining the relationship between China and the US, as they are two nations that share a common ocean.

Joseph D. Ferrara

Packing for Mars: The Curious Science of Life in the Void
by Mary Roach, WW Norton & Co., 2010, ISBN 13: 978-0-393-068474



In *Packing for Mars*, Mary Roach explores the numerous (and often less mainstream) trials and tribulations astronauts in training must undergo before they achieve clearance for travel to outer space.

The book is chock-full of interesting tidbits of information about NASA and its practices and policies. Roach balances the sometimes overwhelming ideas (not overwhelming conceptually, more overwhelming to the senses; an entire chapter is dedicated to discussing the difficulties and dilemmas of liquid and solid excretion in zero gravity) with anecdotal footnotes and a witty, deadpan sense of humor. She exhibits an acute attention to detail and an unparalleled inquisitiveness as she digs into the past, present, and future of space travel. The book is a fast-paced and energetic read, a means for those with little or no knowledge or experience in extraterrestrial affairs to learn a lot about something new.

Among the topics Roach delves into are: the procedures by which potential Japanese astronauts are assessed and tested for desirable qualities by JAXA (the Japanese equivalent of NASA), both in intellect and personality (think solitary confinement and 1000 origami paper cranes, each methodologically analyzed for signs of psychological deterioration in the test subject); the psychology of isolation and confinement, or how NASA attempts to assess how the human brain reacts to extended periods of forced asocial conditions; the effects of space travel on the psyche, or how a number of former astronauts (think Lisa Nowak) have exhibited signs of mental instability following "out of this world" ventures; the dangers of life in zero gravity and the perpetual plague of motion sickness which afflicts many astronauts-in-training and even those who make it to the moon (although Roach does debunk the myth that barfing in a spacesuit will result in death by vomit; astronauts are not supposed to be intoxicated, as Jimi Hendrix was); the careers of two space chimps, Ham and Enos, who were only two of the many non-human mammalian test subjects used for assessing the effects of space travel on the human body; and the nausea-inducing nature of freeze-dried cuisine (tomato paste anyone?) and other aerospace delicacies (corned beef sandwiches + zero gravity = crumb snowstorm). This is not an exhaustive list, merely a glimpse of the breadth and wealth of material Roach covers in her work.

Perhaps my favorite anecdote is that of the NASA crash test dummy. Unlike the creepy mannequins from car commercials, the National Aeronautics and Space Administration uses cadavers. They are frozen after death, and thawed for several days prior to testing. These cadavers are used to provide more accurate information concerning the effects of higher G forces applied laterally, longitudinally, and transversely. It is difficult to simulate the effects of a human body in a crash on a mannequin because of the intricacies of organ places in the abdominal cavity. Also, one of the most important things to study in a crash test is the effect of the crash on the brain (which mannequins do not possess).

All in all, *Packing for Mars* is an engaging and enjoyable read, appropriate for science enthusiasts and other people of a curious nature.

Jeanette S. Ferrara, Princeton, Class of 2015

DAVID SAYRE (1924 – 2012)

When I wrote David to congratulate him on being selected for the IUCr Ewald Prize he replied asking if I knew who was on the selection committee: "Not that I would do anything about it, but I would be very interested to know what might have motivated the selection of the single-particle concept, which to date has produced very little in the way of important science, when crystallography itself is producing such fantastically important science." As I did not know who was on the committee I sent him the text of the announcement of the prize: "The IUCr is pleased to announce that Dr. D. Sayre has been awarded the eighth Ewald Prize for the unique breadth of his contributions to crystallography, which range from seminal contributions to the solving of the phase problem to the complex physics of imaging generic objects by X-ray diffraction and microscopy, and for never losing touch with the physical reality of the processes involved." To which he replied "thanks that helps a little".

To me that exchange represented the quintessential David Sayre and it seemed appropriate to start this appreciation of his life with the article Martin Buerger wrote for *Crystallography in North America* (edited by Dan McLachlan, Jr. and Jenny P. Glusker, ACA, 1983) in which he refers to the fact that in 1950 David was already in touch with the physical reality of the processes involved in our science. Buerger's article also presents the chronology of the formation of the ACA which makes it a fitting addition to our history project in its own right.

Following Buerger's article are three views of David Sayre: a retrospective on his accomplishments by Jenny Glusker and two more personal interactions by Janos Kirz and Ed Lattman.

Judy Flippen-Anderson

Background and Early History of the American Crystallographic Association *

The American Crystallographic Association began life on January 1, 1950. It held its first meeting on April 10-12 of that year at Pennsylvania State College in State College, Pennsylvania. Today, a little over a quarter of a century later (***editors note: this article was written in 1974***), the society holds its 25th meeting in the same locality, and we find that the place is called University Park, the home of Pennsylvania State University.

Six years after its first meeting the origin of the ACA was outlined by William Parrish and Betty Wood in Volume IV of the *Norelco Reporter.* There it is recorded that the ACA is the successor of the American Society of X-Ray and Electron Diffraction and the Crystallographic Society of America (CSA). These two societies had begun their lives as the second world war was beginning to disturb the world. Two separate groups had begun to raise the question of the usefulness of establishing a journal for crystallographic research and this eventually stimulated the formation of the International Union of Crystallography which then not only took over the *"International Tables for X-Ray Crystallography,"* but a short time later established *Acta Crystallographica*. Few of you will recall the birth of the ACA, and even fewer remember the origins and acts of the two societies which eventually merged to become the ACA. It seemed useful, then, while there are a few left who took part in the acts which led to our beginning, to briefly outline the history on this occasion.

One pre-existing branch of the ACA, the CSA, had its beginning as a local organization of crystallographers in Cambridge, Massachusetts and vicinity. As I recall it, at first most of its members were a few mineralogists from the neighborhood who felt that the future of mineralogy lay in understanding the roles of crystal structures in the properties, genesis and relations between minerals. The membership included Harry Berman, Newton Buerger, Martin Buerger, William Dennen, Clifford Frondel, Cornelius Hurlbut and Joseph Lukesh as well as the chemists Cutler West, I. Fankuchen and others. According to a remark in a letter from M. J. Buerger to Paul Kerr dated May 1, 1941, this group began to meet in the winter of 1939 for the purpose of discussing their research results with each other. The meager records which remain show that I. Fankuchen addressed the second meeting, held May 1, 1941 at Harvard University, on the subject "Preparation and Handling of Small Crystals" in which, among other things, the prototype of all twiddlers was described. Volume 95 of *Science,* which appeared on January 2, 1942, contains a note from the secretary of the society, Clifford Frondel, to the effect that after the business meeting of November 17, 1941, held at MIT, Joseph Lukesh addressed the assembled crystallographers on "The Tridymite Problem." At the meeting on April 24, 1942, at MIT, Percy Bridgman gave an invited lecture on a crystallographic aspect of his high-pressure work, which he entitled "Polymorphism at High Pressures." After this there appears to have been a hiatus in the activities of the society due to preoccupation with war work. During this period the society lost its vice-president, Harry Berman, as a casualty of the war. When the war finally ended the society prepared for a large meeting, held at Smith College on March 21-23, 1946. On this occasion the small local society of crystallographers assumed the status of a national society. At the Smith College meeting, papers were presented by Richard S. Bear, J. D. H. Donnay, Howard Evans, I. Fankuchen, Samuel Gordon, Joseph Lukesh, Dan Mclachlan, Benjamin Schaub, Newman Thibault, Edward Washken, Cutler West, and Dorothy Wrinch. The abstracts of their papers were published in the *American Mineralogist,* as were the abstracts of papers given at later meetings.

From the time of the earliest meetings of the Cambridge crystallographers, the possibility of launching a journal of crystallography was considered; indeed an estimate of possible subscribers was made and the financing of the undertaking discussed. Unfortunately it was found that a subsidy would be necessary to begin publication, and the society had no success in arranging for one.

The members of the American Crystallographic Society (ACS), which included biologists, ceramists, chemists, mineralogists and physicists, had banded together to present the results of their crystallographic research to one another because their own professional societies offered them little encouragement and limited discussion. In such meetings their results were overwhelmed by the routine and classical results, and their own results were little appreciated.

Meanwhile certain chemists had found some relief from this situation. Many interested in the new results coming from the study of the atomic arrangement in solid matter were members of the National Research Council's Division of Chemistry, Committee on X-Ray and Electron Diffraction, then chaired by Maurice L. Huggins. Stimulated by the efforts of the ACS to establish a journal devoted to crystallography, Huggins called a conference under the auspices of the NRC Committee on X-Ray and Electron Diffraction to be held at the American Museum of Natural History in New York, June 10-11, 1941. Although no action was taken to go ahead with the journal, the attendants did agree to form a society of structure researchers. The NRC Committee on X-ray and Electron Diffraction (to which I had been appointed in 1940) took the initiative in organizing the society, and its constitution was adopted at the Gibson Island meeting of July 30,1941. Huggins was elected its first president and Warren its first vice- president, to succeed to the presidency the next year. The second meeting was held in Cambridge, Massachusetts, December 31, 1941. Meanwhile, many names had been considered for the new society; the one finally chosen by written ballot from the many submitted was 'The American Society for X-Ray and Electron Diffraction," which was abbreviated ASXRED. Thus this precursor of the ACA took its name from the name of the committee which brought it into existence.

There were now two societies concerned with different aspects of crystallography. Some believed that the societies were in competition and felt it would be to the advantage of both to join forces. Others pointed out that the ASXRED was named after a tool which, though important to crystallographic testing and research, did not begin to represent the whole science of crystallography, and could, indeed, pass out of existence, as did the optical goniometer. In 1948 a joint committee of the ASXRED and the CSA was formed to consider the consolidation of the two societies. Their report was sent to both societies. The membership of the ASXRED discussed the proposal for joining on December 19, 1948 and the CSA on April 8, 1949. Both memberships voted for consolidation. The two societies merged into the American Crystallographic Association on January 1, 1950. The new society held its first meeting on April 10-12 at Pennsylvania State College, as a continuation of the Conference on Computing Methods and the Phase Problem, which had been organized by Ray Pepinsky.

From all this it is apparent that, while the ACA is formally 25 years old, its roots are older. The ASXRED and the CSA are not parents, but earlier divisions of the ACA, so that our beginnings extend back at least to 1938 and 1941.

From this broader point of view, what has been accomplished until now? Perhaps most important is that the interests of the root societies in a journal devoted to crystallography was the stimulus which eventually launched the International Union of Crystallography and *Acta Crystallographica*. This came about in the following way: As president of the ASXRED in 1943, I realized the need of a vehicle to publish articles too long for the ordinary journal. Accordingly, I appointed a committee consisting of J. D. H. Donnay, George Tunell, and myself to see what could be done. We circulated a memorandum to the membership of the ASXRED sounding them out on their interest in a possible monograph series. They authorized us to go ahead. To finance the undertaking, I solicited contributions from companies who were in the business of making x-ray diffraction equipment and received support from The General Electric X-Ray Corp., Machlett Laboratories, North American Philips, and Picker X-Ray Corp. These contributions were placed in a revolving fund. The monographs were distributed free to all members of the ASXRED but sold to all others. Two monographs were published by the ASXRED before the advent of the ACA. The CSA published one monograph during the same period.

On instruction from the membership of the ASXRED, and as chairman of the Monograph Committee, I wrote on October 16, 1944 to H. Lipson, Secretary of the X-Ray Analysis Group of Cambridge, England, telling them of our Monograph Series and informing them of our interest in establishing a journal. I expressed the hope that the X-Ray Analysis Group would join with us in this project. Lipson called a meeting of that group on November 18, 1944 to consider this and other business. Eventually Sir Lawrence Bragg, chairman of the X-Ray Analysis Group, suggested that the Americans send a delegation to England to discuss the possibility of publishing a journal and to consider the formation of an International Union of Crystallography. The meeting was eventually set for July 12 and 13, 1946. The American delegation included Fankuchen, Donnay, Germer, Harker, Wyckoff, McLachlan, Zachariasen and myself. From this meeting arose the International Union of Crystallography, *Acta Crystallographica* and plans for a new edition of the *"International Tables."*

Among the several noteworthy accomplishments of the ACA are the solution of numerous crystal structures whose reports have so filled the pages of *Acta Crystallographica* that the journal had to be split into two parts per volume and other material separated into another journal. It would be interesting to see an analysis of these contributions, but I make no attempt to do that here. I would, however, like to note that in one field of crystallography, the main channel has been outlined by members of the ASXRED, although contributions have come from many countries, namely, the direct methods of crystal-structure analysis.

