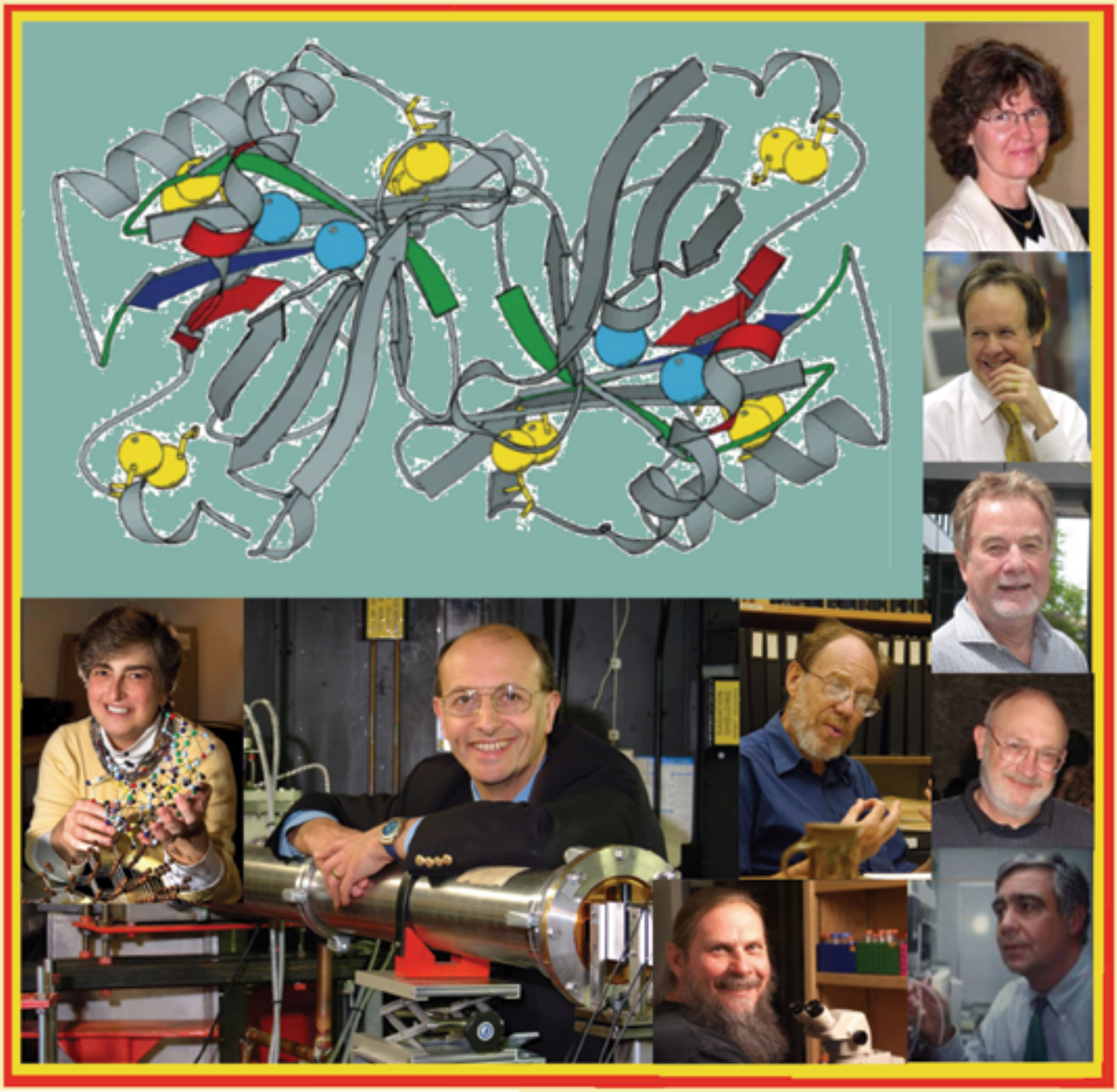
ACA RefleXions

ACA
Structure Matters

Number 1

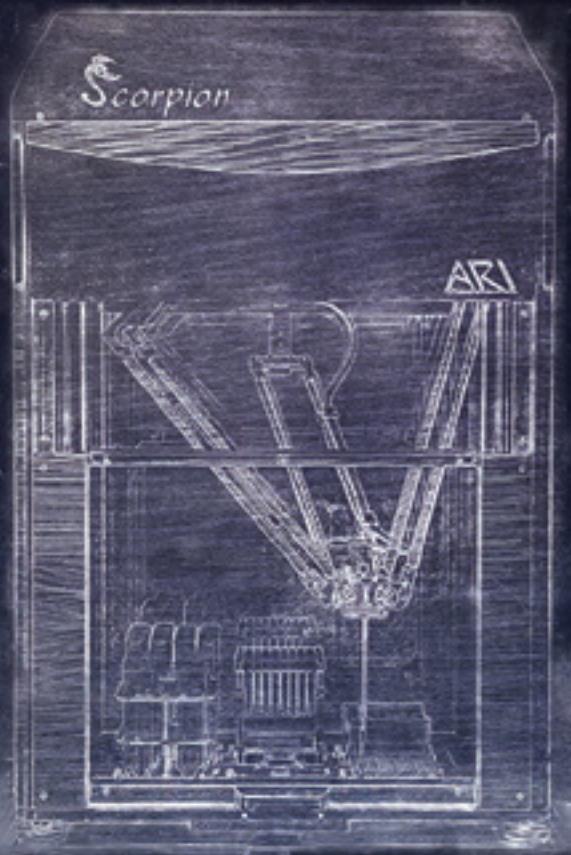
Spring, 2014



Patterson Award at Albuquerque ACA Meeting

TODAY'S LESSON:
What Can A Scorpion Screen Builder Do?

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



Scorpion = Versatility

For more information contact

ARI - Art Robbins Instruments
www.artrobbins.com

ACA RefleXions

ACA
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www.AmerCrystalAssn.org

Spring 2014

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Borden Lacy

Wood Award Winner
Dan Rabinovich

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Puzzle Corner:	Frank Fronczek

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

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President's Column

What a great year to be a crystallographer! And I am honored to be your President. Those of us, "captured for life…by crystals," (Dorothy Hodgkin, Oxford Dictionary of Quotations, 6th edition) and captured by the beauty of atoms and the structure of matter have something to celebrate. This International Year of Crystallography (IYCr) is a year to get the word out that crystallography is not just a tool but also a way to address problems at the cutting edge of our knowledge today. How do proteins and nucleic acids function *in vivo*? How can we make better catalysts? Can we increase the lifetime and efficiency of batteries for electric cars? How do molecules "recognize" one another? There are so many questions.

We are excited to share "what crystallography is" with others. To show them the fun and power of what we do. To explain crystallography's ability to explore the structure of matter to our friends and to our politicians. To volunteer at local schools and excite young people about careers in science through crystallography. To plan events that involve our community in this celebration.

Because crystallography is interdisciplinary, we address issues across the traditional boundaries of academics. Ours is a discipline that can also create understanding between people of very different politics. It can be a mechanism for peace in this conflicted world. Let me tell you what I mean by this.

I had the privilege of attending the Opening Ceremonies of the IYCr in Paris, January 20 and 21, where three young crystallographers who have been involved in leading the ACA's YSSIG accompanied me. I'm grateful for support in part from the US National Committee for Crystallography for Andy Torelli and membership donation for me that enabled our attendance.

A big emphasis of IYCr is on engaging crystallographers in developing countries. We heard from young crystallographers from the developing world, and our own Andy Torelli, former YSSIG secretary, represented the ACA on a Q&A panel during this session. Please read Andy's article in this issue on page 17. We also heard about the formation last November of the Latin-American Crystallographic Association, in part through the tireless efforts of ACA's own CEO Bill Duax. Thank you, Bill!

Delegates to Paris IYCr Opening Ceremonies from USA and Venezuela. L-R; Front: Graciela Diaz de Delgado, Yulia Sevryugina, Cora Lind-Kovacs, Martha Teeter; Rear: Clyde Kovacs, Andy Torelli, Jarrod French, Marvin Hackert. Photo: Bretna Hackert.

It became clear, as Dorothy Hodgkin demonstrated in her diplomacy through science (collaboration with USSR and China during the years of the cold war), that crystallography can catalyze peace on a world level. The new synchrotron facility SESAME in Amman, Jordan, will engage scientists in a war-torn part of our world in peaceful research on the structure of matter. It will generate a carpet of understanding. SESAME stands to open doors to peace worldwide.

And so I urge you to get involved. Visit the ***IYCr2014.org*** website. Our ACA IYCr website will soon be up and running to provide you more tools. Consider training an international student from a developing country to return home to be an ambassador.

Let's get the word out about crystallography at the cutting edge (12.5 % of chemistry and physics Nobel prizes are in crystallography) and the world peacemaking endeavors of crystallography.

Martha Teeter

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From the Editor's Desk

Errata - Winter 2013 Issue of RefleXions (As much as we hate making mistakes it is gratifying to know that we are being closely read).

We inadvertently omitted Thomas Laube from the list of donors to ACA funds. We apologize for the omission, offer belated thanks for the support, and promise to do better in 2014.

J. Michael Bennett pointed out that, in Abe Clearfield's article, we had reversed the captions for the projections of the two structures on page 14. The VPI5 drawing is on the left.

We described Dan Rabinovich (2014 Wood Science Writing Award winner) as being a "Peruvian inorganic chemistry professor with Ukrainian ancestry." However, since Dan has been a US citizen for about nine years, he let us know that he would prefer to be described as, "a Peruvian-American inorganic chemistry professor of Ukrainian descent."

Hawaii Travel Grant Recipient: I am a postdoctoral fellow at the Walter and Eliza Hall Institute, Melbourne, Australia. This was the first ACA meeting I attended, and I thoroughly enjoyed the conference. The program was enjoyably diverse with quite a number of interesting talks and discussions. In particular, the *Career Odyssey Panel* discussion was great. Being chosen to present my work in the *Pathogens* session was definitely a bonus, but losing my laptop minutes before my talk was not so great. The poster sessions and social events were well organized and gave me an excellent opportunity to network. All in all, my experience at the ACA meeting was very positive.

Gyanendra Kumar

Update on the ACA History Site: *Our first testimonial - from Don Caspar.* "I recently stumbled on the wonderful ACA History web site. I was looking at photographs of Dorothy Hodgkin in my browser and noticed the collection included an unlabeled photo of Jenny Glusker and Penny Codding. Curious, I clicked on this photo, which had a link to where it came from. This brought me to Jenny's memoir on the new site, to which I did not pay particular attention since I was interested in the beginning of Jenny's account, which described how she grew up in Birmingham and got interested in science, as did my late wife, Gwladys. Could they have met as schoolgirls? However, it appeared unlikely they had crossed paths since Jenny must be three or four years younger than Gwladys. Having got this far, I read the rest of her memoir with great interest, particularly her account of Dorothy Hodgkins' influence on her career and life; and also her account of her interactions with David Sayre and Kenneth Trueblood."

"When I had finished reading this illuminating history, I noted that the web site also had memoirs by Marjorie Senechal and Jack Dunitz. A few days earlier, I had stumbled on an excerpt from Marjorie's biography of Dorothy Wrinch, describing a Steuben crystal glass truncated tetrahedron, which David Harker had given Dorothy. (I was searching the web to find this Steuben gem, which reflects an icosahedron inside, as a gift for Xiaowei Zhuang who recently presented the second annual Caspar Lecture at FSU, but that is another story.) After reading Jack's intriguing memoir, I finally turned to the ACA web site itself."

"To my surprise, this remarkable web site has historical videos including my account of 'Origins of Structural Biology' from the 2012 ACA meeting. The slides from this talk are wonderfully displayed. … Clearly, I have to write an intelligible account of what I was trying to say to complement the illuminating images. I will do my best to add more text, which can be much more informative than recorded words in this valuable resource. I have agreed to write an account for *Crystallography Reviews* of my discovery of icosahedral symmetry in crystalline viruses and its implications in virus crystal structures. I hope that I will be able to add this to your marvelous web site."

Nobel Laureates. At the 1988 ACA meeting in Philadelphia we had a Nobel session that was moderated by Linus Pauling and included talks by John Kendrew, Dorothy Hodgkin, William Lipscomb, Herbert Hauptman, and Jerome Karle. Helen Berman made arrangements to have the session videotaped and still had the set of original VHS tapes that she recently had transferred to two DVDs. Ilia Guzei has now accepted the challenge to work with the files and get them into shape to be put up on the ACA History site. We are also continuing to collect and add more materials from our own archive of written and oral documents, so keep coming back to the site to see what's new.

Letter from the Editor-in-Chief of Structural Dynamics

Capitalizing on recent experimental and theoretical advances, *Structural Dynamics* aims at providing a forum for the community of scientists working on the development, implementation and use of new tools for the determination of static and time-evolving structures. This community includes scientists dealing with different aspects of structural dynamics in relation to problems in atomic and molecular physics, condensed matter physics and materials science, chemistry and biology, that often use similar experimental (synchrotrons, X-ray free electron lasers, ultrashort pulse UV-visible lasers, ultrashort electron pulses, laboratory sources of ultrashort X-ray pulses, high harmonic generation sources) and theoretical (molecular dynamics simulations, quantum chemical calculations, etc.) tools.

We therefore encourage submissions in areas such as:

- Static structure determination and imaging.

- Dynamical (i.e. time-domain) structural studies with a time resolution from femtoseconds to milliseconds and spatial resolutions from the Å to the micron.

