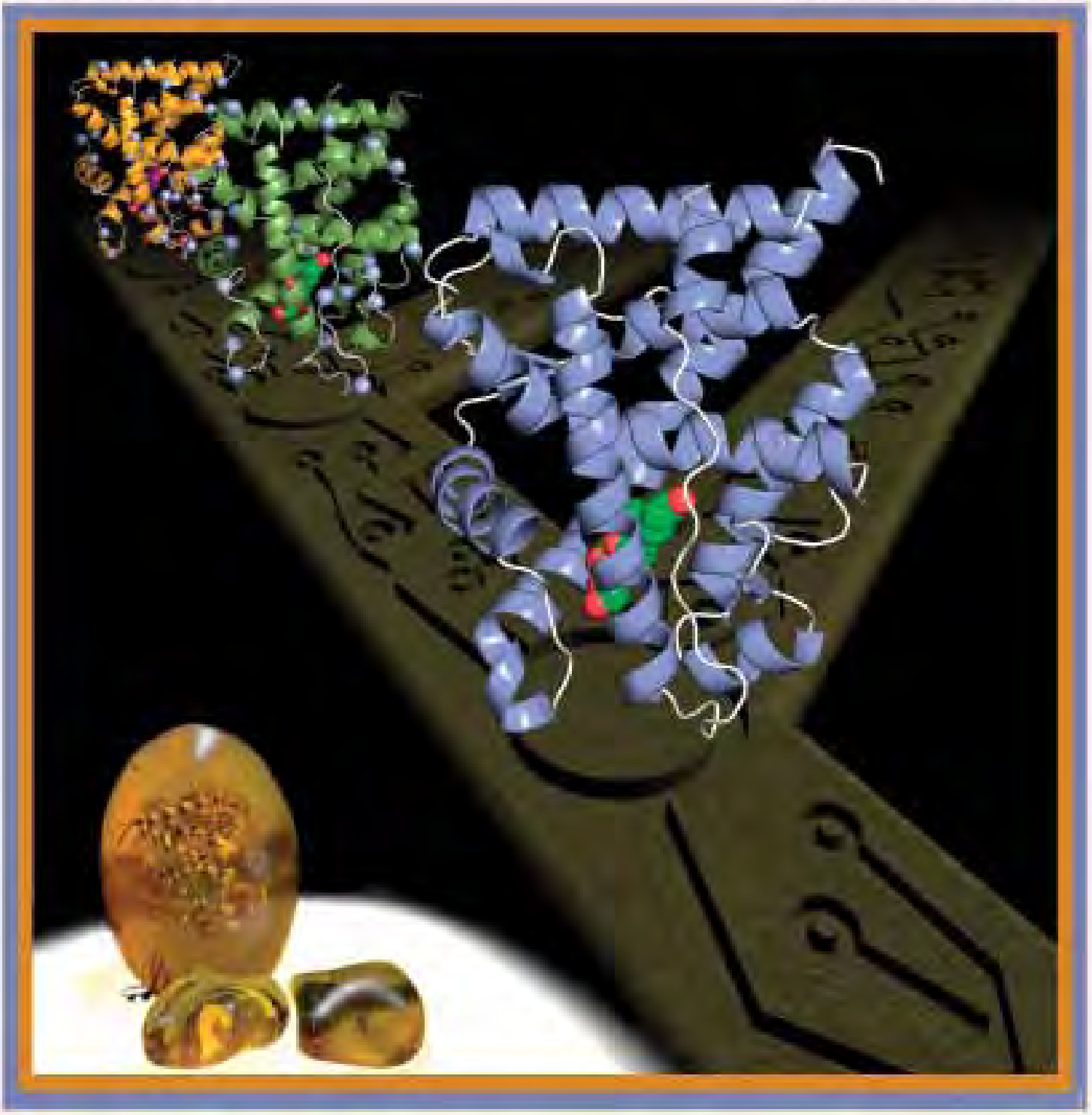
ACA RefleXions

American Crystallographic Association

Number 2

Summer 2013



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ACA RefleXions

American Crystallographic Association

Summer 2013

ACA HOME PAGE: www.amercrystalassn.org

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

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Presidents Column

In the spring issue of *RefleXions*, I reported that Council had decided to go ahead with a joint publishing project with AIP. I am happy to inform you that the contract with AIP has been finalized and the Board of Managers has been formed. The AIP representatives to the Board are Mark Cassar and and Chris McMahon. One of the ACA representatives is Judy Flippen-Anderson who has been involved with the journal project since the idea was first proposed. The other ACA representative is Soichi Wakatuski who recently moved from the Photon Factory in Japan to a joint appointment at SLAC and Stanford School of Medicine. We are thrilled to have two talented and committed scientists represent the ACA as we take this big step forward. The next phase of the project, filling out the editorial and advisory boards is well underway (see page 21).

The Strategic Planning Committee has been hard at work brainstorming and preparing for the Strategic Planning meeting scheduled for the end of May at the AIP. We have been working on a SWOT (strengths, weaknesses, opportunities, and threats) analysis and a vision for the future. Fred Dylla (AIP CEO) will guide us through the process.

I am getting very excited about our annual meeting in Hawaii. It is a great venue and gives our society another opportunity to provide professional growth through workshops and a stimulating scientific program. There will be workshops on Biological SAXS, GSAS-II Crystallographic Analysis System, and the CSD. The *Transactions I* session will be a highlight as we learn about recent advances in high throughput scattering technologies particularly those that aim at characterizing structural changes induced through chemical modification. The *Transactions II* session will focus on supramolecular assemblies and the role of crystallography in studying the structures of large macromolecular complexes that push the limits of current approaches. The scientific program is full of award talks, oral presentations, and posters that span an incredibly broad set of research areas. This is a clear illustration of how pervasive and important crystallography is in so many diverse areas of science.

Plans are underway to develop a strategy for funding, coordinating, and keeping track of International Year of Crystallography activities. Martha Teeter, ACA Vice-President, is leading this effort. She is forming an *ad hoc* committee to coordinate regional celebrations and activities as well as to provide ideas for IYCr14. In addition, she is working with the USNCCr to write a proposal that will be submitted to NSF.

Finally, the ACA is a volunteer-driven organization. With the initiation of a new journal, strategic planning, IYCR14, and our annual meetings, a lot is going on. In order for us to grow and be successful in our new endeavors, we need volunteers. Please consider doing your part to help the ACA. Thanks!

Cheryl Stevens

News from Canada

Research Funding update:

1. NSERC: The National Science and Engineering Council (NSERC) is the federal funding source for essentially all non-macromolecular crystallography as well as much of the macro research. For many years the President of NSERC had been our own Suzanne Fortier. She has now stepped down from that role to take over as Principal at McGill. During Suzanne's tenure, the NSERC funding portfolio shifted partly away from investigator-initiated basic science towards partnerships and industry-matched awards. Some basic programs, such as the RTI (**R**esearch **T**ools and **I**nstruments - the main competition for laboratory equipment) have been eliminated (though the RTI has been resurrected on a smaller scale, following major pushback). There has also been a revision of the peer-review process for the basic science ("Discovery") competitions.

2. CIHR: Biomedically-related crystallography is funded by the Canadian Institutes for Health Research. CIHR is implementing a major revision to their operating grants competition. Currently, most of this envelope is distributed to conventional 3-5 year research programs, evaluated face-to-face by peer-review committees with various specializations (analogous to study sections). The reformed systemwill have two main changes:

a. There will be two parallel competitions. A Project Stream will support proposals somewhat like those currently in place, for 3-5 year projects with definable endpoints, based on 'ideas' instead of applicant track records. These are expected to average about $120K per year. A second Foundation Stream will emphasize applicant track records and fund up to 7 years at higher annual amounts. Holders of Foundation Stream grants will not be eligible to be PIs on project grants.

b. Peer-review will largely be electronic. The goal is to establish a College of Reviewers, at least 10% of whom are international, encompassing the mandate of CIHR. Each proposal is supposed to be reviewed by (ideally) 5 people. These are not part of any committee, but are chosen individually for each proposal. The proposal will then be ranked into 3 groups: an upper group where all the reviews are positive above some threshold (these are essentially funded), a bottom group that is triaged, and a 'grey area' group, which will proceed to a face-to-face discussion by a high level committee, with a much broader constitution than current peer-review committees. There are parallel review processes proposed for each of the Streams.

The current plan for each of the competitions is to phase this new system in over the next 3-4 years. Wish us luck!