I believe I had the honor of presenting the break which led to the hope of developing direct methods. At the Lake George meeting of the ASXRED in 1946 I presented the *implication diagram*. This results from a simple characteristic rotation and shrinking of the Harker section of the Patterson function. It has the property, in favorable space groups, of mapping the locations of atoms in a projection of the crystal structure. In less favorable space groups this desired result is accompanied by certain ambiguities and satellites. I demonstrated the use of the theory by solving the structure of the mineral nepheline, space group $P6_3$. That a structure could be solved by use of reflection

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magnitudes alone was a surprising result and it was greeted with no little incredulity. But Fankuchen immediately pointed out that since this could be done it implied that there must exist phase information hidden among the collection of reflection magnitudes. This was a stunning conclusion, for up to this time it had been believed that since the phases were experimentally unobservable, they were hopelessly missing and there was not any direct route to the solution of a crystal structure. By the time of the next ASXRED meeting at Ste. Marguerite in 1947, the Harker-Kasper inequalities were presented. These provided phase information under certain conditions, so there could no longer be any doubt that phase information was contained in the set of reflection magnitudes.

In subsequent meetings of the ASXRED many kinds of inequalities were reported. It is interesting that at the Conference on Computing Methods and the Phase Problem just preceding the first meeting of the ACA here in 1950, David Sayre showed that the comparison of the electron density with its square revealed that there existed some quite simple relations between the signs of certain structure factors. Sayre's conclusions inspired a spate of theoretical investigations of sign relations between structure factors. These culminated in the statistical work by Herbert Hauptman and Jerome Karle entitled *"The Solution of the Phase Problem,"* published as Monograph No. 3 of the ACA. Later this was followed by a long series of papers, mostly in *Acta Crystallographica* by Isabella Karle and J. Karle, which taught crystallographers a routine called the "Symbolic-addition method" which led to a direct determination of the crystal structure.

Although the "direct" route from diffraction intensities to the crystal structure is commonly thought to occur only in Fourier space, it may also be followed through Patterson space. In the same 1950 conference, I showed that a Patterson function can be decomposed into images of the crystal structure. In another paper in *Acta Crystallographica* entitled "A New Approach to Crystal-Structure Analysis" I presented image-seeking functions by which a Patterson function can be transformed into an approximation to the electron density function. Although many crystallographers have used this "direct" route through Patterson space, the route is less popular than the symbolic-addition method, probably because it has not been reduced to a computing routine. It is, however, a powerful "direct" method which has had no difficulty in solving an inorganic structure which has 15 non-heavy atoms and 20 oxygen atoms per asymmetric unit.

I have presented an outline of how the ACA arose from its two root societies, and some of the achievements of that period. Having solved some of the problems of the past so thoroughly that the solutions are available to other sciences as computer routines, let us not make the mistake of believing that crystallography has reached its zenith and is coasting downhill. Like all other sciences crystallography is open-ended, and the solution of crystal structures by diffraction is not its sole objective. I need only mention another phase problem as an example. It should be possible to theoretically predict the structure of a phase in any phase field, and not have to discover it experimentally. At present we cannot even do this for one-component systems. Understanding phase fields and their structures is one of the many problems which should engage our attention during the next quarter century. Ladies and gentlemen of the ACA, please present your report before the end of nineteen hundred ninety nine.

**** Martin. J. Buerger: Originally presented at the 1974 Summer ACA Meeting, Pennsylvania State University***

It is with great sadness that *RefleXions* reported the death of David Sayre on February 23, 2012. He was truly a visionary scientist. When still a young physics student he realized that it was important to improve our ability to view three-dimensional images of molecules on an atomic scale. During his lifetime he played major roles in several aspects of this goal. This was recognized when he was awarded the Ewald Prize, the highest honor bestowed by the International Union of Crystallography, at the 2008 Congress in Osaka, Japan. With pride in this branch of science he wrote "I have seen a lot of history of our beautiful science. And when I speak of beauty in science, I mean the beauty of science itself, but also mean the beauty of the care that crystallographers devote to it."

David and Anne Sayre visit with Kay Onan (center) at the 1984 Fox Chase Symposium called "A Celebration of the Patterson Function".

David addressed three important scientific problems in his lifetime: (1) how to improve our ability to solve "the phase problem" in crystallography so that good electron-density maps can be obtained from x-ray diffraction data from crystals, (2) how to improve and simplify the communication between crystallographers and computers so that the calculations necessary to obtain electron-density maps will be made easier for the scientist, and (3) how to make it possible, using methods similar to those used currently by crystallographers, to "see" molecules at atomic resolution in non-crystalline (rather than just crystalline) materials.

David, whose father was a scientist, was born in New York City on March 2, 1924. He graduated from Yale University in 1943, aged 19, with a B.S. degree in physics. From there, because of World War II, he took a position as a staff member at MIT in its Radiation Laboratory. His work there on airborne radar involved electronics and circuit design. Once the war was over he joined Raymond Pepinsky's group at Auburn University, Alabama, having, as he wrote, "read one of J. M. Robertson's papers showing

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phthalocyanine, and I could find no one at Harvard who could teach me how to see molecules." In Alabama he was able to use the "X-ray Analogue Computer" (X-RAC) that had been built by Ray Pepinsky to calculate Fourier syntheses and display contour maps. In this way he could view on the X-RAC screen, for a given crystal data set, the results of computed electron-density maps obtained by introducing several different possible phase sets. For his work there at Alabama University David obtained an M.S. degree. He had married Anne Bowns, a writer, and she took a position at nearby Tuskegee Institute. After a while, however, they decided to move to Oxford University in England where David obtained a D. Phil. degree. It was there that Anne got to know Rosalind Franklin and later wrote about her and the structure of DNA.

For his doctoral thesis, which he obtained in the laboratory of Dorothy Hodgkin, David tackled the crystallographic "phase problem," that is the reclamation of the information on the relative phases of the diffracted beams that is lost during data collection. In the early 1950s many crystallographers addressed this problem and David was among them. His previous studies on electrical circuits at MIT and with X-RAC proved to be very useful in this venture. Historically, attempts to relate the atomicity of a structure to the imposition of conditions on possible values for the relative phases of diffracted beams had already been started by Ott in 1928, Banerjee in 1933, and Avrami in 1938. The further requirement of non-negativity in the resulting Fourier summation was successfully used by Harker, Lucht and Kasper in 1948 in the determination of the crystal structure of decaborane. The unexpected three-dimensional structure that they found revolutionized our understanding of the chemistry of the boron hydrides. It also led to an equation involving the relationships of phases of different structure factors to each other (Harker-Kasper inequalities). Karle and Hauptman in 1950 greatly expanded this with a full set of inequality relationships based on positivity.

Sayre's approach, which he called "atomicity-based direct phasing," was to introduce a "squaring-equation method" for use in phase determination. David worked with the general idea that atoms are small and discrete points (relative to the spaces between them) and can act as constraints on the relative phases (relative to the choice of origin) of the diffracted beams. If the electron density within a crystal consisting of equal atoms is squared, the resulting "squared" density is similar to the original density but the peaks have sharper shapes. A general result of Fourier theory is that the "squaring" of any function is equivalent to self-convoluting it. David wrote out the equation for the self-convolution of an array of structure factors and concluded that, for an equal-atom structure, the phase of $F(h)$ is related to that of the product $\Sigma F(k)F(h - k)$. (See equations1.1, 1.2, and 1.3 given in *Acta Crystallographica* **5**, 60-65, 1952. See also his article in ACA *RefleXions*, Winter 2010). This was "Sayre's equation," exact for an equal-atom structure, and a most important advance in our understanding of direct methods. David then applied his conclusion successfully to the determination of the crystal structure of hydroxyproline. In this publication, he wrote to me with respect to structure determination methods, "I gave the basic 3-step process -- examination of triplets to find initial phase sets, use of a convolutional relationship to expand the phase sets, and use of a figure of merit to make a selection -- which remained in use without essential change until fairly late in the 1980s."

$$F_H = \theta_H \sum_K F_K F_{H-K}$$

David then applied his newly found method to the determination of other crystal structures. Back in the United States David went, as a Research Associate, to the University of Pennsylvania in Philadelphia, where he worked with Peter Friedlander on the crystal structure of the carcinogenic molecule 7,12-dimethylbenz[*a*] anthracene. Together they found that this polycyclic aromatic molecule is not planar because of steric overcrowding, a feature that may enhance its interactions with certain biological molecules, such as DNA. At that time, however, a three-dimensional crystal structure determination required extensive and expensive computational assistance in view of the complexity of the equations to be solved. With a welcome offer of some free time on an IBM 701 computer in New York, David wrote a program that impressed Jim Backus of IBM so much that he "borrowed" him for the FORTRAN project in 1955; David stayed there at IBM, mostly at the T. J. Watson Research Center in Yorktown Heights, New York, until he retired in 1990.

At IBM David was the assistant project manager of the group that developed that programming language, Fortran. The aim of the team was to design a device that would translate a language that people readily understood into the binary language of a computer, and vice versa. The programming language that they developed made it easy for scientists and engineers to do their own programming and relieved them of the necessity of assigning experts to do it. Therefore it simplified communication between crystallographers and computers, and crystallographers used it as soon as it was available. David worked on important portions of this project with Dick Goldberg, and details can be found in an article published in ACA *RefleXions* in the summer of 2007. He also wrote the Fortran program manual that, as Backus wrote, "stood for some time as a unique example of a manual for a programming language..." and received much praise for producing an easily understandable book.

The ability to "see" molecules, whether in a crystal or not, continued, however, to intrigue David, and he returned to this problem. He was concerned about the "future of large-biomolecule crystallography," noting that these molecules are fragile in the x-ray beam and do not crystallize readily, if at all. Initially he worked on a possible supermicroscope but the required nature of the lens material, suitable for x-rays, provided a problem. Microscopes based on Fresnel zone plates had produced images, and David worked on these for a while, but then, in 1980, introduced the concept of "lensless imaging." His important contribution was the realization that actual crystallinity is not essential. If the object is non-crystalline (non-periodic), then the intensity pattern is continuous (unlike the pattern, intercepted as spots, from crystals). This continuous diffraction pattern, although weaker in intensity, can be sampled finely enough so that lost phase information can be found by iterative computational methods. The lack of the need for crystallinity makes it possible to

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image structures, such as that of a single biological cell, which are beyond the present capabiliity of x-ray crystallography. The availability of intense synchrotron sources of x-rays has aided this new method of *X-ray diffraction microscopy*. In the 1980's David and co-workers recorded diffraction patterns from several non-crystalline samples. In the 1990's, they were able to apply an iterative algorithm together with oversampling of the diffraction pattern (measuring more diffraction data than a crystal would provide) to find the relative phases for a diffraction pattern. The final breakthrough came when they succeeded in reconstructing a three-dimensional structure from an experimentally recorded diffraction pattern. This achievement opened up the field of *X-ray diffraction microscopy*. David described this work, done in collaboration with many others including Janos Kirz, John Miao, Henry Chapman, David Shapiro and Chris Jacobsen, when he received the Ewald Prize in Japan. He gave his award lecture to a spellbound audience, describing the opportunities that arise "when one can drop the assumption that the specimen in the diffraction experiment must be a crystal."

David has been an interactive and friendly member of ACA, receiving the Fankuchen Award in 1989, and serving several times on the US National Committee for Crystallography. He was President of ACA in 1983. His scientific studies have improved the quality of work each crystallographer can do. David was a great friend and co-edited a book with me and Guy Dodson on Dorothy Hodgkin, the mentor of the three of us. He and Anne were always a treat for Don and me to interact with at meetings. I was particularly touched when he asked me to introduce him when he received the Ewald Award. Therefore I have concentrated here on his science, as I know he would have wished. He will be greatly missed.