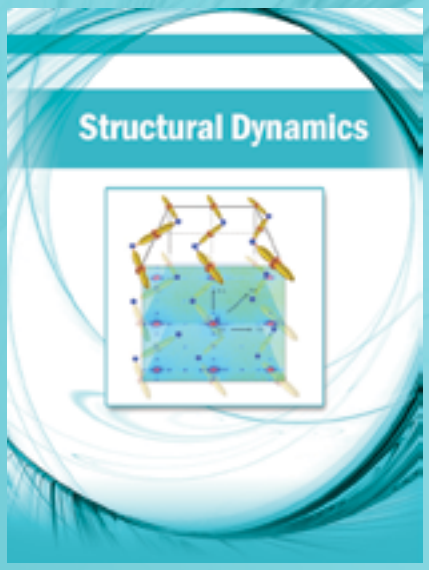
- Electronic structure studies that underlie structures at equilibrium and/or their evolution over time.

- Theoretical modelling and computational studies of all the above.

Structural Dynamics

sd.aip.org

FIRST PAPERS NOW ONLINE JANUARY 2014



Structural Dynamics is a new open access and online-only journal which is now accepting submissions. Co-published by ACA and AIP Publishing, it will highlight research articles on structural determination and dynamics of systems, enabled by the emerging new instruments (e.g. XFELs, electron sources, etc.) and new experimental and theoretical methodologies.

http:/sd-peerx-press.org

TOPICS INCLUDE:

- **Structural dynamics of molecular systems, biological systems, solid materials, liquids and solutions, and surfaces and interfaces**
- **Static structural determination, static imaging techniques and studies using highly coherent sources**
- **Dynamical studies of systems both in and out of equilibrium, with a time resolution from femtoseconds to milliseconds**
- **Spatial resolutions from 1 Å to 1 μm**
- **Electronic structure studies connected to molecular/lattice/protein structure**

FIRST 50 ACCEPTED ARTICLES ARE FREE!

Journal Sections

- *SD Communications:* letter-format papers
- *Topical Reviews:* papers on specific topics in structural dynamics.
- *Articles:*
  - o Theory and Modelling (aspects of theory and data analysis, algorithms, etc.)
  - o Experimental Methodologies (technical and methodological developments)
  - o Materials
  - o Biological Systems
  - o Liquids and Solutions
  - o Surfaces and Interfaces
- *Letters to the Editor:*
  - o Errata
  - o Comments on papers
  - o Reply to « Comments on… »

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ACA
Structure Matters

AIP Publishing

Submissions are also welcome dealing with the methodological aspects of structural studies and their time-dependence, such as:

- X-ray diffraction (crystallography) and X-ray scattering.
- X-ray absorption spectroscopy (XANES and EXAFS).
- Electron diffraction, scattering and microscopy.
- Coherent X-ray imaging.
- Core-level spectroscopies: photoelectron spectroscopy (PS), photoemission, X-ray emission spectroscopy (XES), resonant inelastic X-ray scattering (RIXS), electron-energy-loss-spectroscopy (EELS).
- NMR spectroscopies.
- Vibrational (infrared) and electronic (visible-UV) multidimensional spectroscopies.

The journal thus welcomes articles dealing with scientific questions related to structure determination and dynamics, driven by emerging experimental methodologies and technical developments. The journal will therefore contain the following sections:

- Short Communications
- Theory and Modelling
- Experimental Methodologies
- Materials and Surfaces
- Biological Systems
- Liquids, Solutions and Interfaces

Structural Dynamics will combine high-quality peer review with a streamlined publication process to highlight your results. We very much look forward to receiving your articles.

Majed Chergui - Editor-in-Chief, Structural Dynamics

Report of Canadian Division Representative

Firstly I want to thank those Canadian members of the ACA who voted for me as their representative on the ACA Council in the recent elections. It will be a challenge but also a pleasure to work with the Canadian Division of the ACA and to present the ideas and wishes of Canadian crystallographers and all other material scientists to the ACA Council. Canada has a rich history of crystallography with much of its origins stemming from mineralogy and geology. One of the first crystallographic laboratories was the one headed by William H. Barnes at the NRCC in Ottawa, which was established in 1947 in the Division of Physics. Barnes had studied at McGill University, and subsequent to receiving his doctorate there he spent two post-doctoral fellowship stints at the Royal Institution, London, under the supervision of W. H. Bragg. Barnes returned to Canada in 1930 to an academic position at McGill University where he remained until 1946 when he took a sabbatical at MIT with Professor Martin J. Buerger. Barnes had many excellent scientists to work in his laboratory at the NRCC. One in particular was young David Phillips, who during his time at the NRCC developed the expressions necessary for the spot-shape corrections on Weissenberg photographs. After his stay in Ottawa (1951 – 1955), Phillips returned to the UK to the Royal Institution where he headed the team that determined the first structure of an enzyme, that of hen egg white lysozyme in 1965. Certainly the above brief history illustrates the importance of international collaboration and of exchange of ideas in science, especially for Canadians. This leads me to the main part of my short message. I have taken the opportunity to review the Canadian membership rolls in the ACA. The ACA offices in Buffalo provided me with statistics that are up to date as of January 15, 2014. I also consulted the IUCr World Directory of Crystallographers. Admittedly both of these sources may be out of date, but they do give approximate sets of data on which to ask the following questions: Why are there so few Canadians who are members of the American Crystallographic Association? Is the reason behind this financial? Is it apathy? The statistics that led me to ponder this lack of interest are derived from the above sources. There are 208 people listed in the World Directory under Canada. There are 94 paid-up Canadian members of the ACA as of January 15, 2014 (21 are fully paid up, while 73 were members last year and have probably just forgotten to renew or have been too busy recently). The sad part of the story is that there are 34 who were ACA members in 2011 and/or 2012 but who have let their memberships lapse. Further it means that only 45% of Canadian Crystallographers, or those scientists interested in the structure of materials, are actually members of the ACA. The ACA is our only voice as a scientific body. True, we do have a Canadian National Committee comprising Jim Britten (Chair), Joe Schrag (Secretary), Marie Fraser (Treasurer), Stan Cameron, Lynne Howell, and Lee Groat, but we do not have national meetings through that body; our meetings as a national group of scientists are held in conjunction with the American Crystallographic Association. This is why it is vitally important for Canadians to be members of the ACA, so that our collective voices can be heard.

William H. Barnes was a key figure in bringing the IVth Congress of the IUCr to Montreal in 1957; Louis Delbaere worked very diligently to bring the XXIIIrd Congress and General Assembly back to Montreal this summer in the International Year of Crystallography. In addition to our contributions to the IUCr, Canadians have played important roles in the ACA. Carol Huber was president in 1996; Penny Codding was president in 1998; Louis Delbaere was president in 2005. Several ACA Meetings have been held on Canadian soil: Carleton University in Ottawa in 1971, University of Calgary in Calgary, Alberta in 1980, McMaster University in Hamilton, Ontario in 1986, Montreal, Quebec in 1995, and Toronto, Ontario in 2009. It is clear that Canadians have had a major influence in the ACA. Let's not lose this important connection.

All of this leads me to paraphrase one of the greatest statesmen of the last century, John F. Kennedy, in his Inaugural Address on January 20, 1961. "Ask not what the ACA can do for you, ask what you can do for the ACA." Lets get together and join or renew our memberships!

Michael James
Canadian Division Representative on ACA Council

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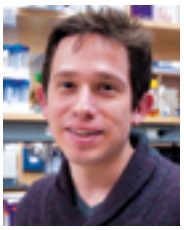

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Nominations for 2015

ACA Awards: Nominations for the **Buerger, Warren Diffraction Physics**, and **Etter Early Career** awards are due by May 1, 2014.

ACA Offices and Committees: In fall 2014 we will elect a new Vice President and one person to each of the ACA Standing Committees (Continuing Education, Communications, and Data, Standards & Computing). To suggest a candidate for one of the above positions, please contact a member of the ACA Nominating Committee: **George Phillips: georgp@rice.edu**, **Carrie Wilmot: wilmo004@umn.edu**, and **Victor Young: vyoung@umn.edu**. Full details describing the criteria for all ACA awards and offices can be found on the website.

2014 Dues are Due: Please renew promptly and remember to support your favorite ACA Award Funds.

NOTE: It is now possible to renew online.

ACA website: www.AmerCrystalAssn.org

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

New ACA Staff Appointment

We are pleased to introduce Jessica Addiss, of Buffalo, NY, as the ACA Bookkeeper.

Jessica graduated from the University of Buffalo in 2007 with a degree in English. She comes to ACA with a wealth of experience in managing a local hostel, and extensive knowledge of nonprofit bookkeeping and QuickBooks. Jessica will attend her first ACA Meeting this May in Albuquerque, and I hope you will all join me in welcoming her to our ACA family.

Marcia Colquhoun
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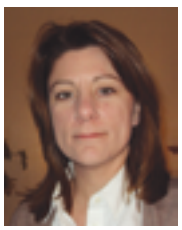

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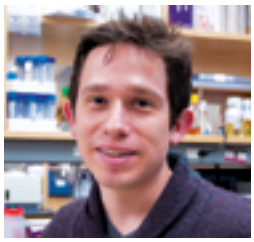
YSSIG Representative on ACA Council



Name: Eric J. Montemayor

Affiliation: Postdoctoral Research Associate, University of Wisconsin-Madison, Madison, WI 53705

Education: Ph.D., Physical Chemistry, University of Texas at Austin, 2008

Professional Activities: 2012 chair of Young Scientist Scientific Interest Group (YSSIG). Session chair at 2012 and 2013 ACA meetings. Co-manager of the YSSIG High School Crystallography Project in Boston (2012), Honolulu (2013), and Albuquerque (2014).

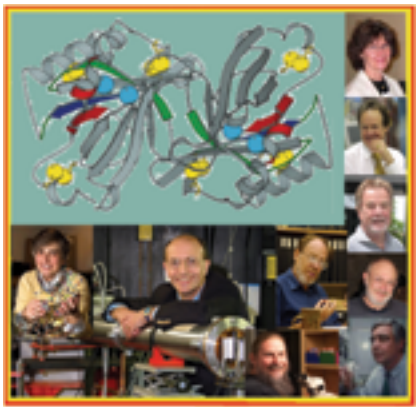
Research Interests: I use *in vitro* biochemistry, X-ray crystallography, and small-angle X-ray scattering to study the structure and function of the spliceosome, a massive and dynamic ribonucleoprotein complex that orchestrates processing of eukaryotic messenger RNA. I am also interested in understanding how the metalloenzyme Dbr1 is able to specifically hydrolyze the unusual 2', 5'-phosphodiester linkage found in lariat introns, a byproduct of spliceosome-mediated mRNA processing.

Statement of goals on council: I am thrilled and honored to represent my YSSIG colleagues this year! My primary goal while on council will be to ensure coordination between the YSSIG and the ACA leadership, so that we can work together in providing career development opportunities for early career scientists and also ensure the long-term sustainability of the ACA by improving retention of young scientists in the Association. I am particularly interested in making it easier for young scientists to attend the annual ACA meetings, either by lowering costs associated with attendance or finding new funding opportunities to expand the limited number of travel awards currently offered by the ACA.

The International Year of Crystallography 2014 (IYCr2014) presents a unique opportunity for increasing our visibility among non-scientists. To this end, the YSSIG has been involved in many outreach activities including three of our members traveling to Paris for the UNESCO IYCr2014 opening ceremonies in January (a trip made possible in large part through the efforts of ACA President Martha Teeter). We also plan to expand the high school outreach project that we initiated in 2012 (see page 25) and fully integrate our outreach activities onto the ACA and IUCr websites.

Eric Montemayor

What's on the Cover?



The **ACA 2014 Patterson Award** will be given to University of Manchester Emeritus Professor **John Helliwell**, currently the Co-Editor of *J. Appl. Cryst.* and Joint Main Editor of *Crystallography Reviews*. The photo on the cover shows him inside the SRS 7.2 radiation protection 'hutch' leaning on the vacuum beam pipe between the monochromator and the crystal sample camera.[1] (See also the summer, 2013, *ACA RefleXions*, when the award was announced.) Above, the apocrustacyanin A1 dimer showing bound Xe atoms in cyan and disulfide bonds in yellow was solved with softer X-rays and their enhanced anomalous scattering signals.[2] United States crystallographers that John especially appreciated collaborating with are, at left: Vivian Stojanoff;[3] center, Michael Rossmann;[4] and, below him, Steve Ealick;[5] on the right side, from the top: Britt Hedman, and Keith Hodgson;[6] Keith Moffat;[7] Howard Einspahr;[8] and Charlie Bugg.[5,9]

For many years John studied protein crystal perfection at SRS, ESRF, and NSLS. At NSLS he collaborated with Vivian Stojanoff as well as with students Eddie Snell, now at Buffalo, and Titus Boggon, now at Yale.[3] Another former student, Ashley Deacon, now at Stanford, worked on the 0.94Å data collection of concanavalin A at MacCHESS. John has served on or chaired various advisory and board panels to review and/or develop synchrotron projects, and in later years also neutron projects. He worked closely with many colleagues, among them Wayne Hendrickson and Denny Mills (APS SAC); Gerd Rosenbaum and B C Wang (SERCAT SAC); Don Bilderback and Bob Sweet (MacCHESS SAC); and Art Schultz (ORNL MANDI). One of John's current interests is neutron Laue diffraction. During the last two decades an interesting synergy between synchrotron radiation and neutron crystallography developed involving the application of Laue diffraction. The use, by the neutron facilities at the Institut Laue Langevin (ILL), at LANSCE (Paul Langan), and most recently at Oak Ridge (Dean Myles), of the Daresbury Laue diffraction images analysis package[11] has led to its use in many neutron protein crystal structures. The most productive instrument in PDB depositions was the SRS wiggler 9.6,[12] and it was used extensively.[2,6,7,11]