David Rose

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CristAL – Crystallography News from Latin America

With this issue of ACA *RefleXions*, we are inaugurating a section to highlight new and exciting things happening in Crystallography in Latin America. We hope to present meeting reviews, information on future meetings and workshops in the region, as well as overviews of Latin American institutions where crystallography is at the center of scientific activities. We welcome reports and contributions from meeting organizers and from representatives of Latin American crystallographic societies. Photos (high resolution) are certainly welcome! You may forward the information to Judy Flippen-Anderson (***acareflexions@gmail.com***), Connie Rajnak (***conniechidester@earthlink.net***), or Graciela Díaz de Delgado (***diaz@ula.ve***).

Latin American Crystallographic Committee

Latin American attendees at the XXII IUCr in Madrid.

During the XXII Congress and General Assembly of the IUCr which took place in August of 2011 in Madrid, a group of participants from Argentina, Brazil, Cuba, Mexico, Uruguay, and Venezuela met with the idea of establishing a committee to coordinate activities to promote crystallography in Latin America. This committee will work on activities to celebrate the International Year of Crystallography and will explore the possibility of creating a Latin American Crystallography Group. Leopoldo Suescun from Uruguay (***leopoldo@fq.edu.uy***), kindly agreed to coordinate this committee and setup a page to host information on meetings, schools, workshops, etc. related to crystallography that will take place in Latin America. For a calendar of activities please visit ***cryssmat.fq.edu.uy/cristAL/calac.htm***. The country representatives and liasons on the committee are: Diego Lamas and Daniel Vegas (Argentina), Iris Torriani and Nivaldo Speziali (Brazil), José A. Chavez and Lauro Bucio (Mexico), José Antonio Henao (Colombia), Ernesto Estévez Rams (Cuba), Alicia Guevara (Ecuador), José Solís and Elvira Zeballos (Perú), Graciela Díaz de Delgado and Miguel Delgado (Venezuela). Representatives from Latin American countries not represented so far will be incorporated soon.

First Latin American Crystallography Meeting, Córdoba, Argentina, October 29 to November 1, 2013

In November of 2011, during the VII Meeting of Asociación Argentina de Cristalografía (AACr) held in Bariloche, with participation of scientists from Brazil, Uruguay, and Venezuela, it was approved to conduct the IX meeting of the AACr in Córdoba, Argentina, and to organize simultaneously the First Latin American Crystallography Meeting. This event will take place from October 29 to November 1, 2013 at Universidad Nacional de Córdoba (UNC). This University, which is celebrating 400 years of existence, is the oldest university in Argentina and the fourth oldest in Latin America. The old campus of UNC was declared a World Heritage Site by UNESCO in 2000. The Chair of the Organizing Committee for the meeting is Raúl Carbonio (UNC). Information about this meeting will be available at ***www.cristalografia2013.com.ar.*** Two satellite events will also take place: a workshop on "Neutron Techniques for the Characterization of Materials" on October 28 and the V School of the AACr which will have as its theme *Structure Solution and Microstructural Analysis from Powder Diffraction Data* from November 4 to 8. Jordi Rius (Institut de Ciencia de Materials de Barcelona, Spain) is among the invited speakers.

Annual Meeting of Asociación Argentina de Cristalografía (AACr) held in Bariloche, November 2-4, 2011.

Country Membership in the ACA

In the last few years, the ACA has offered the possibility of country membership. This type of membership comes with interesting benefits such as: a complimentary, individual membership in ACA for the current president or designated representative of the National Crystallographic Association or group; additionally, two graduate students and one first-year postdoctoral student will each be given a one-year complimentary membership in the ACA and a waiver of registration fees at the annual ACA Meeting. A subscription to all electronic IUCr journals will be granted to one laboratory in the country, identified by the National Association or Group, for one year. The current president or designated representative will be invited to attend the annual meeting of the ACA and the associated Council meeting as a non-voting observer. Argentina renewed their country membership in the ACA for this year and, as a result, three young researchers are going to attend the Hawaii Meeting this July. They are Sebastián Suárez and Jaime Rincón-Cardona (students) and Julian Puszkiel (a postdoc).

We would like to encourage Latin American Crystallographic Societies, Associations or Groups to join the ACA. For information on how to apply for country membership in the ACA and a complete list of benefits, please contact Marcia Colquhoun at ***marcia@hwi.buffalo.edu***.

Graciela Díaz de Delgado

Latin American Seminar of Analysis by X-ray Techniques – SARX 2012

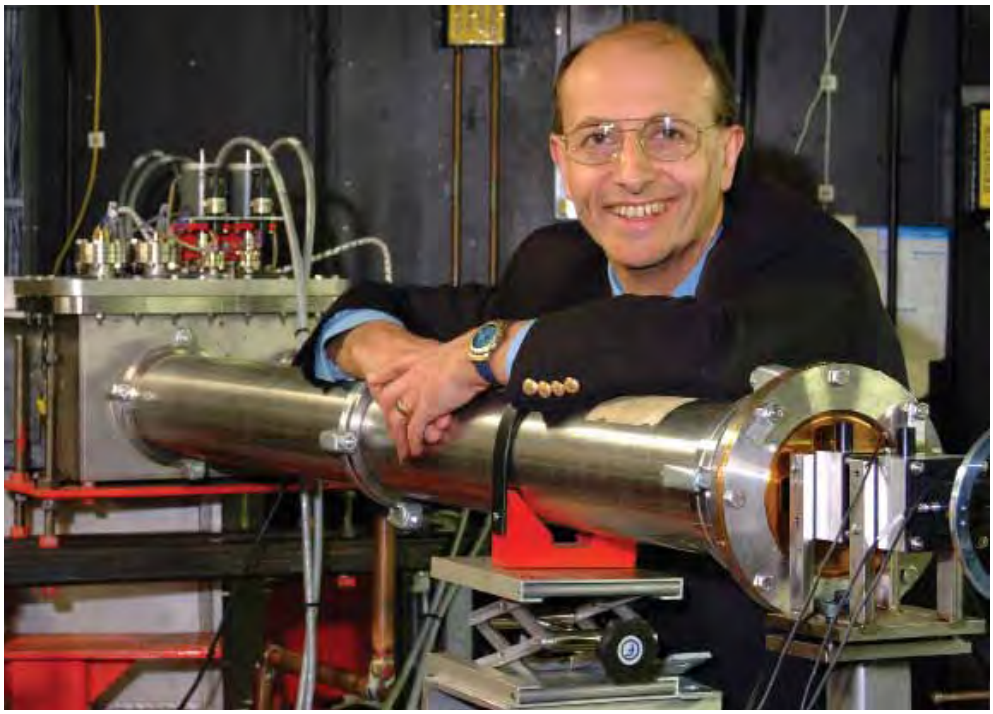
The XIII Latin American Seminar of Analysis by X-ray Techniques (SARX-2012) was held from 18 to 23 of November, 2012, in Hotel Tamacá in El Rodadero, Santa Marta, Colombia. The beaches of El Rodadero attract thousands of tourists from Colombia and from abroad. Santa Marta is the capital of the department of Magdalena and is one of the most important Colombian cities. Its historic downtown offers a passage to the pre-Colombian and colonial times of Latin America. Quinta de San Pedro Alejandrino, a XVII century hacienda dedicated to the production of rum, honey, and brown sugar, is perhaps the most important historic site of the area. Simón Bolívar arrived on December 6 of 1830 with the hope of improving his health. He died here on December 17th after signing his last will and delivering his famous proclamation to Colombians on December 10th. Nearby is the small town of Aracataca, childhood residence place of famous writer Gabriel García Márquez, winner of the 1982 Nobel Prize in Literature, .