Jenny P. Glusker

It was a remarkable coincidence: For 1972-73 I had a Sloan Fellowship that allowed me to take a year off from teaching at Stony Brook University. I decided to use it to learn about biophysics and structural biology. Dorothy Hodgkin kindly offered to host me for the year, and mentioned that she would have one more American visitor.

The other visitor turned out to be David Sayre. He was on leave from IBM. As we met, we were both surprised to learn that our homes were barely four miles apart on Long Island.

My career up to that point was in particle physics. I had never heard of the Sayre equations, of direct methods, or even of David's central role in the genesis of FORTRAN.

Shortly after our arrival in Oxford David gave a seminar on Fresnel zone plates. He pointed out that they could be used to focus x-rays, and that IBM's microfabrication technology could be used to fabricate them with the desired characteristics. This seminar changed my life, and was the beginning of our collaboration that lasted well over 30 years.

David was a most generous collaborator. His visionary ideas guided our work throughout. Once back on Long Island I tagged along on occasion as David went on his daily commute to IBM at Yorktown Heights. David told everyone that the drive through the Bronx took "only" two hours each way, and of course he knew all the shortcuts. Nevertheless, we made it in two hours only once in my experience. But David and his wife Anne had this exquisite house at the Head of the Harbor, and moving closer to IBM was out of the question.

The long commute had advantages for me. In time, David spent more time visiting nearby Stony Brook University, rather than driving to IBM. He was warmly welcomed by faculty and students alike. He became adjunct professor, gave some highly appreciated lectures, and supervised several PhD students. This trend accelerated after his retirement from IBM in 1990. He also participated in our experimental work at the National Synchrotron Radiation Lab in nearby Brookhaven National Laboratory.

When Anne developed a debilitating illness, and David was stricken with Parkinson's disease, the Sayres moved to a retirement community in New Jersey. Subsequently I moved to Berkeley, but our collaboration continued. Our next to last joint paper was published in PNAS in 2005. It was based largely on the PhD thesis of David Shapiro. The young David assisted the old David when the latter delivered his address accepting the Ewald prize in Osaka in 2008.

I last visited David Sayre the day before Thanksgiving of last year. He looked old and frail at the age of 87. He did not make it to 88. He was a wonderful friend and mentor, and I miss him greatly.

Janos Kirz

My remembrance: I first met David Sayre intellectually long before I met him in person. In the early 1960s, when I was in graduate school, I thought that I had found a new way to put x-ray data onto an absolute scale. When I excitedly presented this result to my boss, Warner Love, he gently informed me that the idea had been put forward by David Sayre at least a decade before. To be honest, at that moment I was only dimly aware of who David was. Warner, who had worked for several years with David at the Johnson Foundation in Philadelphia, introduced me to David's work. I then went eagerly to the literature and read, I believe, everything he had published in crystallography up to that time. I was enormously impressed with the clarity of his thinking and with the depth of his insights.

Some years later I finally got to know David through casual encounters at a number of crystallography meetings. Our paths did not start to cross seriously until the early 1980s, a time at which I was contemplating shifting the focus of my research into the nascent area of x-ray microscopy. I discussed with David and Janos Kirz the possibility of doing a sabbatical with them at Brookhaven. But prudence (and my departmental chair) intervened and I stayed put at Johns Hopkins. However, my

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reading in x-ray microscopy, and my obvious interest in the field, prompted David and Janos to invite me to be a member of the advisory committee for their x-ray microscopy facility at the Brookhaven National Laboratory. I served for 3 or 4 years in the middle 1980s; my CV is curiously silent on the exact dates. Through meetings of the board and other conversations I saw close-up the development of several different tracks for x–ray microscopy in which David was involved. There was the work on scanning electron microscopy, made possible by Fresnel zone plates fabricated at IBM. Most exciting to me, however, was the idea of what David called diffraction microscopy, in which a single object, such as a cell, would be illuminated by an x-ray beam, and the continuous diffraction pattern produced by the object would be measured. The belief that such a diffraction pattern could be phased harkened back to a famous paper by David in 1952, entitled "Some Implications of a Theorem Due to Shannon." In this work he showed that for a centrosymmetric crystal one could phase the diffraction pattern if it were sampled at reciprocal lattice points with half-integral as well as integral indices. Both the ideas behind diffraction microscopy and the extremely elegant work needed to create a viable experimental apparatus impressed me greatly. For example, there was the seemingly trivial idea of eliminating scattering from the beamstop by drilling a tiny hole in the detector and putting the beamstop behind it. My advisory committee service ended when Janos Kirz moved on to Berkeley, and David continued his collaboration with him long distance. I kept track of what was going on through the literature and by occasional chats with David. Many of the plans for diffraction studies of single molecules being developed for the Linac Coherent Light Source at Stanford echo the ideas that David put forth a generation ago.

My last interactions with David came about when he hesitantly asked me if I would be willing to serve as the executor of his living will. I viewed this as a great honor and vote of confidence, and of course I said yes. Partly as a result of this agreement, I visited David every 6 months or so in his home in New Jersey to see how he was doing and to make sure that the terms of his living will were what he still wanted. Executor's duties took up only a tiny fraction of the time, and we had wonderful conversations about his work. That stewardship came to an end when I moved to Buffalo, a location too far from New Jersey for me to carry out the duties of executor as promptly as they might be needed.

David is genuinely one of the great intellectual figures in modern crystallography and diffraction, and epitomizes the phrase "a gentleman and scholar." It was a great privilege to know him. I will treasure our friendship forever.

Eaton Lattman

ACA Los Angeles (2001) session on New Computational and Experimental Approaches. From Left to right: Zbigniew Dauter, Janos Hajdu, Tom Terwilliger, David Sayre, Qun Shen, Mike Soltis and Jack Johnson.

In their description of the session Tom Terwilliger and Mike Soltis reported that "David Sayre talked about the oversampling method for phasing and its potential applications to imaging objects sized in the 10 to 3000 nm range. The general idea is to measure the continuous diffraction pattern from a finite object with an approximately known envelope, and use the resulting overdeterimination of the phase information to reconstruct the image. Data collection is accomplished using a fairly conventional diffraction experiment but with considerably larger exposures. Sayre's group has been able to observe 18 nm resolution data from a 3000 nm dried yeast cell at room temperatures. They will soon attempt to collect higher resolution data from a frozen hydrated cell at liquid nitrogen temperature. For studies of small assemblies (proteins and viruses for example), the plan would be to utilize the suggestion of Janos Hajdu based on the intense radiation from a free electron laser x-ray source.".

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Candidates for ACA Offices in 2013

The Nominating Committee (Judy Kelly, Jim Britten and Saeed Kahn) proposes the following candidates for the 2012 elections for ACA offices in 2013

Officers:

Vice-President: **David Rose and Martha Teeter**

Treasurer: **James Kaduk and Virginia Pett**

***Committees*:**

Communicatons: **Nick Silvaggi and Kraig Wheeler**

Data, Standards & Computing: **Chuck Campana and Tom Terwilliger**

Continuing Education: **Graciela Delgado and Richard Staples**

To nominate write-in candidates for any office, write to the ACA Secretary: **Patrick Loll, Dept. of Biochem & Molecular Biol., College of Medicine, Drexel Univ., Philadelphia, PA (pat.loll@drexel.edu).** Letters must be received by September 15, 2012 and must be signed by 5 ACA members and include a signed statement by the candidate describing his or her qualifications. Voting will be by electronic ballot. Statements from all candidates will be available on the election site. The voting window will be open in ***October 2012***.

David Rose - Vice-President

Department of Biology, University of Waterloo, Canada

Education: BA, University of Pennsylvania (1977); DPhil, Oxford University (1981) with David Phillips; Postdoc, MIT, with Greg Petsko.

ProfessionalActivities: ACA: Canadian Rep on Council (2002-2005, 2011-2014), Chair, Canadian Division, Local Chair, Toronto (2009). Canadian Institutes for Health Research: Peer Review Committees, University Delegate for Waterloo, Peer Review for Canadian Cancer Society, Alberta Heritage and others. Graduate Coordinator and Interim Department Chair, University of Toronto (2000-2008), Department Chair, University of Waterloo since 2009.

Research Interests: Macromolecular crystallography, particularly when applied to glycoside hydrolases associated with human health and disease. For many years, my group has been involved in studies of enzymes of the eukaryotic N-glycosylation pathway, specifically Golgi α-mannosidase II and ER α-glucosidase I. We have also been studying the human intestinal glucosidases involved in the processing of nutritional starch.

Statement: For almost my entire career, the ACA has been my professional home. I have been to many other meetings, but the ACA is unique in the way its meetings combine methodology and results. The meetings also provide a platform for cross-fertilization across all branches of diffraction science, interactions across sectors (academia, industry, government), and close contact with vendors. Among the priority areas that I would foster in this leadership position are:

Young scientists: Every generation of scientists has its obstacles. Research in general, including in our field, has, arguably, changed more in the last generation than ever before. Technological developments, front-and-center at ACA meetings, have opened new frontiers and deepened the questions that the next generation can address. At the same time, government-supported universities in most countries have shrinking budgets, job freezes or reductions, and underfunded infrastructure renewal. The private sector is in a state of constant flux. Government research laboratories are downsizing or changing focus. The ACA has historically been an important resource for early-career scientists to gain profile, present their research, make valuable contacts, and have discussions about establishing and maintaining a career in research. I would continue to feature the role of the YSSIG in meeting sessions and events, and in Council participation. They need our advice and encouragement now, more than ever.

Science Policy and Outreach: I group these together because they are so closely intertwined. It has never been more important for science to be seen and to be "relevant" to advancing the welfare of our countries. Professional societies have an important role to play in communicating to politicians and to the general public what science can do to improve our world. A big part of that role is to facilitate communication among ourselves and to synthesize a common vision and voice. ACA meetings provide important means to facilitate those discussions.

Martha Teeter - Vice-President

Professor Emerita (2006-), Chemistry Dept., Boston College, Boston, MA. Volunteer Clinical Faculty (2004-), UC Davis School of Medicine, Sacramento, CA

Education: BA, Wellesley College, (1966), PhD, Penn State Univ. (1973) with Harry Allcock. Postdoc in Biology,

MIT (1974-1976) with Alex Rich and at Naval Research Lab (1976-1977) with Wayne Hendrickson.

Professional Activities: **ACA:** Program Chair McMaster, Canada (1986); distributed bitnet news to ~5000 crystallographers (1988-1994); Chair BioMac SIG (1991); Service awards: (1990, 1994); Computing and Data Comm. (1990-1994, Chair '94). Chaired and organized numerous sessions (1984-2003). **IUCr:** Organized a session Beijing (1993); member IUCr Commission on Electronic Pulbication; US Editor IUCr World Directory (1995). Sabbatical: Max Planck Institut für Biophysik in Frankfurt, Ger. with Helmut Michel (1994-1995). Biophysical Society: Exec. Comm. (1988-1990); Head, Molecular Biophysics subgroup (2004). Plenary Speaker: Mexican Society of Crystallography, Hermosillo, Mexico, (2001). Other: Many study sections and numerous grant and journal reviews. 66 publications from 1971 to 2011.

Research Interests: As the daughter of a physical chemist, I am fascinated by how physical forces – electrostatic and van der Waals – guide molecular interactions. My route to becoming a protein crystallographer was sinuous, and one that gave me appreciation of different fields of crystallography.

In high school, I strongly resisted science, because, well – my father was a chemist. I did take chemistry at Wellesley College, however. It was the summer after sophomore year that decided me about chemistry. I took an NSF Summer Research Assistantship with Emily Dudek, a Wellesley inorganic chemistry professor. At the time, I was struggling with deciding to major in music or in chemistry. But that summer, I fell in love with scientific research and that, as they say, was that.

My first crystallography teacher in graduate school at Penn State was Bob Newnham, a material scientist. I fondly remember homework problems solving 1D Patterson maps of minerals by hand. Later I used the same problems to teach crystallography at Boston University and Boston College.