1) J.R. Helliwell, T.J. Greenhough, P. Carr, S.A. Rule, P.R. Moore, A.W. Thompson & J.S. Worgan, (1982) J. Phys. E. ***15****, 1363-1372.*

2) M. Cianci, P.J. Rizkallah, A. Olczak, J. Raftery, N.E. Chayen, P.F. Zagalsky & J.R. Helliwell, (2001) Acta Cryst. ***D57****, 1219-1229.*

3) T.J. Boggon, J.R. Helliwell, R.A. Judge, A. Olczak, D.P. Siddons, E.H. Snell & V. Stojanoff, (2000) Acta Cryst. ***D56****, 868-880.*

4) M.G. Rossmann & J.W. Erickson, (1983) J. Appl. Cryst. ***16****, 629-636.*

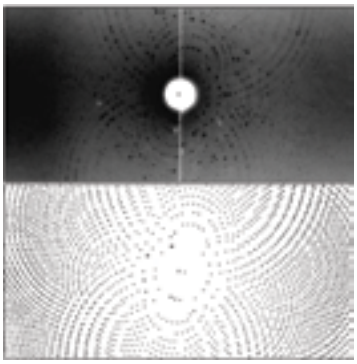
5) S.E. Ealick, S.A. Rule, D.C. Carter, T.J. Greenhough, Y.S. Babu, W.J. Cook, J. Habash, J.R. Helliwell, J.D. Stoeckler, R.E. Parks, Jr., S. Chen & C.E. Bugg, (1990) J. Biol. Chem. ***265****, 1812-1820.*

6) B. Hedman, K.O. Hodgson, J.R. Helliwell, R. Liddington & M.Z. Papiz, PNAS.USA, (1985) ***82****, 7604-7607.*

7) D.W.J. Cruickshank, J.R. Helliwell & K. Moffat, (1987) Acta Cryst. ***A43****, 656-674.*

8) H. Einspahr, K. Suguna, F.L. Suddath, G.Ellis, J.R. Helliwell & M.Z. Papiz, (1985) Acta Cryst. ***B41****, 336-341.*

At right, John's favorite example shows (above) the neutron Laue diffraction done at ILL on a crystal of the plant protein concanavalin A with glucoside bound (unit cell 167 Å) and (below) its spot prediction. The resolution limit is ~3.5 to 4Å.[10]



9) C.E. Bugg, W.M. Carson & J.A. Montgomery, Scientific American, December 1993, 92-98.

10) A.J.K. Gilboa, D.A.A. Myles, J. Habash, J. Raftery & J.R. Helliwell, (2001) J. Appl. Cryst. ***34****, 454-457.*

11) J.R. Helliwell, J. Habash, D.W.J. Cruickshank, M.M. Harding, T.J. Greenhough, J.W. Campbell, I.J. Clifton, M. Elder, P.A. Machin, M.Z. Papiz & S. Zurek, (1989) J. Appl. Cryst. ***22****, 483-497.*

12) J.R. Helliwell, M.Z. Papiz, I.D. Glover, J. Habash, A.W. Thompson, P.R. Moore, N. Harris, D. Croft & E. Pantos, (1986) Nuclear Instrum. and Methods, ***A246****, 617-623.*

ICCBM15

The 15th International Conference on the Crystallization of Biological Macromolecules (www.iccbm15.org) will be held in Hamburg, Germany, September 17 - 20, 2014. ICCBM15 will focus not only on macromolecular crystallization for novel radiation sources, such as the XFEL, but also on advances in CryoEM.

For individuals desiring to learn how to grow crystals, or to acquire new crystallization skills, the conference will be preceded by a workshop on September 14-16 devoted to hands-on instruction on select aspects of macromolecule crystal growth and handling by means of a variety of techniques. New aspects, like preparation and scoring crystals for FEL applications, will be included.

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Howard Einspahr

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IYCr2014 Ad Hoc Task Force Report

In May 2013, Martha Teeter, then ACA's Vice President, convened an *ad hoc* task force to help with celebration of the International Year of Crystallography 2014. The Task Force membership includes 13 regional representatives, a corporate representative, and six consultants. Around once a month, the regional representatives send emails to the 100-200 current or recently active members in their respective areas to share the latest news on IYCr.

The Task Force's goals for the IYCr2014 celebrations are that:

1. The public gains an increased awareness and appreciation for
   - Major contributions of science from crystallography to daily life
   - Symmetry, crystals, crystal growing, and diffraction
   - Nobel laureates in crystallography

2. Elementary, secondary, and university students are excited about and are motivated to learn about crystallography

3. Crystallography units are part of the K-12 science curriculum

4. We attract and retain more young scientists in crystallography

5. Funding for crystallography/science increases

6. Latin American crystallography is supported

7. There is a lasting legacy of appreciation of science.

Specific Task Force projects in support of IYCr include the following:

- An ACA IYCr website (due to launch soon)
- Downloadable files with biographies of crystallographers for library or for school displays
- A 'What is crystallography?' brochure, along with commemorative magnets and bumper stickers
- School outreach projects in Canada, the U. S., and Latin America
- U. S. teacher training in crystallography at the ACA's Albuquerque meeting and at two National Science Teachers Association meetings
- A U. S. national crystal growth contest
- A video contest for grades K-12
- Local/regional IYCr culmination events in October 2014.

Current Task Force regional representatives are: Louise Dawe (Canada), Peter Müller (New England), Miriam Rossi (NY), Curt Haltiwanger (PA Region) – with Jenny Glusker, Jamaine Davis (Washington, DC) – soon to be joined by Chris Cahill, Claudia Rawn (SE States), Cora Lind-Kovacs (OH region), Victor Young (Heartland), Danielle Gray (IL), Marvin Hackert (Southern), Ron Stenkamp (NW and Mountain), Katherine Kantardjieff (CA), and Graciela Diaz de Delgado (Latin America). Jim Kaduk is a corporate representative. Consultants include Camille Jones, Amy Sarjeant, Ilia Guzei, and Jason Benedict. YSSIG representatives are Yulia Sevryugina and Andy Torelli.

Martha Teeter

Ad Hoc Task Force Representatives

Task Force representatives pictured in the right-hand column are (top to bottom and left to right): C. Lind-Kovacs, M. Hackert, C. Cahill, J. Davis, L. Dawe, G. Diaz de Delgado, C. Haltiwanger, P. Müller, J. Glusker, D. Gray, J. Kaduk, R. Stenkamp, K. Kantardjieff, C. Rawn, V. Young, M. Rossi, and M. Teeter.

IYCr2014 Opening Ceremony & Next-Gen Crystallographers Discussion Panel

In January, I had the privilege of attending the Opening Ceremony for the 2014 International Year of Crystallography (IYCr2014) held at UNESCO headquarters in Paris. I was nominated by the ACA IYCr *Ad Hoc* Task Force to serve on a discussion panel as a representative of next-gen crystallographers. At this historic event, I joined a number of ACA members, distinguished speakers, UN officials, many international scientists, and students of all ages – several hundred guests in total – for an inspirational beginning to this celebratory year. The Secretary General of the United Nations, Ban Ki-moon, addressed the assembly by video, followed by Irina Bokova, Director-General of UNESCO, and the heads of multiple international scientific organizations. Keynote speakers included Jenny Glusker, who delivered a rich historical perspective of crystallography, and Brian Kobilka, who recounted his 2012 Nobel Prize work with Robert Lefkowitz involving G protein-coupled receptors. We heard other fascinating talks that included efforts to expand X-ray crystallography in emerging nations, cutting edge technologies, the first extraterrestrial diffraction measurements used to interpret the mineralogy of Mars, and applications of crystallography and symmetry in the study of art.

Panel discussion with talented young crystallographers of the world. Present (L-R): Panel members Rahul Banerjee (India), Maxime Deutsch (France), El-Eulmi Bendeif (France), Andrew Torelli (USA), Malla Reddy (India), Vaughan Maurel (South Africa), Alice Brink (South Africa), Dyanne Cruickshank (South Africa). Moderator: Philip Ball. Selected crystallographers: Adriana Serquis (Argentina), Ji-Joon Song (Republic of Korea), Marcin Nowotny (Poland), Yvon Bibila (Ivory Coast), Anders Madsen (Denmark), Mohamed Eddaoudi (Saudi Arabia), Rumana Akther Jahan (Bangladesh). Not present: Delia Haynes (South Africa). Photo: Marv Hackert.

I was involved in a session that introduced eight selected, early-career crystallographers from around the world, followed by our panel discussion. The main purpose of the panel session, as envisioned by Maciej Nalecz, Director and Executive Secretary of UNESCO's International Basic Sciences Program, was to communicate critical issues facing the next generation of crystallographers to policy makers and sovereign delegations. The young crystallographer group identified these issues:

- the need to emphasize that crystallography, while increasingly commonplace, is at the forefront of so many scientific endeavors
- growing pressures to secure funding with time scales or foci incompatible with basic science agendas
- the scarcity of advanced crystallography training in some world regions
- limited access to scientific journals whose subscriptions are expensive
- the importance of communication to establish mutually-beneficial international collaborations.

The last topic highlights an important theme of the event centered on enabling international collaboration and dialogue. One example, the Open Labs initiative, is a partnership between the IUCr, UNESCO, and major equipment manufacturers to bring X-ray instruments and training to Africa, Latin America, and Asia. I was also moved by the description of the SESAME (Synchrotron Light for Experimental Science and Applications in the Middle East) initiative. This project, nearly operational after decades of planning and partnerships between scientists from countries that could hardly be imagined working together, is proof of the power of science to transcend political and social boundaries. All of us within the crystallography community should be inspired that our science is a basis for cooperation and collegiality in this extraordinary example of collaboration and perseverance.

Overall, the Opening Ceremony was an inspiring start to the IYCr. I have a broadened view of the rich variety of applications utilizing crystallography, and a deeper appreciation for the need to bring the technology and training to emerging and developing countries. This will require not only investment, but also meaningful collaborations, among us – the crystallographers. Fortunately the precedent for the benefits of crystallography to science and humanity is clear, as is the enthusiasm displayed by those who attended the meeting to come together to share ideas. And I left the event with a renewed sense of excitement to be included in a defining science that will have an important role to play in many great achievements of the future.

Andy Torelli

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2014 international year of crystallography IUCr

When I learned of Wally Cordes' death, I had a feeling similar to that of when my parents passed away. In a way Wally was like a parent to me and helped mold me into a productive adult at a point in my life when I really didn't know what I wanted to do.

I have never met a person more interested in teaching – not teaching as a profession, per se, but teaching as a way of life. Wally took his teaching responsibilities so seriously that he never would give the same lecture twice. He would always show up to class with some notes scribbled on the back of a blank computer card, and that was just to remind him to cover all the topics. But I hate to use the word "seriously" because that might indicate that he was too focused and serious. Instead, he instilled a sense of wonder and joy in anything that he taught, and he felt that if you couldn't have fun doing something, then don't do it.

Wally's "teaching way of life" carried over to his family. When Wally and his wife Doris would invite all the students over for a party, their children were always around, and there would be puzzles and games scattered everywhere. Life was a journey of solving puzzles and investigating the unknown and looking for answers. All four of Doris and Wally's children have gone on to successful careers, all involving things that fascinated Wally, like computers or chemistry or architecture. I can honestly say I have never met two parents who did a better job of raising a family.

Wally's enthusiasm and jovial nature created a very conducive atmosphere for graduate school. There was a lot of interaction between the research groups, and graduate students readily helped one another with their research problems. In marketing terminology, he did a great job of branding himself. He was known as a fantastic teacher who was always doing something off the wall to get the students' attention. His eccentricities fascinated students, such as driving around in a jeep without a top, using an umbrella when it rained, and drilling drains in the floorboard.

I found my way into crystallography by accident – literally an accident. I discovered I was not cut out to be a synthetic inorganic chemist after poisoning myself with trimethyl arsine, and decided to quit graduate school and drive a beer truck. Wally begged me to give crystallography a try and I grudgingly did. I fell in love with it immediately and haven't stopped thinking about it since. I discovered that the underlying beauty of nature that crystallography encompasses is what really intrigued Wally, and he really seemed to enjoy teaching me what he knew.

Wally taught experimental crystallography like everything else. It was more important to understand the underlying concepts of crystallography than to see how fast you could produce a structure. The hours spent taking Weissenberg and precession photographs helped cement in my brain the underlying concepts of reciprocal space and gives me a real appreciation of modern instrumentation.

Scattered around the X-ray lab were models Wally had created to illustrate various symmetry elements. I am not sure if he was really an artist who expressed himself through his symmetry sculptures or he became an artist after having fun trying to illustrate crystallographic symmetry through models and sculptures. Not all of his art involved crystallography, as he had replicated some famous sculptures in his yard and hanging from the ceiling.

Many people enjoyed seeing some of his crystallographic models and toys at the ACA meetings, particularly at the San Antonio ACA meeting (see photo opposite), but Wally had been producing these things since the '60's. The more I think about it, I am convinced he was a scientist wrapped around the body of an artist – someone who was internally driven to create objects out of the beauty of nature that he saw through crystallography.

From the beginning of my graduate studies Wally always made sure that there was money set aside to help his students attend at least one ACA meeting each year. Of course in those days there were two meetings each year and it would have been very expensive to go to all the meetings, but we always tried to go to both.

He pushed us to network at the ACA meetings. At the first meeting I attended (Eufaula, AL) I met Wayne Hendrickson at a programming workshop, roomed with David Sayre, and sat through an interesting session where Wayne and Martha Teeter introduced the crambin structure followed by an exciting discussion about anomalous dispersion phasing with Karle and Hauptmann chiming in.