SARX-2012 is the continuation of a series of meetings which started in 1977 in Córdoba, Argentina. Since 1985 the meetings have taken place regularly and they are now held every two years. The Seminar has taken place in Argentina (2004), Chile (2006), Brazil (2008), and Mexico (2010). The meeting was preceded by a one-day course on basic and advanced topics in x-ray diffraction and fluorescence with José Antonio Henao (Colombia), Miguel Delgado (Venezuela), Rodolfo Figueroa (Chile), and Héctor Jorge Sánchez (Argentina) as Instructors. About 150 scientists (young researchers, graduate and undergraduate students from major Colombian and Latin American universities and research centers and invited speakers from France, the USA, and Spain) presented plenary and contributed lectures and posters covering a wide range of x-ray techniques. Topics included powder and single crystal x-ray diffraction, synchrotron radiation, small angle scattering, x-ray fluorescence, electron probe microanalysis, absorption techniques, PIXE, AES, XPS, and x-ray imaging. Plenary lectures were delivered by Rodolfo Figueroa (Chile), Lourdes Infantes (Spain), James Kaduk (USA), Pascal Roussel (France), Héctor Sánchez (Argentina), Leopoldo Suescun (Uruguay), Joaquim Teixeira (Brazil), and Cristina Vázquez (Argentina). Miguel Delgado and Jim Kaduk conducted a workshop on the use of ICDD PDF-4 databases. Bruker, PANalytical, Rigaku, ICDD, and EcoPetrol, as well as several chemical vendors, took part in the commercial exhibit. Colombian crystallographers met during the event to re-establish the Colombian Crystallographic Society and a steering committee composed of representatives from major universities and research centers was set up. The next meeting will be organized by Germán Tirao (Universidad Nacional de Córdoba) and will take place in November 2014.

Graciela Díaz de Delgado

Local Organizing Committee led by José Antonio Henao and Gilles Gauthier of Universidad Industrial de Santander, Bucaramanga, Colombia, and Student Support Team of SARX-2012.

Participants at the SARX-2012 in El Rodadero, Santa Marta, Colombia.



John R. Helliwell has been selected to receive the 2014 ACA Patterson Award for his pioneering contributions to the development of the instrumentation, methods and applications of synchrotron radiation in macromolecular crystallography. A long time member of ACA and Professor of Structural Chemistry at the University of Manchester, UK, John received his undergraduate degree in physics from York University, where he was mentored by Michael Woolfson and Peter Main. He then pursued a PhD in protein crystallography at Oxford, under the supervision of Margaret Adams. He was mentored by Charlie Bugg and Guy Dodson in the laboratories of Dorothy Hodgkin and David Phillips and was involved in the first experiments that used synchrotron radiation for macromolecular structural studies.

Since then his career has been dedicated to exploring new applications of synchrotron radiation and he has worked tirelessly to improve synchrotron and neutron facilities worldwide. Always driven by the desire to innovate and overcome existing limits, John expanded the use of anomalous dispersion techniques to explore new challenges in structural biology. He contributed to solving the phase problem by, among other things, introducing longer wavelength radiation to expand anomalous scattering applications for phasing to a wider range of scatterers. He is also recognized for having pushed forward the development of Laue methods for time-resolved studies and other applications, both in x-ray and neutron crystallography.

The truly innovative nature of his work is demonstrated by the large number of "firsts" encountered in a synopsis of his career. While working in Daresbury, UK, he led the design and realization of the first dedicated synchrotron radiation x-ray source (SRS) instrument for protein crystallography (1981) and of the first protein crystallography synchrotron radiation wiggler instrument (1984).

With USA scientists as his collaborators at SRS notable initiatives were in longer wavelength anomalous dispersion (Howard Einspahr), weakly scattering crystals (Steve Ealick), microcrystal diffraction (Britt Hedman and Keith Hodgson), virus crystal diffraction (Michael Rossman) and Laue diffraction (Keith Moffat). His work at SRS Daresbury was highlighted in *Scientific American*. In the late 80s and into the 90s he led the European working group for macromolecular crystallography for the ESRF Foundation Phase report and became Vice Chair and then Chair of the ESRF Science Advisory Committee.

From 1979 to 1999 he developed two-wavelength anomalous-dispersion phasing techniques using synchrotron radiation, particularly important for their applications in radiation sensitive cases. In 1995 he first demonstrated sharpened crystal mosaicity in microgravity grown protein crystals and in 1998 he conducted one of the first time-resolved Laue protein crystallography studies harnessing fast readout CCD detectors. In 2001-2002 he determined the first *de novo* structure of apocrustacyanin A1, solved with softer x-rays. In 2005 he initiated *ab initio* structure determination by MAD phasing of powder diffraction data and discussed the potential for extending the method to structures of large molecules containing anomalous scatterers.

He is the author of a classic book on protein crystallography *Macromolecular Crystallography with Synchrotron Radiation*, published by Cambridge Univ. Press in 1992 (available in paperback since 2005). He is a founding editor of the *Journal of Synchrotron Radiation* and was president of the European Crystallographic Association (2006 – 2009). He served as Editor-in-Chief of the IUCr journals (1996 – 2005) during which period *Acta Crystallographica Section E* and *Section F were launched*.

He has mentored some of the finest beam line scientists in the world, nurturing a community of researchers devoted to continuously advancing the technological and applicative aspects of synchrotron radiation.

He has traveled widely to promote and support crystallography internationally and has made special efforts on behalf of crystallography in the US. He has fostered several synchrotron and neutron projects in the US and served on many advisory and board panels to review synchrotron projects especially, in the last decade, at the APS. His special relationship with American crystallography and the crucial contributions he has made to improve synchrotron radiation applications from the very dawn of the synchrotron era were key for his selection as the 2014 Patterson award recipient. John will receive the award at the 2014 ACA meeting at Albuquerque, NM.

Chiara Pastore

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AMERICAN CRYSTALLOGRAPHIC ASSOCIATION, INC.
BALANCE SHEET - December 31, 2012 and 2011

	CURRENT FUNDS (2012)		TOTAL	
	Unrestricted	Restricted*	All Funds	
			2012	2011
ASSETS				
Current Assets:				
Cash	180,374		180,374	263,599
Investments	541,841	443,595	985,436	792,599
Inventory	6,393		6,393	5,923
Accounts Receivable	30,214		30,214	6,701
Total Current Assets	758,822	443,595	1,202,417	1,068,8222
Fixed Assets:				
Computers and Printers	0		0	0
Office Equipment	0		0	0
Accumulated Depreciation	0		0	0
Total Fixed Assets	0		0	0
TOTAL ASSETS	758,822	443,595	1,202,417	1,068,822
Liabilities:				
Unearned Revenues	56,432		56,432	49,164
Credit Card Liabilities	1,916		1,916	477
Total Liabilities	58,348		58,348	49,641
Fund Balance:				
Unrestricted	700,474		700,474	585,967
Restricted		443,595	443,595	433,214
Total Fund Balance	700,474	443,595	1,144,069	1,019,181
TOTAL LIABILITIES & FUND BALANCE	758,822	443,595	1,202,417	1,068,822

*** Current Balances in individual restricted funds - *as of March 31, 2013***

Bau Neutron Award	35,456
Buerger Award	37,833
Etter Award	66,052
Fankuchen Award	69,734
History Fund	3,329
Latin American Initiativee	3,353
Patterson Award	45,230
Pauling Award	36,356
Supper Award	12,203
Student Travel Fund	16,541
Trueblood Award	37,962
Warren Award	30,308
Wood Science Writing Award	53,224

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

From the Editor's Desk

On page 8 of this issue you will find the report from our CFO, SN Rao, providing the audited budget report on ACA finances at the end of 2012. Since that time additional donations have come in that bring the overall total for the award funds to $447,581 (fund totals through the end of March 2013 have been included in the report). Most of these donations have come in as part of the membership renewal process that, until recently, has been the only way to donate to your favorite funds. This is certainly an easy way to do it and I would encourage anyone who has not yet renewed to go ahead and renew your membership and consider making a donation at the same time.

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

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

Judy Flippen-Anderson

Errata for spring 2013 issue of RefleXions

Carol Huber wrote : I was extremely sorry to learn of Guy Dodson's untimely death. With Louise Johnson's last year also, we really have lost two wonderful people in the structural biology world. (I also had very high regard for Hugo Steinfink.) I know it wasn't your error on p. 12 of the latest ACA *Reflexions*, but perhaps a correction might be made later. Guy was in Oxford from 1962, not 1967, until he went to York. Ted Baker's article for the IUCr got it right, and an old World Directory of Crystallographers shows that Guy got his PhD in 1962 in New Zealand.

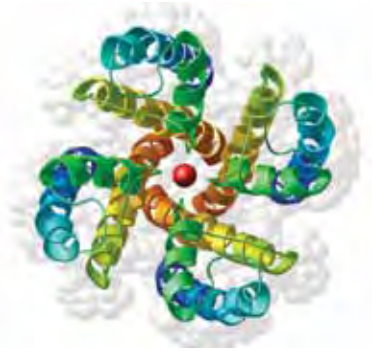
WORLDWIDE PDB PROTEIN DATA BANK

Safeguarding an indispensable archive

July 1st 2013 marks the 10-year anniversary of the founding of the Worldwide Protein Data Bank (wwPDB; ***wwpdb.org***), the international collaboration that manages the PDB archive[1].