Clathrates provided my first research window into diffraction research. I was amazed to find cyclotriphosphazine catechol derivatives spontaneously recrystallized when placed next to a beaker of benzene. These inclusion compounds formed channels only when other molecules were around to fill them, pulling them from the gas into the crystalline phase. And I became an inorganic chemist - a non-metal, inorganic chemistry PhD.

From there, with an NCI fellowship to study shape fitting in polycyclic aromatics with DNA, I spent a summer with Helen Berman on the structure of a thymine dimer. Then, I headed to MIT to postdoc with Alex Rich and wound up switching to macromolecular crystallography – tRNA. Not trusting any molecule that I couldn't understand and visualize every atom of, I determined to eat my lunch next to an 8'x10' tRNA Richard's Box (electron density on plastic sheets with a molecular model fit to the density via a half silvered mirror and model supported by metal rods and piano wire), until I could trace the chain and make sense of it. It was a strange new world for me.

Quite accidentally, when fellow postoc Fran Jurnak and I were looking for a possible protein to crystallize, my attention was caught by a protein diffraction pattern in the article next to the one I was looking up in the *Journal of Phytochemistry*. That launched me into the protein I have worked on for most of my career – crambin from Ethiopian cabbage.

Water, which forms clathrates in its own right, has always intrigued me. And crambin crystals, although a 46-residue hydrophobic protein, contain about 30% water. The structure provides an excellent window into water structure around proteins. Synchrotron data from crambin crystals diffract x-rays to 0.48 Å resolution (the smallest d spacing). This is the world's limit for protein crystals, to my knowledge. Water positions, both single and doubled, are apparent, as well as bonding electron density. Likewise, multiple side chain conformations are found and these can be correlated to water positions. Multiple temperature studies of these crystals provide evidence for a protein glass transition where not only correlated motion of side chains with water but also protein function ceases. Thus, both this research and my additional studies on myoglobin crystals gave crystallographic evidence for the role of correlated substates as critical for protein function. While others such as Greg Petsko had postulated this, I was able to show it at an atomic level. It is these dynamic interactions I find truly fascinating. I continue to research water structure around proteins in retirement.

Graphics – both movies and illustrations of molecular models – have always played a key role in my teaching and research, from making undergraduate lab demos in graduate school to shooting movies of crambin for research to constructing figures for publication. I have continued to explore the visual arts in retirement. I made a short documentary, which was among the top ten at a Sacramento Film Festival in 2008. I have hosted and/or produced over 20 ½ hour interview shows on our local cable station in Davis, as well as several longer productions. My particular favorite was "Teaching College Science through Song". It was an interview with a friend and colleague, a plant, water and soil scientist, who is part of the Art-Science Fusion program at UC Davis as well as a songwriter herself. In her class, students in groups write songs about science and perform them at a public venue. Their songs are about such topics as the water cycle, how soil is formed, and the like.

Teaching is also an important part of my retirement. I teach an applied seminar at UC Davis Medical School. I find it both rewarding and challenging. Spending time to help students learn to think logically, put their clinical learning with basic biochemical principles, and learn to work together on a case is very satisfying. I believe that education in science is something we must take time for at every level possible.

Statement: The IUCr has proclaimed 2014 the International Year of Crystallography (IYCr), in honor of the discovery of x-ray diffraction by Von Laue and the Braggs (father and son). UNESCO and the International Council for Science support this centennial. What an exciting time to be a crystallographer! Proposed IUCr aims for this year include: To increase the public awareness of crystallography; to increase the awareness of the way crystallography underpins most of the technological developments in our modern society; to illustrate the universality of science; to increase the awareness of the way crystallography underpins investigations of cultural heritage artifacts; and to promote education in crystallography and its links to other sciences

As a crystallographer and science educator, I am keenly aware of an anti-science attitude among certain political candidates, corporations and their think tanks, and anti-science educators. I think crystallography provides wonderful opportunities to develop an awe of the natural world and the scientific method for children and adults. For years, I used crystallization in gels demonstrations from the Hauptman-Woodward Institute with elementary and college students alike. I have also used Marge Kastner's program for explaining space groups and many other visual tools for teaching diffraction, such as simulations of interference between two slits. I am an advocate for multi-disciplinary approaches to teaching science as well as for scientific research. I would advocate for the many disciplines of crystallography represented in the ACA.

This juxtaposition of IYCr with anti-science trends presents tremendous opportunities to use crystallography to increase public and political awareness of science and its benefits. I would make this a major emphasis in my term serving the ACA. I envision enabling creation of a series of both short and longer videos and visual aids to bring crystallography before the world and document the accomplishments of diffraction, curriculum units for science teachers to professors, and creation of material to help politicians understand science and its contributions. I hope to elicit the creativity of old and young crystallographers in bringing this message to the world. Further, the IUCr is scheduled for Montreal in 2014, which provides an additional forum to not only hold a symposium on 100 years of diffraction but also to publicize and bring to world attention the accomplishments and the promises for diffraction and for science in solving problems.

Funding for crystallographic research, which is very often interdisciplinary, is another priority for me. I hope to listen and learn from current and past councilors as to other issues facing the ACA at this juncture.

Nomination for VP is a great honor and a chance for me to give back to a society that has provided much for me. Crystallography has been much more than my livelihood. The ACA provided my first professional opportunities to attend international meetings (yes, I was one of those graduate students in 1969 lucky enough to attend the IUCr in Stony Brook on scholarship and show slides for the sessions) and has continued to provide a forum for critical and supportive advances in all levels of crystallography for me. I remember Jim Ibers providing that feedback when I was an outspoken graduate student. Wayne Hendrickson was patient and inventive with this odd crystal crambin, and in the '80's, Håkon Hope cooled a crambin crystal to liquid nitrogen temperatures, as he had done with Ada Yonath's early ribosome crystals. There are too many important people to mention that have mentored me. I am thrilled to have the opportunity to represent a discipline of creative, honest individuals, curious about the science and inventing new crystallographic and computational tools to solve problems. This is a great time to share crystallography with the world

James A. Kaduk - Treasurer

Adjunct Professor of Chemistry, Illinois Institute of Technology, Chicago IL (also President of Poly Crystallography, Inc.)

Education: PhD, Northwestern U. (1977) in Inorganic Chemistry.

Professional Activities: My experience in non-profit management includes: Chair of the Board of Directors of the ICDD (the Powder Diffraction File; just retired from the Board after 20 years) and Chair of the USNCCr; President of the Naperville (IL) Chorus, and member of the Northwestern University Library Board of Governors. I review financial information for many non-profit organizations for the Charitable Contributions Committee at my church. Other activities include: Chair of the ACA Materials SIG; faculty for the ICDD Advanced X-ray Diffraction Clinic, the Short Course on the Rietveld Method, and the ACA Small Molecule Summer Course; Chair of the Powder/Single Crystal Crystallography Proposal Panel at NSLS; member of the Structural Characterization Advisory Subcommittee and review proposals at APS; member of the Neutron Scattering Science Review Committee at ORNL; one of the three main editors of *International Tables for Crystallography: Volume H*; a Co-Editor of *Acta Cryst. B*; member of IUCr Commissions on Powder Diffraction, Crystallographic Nomenclature and the Committee for the Maintenance of the CIF Standard (COMCIFS).

Research Interests: At heart, I'm an old-fashioned crystallographer; I care about knowing where the atoms are, and why. Having spent most of my career in industry (32 years at Amoco/BP/Ineos), single crystals of most compounds were not available, so most of my structural work is done using powder diffraction data. My current work "focuses" on pharmaceuticals, catalysts, corrosion deposits, molecular sieves, and inorganic materials; my interests are broad. Much of my work is at the interface of experimental crystallography and computational chemistry. I am passionate about crystallographic education. My activities during the International Year of Crystallography will center on introducing our science to middle school students (grades 5-8).

Statement: The duties of the ACA Treasurer consist of acting essentially as an internal auditor, representing the ACA on the AIP Comm. of Society Treasurers and the USNCCr. The Treasurer determines the amounts of the annual Travel Grants and is also a member of the ACA Council, thus helping to set policy and strategy, and performs the normal functions of a member of a board of directors. I hope to continue to bridge the gaps between the powder/single crystal communities, as well as the materials/biological communities. The ACA is well run, and an obvious job of the Council is to ensure that it stays that way, and has sufficient reserves to endure any rough patches. I believe in complete transparency, and hope to publish an annual report to summarize the financial and scientific accomplishments of the ACA to the wider world.

Virginia B. Pett – Treasurer

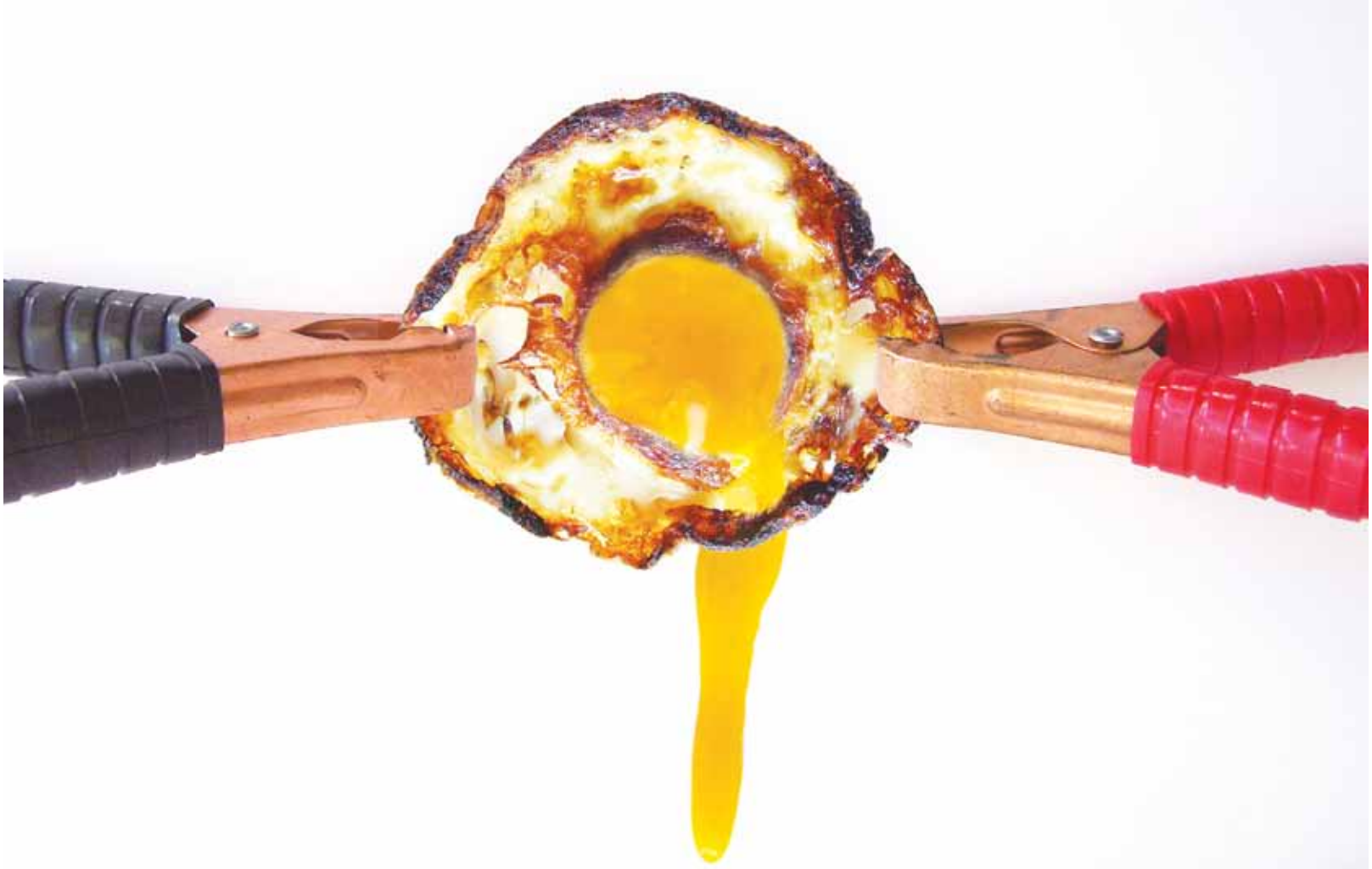
Robert E. Wilson Professor of Chemistry Emerita, Department of Chemistry, The College of Wooster, Wooster, OH

Education: BA, The College of Wooster (1963); MA in History of Science (1972) and PhD in chemistry (1979) with Milton D. Glick and David B. Rorabacher, Wayne State University; NIH Postdoc with Helen M. Berman and Jenny P. Glusker (1979-81), Institute for Cancer Research, Fox Chase Cancer Center, .