I feel truly blessed that Wally entered my life when he did. I can never hope to have the impact on others that he did, but he taught me the importance of enjoying what you do and the joy of discovering the unknown through scientific research.

Paul Swepston

Highlights from 2013 Fall Council Meeting

The 2013 Fall Council Meeting was held at the O'Hare Four Points Sheraton, outside Chicago, on October 23 (the initiative to test a virtual meeting format was postponed until next year, owing to an overly full agenda for this meeting). Much discussion was devoted to the organization's efforts in support of the International Year of Crystallography (IYCr2014). Vice President Martha Teeter chairs a task force devoted to this endeavor, and she presented an impressive list of activities being planned (see page 16 of this issue for additional information on the activities of the IYCr2014 Task Force). Marvin Hackert detailed complementary efforts on the part of the IUCr to support this exciting commemorative year. He also reported that the program for the 2014 IUCr Congress had been completed.

An important international initiative is the effort to strengthen ties between the ACA and Latin American crystallographers. Hackert reported that the IUCr has changed a policy that normally precludes travel awards being used for travel between near neighbors. Thus, IUCr travel awards will be available to Latin American scientists to attend the Albuquerque ACA meeting. In another effort to build bridges, CEO Bill Duax reported plans to travel to Argentina and Mexico to attend crystallography meetings there.

On our northern border, the Canadian Division of the ACA is co-sponsoring a number of sessions at the Albuquerque meeting, where it is also offering the Delbaere poster prize. David Rose will be finishing his term as Canadian Representative on Council, and he reported that two excellent candidates are vying for the right to replace him. We thank David for his outstanding service! (*Editor's Note*: Michael James has been elected as David's replacement, and his report appears in this issue on page 5.)

YSSIG representative Jamaine Davis reported that the SIG is planning to expand its efforts in social networking, as well as to continue its well-received efforts in school outreach and meeting orientation. He also noted that the group was considering ways to increase participation by junior faculty. This meeting was also the last for Jamaine, who has come to the end of his term on Council; his efforts have been greatly appreciated, and he will be missed!

Progress with the ACA journal *Structural Dynamics* was discussed. The first articles are online. As part of the journal's organization, the ACA chooses two members of the management board. One member is Judy Flippen-Anderson, and the second is John Tainer. George Phillips (ACA President in 2012) is one of the Associate Editors, and ACA past-presidents Tom Koetzle and Charlie Carter represent ACA on the AIP Publishing Partnerships Committee.

Treasurer James Kaduk noted ongoing efforts to improve transparency and increase the level of budget detail available to the members through the Council; he is currently working with CFO S. N. Rao and the members of the administrative office to achieve this goal.

Patrick Loll
ACA Council Secretary

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IUCr Awards Tenth Ewald Prize to University of Nijmegen's A. Janner and T.W.J.M. Janssen

Aloysio Janner and T. W. J. M. (Ted) Janssen, Emeriti Professors of Theoretical Solid State Physics at the Radboud University of Nijmegen, The Netherlands, have been awarded the tenth Ewald Prize, "for the development of superspace crystallography and its application to the analysis of aperiodic crystals." The International Union of Crystallography will present the award on August 5, 2014, at the Congress Opening Ceremony, in Montreal, Canada.

A. Janner

Photo courtesy of Erna Gowens, University of Nijmegen.

T. W. J. M. Janssen

Photo courtesy of Erna Gouwens, University of Nijmegen.

Aperiodic crystals are well-ordered materials that lack translational lattice periodicity. They encompass organic and inorganic compounds, metallic alloys, proteins, and minerals. One of the most famous examples of an aperiodic crystal is calaverite, a mineral discovered in the gold mines of Calaveras County, California, at the end of the 19th century. This gold telluride, with a chemical formula of $AuTe_2$, caused much havoc among two very different groups of people: gold prospectors (especially those who lived in Western Australia in the 1890s) and crystallographers. While the sparks and glitters of calaverite attracted the former, it was its unusual internal beauty that intrigued the latter. At the beginning of the 1900's, mineralogists had noticed that the morphology of calaverite's crystal faces did not follow the accepted empirical rule of crystal growth (Haüy's law of rational indices). Sure enough the diffraction patterns of calaverite, recorded after x-ray diffraction techniques took off, also departed from those of a perfect crystal, then defined as an ordered and periodic arrangement of atoms in space.

The mystery of calaverite haunted scientists until 1964, when P. de Wolff noticed that single crystals of sodium carbonate produced similar anomalous diffraction patterns displaying satellite peaks next to the most intense Bragg reflections. Instead of treating these spots as negligible exotic effects, de Wolff gave them the attention they deserved and linked them to the absence of lattice periodicity in Na_2CO_3 crystals. Mathematically, he described these crystals as "incommensurately modulated structures" – they are superimpositions of basic periodic structures, with a symmetry that can be described by a three-dimensional space group along with perturbations of different periodicity. Classical analyses failed to provide an adequate description of these crystals, and de Wolff suggested a multi-dimensional approach to the problem. Janner and Janssen, who were at the time investigating the relationship between symmetry and physical properties in condensed matter, began collaboration with de Wolff. Together they conceived and developed the "superspace" theory, publishing the first complete list of (3+1)-dimensional superspace groups in 1981. For their achievements, de Wolff, Janner and Janssen shared the 1998 Gregori Aminoff Prize awarded by the Royal Swedish Academy of Sciences.

Since that first collaboration, Janner and Janssen have dedicated more than thirty years to expanding the theoretical treatment of aperiodic crystals and have published several seminal papers and monographs on the subject. With their comprehensive studies, they laid the groundwork for the development of methods to solve and refine the structure of aperiodic crystals, with applications to a wide range of disciplines from condensed matter physics to structural biology. Their superspace formalism also applies to the analysis of quasicrystals, a specific class of aperiodic crystals, described in 1982 by Schechtman who won the 2011 Nobel Prize in Chemistry for the discovery. This year's award of the Ewald Prize to Jenner and Janssen is a further recognition of their research and highlights the tremendous impact that their work has had on the development of crystallography.

Michigan State University's Richard Staples Wins Distinguished Academic Staff Award

ACA member Richard Staples is the winner of the 2013 College of Natural Science (CNS) Distinguished Academic Staff Award, a yearly recognition of the career and accomplishments of outstanding academic staff at Michigan State University. The award recognizes individuals who have contributed to the excellence of the University with advising, curriculum development, outreach, research, and teaching.

Richard Staples

At Michigan State, Staples manages the Center for Crystallographic Research in the Department of Chemistry and Chemical Biology. He maintains and operates the diffraction and computational equipment and is responsible for updating the facility's website; he also teaches X-ray crystallography and assists in the evaluation of organic and inorganic chemistry classes.

Staples obtained a Ph.D. in chemistry from The University of Toledo, OH, with Julian Davies, and postdoctoral training at Texas A&M University. Prior to his current position, he managed the Single Crystal X-Ray Diffraction Laboratory at the University of Idaho (1995-1996), and the X-Ray Laboratory at Harvard University, where he also lectured on X-ray crystallography (1996-2007).

Staples' research mainly focuses on improving crystal growth of small organic and inorganic compounds, although he is venturing into the macromolecular world as well. He is author of some 200 peer-reviewed papers and has been invited as an instructor to several X-ray crystallography workshops, summer schools, and webinars. In 2002 and 2003 he chaired the ACA Service Crystallography Scientific Interest Group (SIG) and in 2010 the ACA Small Molecules SIG; in January 2014 he started his term as president of the ACA Industrial SIG. He is founder and director of a company, Crystallographic Resources, Inc., that offers expertise to small pharmaceutical companies and contract research organizations interested in solving the three-dimensional structures of small molecules.

ACA History Portal

In the winter issue of *ACA RefleXions* we announced the launch of the History Portal, the new ACA online website. A brainchild of Virginia Pett, Judith Flippen-Anderson, and Patricia Potter, the History Portal collects multimedia material about notable scientists who contributed to the development of crystallography, and branches off from the Living History series that have been featured in several issues of *RefleXions*.

The History Portal has been up and running since January, 2014, with some pages still under construction (the "ACA Beginnings" and the "Nobel Prizes" pages). To open the portal click the link on the front page of the ACA website or scroll the "Publications" tab, on the same page.

The new website is a pleasure to navigate. On its banner, a collage of four sepia photographs portrays some of the scientists who have made significant contributions to our science. You can guess their names, or find out who they are through the link on the home page. A brief text in the "History Home" page explains the idea behind the History Portal. In the "People" section, readers can browse the written contributions of different scientists and a panoply of other biographical material, while through the "Videos" page they can watch "award" and "historical videos" hosted on YouTube. At the moment (February 2014), two award and two historical videos are available on the Portal. The two award videos are David Watkin's presentation in honor of the 2010 Fankuchen Award and Ronald Hamlin's celebration talk for the Charles Supper Award in 2012. The two historical videos are recordings of the lectures given by Susan Byram and Donald Caspar at the 2012 ACA annual meeting in Boston, entitled respectively, "Evolution of Small Molecule Instrumentation in North America," and "Origins of Structural Biology and Trials and Errors in its History: An Idiosyncratic View."

The History Portal is an ongoing project and is in constant evolution. It will continue to expand in the coming months, with the addition of more Living History articles and videos. As the crystallography community becomes aware of the project, we expect that an even larger number of compelling stories and videos will fill its pages, transforming it into a powerful virtual archive. Its maintenance and development is possible thanks to the kind donations of ACA members.

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YSSIG Activities

The Young Scientist Scientific Interest Group (YSSIG) community has been busy planning events for this year's ACA meeting in Albuquerque. We are also planning a number of outreach activities that will extend our involvement beyond the annual meeting.

Ready for Albuquerque:

We are excited to chair or cochair several scientific sessions this year. Yulia Sevryugina (YSSIG chair) will organize the Etter Early Career Symposium, which will focus on the work of early career scientists (undergraduates, graduate students and post docs, or in other words… YSSIG). Andy Torelli will cochair the fifth installment of the highly popular Blackboard Sessions; this year's focus revisits processing data sets with commonly encountered challenges. George Lountos (YSSIG chair-elect) will cochair a session featuring industrial research from young scientists, and Daouda Traore will cochair the 'Exciting Structures' session.

We are also organizing several networking and career development events at the meeting. For example, Kate Page will host a 'YSSIG Orientation' that will help first-time attendees get the most out of the meeting (networking events, local attractions, etc…). Martin Donakowski has organized a Career Odysseys Panel that will involve a Q&A session with established scientists, to sample a diverse set of career paths in crystallography, and Yulia Sevryugina has scheduled our annual mixer at the rooftop Ibiza bar at Hotel Andaluz, which is a short walk from the conference hotel in Albuquerque. For the first time this year, YSSIG and the Society of Physics Students will together host a reception highlighting undergraduate research. Initiated and organized by Krystle McLaughlin, this event will showcase undergraduate student poster presentations with a special MiTeGen-SPS poster prize.

Rooftop bar at Andaluz hotel in downtown Albuquerque, the location of YSSIG's annual mixer event in 2014.

Finally, if you are an early career scientist, please attend our YSSIG planning meeting in Albuquerque. This is where we will arrange next year's events and will nominate individuals for 2015 secretary and chair-elect (the latter of whom will become full chair in 2016). This is also where we will accept volunteers to cochair the YSSIG-sponsored scientific sessions for 2015. It's a great opportunity to make important connections within the ACA and to develop valuable experience for your CV.

High School Outreach Project:

We are pleased to report the High School Outreach Project pioneered in Boston in 2012 is both growing and thriving! This project entails an in-class crystal growth experiment and a subsequent field trip to a local X-ray diffraction facility and wet lab, thus allowing high school science students to not only see the process of crystal structure determination, but also to appreciate the context for how crystallography fits into the big picture of science. The project was also held during the 2013 ACA meeting in Hawaii with participation of students from two high school classes from Oahu. This year, Tom Terwilliger, Javier Gonzalez, and John Bacik at Los Alamos National Labs will host a similar event involving students at Los Alamos High School.

2012 High School Outreach at Boston University. Students from Aaron Mathieu and Brian Dempsey's AP Biology class on a field trip to Karen Allen's laboratory.

2013 expansion of the High School Outreach at University of Hawaii-Manoa. Students from Namthip Sitachitta's class on a field trip to Ho Leung Ng's laboratory.

The project seeks to advance the ACA's goal of presenting crystallography to a young audience and will complement other outreach activities during the upcoming International Year of Crystallography in 2014 (IYCr2014). The project was made possible in large part through generous financial support from Hampton Research and Laboratory Research Products.

Speaking of outreach, we are also very grateful for the ACA's support in helping three of our members attend the Opening Ceremonies for IYCr2014 at UNESCO headquarters in Paris this past January (see Andy Torelli's article in this issue on page 17).

Eric Montemayor

The High School Outreach Project was made possible through the generous financial support from Hampton Research and Laboratory Product Sales.

BioSAS 2013 Honolulu Workshop Report

Richard Gillilan

Edward Snell

WK.01: Biological Small Angle Solution Scattering – Theory and Practice

Since its inception in the 1930's, when a young aspiring graduate student named André Guinier looked behind the beam stop, small angle solution scattering (SAS) has contributed greatly to our understanding of the structure of matter in a wide range of physical systems. Although SAS had been applied to biological samples almost from the start, the particular power of the method to complement crystallography, NMR, and other biophysical techniques has only become widely evident to structural biologists in recent years. As a consequence, there has been a rapid influx of novice users into the field, with regional training workshops frequently filled to capacity. Because SAS data does not provide sufficient restraints to build atomic models on its own, and is often combined with crystallographic and other data, there is a serious need to educate new users as to the method's limitations, its proper use, and how to critically interpret and report results. In addition to the large group of potential new users, there is a growing base of experienced users ready to navigate the world of advanced and emerging SAS modeling techniques. With this in mind, we assembled an organizing committee composed of academic, government lab, and industrial/corporate SAS experts to plan a dual-track training workshop at the 2013 ACA Annual Meeting in Honolulu. One track would be devoted to basics, while the other would focus on proper application of advanced methods combining SAS with crystallographic, NMR, and other data. As an additional benefit, we envisioned a national workshop as a first opportunity for representatives of multiple facilities with their own training programs to work together on a single body of educational material.