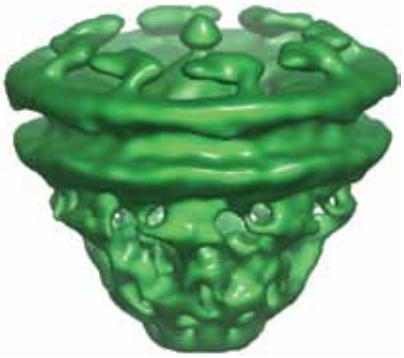
From modest beginnings: Starting from just 7 protein crystal structures in 1971, the PDB archive has grown rapidly over the past 42 years. Last year alone, 9,972 new structures were deposited, more than in the first 25 years of the PDB combined. Today, the archive contains over 90,000 structures and at its current rate of growth will reach the 100,000 structure mark in 2014, the International Year of Crystallography.

On July 1st 2003, the way in which the PDB archive was managed was transformed by the founding of the Worldwide Protein Data Bank organization. From its inception, the PDB has been an international archive and the establishment of the wwPDB ensured that these valuable data will continue to be stored, managed and kept freely available for the benefit of scientists worldwide.

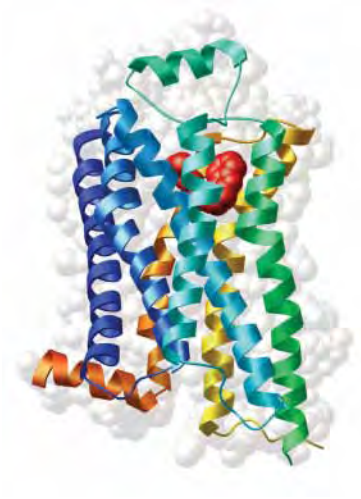


The wwPDB organization nowadays consists of four partners: the Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB; ***rcsb.org***) and BioMagResBank (BMRB; ***bmrb.wisc.edu***) in the USA, the Protein Data Bank in Europe (PDBe; ***pdbe.org***) and the Protein Data Bank Japan (PDBj; ***pdbj.org***).

wwPDB activities: The wwPDB partner sites each act as deposition, processing and distribution centers for PDB data. They work together and in consultation with the wider community to define deposition and annotation policies, and file formats and validation standards for structural data. This close collaboration between the member organizations is vital because it guarantees that the global community of PDB users is provided with reliable and consistent data.



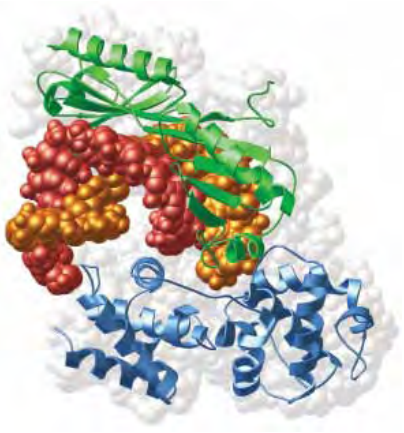
While working jointly on all aspects of data representation and processing, each partner site also offers independent tools and services that help make the wealth of data about structure and function easily accessible to the user community.



wwPDB activities are overseen by an international advisory committee comprised of experts in x-ray crystallography, 3D-EM, NMR, and bioinformatics.

Future challenges: The increasing volume, diversity and complexity of biological data being deposited in the PDB and the emergence of hybrid techniques to obtain structural insights into biologically relevant molecules, complexes and molecular machines all present major challenges for the management and presentation of structural data.

To address these challenges, the wwPDB partners are jointly developing a software system that will allow deposition, validation and annotation of complex and diverse macromolecular structures along with the underlying experimental data using a single interface. This new system will go into full production at all the wwPDB deposition sites early in 2014 and will then be able to handle depositions of structures of any size, determined using diffraction, NMR and/or EM methods.



Validation will be an integral part of the new deposition and annotation system. Assessment of coordinates, experimental data and associated meta data at the time of deposition is vital for improving the quality of the archive. In addition, it will help users with no or limited structural biology background select the most appropriate structural models for their purposes.

Whatever new challenges the next 10 years will bring, the wwPDB will remain committed to maintaining high standards of quality, integrity and consistency of the macromolecular structure archive and to making it freely available to a large, diverse and demanding global community of users.

wwPDB Milestones Through the Years

2003: wwPDB established.

2004: First x-ray crystal structure from Africa is released in the PDB (1ydk[2]).

2005: PDB data available in PDBML/XML format.

2006: BMRB joins the wwPDB.

2007: First archive-wide remediation includes updated sequence information and primary citations, improved representation of virus assemblies, and standardized chemistry and nomenclature for monomers and ligands.

2008: 50,000 entries in the PDB archive - experimental data are mandatory for deposition - X-ray Validation Task Force (VTF) is convened[3].

2009: Second release of remediated data includes details about the chemistry of polymers and the ligands bound to it, biological assemblies, and binding sites of ligands and metal ions - NMR VTF is convened - deposition of chemical shifts mandatory for NMR structures.

2010: Provision of wwPDB validation reports becomes a requirement for manuscript submission, starting with the IUCr journals - 3DEM VTF is convened[4].

2011: PDB40 symposium commemorating 4 decades of the archive held at Cold Spring Harbor Laboratory; the PDB is now the oldest electronic archive of biomolecular data - at a wwPDB workshop, the major developers of x-ray structure-determination software agree to adopt PDBx/mmCIF as the principal format for structure deposition.

2012: PDB data and EMDB maps become part of the same ftp tree, simplifying distribution of these two important structural archives - SAS Task Force is convened[5].

2013: 10,000th NMR structure is released - PDBx/mmCIF becomes the standard format for deposition and distribution of PDB data- updated wwPDB Charter goes into effect on July 1, starting the second decade of the wwPDB.

References:

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Images:

Left column : **1BL8**: DA Doyle, J Morais Cabral, RA Pfuetzner, A Kuo, JM Gulbis, SL Cohen, BT Chait, R MacKinnon (1998) The structure of the potassium channel: molecular basis of K+ conduction and selectivity, *Science* **280**: 69-77. **EMD-1097** M Beck, F Forster, M Ecke, JM Plitzko, F Melchior, G Gerisch, W Baumeister, O Medalia (2004) Nuclear pore complex structure and dynamics revealed by cryoelectron tomography, *Science* **306**: 1387-1390.

Right column: **2RH1**: V Cherezov, DM Rosenbaum, MA Hanson, SG Rasmussen, FS Thian, TS Kobilka, HJ Choi, P Kuhn, WI Weis, BK Kobilka, RC Stevens. (2007) High-resolution crystal structure of an engineered human beta2-adrenergic G protein-coupled receptor. *Science* **318**: 1258-1265. **1VOL**: DB Nikolov, H Chen, ED Halay, AA Usheva, K Hisatake, DK Lee, RG Roeder, SK Burley. (1995) Crystal structure of a TFIIB-TBP-TATA-element ternary complex. *Nature* **377**: 119-128. **1PCQ**: C Chaudhry, GW Farr, MJ Todd, HS Rye, AT Brunger, PD Adams, AL Horwich, PB. Sigler. (2003) Role of the gamma-phosphate of ATP in triggering protein folding by GroEL-GroES: function, structure and energetics. *EMBO J* **22**: 4877-4887.

Members of the PDB, past and present, in attendance at the PDB40 Symposium (www.wwpdb.org/PDB40.html): Photo by Constance Brukin.

Jack Dunitz -- The Early Years

In this autobiographical narrative Jack D. Dunitz describes his education and early "itinerant" research at Oxford, Caltech, and the Royal Institution. After these experiences he went on to an illustrious career as Professor of Chemical Crystallography at the Swiss Federal Institute of Technology (ETH), retiring in 1990 after 33 years. Jack is a Fellow of the Royal Society of London and the American Association for the Advancement of Science; he is a Foreign Associate of the US National Academy of Sciences and a Foreign Member of the American Philosophical Society. Among his many honors are the Paracelsus Prize (Swiss Chemical Society), the Arthur C. Cope Scholar Award (American Chemical Society) and the Buerger Award (ACA). He has published more than 350 articles. He is the author of the classic "X-ray analysis and the structure of organic molecules" and the co-author with Edgar Heilbronner of "Reflections on symmetry: in chemistry-- and elsewhere".

Jack receiving the 1991 ACA Buerger Award from Judith Flippen-Anderson.