Professional Activities: ACA Secretary (1997-99); ACA Historian (2010-); AIP, Advisory Committee on History of Physics (2012-14).

Research Interests: As a physical chemist at an undergraduate liberal arts institution (1981-2009) my research included both educational methods and chemical exploration. With funding from the ChemLinks Coalition I designed teaching modules for organic chemistry that emphasized active learning and group collaboration, and I applied these teaching approaches to introductory chemistry courses and in teaching crystallography to physical chemistry students. In the laboratory students and I synthesized and determined the structure of organo-cobalt complexes that serve as model compounds for B_{12} coenzyme. Later on, my research interest changed to investigating the properties and chaperone capabilities of small heat shock proteins isolated from maize. I was fortunate to have five research leaves: Laboratory for the Structure of Matter, Naval Research Laboratory, Washington, DC (1987-88 and 2002-03); Case Western Reserve University School of Medicine, Department of Biochemistry (1991-92); Structural Biology Section of the Laboratory of Molecular Structure of NIAID, Rockville, MD (1996-97); The College of Wooster (2006).

Statement: I have been a member of the ACA since I began teaching at The College of Wooster in 1981. ACA meetings have been crucial in sustaining my love of crystallography, keeping up with new techniques, and broadening my crystallographic interests to include protein crystallography as well as small-molecule crystallography. I'm delighted to contribute back to the professional organization that has meant so much to me in my professional career. Previously, I served as ACA Secretary; currently I am the ACA Historian. If I am elected Treasurer, I look forward to serving on the ACA Council again.



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The duties of Treasurer have recently been redefined and clarified as follows — reviewing monthly reports from the Buffalo office and working with the ACA CFO, S. N. Rao, serving on the ACA Financial Review Committee, reporting to the ACA membership at the annual meeting, determining Travel Grant amounts, and serving on the USNCCr as one of ACA representatives. My experience as Department Chair, handling a Department budget has prepared me to carry out these responsibilities.

If elected, I would gain a detailed understanding of ACA finances in order to become a resource person for the ACA Council and the Financial Review Committee. My goals would be to evaluate the current financial situation, suggest any needed changes, and ensure the long-term financial health of our professional society. I would strive to communicate the ACA financial status to the membership in the clearest possible terms.

Graciela Díaz de Delgado, - Communications

Professor of Chemistry, Departamento de Química, Facultad de Ciencias, Universidad de Los Andes (ULA), Mérida, Venezuela

Education: MA (1985) and PhD (1988) in Chemistry, Brandeis University, USA; *Licenciatura* (1982) Universidad de Los Andes, Mérida, Venezuela.

Professional Activities: Chair of the Materials Science Program in the Chemistry Graduate Division, ULA; member of the Steering Committee to establish the Latin American Union of Crystallography and to plan Latin American activities for the International Year of Crystallography. Chair of the Grant-in-Aid Committee of the ICDD; member of the ICDD Ludo Frevel Scholarship Committee; member of the Editorial Board of *J. Chem. Cryst.* and reviewer for several journals. Member: The IUCr Subcommittee on the Union Calendar (2002-2011); advisory committees of the Venezuelan Academy of Sciences; the Committee for activities of the International Year of Chemistry (2011); and the international advisory board of ICCOSS. Organizer: Courses; workshops; national and international meetings in chemistry and crystallography; the Venezuelan Chemical Society (2005), ICCOSS (2007); and a Latin American Symposium on Organometallic and Coordination Chemistry (2009). Chair and Co-Chair of sessions and symposia at ACA, IUCr, and Latin American chemistry congresses.

Research Interests: Solid state reactivity of unsaturated carboxylic acids and their metal derivatives. Relationship between their structures and reactivity. Structural characterization of Active Pharmaceutical Ingredients (APIs) and natural products isolated from plants used in Venezuelan folk medicine. Polymorphism in these compounds.

Statement: The American Crystallographic Association has sustained a continuous effort to incorporate new and better ways of communication within its community and with the society in general. The publications produced by the ACA have increased the presence of the Association in the scientific community and should continue to grow in quality and scope. In today's world, any ideas and proposals coming from people of different latitudes should be welcome to better disseminate the important role that crystallography has played for decades in the improvement of our quality of life. As a South American member of the ACA since 1987, I would like to contribute, through the Communications Committee, to the important task of making more people aware of the impact that crystallography has had and will continue to have in our lives. I will actively participate within the ACA organization in the promotion of the activities to be organized for the International Year of Crystallography (IYCr). Being a member of the steering committee established to organize the Latin American Union of Crystallography and to plan activities for the IYCr in Latin America, I will take the opportunity to strengthen the relationship between the ACA and the Latin American crystallographic community.

Richard J. Staples - Communiations

Academic Specialist, Crystallographer, Department of Chemistry, Michigan State University, East Lansing, MI

Education: PhD, Chemistry (1989) University of Toledo.

Professional Activities: Webinar presentation on *Crystal Growth and Mounting* Bruker (2010); Chair of ACA Small Molecule and Service Crystallography SIGs (2002, 2003); instructor for summer school *X-ray Crystallography for Industrial and Academic Chemists* (2007); Bruker/MIT Symposium workshops (2005 and 2006); summer school *X-ray Crystallography for Industrial Chemists* (2005); and ACS summer school *X-ray Crystallography for Organic Chemists* (2004). Reviewer: NIH and NSF panels, proposals for ALS, various journals. Memberships: ACA, ACS, AAAS, AAPS and Protein Society. Publication of over 200 peer reviewed papers; Distinguished Service Medal, Harvard U., Dept. of Chemistry.

Research Interests: Recent interests involve the development of crystallization techniques and procedures that can provide single crystals of small organic or inorganic compounds quickly and efficiently. I present this information to chemists by way of course and web interactions so as to help them understand the importance of small molecule crystallography. This includes the formation of a laboratory section of the x-ray course to include crystal growing of simple organic compounds and expansion to macromolecular x-ray diffraction.

***Statement*:** Communication of scientific results has long been one of the most important aspects of a researcher's career and progress, but in today's new internet society it is even more important to be sure our results reach a wide general audience in such a way that they understand the significance of the results. Our ability to project a sense of great accomplishment is vital to our ability to continue to help drive the social and political landscape that keeps the funds flowing. This ability to make the general public aware of the how and why we need to continue research in these areas is essential to the foundation of an advanced society. We must have a strong and focused PR in the ACA if we are to continue to convince those involved that the science we generate is a necessity. This will have profound effects on our funding and ability to attract talented individuals to continue to explore the exciting world that encompasses the broad activities of the ACA.

Nicholas Silvaggi - Continuing Education

Assistant Professor, Department of Chemistry and Biochemistry, University of Wisconsin-Milwaukee, Milwaukee, WI

Education: PhD (2003) University of Connecticut, Department of Molecular and Cell Biology; BS/Biology (1998) Rensselaer Polytechnic Institute.

Professional Activities: ACA member since 2000; Chair, Young Scientists SIG (2001-2002); ACS member since 2008.

Research Interests: Nonribosomal peptide biosynthesis and developing enzymes as tools for organic synthesis. My lab uses traditional structural biology and mechanistic enzymology methods, supplemented with a number of complimentary biophysical techniques, to determine the structures and catalytic mechanisms of enzymes involved in the biosynthesis of bacterial secondary metabolites.

Statement: I am honored to accept this nomination to the Continuing Education Committee. It is increasingly common that researchers in fields outside of the various crystallographic disciplines are incorporating crystallography into their laboratories. This positive trend is tempered by the fact that university courses in x-ray diffraction theory are becoming less common. As a result, we now have more people using the technique and fewer who thoroughly understand it. I believe the ACA can do a great deal to help remedy this situation.

The ACA meetings, and especially the workshops, provide valuable and vital training opportunities that benefit novice crystallographers, and keep more established investigators current. These meetings also provide some of the only interactions many of us have with crystallographers in other sub-disciplines. But beyond these traditional benefits of the ACA meetings, I think we can do more to support and facilitate education in crystallographic theory and practice. If elected to the Continuing Education Committee, I will work to not only ensure that we continue to provide high quality educational experiences at the annual meeting, but also to leverage the tremendous existing resources to reach larger numbers of students and researchers.

Kraig Wheeler – Continuing Education

Professor, Department of Chemistry, Eastern Illinois University, Charleston, Illinois

Education: BA, Chemistry, University of Minnesota (1987); PhD, Chemistry, Brandeis University (1992); postdoctoral fellow, University of Texas, Austin (1993).

Professional Activities: Chair, Small Molecule SIG (2007); Co-organizer, *Transactions Symposium* (ACA12), *Crystallography at Undergraduate Institutions* (ACA12), *Supramolecular Chemistry* (ACA07), Midwest Organic Solid State Chemistry Symposium (2011), ACS-PRF Crystallography Summer Workshop for Organic Chemists (2004, 05, 07); USNCCr (2012); Councilor, Council on Undergraduate Research (2007-present).

Research Interests: Organic supramolecular chemistry, enantio-controlled solid-state reactions, crystal transformations, quasiracemic materials, molecular topology, noncentrosymmetric molecular assemblies, and molecular recognition processes.

Statement: Continuing Education within the context of the ACA describes a wide range of educational initiatives directed at entrenched practitioners to those just starting out with their careers. The ACA's Continuing Education Committee (CEC) serves as one of the critical service arms of the organization. How critical? In 2001, the ACA council consolidated the assortment of standing committees to three – Continuing Education; Data, Standards and Computing; and Communication – to provide more continuity and focused leadership for the emerging issues in our changing discipline. The CEC is distinguished as the only standing committee responsible for providing readily accessible professional development and thus its success (or demise) has far reaching implications to the crystallographic and scientific communities. This committee's rich history of sponsoring educational opportunities is quite evident by its support over the last several years of crystallographic summer schools and ACA national conference activities (e.g. workshops, sessions, and travel grants).

I am honored to be nominated to serve on the CEC. My past service to the ACA has been enriching and I am excited by the opportunity and new challenge of serving on this standing committee. For the last 18 years, my experience as a faculty member at a predominantly undergraduate institution has provided many opportuni-

ties to explore and support the teaching of x-ray crystallography. Inspiring students through purposed instructional activities and research programs still holds much interest to me. This passion coupled with outreach activities (collaborations, workshop and session organizer) and managing a small-molecule single-crystal x-ray facility offer a unique perspective that should be of benefit to the ACA community.

CEC continues to make its mark on the ACA. Given the changing climate of the crystallographic community (instrumentation, software, and users), it is imperative that the Committee develop accessible high-impact programs that reach a broad demographic of users. Two key areas that will likely need attention include:

(1) Workshops and summer schools. The current offerings of ACA sponsored workshops and summer schools provides significant opportunities to train novice to seasoned users on the various aspects and depths of crystallography. Because such activities are foundational to the mission of the committee, evaluating existing practices and extending current directions to other projects would provide excellent opportunities to foster innovative instruction.

(2) Next generation users. The success of future crystallographers and users will require formal instruction and hands-on experiences with crystallographic theory, data, and instrumentation. Though this group most often includes post docs and graduate students, it is now increasingly apparent that there is considerable value in capturing an even younger crowd such as undergraduates and high school students. Academic and industrial institutions often serve as the initial point of exposure to our field; however, the ACA (the leading voice of crystallography in the Americas) should also play a pivotal role in the development of the next generation of x-ray users. How to most effectively train and support these demographic groups, as well as their integration into organizational activities should be explored with best practices implemented.