Workshop website containing lecture notes, software links, installation instructions, tutorials, example data, and links to other valuable SAS resources: meetings.chess.cornell.edu/ACABioSAS/index.html.

Biological Small Angle Solution Scattering (WK.01) consisted of two parallel workshop sessions in adjoining rooms – Track A: Getting Started in Biological Small Angle Solution Scattering: Your Practical HOW TO Guide, and Track B: Using Advanced Methods in Biological Small Angle Solution Scattering, 'Master Class in BioSAXS'. Although the workshop primarily covered X-ray scattering, an introduction to neutron scattering was also provided. The workshop also included a strong component on laboratory-source data collection through talks by several industry experts. Since students were expected to perform the tutorials using their own laptops, we set up a web site in advance of the meeting to act as a clearing house for software installation instructions, online computing links and information resources, tutorial data, examples, and ultimately lecture notes.

Despite the remote location for this meeting, response to the workshop was outstanding, with over 80 students registered. Some 72% of the group attended the introductory session (Track A). Track A started off with a lecture on scattering basics by

Srinivas Chakravarthy (APS) lectures to Track A students on the importance of proper sample preparation.

Angela Criswell (Rigaku), who also conducted the first tutorial on evaluating data quality. **Javier Pérez** (Soleil Synchrotron) continued the basics, moving into molecular weight estimates, assessing flexibility, and P(r) functions. Javier's talk was also followed by a second hands-on tutorial. **Srinivas Chakravarthy** (Advanced Photon Source) took a break from data analysis to focus on the vital subject of sample preparation. Sample polydispersity, instability, and concentration effects are leading causes of failure in SAXS experiments, but careful technique can dramatically improve success. In preparation for the final tutorial, **Edward Snell** (Hauptman-Woodward Institute) covered pitfalls and proper interpretation of molecular shape reconstructions … including a humorous cautionary tail about over-interpretation of bad data. **Richard Gillilan** (Cornell High Energy Synchrotron Source) finished the tutorial sessions showing students how to reconstruct shapes from experimental data.

In the afternoon, Track A offered a special sub-session entitled, "Do try this at home: home source data collection," taught by **Andreas Keilbach** (Anton Paar), **Angela Criswell** (Rigaku), and **Matthew Benning** (Bruker AXS). Finally, **Jill Trewhella**

(University of Sydney) wrapped up this session with two lectures. The first, "Going beyond SAXS with SANS," was a whirlwind introduction to neutron small angle solution scattering. This was followed by, "Publishing your first SAS data: what you should know," which provided important guidelines for data reporting that every student should understand.

That 28% of students considered themselves ready for advanced topics in SAS shows that individual institutions, and neutron and X-ray facilities, along with industry have already been quite busy educating the crystallography community. The Track B advanced class began with **Robert Rambo** (SIBYLS, Advanced Light Source) giving a brief review of basics and an introduction to the new software package ScÅtter. **Michal Hammel** (SIBYLS, Advanced Light Source) introduced the software modeling packages FOXS, MES, FoXSDOCK, and AllosMod-FOXS to be used in the session's first tutorial. Following this introduction **Rambo** and **Hammel**, together with **Greg Hura** (SIBYLS, Advanced Light Source), walked users through the first tutorial set. In contrast to Track A, where students ran software on their laptops, students in Track B ran a number of tutorials through compute servers online.

Following lunch, **Kushol Gupta** (Perelman School of Medicine, University of Pennsylvania) discussed analysis of an example flexible system, prototype foamy virus integrase, as he introduced students to the SASSIE program. **Emre Brookes** (University of Texas Health Science Center at San Antonio) next discussed integration of size exclusion chromatography with SAXS and a new methodology to analyze resulting experimental data implemented within the US-SOMO software suite.

Greg Hura lectured on strategies to obtain inference-free data and introduced his new high-throughput data analysis method called the SAXS Similarity Map (SSM). The integration of NMR data with SAXS data is an area of much recent interest. **Alex Grishaev** (NIH/NIDDK) covered current approaches to this very productive area. In the second and final tutorial of Track B, **Hura**, **Rambo**, and **Hammel** focused on modeling flexible systems in solution: ensembles, *ab initio* residue-level approaches.

As in Track A, a special sub-session was devoted to laboratory data collection. As an advanced topic for Track B, however, speakers emphasized more technological subjects associated with choosing, building, and maintaining home SAXS facilities. **Jürgen Graf** (Incoatec GmbH) covered optical elements and source types. **Matt Benning** (Bruker AXS) reviewed detector types and sources. **Angela Criswell** (Rigaku) described SAXS camera design concepts and signal-to-noise considerations. **Andreas Keilbach** (Anton Paar) gave a talk on collimation types and an overview of instrument broadening, a subject of potential value to synchrotron users as well.

The course website was created with help from CHESS, the Cornell High Energy Synchrotron Source (**Kristen Tierney**) and will continue to remain online as a future resource for SAXS students and researchers. In addition to our speakers, we thank the non-lecturing members of the organizing committee for valuable insight and behind-the-scenes help: **Mark van der Woerd** (Colorado State University), **Thomas Irving** (APS, IIT), **Lin Yang** (NSLS), **Thomas Weiss** (SSRL), and **Gerd Langenbucher** (Anton Paar). Thanks also to **Andrew Whitten** (University of Queensland) for assisting students and to **Jane Tanamachi** (SIBYLS, ALS) for onsite help with Track B.

These two training workshops would not have been possible without the generous support and participation from our corporate sponsors: **Anton Paar**, **Bruker**, **Dectris**, **Incoatec**, **Rigaku**, **Wyatt Technology Corporation**, and **Xenocs**. Thanks to all!

Richard Gillilan and Edward Snell

NetfleXions – Spring 2014

At long last the International Year of Crystallography (IYCr) is upon us! Hopefully by now you've extolled the virtues of crystallography to friends, family, and colleagues far and wide. If not, are you looking for resources to help spread the word? Perhaps you're wondering what events are planned to celebrate this commemoration of crystallography. Have you planned an event and are looking for an avenue to advertise it? Or maybe you just want to participate on some level, but don't know where to begin. As always, *NetfleXions* is here to help, by directing you to the best resources on the web for everything about the International Year.

The IUCr is maintaining the website ***www.IYCr2014.org***, which is the main portal to all things related to the IYCr. There you can look up news articles on crystallography, search for links to educational resources, and find contests and events in your neck of the woods. A Twitter feed scrolls across the bottom of the site, so if you're Tweeting your IYCr news, be sure to include **@IYCr2014**. Click on the "events" tab to see a global list of events by month. The "learn" tab includes an interactive crystallography time line, links to audio and video clips by famous crystallographers, and even an iOS game to learn more about crystallography! The site also includes an enchanting video on how to grow a single crystal, which is a must-have tutorial for anyone planning to participate in a crystal growing competition!

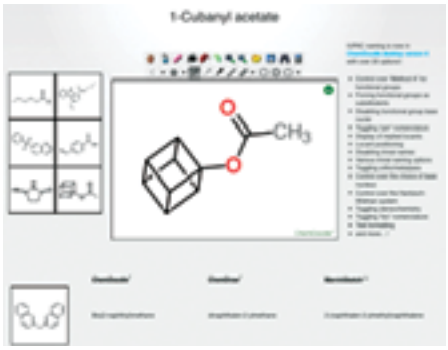
Even better, if your focus is more on North America, the ACA is maintaining its own site under the framework of the main IYCr2014 site at ***www.IYCr2014.org/ACA***, which contains educational resources, historical documents, and links to local and national contests. Any resources you may have to contribute to the IYCr effort can be submitted to the IYCr2014-ACA site, if pertinent to ACA members, or to the main IYCr2014 site if geared toward the global audience. Events submitted to the ACA

site will automatically be posted on the main IYCr events page as well. As the IYCr progresses and you have news or other content to share with the community on the IYCr2014-ACA site, please send it to Danielle Gray at ***dgray@illinois.edu***.

We all know the crystallographic community is broad and diverse. These sites will ultimately contain a large collection of insights and resources on crystallography that can be used for years to come. Make sure you browse over to ***www.IYCr2014.org*** and ***www.IYCr2014.org/ACA*** and get involved today!

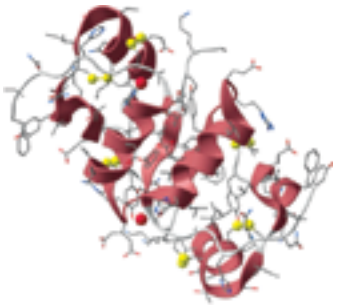
...

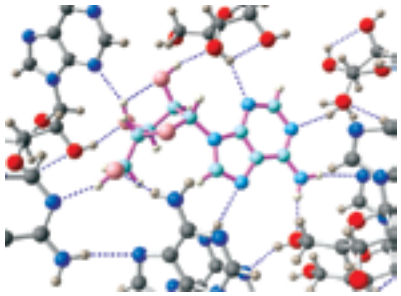
On to app reviews! Are you a ChemDoodle user? If you've been using this desktop application to produce 2D figures, calculate molecular data, or reproduce NMR spectra, you may be happy to know that these same functions are available using the ChemDoodle mobile app available for download from the Apple App Store or Google Play. Customers can enter their login credentials for full accessibility, or use the app as a guest. Licensed customers can take advantage of an IUPAC name generator through the mobile app, and this handy feature is also available on-line. Simply browse to ***http://web.chemdoodle.com/demos/iupac-naming*** for a demonstration. Many thanks to reader Allen Oliver for bringing ChemDoodle Web Components to the attention of *NetfleXions*!

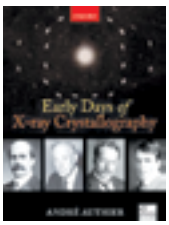


And finally, an update: CrystMolPad has been released for the iPad and is available for download from the App Store. Developer Dave Duchamp sent along a couple of screen shots of his app, which are shown below.

Amy Sarjeant







Early Days of X-ray Crystallography: André Authier, Oxford University Press, Oxford, UK, 2013, 441 pp, ISBN 978-0-199-65984-5.

We crystallographers have just finished celebrating the 100th anniversary of the first diffraction experiment, which took place in 1912, and we are now celebrating the International Year of Crystallography (IYCr). Thus, this book could not have been published at a more opportune moment. It is very clear that Authier has labored long and hard and as a result has done a good job presenting a history of crystallography.

The author set out to describe the early days of X-ray crystallography and succeeds nicely. However, a more appropriate title might have been "Early Days of Crystallography," and I will touch on this in a few paragraphs.

Intriguingly the author chose not to follow a strict time line, instead leading off with a short description of the Laue and Bragg experiments of 1912 and the significance of the actual wavelength of X-rays and the scale of crystal lattices. To pique the reader's interest, Authier provides a list of all the crystallography-related Nobel Prizes, thus demonstrating the importance of the method to science.

The next two chapters provide background on the concepts of a space lattice and the dual nature of light, as both are important in understanding the diffraction experiment at its core. Authier then takes us through the history of the discovery of X-rays by Röntgen in 1895. All this sets the stage for a detailed history of the original diffraction experiment by von Laue in 1912. In 1913 W. L. Bragg started using the diffraction method to determine the structure of simple materials, such as diamond and sodium chloride, which laid the groundwork for our current understanding of the solid state. Authier then explains the X-ray experiment as a branch of optics in the context of the period from 1913 to about 1931, covering kinematic and dynamical theory in easy to understand language.

In the final chapter of this part of the book Authier highlights the work done by the luminaries of structural studies up to the early fifties including Pauling, Hull, Bragg, and Astbury, along with many more chemists, metallurgists, material scientists, and biologists.

In Chapter 11, Authier travels back to ancient Greece, describing the history of crystallography up to 1783. Chapter 12 starts in 1784 with the space lattice concepts of Haüy, who solved the structure of calcite by logic, and ends with the derivation of the 230 space groups by Fedorov, Schoenflies, and Barlow in the 1890's. Along the way we learn about the contributions of many others, including but not limited to Miller and Bravais.

Some of the concepts are explained with mathematics, but the lay reader could skip the equations without any loss in appreciation of the history presented. The book is well referenced with detailed footnotes and short inset biographies of people discussed in the text. It was actually quite nice to learn more about some of the less famous contributors to our science. There is an extensive set of references and a full index.

Unfortunately, there are a few typos in this edition. There is a misspelling of Dorothy Hodgkin's maiden name, Crowfoot, and a wrongly assigned Nobel Prize. One equation has an error in placement of a parenthesis, but it does not change the result. I will leave it to others to catch any other errors and report them to the author.

Joe Ferrara

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Notes of a Protein Crystallographer: The 'Rose Windows' as a Unique Treasure of Symmetry, Art, and Cultural Heritage

The ceremony and events related to the opening of the IYCr2014 in Paris this January were indeed a happy occasion to re-encounter old friends, colleagues, and practitioners of crystallography from France and abroad in the unique venue of the UNESCO building and gardens in Paris. That was one of the reasons to visit Paris this year. There was, however, a further motivation that had been ignited by re-reading the brief book *Symmetry* written by Hermann Weyl (1885-1955). In this marvel of conciseness there is a quote that indirectly also steered my visit to Paris this year: 'Magnificent examples of such central plane symmetry are provided by the rose windows of Gothic cathedrals with their brilliant-colored glasswork' (p 58). Paris (Notre Dame, Sainte Chapelle, St. Merry) and its surroundings within L'Ile de France (Chartres , Rouen, and Amiens, among many others) harbor many magnificent examples of Gothic cathedrals with their magnificent rose windows (**Fig. 1**).