I have had the enormous good fortune to spend my time more or less as I liked to spend it — in inventing and solving scientific problems, mainly in structural chemistry — problems that to the best of my knowledge have had no practical relevance, either for good or for evil. The last half-century has probably been the only time in history when such a thing was possible; when a person of modest abilities could enjoy a comfortable existence doing whatever seemed interesting. I feel I have been tremendously fortunate.

I do not remember ever having made a conscious choice or decision to follow a career in science. It just happened, as in a dream. In a dream you don't do things, things happen to you. Near the beginning, during the early 1940's, I was a student of chemistry at Glasgow University, ignorant not only of chemistry but of almost everything else, an innocent in every way one can imagine. I did not choose chemistry. My mother would have liked me to study medicine, my headmaster tried to push me into the study of classics. I did not much fancy either of these possibilities. The science teacher at my school, John McLennan, chose chemistry for me by making it interesting. Likewise, I did not choose crystallography. Crystallography chose me. As a frustrated mathematician, my interests were mainly in physical chemistry. After a somewhat compressed wartime three-year crash course in chemistry, most of the Phys. Chem. students were funneled off for work about which they were not allowed to talk (now we know it was radar research), but in 1943 John Monteath Robertson returned to Glasgow as newly appointed Gardiner Professor and needed a few doctoral students to carry out work in x-ray crystallography and molecular structure studies. At that time and place, there was no question of a student choosing a research supervisor or a line of research. It was still wartime. "You, you and you will report for duty at such and such a locality, you, you and you will stay on here and work for Robertson" and so it was that I came to chemical crystallography. As Robertson was much away on official duties, and as there was no formal post-graduate course of study, we doctoral students taught one another what we had taught ourselves about the theory and practice of crystal structure analysis.

After my arrival as a post-doctoral researcher in Dorothy Hodgkin's laboratory at Oxford in late 1946, I practiced my skill in trial-and-error analysis by determining the crystal structure of the centrosymmetric isomer of 1,2,3,4-tetraphenylcyclobutane in projection down the short (5.77 Å) monoclinic axis and then also tested my endurance by calculating lines and sections of the three-dimensional electron density distribution, based on visual estimates of all photographically recorded reflections within the CuKα sphere of reciprocal space. From today's perspective, when the measurements could be made in a few hours and the calculations in a few seconds, it is hard to imagine how much drudgery was involved in such an exploit in those days, working with paper, pencil and Beevers-Lipson strips. Why on earth did I take it on, and why did I persist? No one was pushing me. Perhaps I merely wanted to show that I could do it.

My tetraphenylcyclobutane work did not bring me fame but it did bring me to Caltech. Indirectly. From my results, the bond distances in the cyclobutane ring appeared to be longer than the standard carbon-carbon single-bond distance of 1.54 Å, while those in the phenyl groups were normal for benzene rings. However, according to the recently developed "bent bond" model, bonds in small carbocyclic rings were expected to be slightly shorter than the 1.54 Å, as had been found, indeed, for cyclopropane and spiropentane from gas-phase electron diffraction. Were the long bonds found in tetraphenylcyclobutane an intrinsic property of the cyclobutane ring? Or were they in some way connected with the presence of the four phenyl substituents? Or were they merely attributable to experimental error? When I discussed this problem with Verner Schomaker during his visit to Oxford in the early summer of 1948, we decided that the problem called for a gas-phase electron diffraction study of cyclobutane itself. I was interested in learning this technique, and, through Schomaker's intervention, Pauling offered me a research fellowship to come to Caltech.

Jack at Caltech, 1948 (from the Ava Helen and Linus Pauling Papers, Special Collections & Archives Research Center, Oregon State University).

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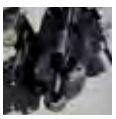

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Our gas-phase electron-diffraction study of cyclobutane confirmed my supposition that the carbon-carbon bonds were long. Moreover, contrary to what had been generally assumed until then, the four-membered ring was not a planar square but was buckled (D_{2d} rather than D_{4h} symmetry). The reason for the striking difference between the C—C bond distances in cyclopropane (1.51 Å) and cyclobutane (1.57 Å) is that in the former there are no non-bonded 1,3-interactions, whereas the four-membered ring shows the strongest possible interactions of this type, which are, of course, strongly repulsive. It was a great experience to work with Verner Schomaker, to argue with him, and, more than anything, to share with him the writing of a scientific paper. Our cyclobutane paper took ages to write, but, as compensation, after almost 50 years, I am still pleased with the result. Among other things, that publication contained what must have been one of the earliest force-field calculations, and also a carefully qualified sentence defining what we meant by the term "bent bond": "It appears that this argument might be expressed in terms of the significant existence of a bond line, to be distinguished from the internuclear (straight) line, which more or less follows a line of maximum density of the bonding electron distribution, and which, in the bent bond, tends to retain a fixed length, thereby possibly causing the internuclear distance to be shortened in spite of the resulting increased internuclear repulsion."

Model of cyclobutane showing the puckered ring - courtesy of Jeff Deschamps.

More than thirty years later, when bent bonds had become fashionable and had showed up in Bader's theory of chemical bonding, this definition received a seal of approval when it was reproduced in one of Bader's papers. Not many sentences in the scientific literature are deemed to be worth repeating after thirty years.

Pauling had a feeling for drama. At the lecture where Pauling first publicly announced his stable hydrogen-bonded model structures for polypeptide chains, on the table in front of him stood bulky columnar objects shrouded in cloth, which naturally excited the curiosity of those in the packed auditorium. Only after describing in detail the structural principles behind the models did he turn to the table and unveil the molecular models with a characteristic theatrical gesture. There were the two structures, the three-residue and the five-residue spirals, later dubbed the α- and γ-helices! I was immediately converted, a believer right from the start.

While my own work at Caltech had nothing to do with protein structure, Pauling used to talk to me occasionally about his models and what one could learn from them. In his lecture, he had talked about spirals. In conversation a few days later, I told him that for me the word "spiral" referred to a curve in a plane. As his polypeptide coils were three-dimensional figures, I suggested they were better described as "helices". Pauling's erudition did not stop at the natural sciences. He answered, quite correctly, that the words "spiral" and "helix" are practically synonymous and can be used almost interchangeably, but he thanked me for my suggestion because he preferred "helix" and declared that he would always use it henceforth. Perhaps he felt that by calling his structure a helix there would be less risk of confusion with the various other models that had been proposed earlier. There was no going back. A few years later we had the DNA double helix, not the DNA double spiral. The formulation of the α-helix was the first and is still one of the greatest triumphs of speculative model building in molecular biology, and I am pleased that I helped to give it its name.

Friends from Caltech days, Jim Ibers and Jack in Zurich (summer 1989, courtesy of Carol Brock).

Back in Oxford in Dorothy Hodgkin's lab, I came across an astonishing proposal from a group of Harvard chemists (Wilkinson, Rosenblum, Whiting, and Woodward) for the structure of the recently obtained compound, $C_{10}H_{10}Fe$: two parallel cyclopentadienyl rings with the iron atom sandwiched between them. The only physico-chemical evidence offered for this unprecedented structure was the infrared absorption spectrum, which contained, in the 3-4 μ region, a single, sharp band at 3.25 μ, indicating the presence of only one type of C—H bond. It may be difficult today to appreciate just how surprising, unorthodox, even revolutionary, this structure was at the time. At any rate, my first reaction was one of extreme skepticism. On my way out of the library I met my friend Leslie Orgel, at that time holder of a research fellowship at Magdalen College, and asked if he had seen the remarkable structure proposed in the latest *JACS* number. We retrieved the journal and re-read the article together. He was as skeptical as I was. When we learned that the compound was relatively easy to prepare in crystalline form, we decided to make it and determine the crystal and molecular structure. Or rather, since neither of us had access to facilities in a synthetic laboratory, we decided to try to persuade a friendly organic chemist Hugh Cardwell to carry out the relatively straightforward synthesis.