As with any organization, developing excellent training programs requires effective planning, promotion, oversight, and execution by a dedicated group of individuals. I see the ACA Continuing Education Committee as vitally important to the progress of our organization and profession and as such, if elected, I will commit to support and strengthen existing initiatives in addition to help identify strategies to initiate new programs and resources.

Charles Campana - Data, Standards, and Computing

Senior Scientist, Bruker AXS Inc., Madison, WI

Education: BS (1970) Chemistry, Montana State University; PhD (1975) Inorganic Chemistry; University of Wisconsin – Madison; Postdoc (1975 to 1976) University of Alberta.

Professional Activities: Assistant Professor of Chemistry, University of New Mexico (1976 -1980); Consultant, Sandia National Laboratory (1976-1980); Senior Applications Scientist for single-crystal x-ray diffraction product lines - Nicolet Instrument Corporation, Siemens Analytical X-Ray Instruments, Inc., and Bruker AXS, Inc (1980-present); Instructor at ACA Summer Schools at University of Pittsburgh (1993-1996), University of Georgia (1997-2002) and Indiana University (Pennsylvania) (2004 and 2005); Instructor in Crystallography Workshops at UCSD (2004, 2007), California State University – Fullerton; Cal Poly – Pomona (2011); Indian Institute of Science (Bangalore - 2004), UNAM (Mexico City - 2007) and Universidad de Santiago (Chile- 2003); problem structures workshops – Taiwan, China, Hong Kong, University of Nevada – Reno, University of Tennessee, Mexico City; instructor at Canadian Chemical Crystallography Workshop; Bruker / MIT Symposium (1995 to present); co-author of several hundred crystallographic papers; presented many papers at ACA, ACS and IUCr meetings ; reviewer for crystal structure publications in ACS journals.

Research Interests: Development and testing of new hardware and software for commercial chemical crystallography instruments. Production of technical documentation and training materials for commercial crystallographic systems. Solution and refinement of difficult crystal structures.

Statement: During the past few decades we have witnessed the remarkable transformation of the field of x-ray crystallography brought about by the introduction of reliable low-temperature devices, micro-sources and new two-dimensional detectors, such as image plates, and CCD and CMOS detectors. Coupled with improvements in computer hardware and new software algorithms, these advances in diffractometer technology have resulted in enormous increases in efficiency and productivity. The improvements in data quality and the speed of data collection offered by new instrument technology have also extended the use of x-ray crystallography to a further level by facilitating structure determination on very small specimens, and twinned and aperiodic structures. Charge-density studies, which were previously limited to very small molecules due to long data collection times (typically three to six months on conventional instruments), may now be carried out in less than one week on much larger molecules.

I believe that the ACA DSC Committee must play an active role in developing standards for validation, publication and archiving of modern crystallographic data. This committee should help to facilitate the adoption of CIF extensions and validation programs for twinned and modulated structures and work with external groups to ensure that proper standards for validation and review of crystal structures are also adopted by non-IUCr journals. This committee should continue to support educational ACA activities, such as workshops and tutorials to train new users to properly use the latest technology to collect high quality experimental data and to carry out proper analysis of this data. In addition, ACA must take advantage of outreach opportunities to promote the proper use of crystallography by non-crystallographers (e.g., chemists and molecular biologists) in their research.

Thomas C. Terwilliger - Data, Standards, and Computing

Los Alamos National Laboratory Fellow, Los Alamos, NM 87545

Education: PhD (1981), Molecular Biology, UCLA; AB (1978), Physics, Harvard.

Professional Activities: ACA member; IUCR Commission on Biological Macromolecules; IUCR Diffraction Data Deposition Working Group; Co-editor, *Acta Crystallographica section F*; Co-Editor, *Journal of Structural and Functional Genomics*; Executive Committee, International Structural Genomics Organization.

Research Interests: Development of algorithms and software for macromolecular structure determination; structure determination of potential drug targets from pathogens including *M. tuberculosis*; development of methods for modifying proteins to increase their suitability for crystallization and structure determination.

Statement: I would be pleased to help represent the ACA in the current international discussions of two major ideas for crystallographic data deposition and data interpretation. The first discussion is on the issue of deposition of diffraction images as a standard part of a PDB deposition. My personal view is that this is highly desirable if it can be accomplished with relatively low cost and relatively low burden to the investigators. I initiated the discussion in the fall of 2011 on the CCP4 bulletin board on this subject (see summary at ***http://forums.iucr.org/viewtopic.php?f=21&t=79***), and I will continue to listen the views of ACA members as the discussion continues. The second discussion, related to the first but separate, is on continuous improvement of macromolecular crystal structures. The idea is that methods continually improve, so applying today's methods can improve yesterday's structures, and applying tomorrow's methods will improve today's structures. The question is whether it would be useful to change our paradigm of having a fixed interpretation of a crystallographic dataset into one where both the original and improved models might co-exist. Depending on the question that is being asked, the most appropriate model could be used.

Thomas Terwilliger named as the recipient of the 2013 ACA Ken Trueblood Award

The ***ACA Trueblood Award*** recognizes exceptional achievement in computational or chemical crystallography. ***Thomas C. Terwilliger*** has made brilliant contributions to the community of crystallographers through his software that permits the near-automatic determination of molecular structures. His deep understanding of chemical crystallography, statistics, and computer codes has enabled him to produce a string of programs that have helped to transform the field of macromolecular structure determination.

Among his innovations are the following: ***HASSP:*** First automated analysis of difference Patterson functions to find heavy-atom sites. ***SOLVE:*** first Bayesian estimates of heavy-atom structure factors from MAD data; analysis of MIR phasing including correlated non-isomorphism; and automated structure solution (finding sites through calculation of an electron density map) for macromolecular structure solution by MIS/MAD/SAD. ***SOLVE, PhenixAutoSol wizard***: first systematic set of criteria for automatic assessment of the quality of electron density maps. ***RESOLVE:*** first rapid and automated procedure for finding non-crystallographic symmetry from heavy-atom sites. ***RESOLVE maximum-likelihood density modification:*** first Bayesian approach for density modification. ***RESOLVE build script:*** first procedure capable of map improvement at moderate resolution (2.5-3Å) by iterative model-building, density modification and refinement.

Tom's programs execute with a minimum of required intervention. He has achieved this by incorporating statistical deicision making ("Wizards") into the software. His programs, along with advances in instrumental automation, are one of the major reasons that the structural genomics side of macromolecular crystallography has been able to move ahead. One or more of his programs has been used in many of these structures, as demonstrated by the number of research papers that cite his work.

Ken Trueblood, while brilliant and multitalented, was modest, generous, and devoted to community. He sent out his programs to any scientist who asked and he loved to teach, always making students' needs his first priority. Tom Terwilliger has also been known to put his research aside and help anyone who comes to him for help with one of his programs or some crystallographic problem. He has been dedicated to the dissemination of his work for the benefit of others and has worked in the community to bring about the successes of structural genomics.

Tom has been selected for this award partly because he fits the Trueblood model of generosity and service, but even more because of his brilliant contributions to crystallographic computing.

Richard Dickerson named as the recipient of the 2013 ACA Isadore Fankuchen Award

The ***ACA Fankuchen Award*** was established in memory of I. Fankuchen, professor of physics at the Polytechnic Institute of Brooklyn, to recognize contributions to crystallographic research by one who is known to be an effective teacher of crystallography. The honoree delivers a lecture at an ACA meeting and at the recipient's home institution or at another institution of the recipient's choice. In 2013 the Award will be presented to ***Richard (Dick) Dickerson.***

Dick Dickerson (far right) enjoying the IUCr meeting in Seattle (1996) with Helen Berman, Olga Kennard and Stephen Neidle.

Dick did his PhD with Bill Lipscomb on the structures of boron hydrides. Following that, as post-doc, he had the great good fortune to work with Kendrew and Perutz on the first high resolution structure of myoglobin (Kendrew et al., *Nature* (1960) **185**, 422). An excellent account of those years is in included in "Fifty Years of Protein Structure Analysis" (Strandberg, B, Dickerson, RE and Rossman, MG, *J. Mol. Biol.* (2009) **392,** 2).

Dick began his academic career in 1959 at the University of Illinois and moved to the California Institute of Technology in 1963 where he spent the ensuing 18 years. During this time his analyses of the structures of cytochromes c from mammals, fish and bacteria allowed him to demonstrate the principles of evolution at the molecular level. As a consequence, he served as an expert witness in trials challenging the imposition of creationism on our science curricula, and lectured on the threat of creationism to science teaching. His structure of cytochrome c550 (Tikovich, R and Dickerson, RE, *J. Biol. Chem.* (1976), **251**, 4033) was also among the earliest depositions to the Protein Data Bank. In 1981 he moved from Caltech to UCLA with a joint appointment in the Division of Chemistry and Biochemistry and the Institute of Geophysics and Planetary Physics, the latter a consequence of his evolution *vs.* creationism interests. Dick was the first to carry out a single-crystal structure analysis of B-DNA, with what has become known as the "Dickerson dodecamer": C-G-C-G-A-A-T-T-C-G-C-G. At UCLA he continued his investigations of the structures of A- and B-DNA, and of complexes between DNA and drugs or proteins.

He was elected to the National Academy of Sciences and American Academy of Arts and Sciences in 1985 and is the author or co-author of 200 scientific papers and seven textbooks, many of which have been translated into eight languages.

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Lisa Randall named as 2012 recipient of the AIP Andrew Gemant Award

The ***Andrew Gemant Award*** recognizes a person who has made significant contributions to the cultural, artistic, or humanistic dimension of physics is given annually. The 2012 citation honoring ***Lisa Randall*** states that she will receive the award because her excellence in research and her extraordinary public outreach through popular books, colloquia, public lectures, and television interviews, has increased public awareness of physics and cosmology and has made her a role model for future scientists and science communicators

The ACA was ahead of the game when it recognized Lisa in 2007 with the ACA ***Elizabeth Wood Science Writing Award*** which is given to those who excel in bringing science to the attention of a wider audience. She gave an impressive presentation at the banquet in Salt Lake City on the research behind her book *Warped Passages: Unraveling the Mysteries of the Universe's Hidden Dimensions*.

Her most recent book, *Knocking on Heaven's Door*, was reviewed by Jeanette Ferrara in the spring 2012 issue of ACA *RefleXions*.

Accolades to Helen M. Berman

The 2012 Carl Brändén Award, sponsored by Rigaku Corporation, is given to an outstanding protein scientist who has also made exceptional contributions in the areas of education and/or service to the science. The 2012 award will be presented to ***Helen Berman*** for her accomplishments toward enabling a freely available and uniform worldwide (***www.wwpdb.org***) archive of 3D structural information for biomedical research and education. She was nominated because her passion for making structural data accessible and understandable by a broad community has driven the development of the Protein Data Bank into a vital and accessible international resource for biology. In the early 1970s she was one of the first voices for open access of scientific information; albeit obvious today, the concept at that time of open access was truly visionary.

Helen was also one of finalists for the ***Benjamin Franklin Award for Open Access in the Life Sciences***, a humanitarian/bioethics award presented annually by Bioinformatics.org to an individual who has, in his or her practice, promoted free and open access to the materials and methods used in the life sciences. She was nominated for her passion for making structural data accessible and understandable by a broad community has driven the development of other bioinformatics resources. These include the ***Electron Microscopy Data Bank (EMDB- www.ebi.ac.uk/pdbe/emdb/)***, a global deposition and retrieval network for cryoEM map, model and associated metadata; the ***Nucleic Acid Database (NDB - ndbserver.rutgers.edu/)***, a resource for information about nucleic acid structure; and the ***Structural Biology Knowledgebase (SBKB - sbkb.org)***, a comprehensive resource that integrates the results of structural biology and genomics efforts with other publicly available biological information to facilitate further research.

She was also named one of ***Jersey's 20 Biggest Brains*** by the *New Jersey Star Ledger*, February 20, 2012.

Golden Mouse Award - Crystallography on iPhone.

The Award, given by two of Sweden's most prominent magazines, *Affärsvärlen* and *Computer Sweden,* in cooperation with IT-företagen, Invest in Sweden Agency and Comdex Scandinavia is given to a product that is technologically advanced and has received attention beyond the Swedish borders. It can be hardware, software, or a combination of both.