Fig. 1. Notre Dame Cathedral, North Window. ***The magnificent rose window of the North Transept of Notre Dame Cathedral in Paris. The symmetry of the stone tracery is 16mm by duplication of the 8mm symmetry of the innermost circle. High quality image extracted from the website www.therosewindow.com. Photo courtesy of P. Cowen.***

I have been looking at rose windows with the 'eyes of a crystallographer' for some time now, looking for planar symmetry groups and other geometrical subtleties. Following the trail of other investigators, I found the superb compendium of images available in the book *The Rose Window: Splendor and Symbol*, by Painton Cowen (Cowen, 2005), as well as the accompanying website ***www.therosewindow.com***. The book and the website provide an amazing resource to examine and study hundreds of windows with the corresponding stained glass work. After reading and studying these materials I also wanted to meet Mr. Cowen, once I learned that even though he is a British citizen he lives in Paris. The impetus for a visit to Paris was irresistible.

The tangible result of my initial analysis of the material cataloged and summarized by Cowen is a brief essay recently published in *Acta Crystallographica D* (Abad-Zapatero, 2014) that I would like to briefly recapitulate here.

Painton Cowen's work presents among the notes an interesting table (Cowen, 2005; p 273) with a survey of the basic geometry of the 524 windows that he has studied. The results are shown in **Fig. 2** and clearly document that the most common arrangements are based on 4, 6, 8, 12, or 16 repetitions around the central point. Rather uncommon are the ones based on 5, 10, or 20-fold patterns. A possible reason for this is the inherent difficulty of inscribing a regular pentagon (and related double multiples) in the circumference using the tools available to the artisans of the time, namely, a compass and straightedge. Euclid had shown in his *Elements* (third century B.C.E.) that it was possible to divide the circle into 2, 3, 4, 5, 6, 8, and 12 parts using only those tools; importantly, not 7, 9, 11, or 13 parts. A complete discussion of this subtle difference is related to studies by the great mathematician C. F. Gauss (1777-1855) and his discovery that it was possible also to divide the circle in 17 parts, made when Gauss was only nineteen.

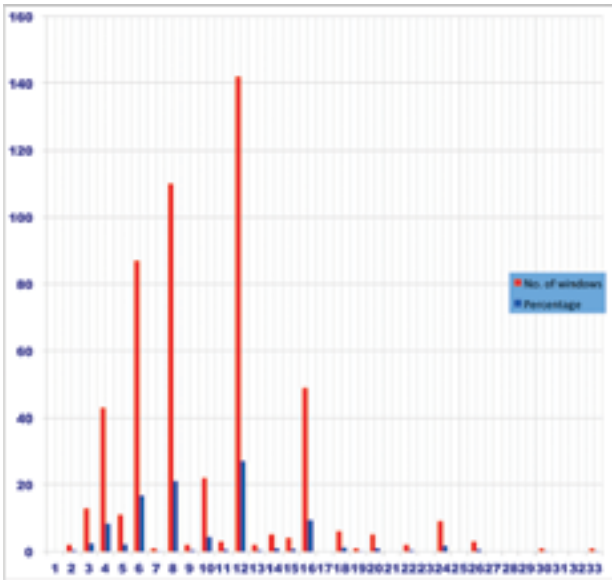

Fig. 2. Summary histogram of the main symmetry of rose windows summarized in Cowen's survey (524 windows). ***The histogram represents the number of windows in red (ordinate) vs. the number of 'rays' or 'spokes' (abscissa). The data are extracted from The Rose Window: Splendor and Symbol by P. Cowen. Blue: percentages. (Cowen, 2005, table on p 273). Reprinted with permission from Acta Cryst. D (Abad-Zapatero, 2014). Copyright, International Union of Crystallography.***

The *Acta Cryst. D* article illustrates with a few examples how the different types of symmetry can convey a different message to the viewer. As shown, the pattern based on 12 rays (cyclic 12-fold repeat) is one of the most common motifs. The number 12 has many resonances in human culture, such as the hours of the day, months of the year, zodiac symbols, and in the Christian context the number of apostles and prophets; thus, it is easy to understand the frequent presence of this pattern. However, a

12-fold repeated pattern can be presented in two radically different ways that can be related to two distinct types of symmetry. These are illustrated in **Figs. 3a,b**. The first (**Fig 3a**) presents the

Fig. 3a. View of the rose window in the main façade of the church of Santa María del Pi in the Cita Vella of Barcelona. ***The construction and symmetry is very similar to the one found in the upper rose window at the main entrance to Reims Cathedral in France. From the central 6-fold repeat the number of 'rays' doubles (left-right) as it expands out to 12 'petals' and contains 24 curved triangles on the outmost edge. Ignoring the innermost hexagon, the rose has symmetry C_{12v} (12 mm). Image from the author's personal collection.***

Fig. 3b. View of the rose window inside the Chapel of the Bourbon in the Cathedral of Lyon, France. ***The pattern exhibits only cyclic 12-fold symmetry (C_{12}). Further details can be found at the site and also in the book by Painton Cowen (Cowen, 2005). Image obtained from the website www.therosewindow.com. Reproduced from the website with permission. Courtesy of Painton Cowen.***

most common division of the circle in 12 parts with the left half balanced by the corresponding right part related by bilateral (or mirror) symmetry (12 mm). In the plane, the balanced symmetry can also be accomplished by the inclusion of 2-fold axes (180° rotations) perpendicular and intersecting the main axis at regular intervals (360/n), described by the 'dihedral' planar symmetry groups D_n, with n being the high-symmetry axis (n=2,3,4,5,6…).

The second (**Fig. 3b**) is certainly a rare pattern that cannot be discerned by the classification in Cowen's summary. It presents a wheel (or spiral, as it is described) of 12 curved leaves or 'mouchettes' packed around the central point. Neither the reflection (mirror symmetry) nor the two-fold repeat are present in the image. Thus the resulting image is strikingly different: it possesses only cyclic C_{12} symmetry (12-fold). The immediate image that comes to mind is that of a rotating windmill or vortex, spinning unrelenting as in the flow of time or life or even a wheel of fortune. Possibly the 12 petals might symbolize the months of the year or the flow of time, but without further investigation it is difficult to come to a definite conclusion.

It is important to emphasize now that the stone tracery of the 'Rose Window' provides only the geometrical (symmetrical) framework; the content is provided by the stained glass panels that are another marvel on their own (see also the discussion by Painton Cowen in the resources mentioned above (Cowen,

Fig. 4. Views of the rose window of the Lausanne Cathedral in Switzerland: Imago Mundi.

Fig. 4a. External view of the stone tracery (c. 1205). ***The design is essentially tetragonal, but the alternating elements of circles and squares add variety within a perfectly balanced composition (C_{4v}, or 4mm). The various 4-fold encircling motifs are labeled clockwise: A; B-E; F-I; J-M; N-U and refer to the stained glass content explained in the text under Fig. 4b.***

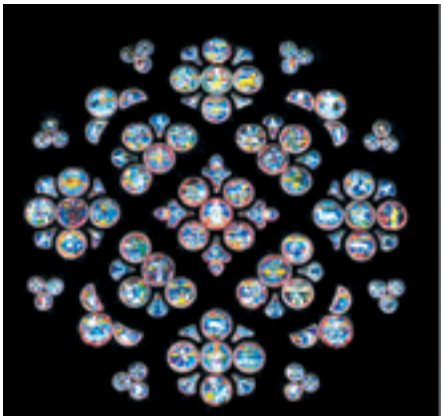

Fig. 4b. Internal view and images of stained glass (c. 1230) ***The central square (A) representing the creation is surrounded by clusters of figures (B-E), (F-I), (J-M), and (N-U) that provide an Imago mundi. Figs. 4a, b reproduced with permission from the website and adapted for description. Courtesy of P. Cowen. See website for details.***

2008)). Indeed, two windows with the same overall symmetrical pattern can be decorated by a different stained glass content providing a different meaning. The brilliant colors of stained glass material are provided by the amorphous structure of quartz along with the heavy metals and ions present. In this context it is significant to highlight the inimitable window of the Cathedral in Lausanne, Switzerland **(Fig. 4)**. Details of this masterpiece can be found in the *Acta Cryst. D* article and also in Cowen's work. The Lausanne window is over eight meters in diameter and is based on a 4-fold repeating pattern around a central circle (**Fig. 4a**) with bilateral symmetry balance (C_{4v} or 4mm). The 'glass' and iconic content for each individual group may be found at ***www.therosewindow.com/pilot/Others/Lausanne-Frame.htm***.

Suffice it to say that this window represents an *Imago Mundi* of the medieval world, a graphical summary of all the knowledge of the universe at the time. Around the central image, (A), there are four circles in the central square representing the Creation; clockwise around them, the seasons and the months (B-E). Alternating around them (F-I) are the four elements of antiquity (Earth, Water, Air, Fire) and the Zodiac signs. Illustrating also the geography of the biblical world, the four square corners (J-M) include the four rivers of Paradise and the mythical worlds with the imaginary creatures in them. Finally, the outermost eight trefoils (N-U) represent the eight winds of the Cosmos (**Figs. 4a-b**, Cowen, 2005).

What can we offer now to counterbalance this masterpiece of the Middle Ages? Readers can select their own iconic representations of the world, but in this context, and as a macromolecular crystallographer and structural biologist, my choice is the 'Atomic Rose Window' that appeared on the cover of *Science* on Feb. 13, 1981 (**Fig. 5**). Those were the times when the computer and computer graphics were beginning to impact the analysis of the structure and function of biological macromolecules at the atomic level. At that time, the ground-breaking work of Langridge, Ferrin, Kuntz, Connolly and others in molecular graphics succeeded in integrating the structural knowledge, beauty, and mystique of the structure of B-DNA in an 'Electronic Rose Window' that produced an *Imago Vitae*, comparable in the writer's view to the cosmological view of the Middle Ages. It was also this pioneering effort in computer graphics that gave us our molecular graphics tools to build and refine structures, most notably FRODO among them (see Langridge, 1995, for a historical perspective).

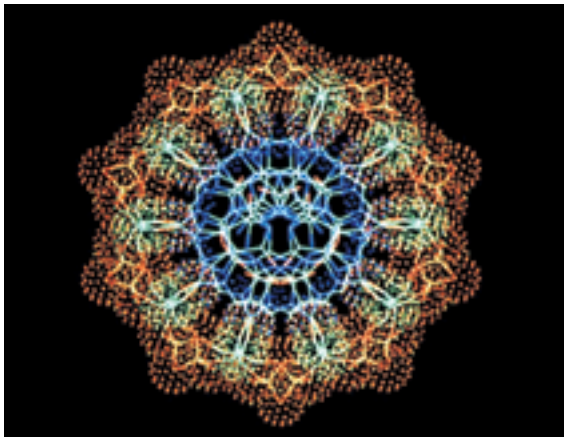

Fig. 5. Iconic images of the biological atomic world: Imago Vitae. The B-DNA 'Atomic Rose Window'. The structure of DNA is undoubtedly one of the icons of the atomic description of the biological world in the 20th century. The symmetry of this projection of the B-DNA structure is 10 22. Reproduced from Science with permission. Copyright, AAAS.

Prof. Weyl in his book also discusses the possible meaning of symmetry, and he alludes to the difference in content of the cyclic patterns containing bilateral symmetry versus the ones containing only the rotational arrangements. He quotes Dagobert Frey in an article entitled *On the Problem of Symmetry in Art* (Weyl, 1952):

'Symmetry signifies rest and binding, asymmetry motion and loosening, the one order and law, the other arbitrariness and accident, the one formal rigidity and constraint, the other life, play and freedom'. (Included in the book *Studium Generale*.)

The preliminary analysis of the stone tracery and stained glass content of the rose windows suggests that they are iconic images of their age comparable to our own macromolecular insights of the world that surrounds us. The windows should be considered unique examples of planar symmetry, beauty, and Art, and represent one of the pinnacles of our human Cultural Heritage and that of our ancestors. The incorporation of the mathematical tools of symmetry to describe them, and the application of advanced techniques of analysis, composition, and conservation science to the stained glass in order to understand and maintain them (Artioli, 2010), can only add to their value for future generations.

Acknowledgments

The summary and expanded view of the *Acta Cryst D* article presented here has benefited greatly from personal discussions with Painton Cowen at the Pompidou Center, during my stay in Paris to attend the ceremonies of the opening of the IYCr2014. His contributions to the study of rose windows and stained glass are greatly appreciated.