I made optical measurements on crystals of the new compound on June 9th, 1952 and began to make preliminary x-ray photographs the following day. I soon found that the crystals slowly sublimed in the atmosphere at room temperature and had to be sealed into glass capillary tubes. From the space group alone it was evident that the molecule must sit at a crystallographic center of symmetry. By the end of the following week, I had made enough intensity measurements to produce two electron-density projections down mutually perpendicular directions. This was possible because, fortunately for me, there was a slack period in the laboratory so that not only one but two x-ray Weissenberg cameras were free for my use. Of course, to get all this done on my own, I had to work long hours, during the evenings and over the weekend too. As the structure began to emerge from the electron-density maps, calculated with Beevers-Lipson strips with the aid of an adding machine, I was becoming so excited that I was working through most of the night as well. By the end

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Crystallography

of the following week, the structure was solved. Extraordinary as it seemed to me, the Harvard proposal was correct. The rings were parallel, with the iron atom sandwiched between them at a crystallographic centrer of symmetry. There was no doubt about it. That was the marvelous thing about crystal structure analysis. When it worked, the result had a satisfying definiteness about it. Even though this aura of definiteness could sometimes be misleading! The crystalline structure of ferrocene occupied me, on and off, for more than thirty years. Later, the apparently staggered orientation of the cyclopentadienyl rings was revealed to be an artifact resulting from crystal disorder. Ferrocene turned out to be trimorphic — at least — and the ring orientation in the low-temperature stable polymorph is eclipsed not staggered.

Back to 1952; there was still the question of how to account for the new kind of bonding in this extraordinary molecular structure. How can the iron atom simultaneously make ten Fe—C bonds? How could the tenfold symmetry be reconciled with the well known tendency of Fe^{2+} to form 4- or 6-coordinated complexes? Faced with this challenge, within a few days Leslie developed an explanation based on orbital symmetry properties, on the relationships between the symmetry properties of the d-orbitals of the metal atom and the π-molecular orbitals of the cyclopentadienyl rings. This was new terrain. This new type of molecule required a new type of description of its bonding, and Leslie's model, formal and over-simplified as it was, expressed the essence of this. When it was first explained to me I did not understand a word, but by the end of the week I had picked up enough of the group theoretical background of this new language to construct simple statements on my own. In particular, I could see that the model was a generalization of the standard molecular orbital (MO) model of benzene and other aromatic systems. So we wrote a paper, covering both the structure determination and the new theoretical model, and sent it off to *Nature* on July 2nd, less than a month after we had the crystals, under the provocative title, "Bis-cyclopentadienyl Iron: a Molecular Sandwich". That was the first time, I believe, that this gastronomic epithet had been used in the title of a chemical publication. The name certainly stuck.

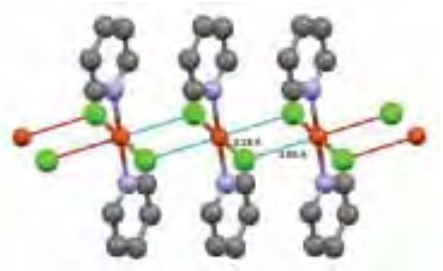
Jack and Barbara Steuer were married in 1953 (summer 1985, courtesy of Carol Brock).

Since the same symmetry arguments as we applied to ferrocene could be applied *mutatis mutandis* to the then still unknown and scarcely imagined molecules dibenzene chromium and dicyclobutadiene nickel, Orgel wanted to include in our paper his prediction that these molecules would turn out to be stable species. I argued that it would be a pity to spoil a good, solid paper by what could be regarded as risky speculation and managed to persuade him to omit the additional paragraphs. As Leslie later ruefully remarked, one characteristic of our collaboration was that we sometimes succeeded in shooting down each other's best ideas.

Besides our work on ferrocene, Orgel and I wrote a paper about hydrogen bonds. It was then generally considered that O-H···O hydrogen bonds were unsymmetrical, with the hydrogen atom closer to one oxygen atom than to the other. We proposed that the acid maleate anion should have an unusually strong, symmetrical hydrogen bond, and backed this up with spectroscopic observations on crystalline potassium hydrogen maleate. Our proposal was subsequently confirmed by neutron diffraction studies. This may be the first example of what came to be known much later as a low barrier hydrogen bond.

In April 1955, Sir Lawrence Bragg offered me a five-year appointment as Senior Research Fellow at the Davy-Faraday Research Laboratory at the Royal Institution. There I decided to study the crystal structures of cobalt dipyridine dichloride, $CoPy_2Cl_2$ and its copper analogue $CuPy_2Cl_2$. There were two known forms of the cobalt compound, one violet colored, the other blue. The blue form was known to contain discrete molecules with tetrahedral bonds at the cobalt atom, while the violet form was believed to contain polymeric chains with octahedral bonds at the cobalt atom, each chloride ion linked to two cobalts, each cobalt to four equidistant chloride ions and to the pyridines. Indeed, this turned out to be the case. The copper compound was found to have a very similar structure, except that the four chloride ions were not equidistant from the metal atom; instead, there were two short Cu–Cl bonds and two long ones.

This result led to another collaboration with Leslie Orgel, who, a couple of years earlier, had suggested that such distortions of octahedral complexes could be interpreted in terms of crystal-field theory as structural expressions of the Jahn-Teller effect. The differences between the octahedral coordination in the cobalt compound and the distorted octahedral coordination in the copper compound seemed a perfect illustration of this, and I soon found that similar differences between other pairs of structurally related compounds occurred according to a quite regular pattern. We also saw that crystal field theory could be applied to minerals with the spinel structure. Spinel is a mineral with composition $MgAl_2O_4$, built from a cubic close-packed arrangement of oxygen atoms with the Mg^{2+} ions at tetrahedral cavity sites and the Al^{3+} ions at octahedral ones. There are many other AB_2O_4 minerals with essentially the same structure, with the A^{3+} ions in tetrahedral sites and B^{3+} ions in octahedral ones. However, in "inverted" spinels the tetrahedral sites are occupied by B^{3+} ions, with the A^{2+} ions and the remaining B^{3+} ions distributed at random over octahedral sites. We found we could explain all the known experimental evidence on the metal ion distributions in the normal and inverted spinels. Moreover, the existence of tetragonally deformed spinels could also be explained by our theory in terms of the Jahn-Teller distortions expected to occur when certain metal ions were present. When I told Bragg about these results he



The structure of $CuPy_2Cl_2$ showing two Cu—Cl distances (drawn by Jeff Deschamps from CSD PYRCUC01).

was delighted. He was just then working on a new edition of his classic *The Crystal Structures of Minerals* and could now include an explanation of the problem of the inverted and tetragonally distorted spinels.

Jack with A.I. Kitaigorodskii and Olga Kennard, 1970s (from the Jack Dunitz Papers, Special Collections & Archives Research Center, Oregon State University).

In December 1956 Edgar Heilbronner telephoned out of the blue to ask if I could come to Zurich to talk to Professor Leopold Ruzicka about the possibility of my starting a crystal structure analysis group at the Swiss Federal Institute of Technology (ETH Zurich). Ruzicka was due to retire the following October from his position as Professor of Organic Chemistry. Impressed by Dorothy Hodgkin's success in deciphering the structure of vitamin B_{12}, he saw that a strong organic chemistry team would be incomplete without this new method. Ruzicka offered me a post as associate professor and gave me fourteen days to decide. A few days before the end of the year I sent a telegram to Ruzicka to accept the offer. Thus, after only a year and a half in London, I landed in 1957 at the Organic Chemistry Laboratory of the ETH in Zurich, to join an illustrious group of natural philosophers there, my friends and colleagues for the last fifty years and more, during which we have argued and discussed and learned together about chemistry and molecular structure and about everything else under the sun.

Jenny Glusker, Jack, and Carol Brock at the 40th anniversary celebration of CCDC (2005, courtesy of Carol Brock).

Editor's note: *An extended version of this narrative appeared recently in Helvetica Chimica Acta (2013, **96**, 545). Also see* ***scarc.library.oregonstate.edu/coll/dunitz/primavera/page1.html****. The complete version of Jack's narrative for ACA will be deposited at the Niels Bohr Library & Archives and will also appear on the planned ACA History website.*

Harold Glenn Smith (1927-2012)

Our dear friend and colleague Hal Smith passed away on October 9, 2012 in Oak Ridge, Tennessee. After graduation from Lafayette High School in 1944, Hal joined the US Navy to become an air crewman Petty Officer 2nd class in World War II. Under the GI Bill he graduated with honors in physics from the University of Louisiana-Lafayette in 1949. He married Marion (Sal) Batty in 1950 in New Orleans and graduated from Tulane University (MS Physics - 1951). He worked as an x-ray crystallographer in the Ames Laboratory at Iowa State University (1951-1954) where he pursued his PhD in physics (1954 -1957). In that year he joined Bill Busing and Henry Levy in the neutron diffraction group at Oak Ridge National Laboratory (ORNL) Chemistry Division where he studied the structure of crystals at the Graphite Reactor and the Oak Ridge Research Reactor (ORR). In 1962 he joined Mike Wilkinson to set up a new inelastic neutron scattering program at ORNL's Solid State Division to investigate the dynamical properties of atoms in solids. This group was later expanded to include Robert Nicklow, Herbert Mook and Nobuyoshi Wakabayashi. The group constructed the first triple-axis spectrometer in the US at the ORR, which was based on an instrument developed at the Chalk River Laboratory in Canada by Bertram Brockhouse, and then similar instruments at the High Flux Isotope Reactor.