The e-learning application *Escher Mobile for iPhone* was named as one of the recipients of the Golden Mouse Award. The application was developed by ***Ivan Orlov (right)*** and ***Gervais Chapuis (left)*** and is presumably the first e-learning app for crystallographers. It is free, compatible with the iPhone, iPod Touch and iPad, and simulates the symmetry environment of the 17 two-dimensional (planar) symmetry groups which can be decorated with various objects according to anyone's fantasy. ***itunes.apple.com/us/app/escher-mobile/id360530191?ls=1&mt=8***

New travel award available from the ICDD

The International Centre for Diffraction Data is pleased to announce the ***Robert L. Snyder Student Travel Awards***, which honor the life and work of ***Robert (Bob) L. Snyder.*** These awards offer limited travel support which allows undergraduate and graduate students to attend the Annual Denver X-ray Conference. Bob devoted a great deal of energy to cultivating future x-ray analysts, and it is with this award that the ICDD strives to continue his mission. Students granted the award must participate in the technical program of the conference by submitting an abstract for oral or poster presentation. Grants in the amount of $500 will be awarded to students living in the USA, and those living outside of the USA will receive $1,000. Applications are reviewed on a competitive basis. To apply for a student travel award, students must submit an application, a copy of the abstract for oral or poster presentation at DXC, and a supporting letter from an advisor. The deadline to apply is 1 May each year.

As an outstanding educator and researcher, Bob was Professor Emeritus of Ceramic Science at Alfred University, Chairman of Material Science and Engineering at The Ohio State University, and co-chair of the School of Materials Science and Engineering at Georgia Tech. He also served as chairman of both the ICDD and the Denver X-ray Conference. Bob was known for his passion for science and life, which was evident in his extensive travel and interactions with scientists from around the world.

Submit an application to: ***dxctravelgrants@icdd.com***

The AIP State Department Science Fellowship

Most of the foreign policy issues faced by the US Department of State have a scientific or technical component. This fellowship is intended to enhance the S&T capacity of the Department by enabling at least one scientist annually to work at the Department's Washington, DC headquarters for a one-year term.

This is a unique opportunity for a scientist to contribute scientific and technical expertise to the Department and raise awareness of the value of scientific input. In turn, scientists broaden their experience by interacting with policymakers in the federal government and learning about the foreign policy process.

Application deadline: November 1 of the year prior to the fellowship term of the year applied for.

The AIP Congressional Science Fellowship Program

The American Institute of Physics, in partnership with the Acoustical Society of America (ASA), annually sponsors one scientist to spend a year providing analytical expertise and scientific advice to Congress. A second fellowship is sponsored by the American Physical Society. The program enables scientists to broaden their experience through direct involvement with the legislative and policy processes.

Fellows gain a perspective which, ideally, will enhance not only their own careers but also the physics community's ability to more effectively communicate with its representatives in Congress.

Benefits: Stipend of $70,000 - $72,000 per year. Relocation allowance. Allowance for in-service travel for professional development. Reimbursement for health insurance premiums up to specified maximum.

Application deadline: January 15 of the year of the fellowship term. Fellowships are for one year, usually running September through August.

Scientists at all career stages, including mid- and late-career professionals, are encouraged to apply. Although the fellowship is a full-time position, arrangements to supplement the stipend by continuing to receive a salary from a current employer while taking a sabbatical or leave of absence during the fellowship term may be worked out on a case-by-case basis.

www.aip.org/gov/fellowships/both_apply.html

New ACA Poster Prize Descriptions - January, 2012

Pauling Poster Prize: was established by the ACA and is supported by member contributions, to honor Linus Pauling. Pauling was one of the pioneers in American structural research and was a very supportive member of the ACA for many years. At each meeting the five best graduate or undergraduate poster presentations receive Pauling awards that consist of $200, a complimentary banquet ticket, and a copy of a Linus Pauling book.

Herman R. Branson Pauling Poster Prize: recognizes the contributions of Herman Russell Branson, one of the first African American physicists to make crystallography the focus of his research.

Muttaiya Sundaralingam Pauling Poster Prize: recognizes the ground-breaking crystallographic research on the stereochemistry of nucleotides and nucleic acids done by Muttaiya Sundaralingam and his colleagues.

Louis Delbaere Pauling Poser Prize: sponsored by the Canadian Division of the ACA and the Canadian National Committee of the IUCr. The prize will be given to the highest ranked graduate or undergraduate poster from a Canadian laboratory.

IUCr Pauling Poster Prize: sponsored by the IUCr, to be given to a ranked graduate or undergraduate poster. The award is complimentary online access to all IUCr journals for one year or a complimentary volume of *International Tables* or other IUCr publication.

Journal of Chemical Crystallography Prize: sponsored by Springer's *Journal of Chemical Crystallography* to recognize the best student poster presentation in the area of chemical crystallography or small molecule structure determination and analysis. The winner will choose a book from Springer's extensive portfolio of titles

AIP Undergraduate Research Prize: **t**he winning presentation must describe research with a significant crystallographic component. Students must demonstrate a command of the science, and must have completed the majority of the work being presented.

RCSB Protein Data Bank Poster Prize**:** this prize recognizes a student poster presentation involving macromolecular crystallography. The award will be two educational books that will be mailed to the winner after the meeting. An announcement will appear on the RCSB PDB website and newsletter. For more information, see ***www.rcsb.org/pdb/static.do?p=general_information/about_pdb/poster_prize.html.***

CrystEngComm Poster Prize: *CrystEngComm* (published by the Royal Society of Chemistry) is very pleased to sponsor a prize for the best student poster presentation in the area of crystal engineering /supramolecular chemistry. The winner will receive an RSC book voucher and an announcement will be posted on the *CrystEngComm* website (***www.rsc.org/Publishing/Journals/CE/about.asp***).

Oxford Cryosystems Low Temperature Poster Prize: this prize is open to all participants and is awarded to the best poster describing work in low temperature crystallography. The winner will receive a cash prize donated by Oxford Cryosystems, Inc.

Scientific Controversies and Crystallography

Scientists love to read an upbeat account like the discovery of x-ray diffraction and its rapid acceptance. We also love to read stories about embattled scientists like Galileo and Darwin who were assailed by non-scientists for unscientific reasons but ultimately prevailed. Far more painful are stories about scientists who put forward correct new ideas that were attacked and ridiculed by their own fellow scientists. Two such figures from the last century were Alfred Wegener and Barry Marshall. Their biographical details are well presented on Wikipedia. Incidentally, I used the English-language Wikipedia for my initial research; but when I attempted to follow it up on January 18, this source had closed down for the day. Reading the German-language www.wikipedia.de instead I found that significant factual information was available on one of the Wikipedias but not the other.

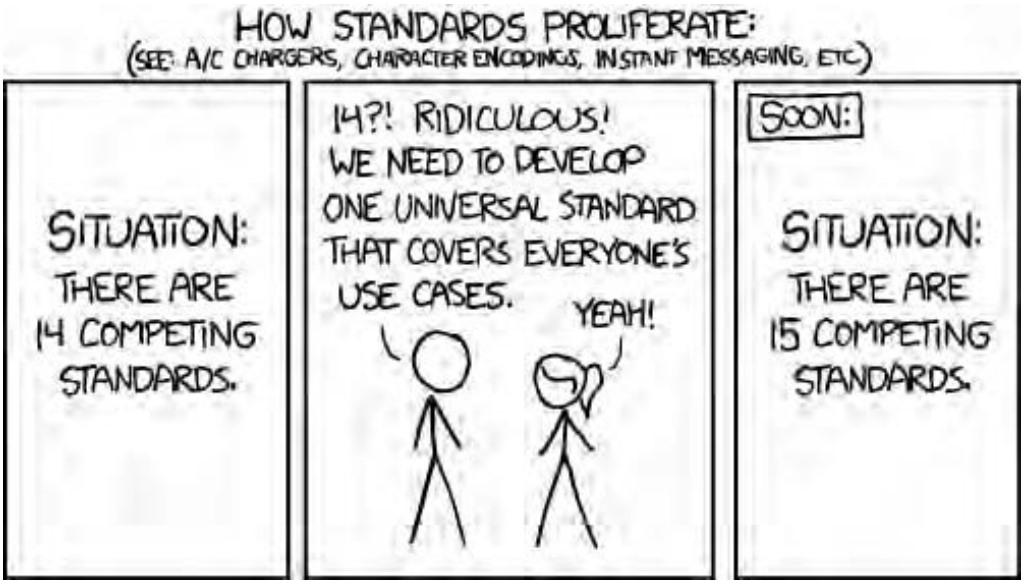
Wegener proposed the theory of continental drift, which ultimately led to plate tectonics. Initially he noted the shape complementarity of Europe, Africa and the Americas and suggested that they had once formed a supercontinent before drifting apart. Critics quite reasonably countered that the shape match could be fortuitous. Wegener provided a detailed analysis of rocks and fossils, showing that they were very similar across the joints in his proposed supercontinent. His blinkered opponents could only imagine the continents sailing through the viscous mantle like ships sailing through treacle, and they continued to ridicule Wegener. He went on to make his name in Arctic meteorology. In 1930 he led an expedition to establish an observing station to measure winter weather conditions in the middle of Greenland. Bad autumn conditions prevented the transport of sufficient supplies to the station. Having been funded by the German government at a time when some Germans were starving, Wegener felt a strong obligation to make the expedition a success. When winter had already started, he and a colleague took a dog-sled with the missing supplies to the station. On the way back, to lighten the load on the sledge when they only had a minimal number of dogs, Wegener proceeded on skis, but the exertion was too much for this 50-year-old smoker; and he died, presumably of a heart attack.

By the early 1980s most medical scientists believed that gastric and duodenal ulcers were a mature research field not requiring further investigation. It was an established dogma that bacteria could not survive in the strongly acidic contents of the stomach. Ulcers were attributed to excessive acid secretion induced by stress, spicy food and smoking, augmented by a hereditary predisposition. In fact, a few microscopists identified Helicobacter pylori in gastric washings from ulcer patients and animals at the end of the 19th century, but it was dismissed as a contaminant or a transient harmless commensal.

More systematic studies by the pathologist and surgeon **Georg** Ernst Konjetzny from the 1920s to the 1940s found *H. pylori* in samples from many patients. However, unlike the courageous and principled Max von Laue, who shunned Nazi science, Konjetzny joined the Nazi party. Possibly because of his nasty political affiliation, his work was not followed up after the war. In Perth, Australia, in 1981, microbiologist Barry Marshall and pathologist John Robin Warren established an association between ulcers and the bacteria with impressive statistical validation. However, their results were not generally accepted, and one reason was that they had not yet satisfied all of Koch's postulates. It was necessary to show that starting the infection in a healthy subject induced the disease. Marshall administered the bacteria to piglets, but they grew into inconveniently large healthy pigs with no sign of *H. pylori*. Marshall solved the problem by drinking a culture himself. Within a few days he developed severe gastritis, and a biopsy showed large numbers of *H. pylori* and pus cells. It took until 1989, but Marshall and Warren's methods of diagnosis and treatment were finally accepted, and they received a Nobel Prize in 2005. Marshall's Nobel Lecture, complete with a comic book illustration, is very entertaining.

By now you are probably wondering what all this has to do with crystallography. Geologists and medics may be prejudiced, but surely crystallography is so evidence-based and crystallographers are so open-minded that it could never happen to us. Well, it could and it did! Exactly 50 years ago **D. June Sutor** published a paper in *Nature* that presented a geometrical analysis of C-H...O interactions in crystals that was intended to confirm the presence of hydrogen bonding. However, the idea of C-H...O hydrogen bonding was condemned by some prominent crystallographers in the 1960s. For the next two decades only the bravest authors referred to "C-H...O hydrogen bonding". Others tiptoed around the subject with terms like "C-H...O interactions". I have published a *Crystallography Reviews* (2012, 1–16, iFirst) article about this controversy, including an analysis of the evidence available in the 1960s.