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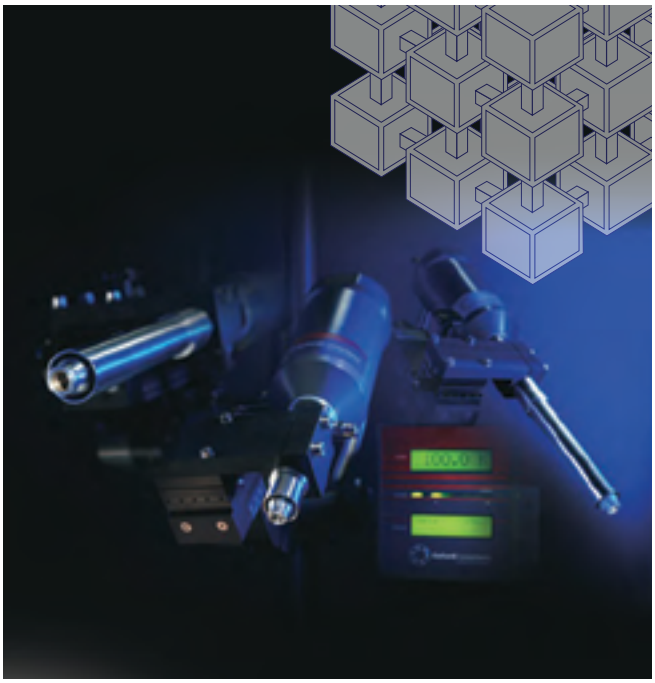
Cele Abad-Zapatero



Puzzle Corner

Frank Fronczek
Puzzle Corner Editor

Cubes within Cubes

Consider a cubic stack of unit cubes, four on an edge. How many cubes of various sizes are contained in it? (Adapted from Marilyn vos Savant's column in Parade magazine, as suggested by Loren Booda).

Solutions to Winter 2013 Puzzles

The solution to the winter issue's DISORDERED puzzle is given, along with a new DISORDERED puzzle. The identities of the crystallographers in Joe Reibenspies's periodic table are given on the facing page. Joe's periodic table can be seen in the winter issue of ACA RefleXions, and at ***http://xray.tamu.edu/ptable.***

DISORDERED

Deconvolute these crystallographic words to find an ordered solution

ILICITCRN	TRICLINIC
TYROPAIL	POLARITY
CUSTURRET	STRUCTURE
DELAW	EWALD

Answer: CRYSTAL CLEAR

DISORDERED

Reorder these words to find the missing answer.

TIREMYBUT	
TILESTAC	
GREENCINT	
YELSIN	
ACRAPSIT	

Answer:

Crystallographers in Joe Reibenspeis's Periodic Table from Winter 2013 Issue

1 **H** Herbert Hauptman
2 **He** Carl Hermann
3 **Li** William Nunn Lipscomb
4 **Be** J.D. Bernal
5 **B** Martin Buerger
6 **C** Francis Crick
7 **N** John H. Northrop
8 **O** Yuji Ohashi
9 **F** Howard Flack
10 **Ne** Nikolai V. Belov
11 **Na** David Sayre
12 **Mg** Charles-Victor Mauguin
13 **Al** F. Albert Cotton
14 **Si** Yuri Struchkov
15 **P** Paul Ewald
16 **S** Dan Shechtman
17 **Cl** William Clegg
18 **Ar** Armel LeBeil
19 **K** John Kendrew
20 **Ca** Carol Brock
21 **Sc** Authur Schoenflies
22 **Ti** Theo Hahn
23 **V** Venkatraman Ramakrishnan
24 **Cr** Durward Cruickshank
25 **Mn** Richard Marsh
26 **Fe** Yevgraf Stepanovich Federov
27 **Co** Philip Coppens
28 **Ni** Nicolaus Steno
29 **Cu** Georges Charpak
30 **Zn** William H. Zachariasen
31 **Ga** Mike Glazer
32 **Ge** George Sheldrick
33 **As** Anthony Spek
34 **Se** William H. Stein
35 **Br** WH & WL Bragg
36 **Kr** Jerome Karle
37 **Rb** Roger D. Kornberg
38 **Sr** Wendell M. Stanley
39 **Y** Ada Yonath
40 **Zr** Zdzislaw Galdecki
41 **Nb** N. Kato
42 **Mo** Stanford Moore
43 **Tc** Thomas C. Furnas
44 **Ru** Arnold Rheingold
45 **Rh** Robert Hooke
46 **Pd** Max Perutz
47 **Ag** Peter Agre
48 **Cd** Clinton Davisson
49 **In** Isabella Karle
50 **Sn** Robert Snyder
51 **Sb** Christian Anfinsen
52 **Te** Torahiko Terada
53 **I** James Ibers
54 **Xe** Häkon Hope
55 **Cs** John M. Cowley
56 **Ba** Charles Glover Barkla
57 **La** Kathleen Yardley Lonsdale
58 **Ce** Radovan Cerny
59 **Pr** Charles Keith Prout
60 **Nd** Paul Knipping
61 **Pm** Peter Main
62 **Sm** Sydney Hall
63 **Eu** Elizabeth A. Wood
64 **Gd** Gautam Radhakrishna Desiraju
65 **Tb** Kenneth N. Trueblood
66 **Dy** Peter Debye
67 **Ho** Dorothy Hodgkin
68 **Er** Margaret C. Etter
69 **Tm** Joseph Thompson
70 **Yb** Jenny Glusker
71 **Lu** Max von Laue
72 **Hf** Judith Howard
73 **Ta** Thomas A. Steitz
74 **W** James Watson
75 **Re** René Haüy
76 **Os** Oksana I. Bodak
77 **Ir** Jean-Baptiste Louis Romé de l'Isle
78 **Pt** Pliny the Elder
79 **Au** Judith Flippen-Anderson
80 **Hg** David Harker
81 **Tl** David H. Templeton
82 **Pb** Robert J. Lefkowitz
83 **Bi** Johannes Martin Bijvoet
84 **Po** W. J. Pope
85 **Ar** Andre Geim
86 **Rn** Ralph Wyckoff
87 **Fr** Rosalind Franklin
88 **Ra** G.N. Ramachandran
89 **Ac** Arthur C. Wilson
90 **Th** Theophrastus
91 **Pa** Arthur Lindo Patterson
92 **U** Uli Arndt
93 **Np** Mario Nardelli
94 **Pu** Linus Pauling
95 **Am** Oren Anderson
96 **Cm** Carmelo Giacovazzo
97 **Bk** Auguste Bravais
98 **Cf** Abraham Clearfield
99 **Es** Erwin Parthe
100 **Fm** Walter Friedrich
101 **Md** Maurice Wilkins
102 **No** Konstanin Novoselov
103 **Lr** Lawrence Dahl
104 **Ru** Hugo Rietveld
105 **Db** Louis de Broglie
106 **Sg** Robert Sparks
107 **Bh** Robert Bau
108 **Ha** Hugo Steinfink
109 **Mt** Eilhard Mitscherlich
110 **Ds** Jack Dunitz
111 **Rg** Wilhelm Roentgen
112 **Cn** Charles Campana
113 **Uut** Lachlan Cranswick
114 **Fl** Edith Flanigen
115 **Uup** Albert Hull
116 **Lv** Lieselotte “Lilo” Templeton
117 **Uus** Edward Wesley Hughes
118 **Uuo** A. I. Kitaigorodskii

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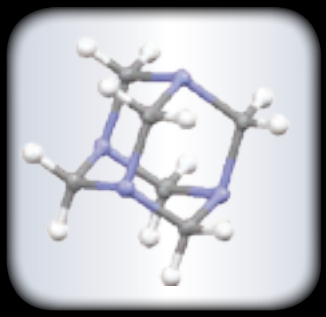

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Travel Fellowships for XXIII IUCr Congress, Montreal, Canada, August 5-12, 2014

The U.S. National Committee for Crystallography (USNC/Cr) is providing partial travel support for the International Union of Crystallography (IUCr) Congress in Montreal, Canada http://www.iucr2014.org/ to undergraduate students, graduate students, post-doctoral fellows, untenured faculty, and other recent graduates employed in any of the crystallographic, diffraction, and imaging sciences affiliated with the IUCr. Applicants must be studying or working at a U.S. institution. Applications from underrepresented minorities are especially welcome. Recipients are required to attend most of the meeting, a Mentoring Dinner, possible networking events sponsored by the USNC/Cr, and submit a short report after the meeting(*).

An application should include the following:

- Cover page indicating name, academic program, graduation year (if applicable), and contact info. for the applicant and academic advisor;
- A current Curriculum Vitae;
- Abstract including title and authors, with applicant as presenter, submitted for presentation at the 2014 IUCr Congress or to be submitted if fellowship is awarded;
- A paragraph by the applicant describing where they are in their career and why they want to attend the Montreal meeting;
- Under separate cover: A letter of recommendation from the academic advisor detailing the group's travel funding and explaining why funds from the USNC/Cr are needed;
- Applicant must process the appropriate entry visa to Canada (3 months in advance).

The award will not exceed $1,500. (*) By accepting this award, the awardee agrees to complete a short questionnaire within 2 months of the end of the meeting.

This award is possible through the generous support provided by the National Science Foundation.

Application Deadline: April 10, 2014

Send applications to:

Amy Sarjeant
Department of Chemistry
Northwestern University
2145 Sheridan Rd. Evanston IL 60202
asarjeant@northwestern.edu

A Crystallographic 4-Simplex – Edgar Meyer

In 2003, when Edgar Meyer retired from the Department of Biochemistry & Biophysics at Texas A & M, where he had been a crystallographer for over 36 years, he moved on to the next phase of his career, as a sculptor. He had been a pioneer in 3D computer graphics and database searching, both of which were crucial for the early success of the PDB. Now Edgar devotes his energies to the combination of science and art, to his family, and to his vegetable garden.

A simplex is the simplest object that can be drawn in a given space domain; "a *k*-simplex is a *k*-dimensional polytope – or – the smallest convex set containing the given vertices." For example: the dot, line, and triangle are simplices in 0, 1, and 2D space.

Several threads anchor and define my life: near-death from a childhood accident, fascination with the beauty of crystals, my wife Catarina and our family, and a pervasive urge to create. At age six, I had a life-threatening burn accident with three months in a hospital; survival stamped me with a spiritual sense of purpose. In middle school I remember really enjoying wood shop. In high school, geometry, chemistry, and world history made me excited about learning.

As a teaching assistant in chemistry at North Texas State my senior year, I had the chance to show a movie about crystals and crystal growth. Some in the class may not have appreciated the movie's reference to God as the source of cosmic order, with crystals as a prime example, but crystalline order and beauty was life changing for me – I had to become a crystallographer.

In graduate school at the University of Texas (Austin), I was given a project by Stanley Simonsen. His only crystal of an organometallic complex (bis(3-hydroxyl-1,3-diphenyltriazine) palladium(II)) was mounted, and I set about measuring diffraction intensities from Weissenberg photographs with a densitometer. After accidentally knocking off the crystal, I spent two years learning crystal growth so that I could complete the project; this skill was useful throughout my career. I learned Fortran and assembly language programming and was exposed to scientific computing on the IBM 650 and CDC 1604.

At my first ACA meeting in Boulder (1961) I met and had a beer with Peter Pauling, who referred me to Jack Dunitz for a post-doc. My two years at the ETH in Zürich with Jack were crucial: 1) the study of the corrin (porphyrin-like) tetrapyrrolic macrocycle of vitamin B12 being synthesized by Eschenmoser and his group – I continued studying porphyrins and polypyrollic structures for the next 10 years; *and* 2) Catarina Pestalozzi – we have been married for 49 years – Catarina's charm and vitality and wisdom are unchanged with time, even when challenged by my occasional unpredictability. We are enormously proud of our three children and their families.

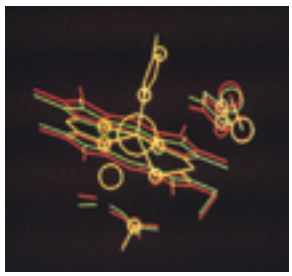
Jack Dunitz at Texas A&M (January, 1980).

Edgar Meyer using the KLUGE display at Project MAC (MIT, 1967). Photographer's identity not known.

After a year at MIT trying to solve a triclinic structure with mis-indexed upper-layer Weissenberg data I measured by eye, I jumped at the chance to join Cy Levinthal's group, working with the first interactive, real-time computer graphics system available (MIT's Project MAC). I had the chance to write my first graphics program to draw and manipulate molecular structures in 3D.

In 1967, with a growing family, I accepted an offer to be an assistant professor at Texas A&M University (TAMU), College Station, Texas, setting up a laboratory studying metalloporphyrin structures. I met Walter Hamilton at the 1968 Tucson ACA meeting, and on short notice Walter arranged for me and my family to spend the summer of 1968 at Brookhaven National Laboratory so that I could use the new Brookhaven RAster Display (BRAD). Starting with crystallographic coordinates, my program DISPLAY drove a color television monitor to draw red/green 3D images of up to 256 atoms, which was crucial for the founding of the Protein Data Bank (PDB) at Brookhaven in 1971. Walter was very supportive, and these summers (1968-1974) at Brookhaven were enormously productive. So, the 3D interactive display of molecular structures was the first apex of the crystallographic simplex and connected immediately with the second apex, the nascent PDB.

Teaching duties at TAMU caused me to miss the crucial 1971 Cold Spring Harbor Protein meeting. As things turned out, I could spend only the last six weeks of that summer at Brookhaven to finish program SEARCH, which offered various non-textual search and retrieval tools for studying complex protein structures. With SEARCH and the PDB linked, this was the most productive year of my scientific career. While virtually all search procedures up to this time were text-based, SEARCH could query a structure file for atomic properties. I had at my fingertips, for the first time, a search engine that completed the triangular simplex of structural biology: a database, a search program, and a display to visualize the results in 3D. Walter Hamilton was busy that summer, and so I could not demonstrate the program at Brookhaven. Rather, when he visited me in Texas at the beginning of September, I could run the program remotely at Brookhaven and thus demonstrate the first use of networking in the life sciences (and probably also in chemistry) by remotely selecting a structure (myoglobin) from the PDB database at Brookhaven, defining a search atom (Fe), and extracting all atoms within a chosen radius.



7.5 Å scoop around the Fe atom in myoglobin – red/green 3D image prepared using SEARCH and DISPLAY.

Walter and I obtained a NSF grant to fund a networking project,

CRYSNET, linking Brookhaven with TAMU and Fox Chase Cancer Center. While the prevailing graphics technology at the time was monochromatic (black & white), the BRAD system showed the power of color raster graphics directly on the screen.