The materials that Hal studied included metals such as Cu, Au, Ti, Co, Tc and rare-earth metals; ionic materials including LiF, AgCl and TiO_2, superconductors like alpha-U, and semiconductors like MoS_2 and graphite to name only a few. His work included studies of phase transitions in alpha-U and alkali metals Na and Li, and also studies of alloys in which the theoretically predicted localized and resonant modes of vibrations observed were found to be due to the influence of disorder on the dynamical properties of crystals. His work added significantly to the understanding of the nature of interatomic interactions in solids. At Oak Ridge Hal developed the x-ray and neutron sensitive Polaroid camera, which was used worldwide for many years.

Hal at the HB-3 triple axis spectrometer at the HFIR in the 1960s.

Over the years he held many posts, he was a guest scientist at AERE, Harwell, England (1961 - 1962) and at the Institute Laue-Langevin in Grenoble, France in the 1980s. He was a member, then Chair of the Neutron Diffraction Commission of the IUCr. He was the ORNL correspondent for *Neutron News* (1990 - to 1994). Hal retired from ORNL in September 1993.

Hal had a distinguished scientific career; he was author or co-author of numerous scientific papers, book chapters, and review articles. He published in the areas of physics, materials science, crystallography and metallurgy. After retirement he formed a small consulting company, Neutronics of Oak Ridge, where he purchased and assembled parts for neutron-sensitive CCD cameras for various reactor groups in this country and Canada.

Hal will be remembered by his friends and colleagues as a fine scientist, a wonderful human being and a true gentleman. In his private life, he was absorbed with conservation efforts of wild lands in Tennessee, photography, and hiking. He is survived by his wife of 62 years, Marion (Sal), daughter Lorie James and her husband Lyle, a son, Brian Smith and his wife, Sandra, and two grandchildren, Daniel and Clara. A daughter, Lynette Smith preceded him in death in 1977.

R. M. Nicklow - J. A. Fernandez-Baca

John Woolcock (1956-2013)

With great sadness I announce the passing of John C. Woolcock after a battle with pancreatic cancer on January 29, 2013 at the age of 57. John joined the IUP Dept of Chemistry in 1984 after receiving his PhD in inorganic chemistry from UC, Riverside. At IUP, he proved to be a highly dedicated teacher-scholar who served as a role model for numerous students as well as faculty colleagues. His dedication and love for science were acknowledged in 2012 when the University created the "John Woolcock Teacher/Scholar Award" in his honor. This annual award is to be presented to an IUP faculty member who demonstrates excellence in the teacher/scholar model.

John was very passionate about providing students with the best possible educational opportunities and was always seeking methods to inspire students. This passion led John to attend the ACA Summer Course at the University of Pittsburgh in 1995. While attending this course, he developed a vision of bringing crystallographic education and research to IUP. His vision became reality in 1998 when John was able to attract Bryan M. Craven to IUP as a Professor Emeritus. John and Bryan served as the nucleus that grew into a very dynamic, prosperous crystallography program at IUP. Since that time, John made many contributions to the crystallographic community including serving as a faculty member of the ACA Summer Course from 2003 - 2011 and serving as the President-Elect of the Pittsburgh Diffraction Society 1998 - 1999. John's excitement for crystallography was evident from a quote he proudly displayed on his office door stating "*I am extremely happy. I shall soon publish a paper on crystallography. L. Pasteur, 1847*". He is survived by Ruth, his wife of 34 years and his daughters Sara and Lindsey.

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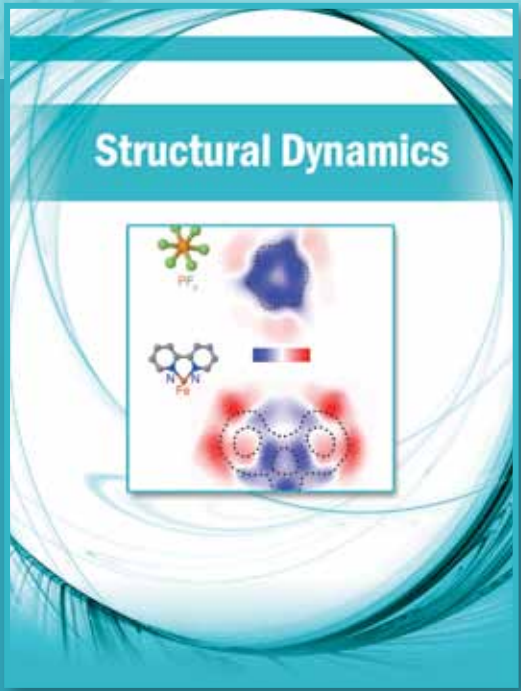

Structural Dynamics

Structural Dynamics is a new open access and online-only journal which will begin accepting submissions in the fall of 2013. 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.

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- 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

EDITOR

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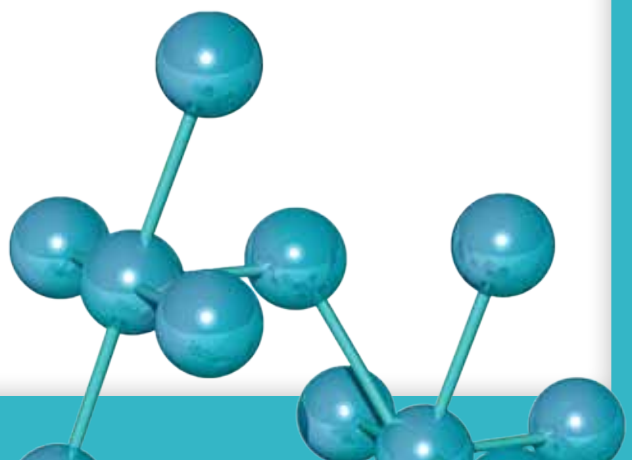
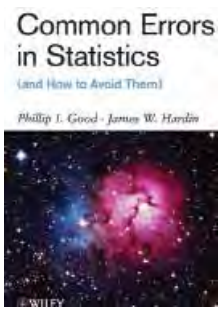




Common Errors in Statistics (and How to Avoid Them) by Phillip I. Good and James W. Hardin, John Wiley and Sons, Inc., 2012, ISBN 978-1-118-29439-0.

I saw a review of this book in *Scientific Computing a*nd thought it looked interesting. I did not read the review to avoid any bias, but had I read it, I might not have bought the book. Don't get me wrong it is a very good book, and there is much to be learned if you are willing to stop and think as you read it. The focus of the book is on the application of statistics to the medical field, mostly in the context of the effects of treatments on patients. There are points that may even be confusing to a crystallographer. For example, there is a short diatribe (funny too) on maximum likelihood that, while correct, does not apply to its usage in crystallography, since we generally work with normal distributions. There is also a section on how not to create bogus priors for Bayesian analysis. The scary part is the judicial system allows falsely generated priors to affect the outcome of civil and criminal cases to no good.

The authors are adamant about designing an experiment such that one can extract the information needed to test the original hypotheses at the end of the trial. The authors point out the fallacy of stopping studies in the middle or extracting information that was not originally planned because it can introduce a bias. If one sees an unexpected trend, one should go back and design a new trial to properly test the new hypothesis.

CES is not an introductory text and requires a basic knowledge of statistics. In the first part of the book, "Foundations" the authors cover the topics of sources of error, hypotheses, and collecting data. With each chapter, the authors provide a descriptive "for further reading" as well as copious references to enhance the topics covered.

In the second part of the book, "Statistical Analysis", data quality assessment, estimation, testing hypotheses, strengths and limitations of procedures, reporting results and interpreting and presenting results are covered.

The third section, "Building a Model" covers univariate, multivariate and alternate forms of regression, modeling counts and correlated data and validation. The authors discuss data analysis, reporting, and presentation and provide useful guidelines for each of these topics.

There some very funny lines, I won't spoil them all but one I particularly like is "What is the sound of one hand clapping?". The answer is the same as an experiment without a control. Another bon mot "a picture is worth a 1000 words only if does not take a 1000 words to describe it". That said, there is a very good discussion, *a la* Tufte, on the display of numerical data: how to draw useful and informative graphs as well when to use a table instead of a graph.