Carl Schwalbe - from the March 2012 issue of BCA Crstallography News.



Office of Science and Technology Policy Unveils Big Data Initiative

In March (2012), the White House Office of Science and Technology Policy (OSTP), in collaboration with several federal departments and agencies, announced the creation of a *Big Data Research and Development Initiative* to a packed auditorium at the American Association for the Advancement of Science.

The goals of this initiative are *"to advance state-of the-art core technologies needed to collect, store, preserve, manage, analyze, and share huge quantities of data; harness these technologies to accelerate the pace of discovery in science and engineering; strengthen our national security; transform teaching and learning and to expand the workforce needed to develop and use Big Data technologies."*

OSTP Director John Holdren began the event by emphasizing *"it's not the data per se that create value, what really matters is our ability to derive from them new insights, to recognize relationships, and to make increasingly accurate predictions. Our ability, that is, to move from data to knowledge to action."*

Though the private sector will take the lead in developing Big Data systems, Holdren stated that the government will play a large role in supporting research and development by investing in a Big Data work force, using new approaches to make progress on key national challenges, and shaping policies on issues such as electronic privacy.

Subra Suresh (NSF), outlined the strategies being implemented at NSF used to derive knowledge from Big Data: to develop infrastructure to manage, curate, and serve data to communities; and to build education and workforce opportunities.

NSF's Big Data interdisciplinary efforts include: a collaborative project between NSF and the NIH to advance Big Data science and engineering, funding a $10 million Expeditions in Computing project based at UC Berkeley; integrating human knowledge and computer algorithms and machines to develop a new understanding of these Big Data. NSF will also encourage research universities to develop interdisciplinary graduate programs in Big Data and will provide the first round of grants to support "EarthCube" which is a system that will allow geoscientists to access, analyze, and share information about earth. In addition, NSF will issue a $2 million award for undergraduate training in complex data, provide $1.4 million to support a group of statisticians and biologists to study protein structures and biological pathways, and create an "Ideas Lab" forum to enhance efforts to understand teaching and learning environments.

Francis Collins (NIH) described a new collaboration between the National Human Genome Research Institute, the National Center for Biotechnology Information and the European Bioinformatics Institute to put the largest set of data on human genetic variation, produced by the international 1000 Genomes Project, on the Amazon Web Services Cloud. The 200 terabytes of data from this project had become so massive that user access was very challenging. Therefore having the data in the cloud, and making it freely available, has benefited the science community by granting improved access to the data.

Marcia McNutt (USGS) announced projects on climate change, earthquake recurrence rates, and ecological indicators.

Zach Lemnios (DOD) stated that they will invest approximately $250 million annually, with $60 million available for new initiatives projects. He described Big Data challenges such as the capability to use the large amounts of generated data and how scientists perform computations and employ data capacity. DOD areas of focus include data-to-decision projects focused on reasoning and inferences, autonomy research to develop ways to adapt to "real world" scenarios, and human-system research such as the need for new technological interfaces.

Ken Gabriel, Defense Advanced Research Projects Agency (DARPA) announced that the agency is beginning the XDATA program, which will invest approximately $25 million annually for four years to develop computational techniques and software tools for analyzing large volumes of data. The goals of this project are to develop scalable algorithms for processing data and to create effective human-computer interaction tools.

William Brinkman (DOE) Office of Science (SC), spoke about the need to store, analyze, and use Big Data. One of the roles of SC will be to operate and maintain facilities at national laboratories including supercomputers, x-ray light sources, advanced light sources, nanoscience and systems biology laboratories. The data at these facilities is rapidly generated and there is a need for a way to better manage this Big Data. Brinkman announced that SC is establishing the Scalable Data Management, Analysis and Visualization (SDAV) Institute to bring together six national laboratories and seven universities to develop tools to help scientists manage and visualize data on DOE's supercomputers.

Aline D. McNaull - AIP

2012 Travel Awards

Argentina
Cristian Huck-Iriart
Institute of Inorganic Chemistry, Material Science and Energy

Canada
Halil Aydin
University of Toronto
Jonathan Cook
University of Toronto
Sergei Kalynych
McGill University
Timothy Munsie
McMaster University
Brahm Yachnin
McGill University

New Zealand
Sanaz Khorasani
University of the Witwatersrand

Spain
Elena Forcen-Vazquez
University of Zaragoza

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D. Sean Froese
University of Oxford
James Hall
University of Reading
Allan Pang
Queen Mary University of London

United States
Elena Aksel
University of Florida
Keith Alquist
Kansas State University
Srinivas Aripirala
Johns Hopkins University
Shyamosree Bhattacharya
University of Wisconsin Madison
Faye Bowles
UC Davis
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Richa Dhatwalia
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HHMI at the Rockefeller University
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Bhupinder Sandhu
New Mexico Highlands University
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University of Missouri-Columbia
Jason Stagno
NCI/NIH
Vitali Stanevich
University of Wisconsin - Madison
Shraddha Thakkar
University of Arkansas for Med. Sci.
William Wan
Vanderbilt University
Wenhua Wang
University of Rochester
Matthew Whitley
University of Pittsburgh
Marni Williams
Yale Univ.
Mario Wriedt
Texas A&M University

2012 Margaret Etter Awards

Etter Early Career Award
Emmanuel Skordalakes
University of Pennsylvania

Etter Student Lecturers

Bio-Mac SIG
Eugene Chun
Scripps Research Institute

General Interest SIG
Karim Sutton
University of Oxford, UK

Powder Diffraction SIG
Andrey Yakovenko
Texas A&M University

Small Angle Scattering SIG
Allan Pang
Queen Mary University of London, UK

Fiber Diffraction SIG
Simon Goodson
Cardiff University, UK

Synchrotron SIG
Christopher Dettmar
Purdue University

Industrial SIG
Shraddha Thakkar
University of Arkansas

Neutron SIG
Elena Aksel
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ACA 2013 – News Flash

ACA will be returning to the Sheraton Wakiki in Honolulu, Hawaii for our 2013 meeting. This will be our second meeting on the 4 day schedule that will debut in Boston.

Save the Date: July 20-24, 2013

Deadlines:

Abstracts	March 31
Travel Grants	March 31
Early Registration	May 31
Hotel Conf. rate	July 5

Awards:

Trueblood	Tom Terwilliger
Fankuchen	Richard Dickerson
Bau	to be announced
Etter Early Career	to be announced

Program Chairs:

Jeanette Krause

Allen Oliver

Photos: Hawaii Tourism Authority (HTA) / Tor Johnson

JULY 2012

28-1 **ACA2012, Westin Boston Waterfront Hotel, Boston, MA.** *Program Chairs: Bruce Foxman and Bruce Noll; Local Chair: Peter Mueller*

Bruce Foxman

Bruce Noll

Peter Müller

NOTE: New meeting format - Workshops still on Saturday but then 4 days instead of 5 - beginning on Sunday, July 29 and concluding on Wednesday, August 1st.

AUGUST 2012

7-11 **ECM-27**, Bergen, Norway. *www.ecanews.org/meetings.php*

SEPTEMBER 2012

9-13 **EMC 2012**, European Mineralogical Conference, Johann Wolfgang Goethe-University, Frankfurt, Germany

NOVEMBER 2012

25-30 **2012 MRS** Fall Meeting and Exhibit, Boston, MA *www.mrs.org/fall2012/*

NOVEMBER - DECEMBER 2012

25-3 **MaThCryst International School on Fundamental Crystallography (ISFC2012)** Uberlândia Brazil. *www.crm2.uhp-nancy.fr/mathcryst/uberlandia2012.php*

DECEMBER 2012

2-6 **AsCA'12 and Bragg Symposium** Adelaide, Australia. *www.asiancrysassn.org*

Index of Advertisers

JULY 2013

20-24 **ACA2013,** Sheraton Waikaki, Honolulu, HI.

AUGUST 2013

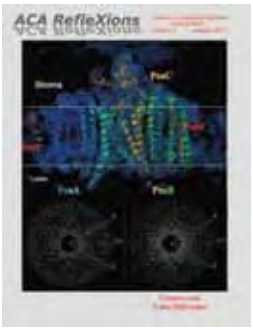
6-13 **ECM 28** Univ of Warwick, Coventry UK, *ecm28.org/*

11-16 **XXII International Materials Research Congress** Cancun Mexico, *www.mrs.org/imrc2013/*

AUGUST 2014

5-12 **XXIII Congress and General Assembly of the IUCr,** Montreal, Quebec, Canada: *www.cins.ca/cncc/montreal/2014iucr*

What's on the Cover



The illustrations used for the cover of this issue of *RefleXions*, provided by *John Spence*, are from results described in the paper titled *Structure-factor analysis of femtosecond microdiffraction patterns from protein nanocrystals* (Kirian et al., *Acta Cryst.* (2011) **A67**, 131-140). (For a full list of the many collaborators who contributed to this project, see *Femtosecond X-ray protein nanocrystallography* by Chapman et al., *Nature* (2011) **470**, 73-77). The authors reported that a complete set of structure factors had been extracted from hundreds of thousands of femtosecond single-shot x-ray microdiffraction patterns taken from randomly oriented Photosystem I nanocrystals prepared in the laboratory of Prof P. Fromme. Monte Carlo integration over crystallite size and orientation was used to arrive at the structure factors without prior knowledge of the particle-size distribution. The data, collected at the Linac Coherent Light Source (the first hard-x-ray laser user facility), are single 'still' diffraction snapshots, each from a different nanocrystal with sizes ranging between 100 nm and 2 mm, so the angular width of Bragg peaks was dominated by crystal-size effects. The protein nanocrystals were sprayed in single file across the pulsed x-ray beam using a novel type of micron-diameter liquid stream and droplet beam in vacuum. These results were compared with single-crystal data recorded from large crystals of Photosystem I at the Advanced Light Source and the quality of the data was found to be similar.

Cover images: Top - Density map for PSI obtained by combining this LCLS nanocrystal diffraction data with data in the PDB. Some of the 12 proteins in each monomer are labeled PsaA etc. Lines across the figure indicate the position of the membranes. *Lower left* - Calculated precession image of the [001] zone extracted from single crystal data obtained at the Advanced Light Source. 50% twinning has been applied. *Lower right* - Calculated precession image of the [001] zone extracted from PSI nanocrystal data collected at the LCLS following indexing by MOSFLM. The data set consists of 16,374 single snapshot diffraction patterns of 70 fs pulse length collected at the AMO beamline at LCLS at 6.9 Å wavelength. The space group was $P6_3$, but $P6_322$ symmetry was imposed by autoindexing ambiguity, resulting in an apparent twin fraction of 0.5 for this data set. The integration domain radius was $\delta = 7.3$ mm^{-1}.

See what U'V been missing

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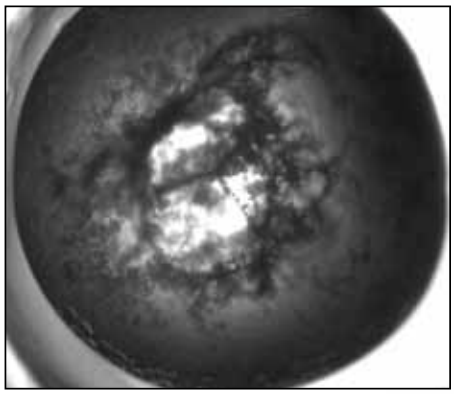

Visible image of microcrystals in precipitate

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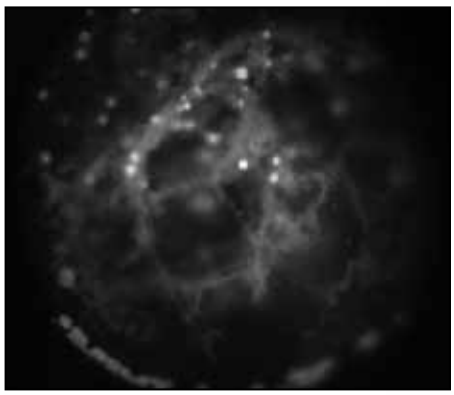

UV image of microcrystals in precipitate

Which leaves one question:

What will you see with your new Minstrel DT UV?

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Crystallography

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