Walter Hamilton visiting Syntex Analytical (Palo Alto, CA, 1971). L-R: Bob Sparks, Tom Workman, Neville Crooke, Walter Hamilton.

Around this time we began a collaboration with Bob Sparks at Syntex Analytical in Palo Alto.

Simultaneously, with the lads in the lab, especially Dave Cullen and Carl Morimoto, we were studying metalloporphyrin structures. The last and one of the most unusual structures was a porphyrin-phosphorus(V) structure studied by Stefano Mangani (now at the Universities of Siena and Florence).

Up to this time the majority of macromolecular structures were solved by building a mechanical (Kendrew=brass) model to fit hand-drawn electron density maps in a device called a Richards Box. In 1975, a graduate student, Marge Legg, working in the laboratory of Al Cotton at TAMU, built the first model of a new protein, staph. nuclease, with interactive 3D graphics, using the visual and manipulative tools of program FIT, begun in my lab by Carl Morimoto and brought to completion by Stan Swanson. Next, in September of 1976, Jim Hogle, a graduate student of M. Sundaralingam's (University of Wisconsin) built the models of both molecules in the asymmetric unit cell of monoclinic lysozyme. A full year passed before another graphics system accomplished a similar feat.

The tools and facilities offered by program FIT thus extended the crystallographic simplex to the next dimension: the tetrahedron. It is easy to overlook the limitation that up to this time the maximum addressable computer memory available was

Early program FIT demo, at Brookhaven, in 1972 or 1973. L-R: David Klunk (at console), Tom Koetzle, Edgar Meyer, Herbert Bernstein, Tom Willoughby (partially hidden). Photographer's identity not known.

December 12, 1975 cover of Science showing a 3D image of a tripeptide backbone rotating in space. Copyright, AAAS.

32 thousand words (vs. 16 gigabytes on my iMac).

The issue of *Science* in 1975 that describes program FIT shows on the cover a stereo tripeptide backbone rotating in space to sculpt out an ethereal image: the first of my virtual sculptures.

Thanks to an EMBO grant and the hospitality of Robert Huber at Max Planck Institute for Biochemistry (MPIB – Martinsried, Germany), Wolfram Bode of MPIB introduced me to protein chemistry and crystallization. A collaboration with Jim Powers (Georgia Tech) and Jay Fox (Virginia) led to the study of proteolytic enzymes. I was able to spend 10 consecutive summers in Martinsried studying proteolytic enzyme complexes. Short of funds, my lab in Texas had no data collection capability, so I collected enough data each summer to keep the lab busy for the coming year.

1999 Gordon Research Conference – Matrix Metalloproteinases: (Colby-Sawyer College, New London, NH). L-R: Edgar Meyer, Xavier Gomis-Rüth, Wolfram Bode. Photo most likely by Walter Stocker.

Computationally, in the late 1980s, the NSF gently urged me to explore molecular dynamics, and I was fortunate to be joined by Bogdan Lesyng and Maciek Geller (University of Warsaw). They, and a graduate student, Gail Carlson (University of Illinois) with the help of Stan Swanson, struggled successfully with supercomputer resources just emerging at that time. Molecular dynamics videos were an eye-opener, but do not qualify as an apex of the simplex for us.

Istvan Botos (NIH), Dachuan Zhang (National Library of Medicine) and my son, Erik (GlaxoSmithKline) were studying metalloproteins from rattlesnake venom (with Jay Fox and Wolfram Bode) and branched out to the study of fire ant chymotrypsin (with funding from the State of Texas). The final structures studied in my lab by Shahram Khademi were a fungal cellulase and the first insect cellulase – of course, from termites, even though the textbooks said they were not supposed to make their own cellulase.

Meyer lab group photo, TAMU, ca. 1988. L-R: Edgar Meyer, Stan Swanson, Radhakrishnan Rathnachalam (India), Rosie Swanson, Bogdan Lesyng (Poland), Dick Rosenfeld, Gail Carlsen, Andi Karrer (Switzerland), Lori Takahashi, Harly Hansen (Denmark).

Over these 36 years at Texas A&M, two things kept my lab alive: 1) a sustaining grant from the Robert A Welch Foundation, and 2) a steady flow of bright, energetic students, post docs, and some visiting faculty. La bella Catarina and our children provided stability at home, and for 30+ years Stan Swanson (plus his wife, Rosie) were the brains of the lab when difficult problems came along. Our pursuit of computational and structural biochemistry did not always resonate with the goals of my college (agribusiness), but the internal momentum of the lab made this a pleasant place to work, dream, and create. I taught biochemistry, graduate crystallography, and an honors course, 'Science in Literature,' for many years. I used 3D graphics to make biochemistry teaching more vibrant.

As Catarina and I contemplated the prospects of retirement, we considered moving to Taos, New Mexico. I had always been interested in the art-crystallography connection. So I wrote program SCULPT to generate gcode to control a CNC milling machine. A NSF grant made it possible to install an aged CNC machine donated by Los Alamos National Lab and, after setting up a wood-working shop in Taos, to install a modern machine together with necessary woodworking tools.

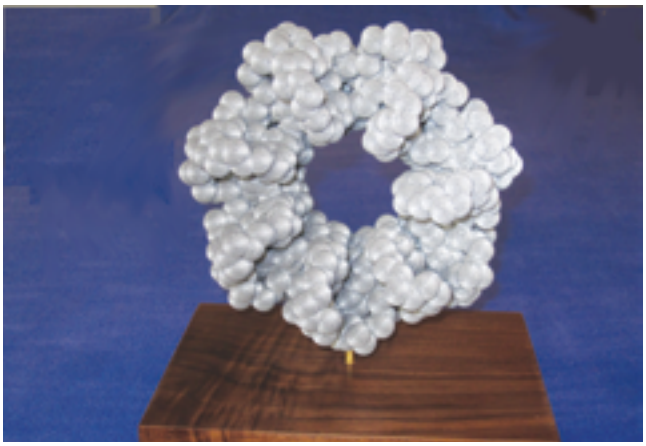
Molecular models have been around since 1866, but to have the opportunity to carve a noble hardwood to depict a molecular structure was, and is, a unique blessing. I carved sculptures of amino acids, nucleic acids, and specific compounds as memorials and tributes, some of them privately commissioned. The simplex reaches into the fifth dimension with the addition of molecular sculptures to the apices described above, but the art market has been slow to catch on.

Then, the Smithsonian (National Museum of American History) commissioned a precisely scaled bronze sculpture of the polio virus capsid and the capsid+receptor complex (Jim Hogle lab, Harvard Medical School) as part of the sesquicentennial celebration (2005) of the Salk polio vaccine: ***www.molecular-sculpture.com/Castings/Polio-bronze/Polio-bronze.html.***

A firm in California made the plastic maquettes, and I worked with the Shidoni Foundry in Santa Fe to make the wax models, molds, and bronze castings for the exhibit.

Edgar Meyer with polio virus sculptures at the Shidoni Foundry, Santa Fe, New Mexico, 2005. Photo by Catarina Meyer.

Does 'everyman' know what a vital nutrient or life-saving drug actually looks like (appropriately scaled of course)? And what will future generations know of this "golden age" of crystallography, which successfully elucidated the structures of the major building blocks of life? My answer: we need to place large (2m or taller) precisely scaled bronze or stainless steel sculptures of monumental molecules in public spaces – penicillin in the lobby of a hospital, a block-buster drug at a pharmaceutical laboratory, a carbohydrate, nucleic- or amino-acid model before an athletic field or stadium.



3D sculpture of co-chaperonin (PDB ID 1G31) – Taos, NM, 2014.

What would such a sculpture look like? And how would it fit in a public space? The same software I use to generate files for rapid prototyping and sculpting also generates high-resolution video files that I have used to make movies of virtual sculptures ***www.molecular-sculpture.com/WebSampler/Sampler.html***.

Imagine placing such a sculpture of your structure in front of your building. Imagine children playing on it. Imagine someone asking, "What is it?" = a rare teaching moment.

So, our simplex has five apices, each depicting an adventure in a new direction. Each modest but collectively useful. Nothing original – any of you could have done it – but it was my calling in life and my joy to have the privilege – and honor – to have been associated with gifted, dedicated colleagues and to have contributed in a small way to our discipline as it matured.

Edgar Meyer

Editor's Note: All photos are by the author except where noted otherwise.

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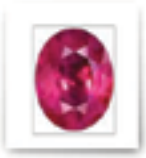

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for meeting sponsor information, abstracts, on-line registration, and details including room sharing feature for students see
www.AmerCrystalAssn.org/2014-homepage

The meeting will conclude Wednesday, May 28, following the awards banquet.

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Award Symposia

Patterson Award in honor of John Helliwell
Etter Early Career Award Award in honor of Borden Lacy
Wood Science Writing Award in honor of Daniel Rabinovich

John Helliwell
Patterson Award

Borden Lacy
Etter Early Career Award

Daniel Rabinovich
Wood Science Writing Award

Christine Beavers
cmbeavers@lbl.gov

Peter Zwart
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Program Co-Chairs

Poster Chair
Ilia Guzei
iguzei@chem.wisc.edu

Session Photos
Jeff Deschamps
deschamps@nrl.navy.mil

Workshop
Joint X-ray & Neutron Refinement with PHENIX
Organizers: Zoe Fisher, Marat Mustyakimch & Pavel Afonine

Plenary Lecture
Women in Crystallography – Jenny Glusker

Transactions Symposium
100 Years of Crystallography
Organizers: Eddie Snell &Stephen Ginell

Evening Session: *Would You Publish This?*
Chairs: Christine Beavers & Kevin Gagnon

APRIL 2014

21-25 **MRS Spring Meeting & Exposition**. San Francisco, CA. ***www.mrs.org/spring2014***

23-26 **44th Mid-Atlantic Macromomolecular Crystallography Meeting & 11th Annual SER-CAT Symposium.** University of Maryland, IBBR Shady Grove Campus. ***www.mid-atlantic.org***

MAY 2014

18-21 **Molecular Machines: Lessons from Integrating Structure, Biophysics and Chemistry.** EMBO EMBL Symposium, Heidelberg, Germany. ***www.embo-embl-symposia.org/symposia/2014/EES14-03/***

24-28 **ACA 2014 Annual Meeting**. Albuquerque, NM. ***www.AmerCrystalAssn.org/2014-homepage***

30-8 June **Intl School of Crystalography. 47th Course – Structural Basis of Pharmacology: Deeper Understanding through Crystallography**. Erice, Sicily. ***www.crystalerice.org/Erice2014/2014.htm***

JUNE 2014

1-5 **Amer. Conference on Neutron Scattering**. Knoxville, TN. ***www.mrs.org/acns-2014/***

13-15 **11th Midwest Organic Solid State Chemistry Symposium – MOSSCS XI**. University of Iowa, Iowa City, IA. Contact: L. MacGillivray. ***www.chem.uiowa.edu/faculty/macgillivray/index.html***

JULY 2014

9-11 **Emerging Photon Technologies for Chemical Dynamics**. Sheffield, UK. ***www.rsc.org/conferenc-esandevents/rscconferences/fd/fd171/index.asp***

AUGUST 2014

5-12 **XXIII Congress and General Assembly of the IUCr.** Montreal, PQ, Canada. ***www.iucr2014.org***

SEPTEMBER 2014

17-20 **15th International Conference on the Crystallization of Biological Macromolecules – ICCBM15**. Hamburg, Germany. ***www.iccbm15.org***

OCTOBER 2014

26-28 **72nd Annual Pittsburgh Diffraction Conference**. University of Georgia, Athens, GA. ***pdc14.bmb.uga.edu/Home.html***

JULY 2015

25-29 **ACA 2015 Annual Meeting**. Philadelphia, PA, Sheraton Philadelphia Downtown. Program Chairs: Kraig Wheeler & Louise Dawe. ***www.AmerCrystalAssn.org***

AUGUST 2015

23-29 **19th European Crystallographic Meeting, ECM29**. Rovinj, Croatia. ***ecm29.ecanews.org***

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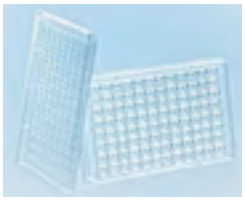
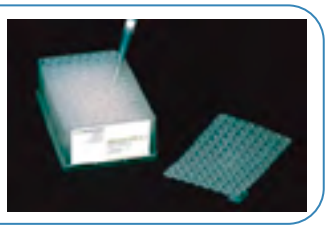
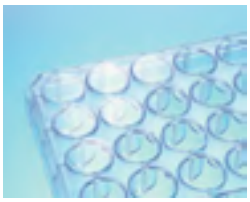
Screen

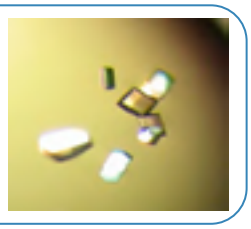


Optimize

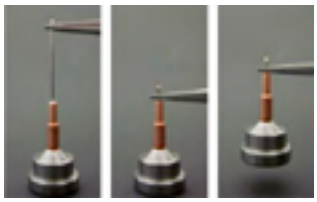
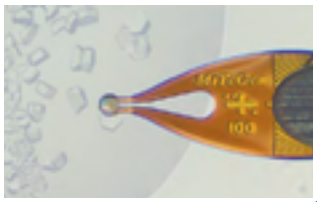






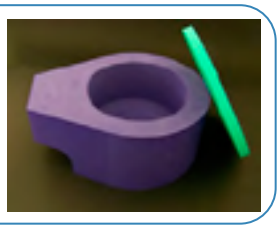
Harvest



Freeze



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