As an aside, if you want to read something laugh-out-loud funny, try Dave Barry's *Insane City*. But, don't read it on an airplane or your cabin mates might think you've lost it.

Joe Ferrara

Let's keep evolving

Thanks to campaigns organized by activist Zack Kopplin to repeal the 'academic freedom' bill in his home state of Louisiana (***www.repealcreationism.com/about/***), the debate between creationism and evolution is getting renewed attention from the general public. Academic freedom bills *de facto* allow creationism to be taught in public schools alongside evolution, as a plausible 'scientific theory'. They are a reality in Louisiana and Tennessee, and were on the table in several other states in February 2013 (***ncse.com/creationism/general/chronology-academic-freedom-bills***). This strikingly anachronistic debate leaves me deeply puzzled. The US is 'the' country where innovation, creativity, great ideas and scientific development have been praised and encouraged and where rationality and forward thinking was once the motor of social and economic growth. Nonetheless, in 2012, 46% of the people participating in a Gallup poll believed that God created human beings in their current form; 32% that we evolved with God's help and only 15% that we evolved without help from God (***www.gallup.com/poll/21814/evolution-creationism-intelligent-design.aspx***). In an online debate, published on ***Debate.org*** in 2012, 36% of the participants supported teaching of creationism in public school alongside evolution (***www.debate.org/opinions/should-public-schools-teach-creationism-alongside-evolution-in-science-classes***). Most reasoned that creationism and evolution are both 'theories' and that children should be left free to make up their own minds. As an active scientist, comparisons between creationism and evolution make me cringe. 'Creationist Science' is an oxymoron. Since there are no experimental proofs or reproducible data that can support it, creationism does not share anything with science and it is deceitful to state otherwise. A scientific theory is not the product of a single experiment, from a single research group, but rather the result of discussions, collaborations, criticisms and interpretations by the experts in the field. Evidence gathered from different disciplines including biochemistry and anthropology point to a single unifying theory. This theory is not debatable and must therefore be considered a fact.

Shockingly, a large percentage of Americans do not agree with this, but rather think that evolution, and by extension science, is a matter of opinion, giving it the same weight as that given to religion. This type of thinking minimizes the role that science plays in our society and undermines the possibility of developing the adequate scientific resources needed to face the environmental, energetic, health and medical challenges that the future will present. For this to change, formal public education has to play a major role. It is crucial that today's students in K-12, without discrimination of means, receive strong, sound and reliable training in STEM (Science Technology Engineering and Mathematics) disciplines, even at a basic level. The development of a framework that delineates the guidelines for science classes, placing evolutionary biology at the core of science curricula (***www.nas.edu/evolution/***), does not seem enough to reach this goal. The first step is to train science teachers that are up to the task and that possess a deep understanding of evolution and the scientific method. The urgency of this need is clear from the data in the 2012 paper by Berkman and Plutzer (M. Berkman and E. Plutzer. *An Evolving Controversy. The Struggle to Teach Science in Science Classes, American Educator*, Summer 2012). According

to a survey conducted in 2009, only 28% of high school teachers present evolution as an accepted scientific fact and draw clear lines between religion and science, understanding that they answer different questions. 13% of the teachers minimize teaching of evolution and claim that both evolution and creationism are plausible models. 60% of the teachers, called the 'cautious middle', are ambivalent towards teaching evolution, even if they believe in it, and compromise by excluding the most controversial aspects of evolution, such as 'micro' *vs* 'macro-evolution'. They are not confident enough in their own expertise to teach evolutionary biology in a rigorous manner and to be able to stand up for their teaching in front of the community; they find it too stressful, and therefore prefer to resort to compromising strategies. Berkman and Plutzer's research also shows that the level of confidence in teaching evolution depends on the number of biology classes that the teachers took in college, and in particular if they completed a thorough course in evolutionary biology. A possible solution to the teachers' reluctance to teach evolution might be to make it compulsory for future science teachers to enroll in at least one course the covers evolution. This would boost their confidence by providing concrete tools to counter arguments for teaching creationism that arise in their communities as well as increasing the standards of science classes.

Chiara Pastore

2014 ACA Etter Early Career Award to D. Borden Lacy

D. Borden Lacy (Vanderbilt University Medical Center) is a structural biologist and biochemist. Some of her outstanding achievements include the determination of the structure of the botulism neurotoxin during her graduate studies at UC Berkeley, broadly enabling both basic and applied research targeting this pathogen. Her postdoctoral studies with John Collier were equally productive and are best described by Walter Chazin as a *tour de force examination of the molecular basis of anthrax toxin pathogenesis*. As an independent investigator, she has also contributed tremendously to Vanderbilt University as well as to the overall scientific community. She has trained a number of students and has contributed to a number of courses. She has served on multiple committees both within and outside the university. She is exceptionally well-funded: she has won the Burroughs Welcome Award for the study of the pathogenesis of infectious diseases as well as several NIH grants. She was also well funded, with numerous fellowships and awards, during her training years. On a personal level, she is known for her outstanding personality, and for being a caring mentor and a role model for women in science. She is successful by all measures and embodies the spirit of Margret C. Etter.

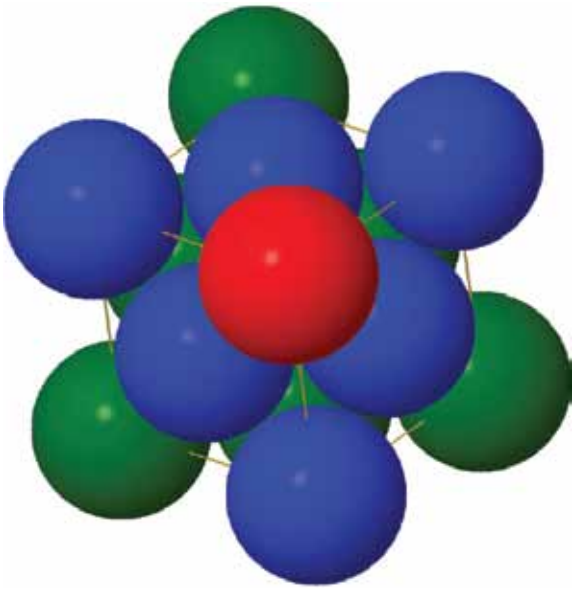
Eric Ortlund / Emmanuel Skordalakes

Net RefleXions

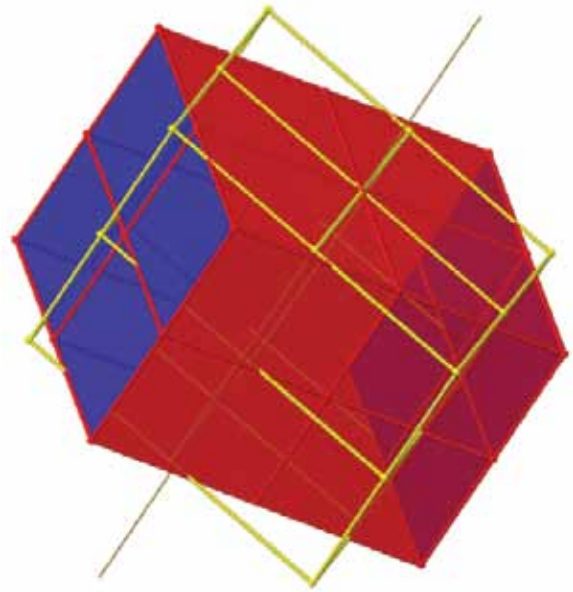
What do you do in those mere minutes while waiting for your data collection to finish? How do you spend the spare seconds between refinement cycles? If you're like most folks out there with some time to waste, you're either surfing the Net or playing solitaire on your smartphone. While improving your score in Bejeweled is a worthy endeavor and lolcats are always a cute distraction, there are better things to do with all this great technology. In this column, I'll spend some time introducing you, gentle reader, to web sites and smartphone apps for the modern-day crystallographer. Hopefully you'll find something new and useful here. Should you have any suggestions or requests for sites you'd like reviewed, please send them to me at ***asarjeant@northwestern.edu***.

For my first foray into web and tech review, I'll focus on symmetry visualization. Those of us who have struggled to show a 4-fold rotary inversion axis to a classroom of sleepy students might want to browse over to ***crystals.otterbein.edu/***. This site is written and maintained by Dean Johnston of Otterbein University

and includes wonderful tools to help students grasp the symmetries involved in point groups, space groups and crystal packing. A desire to bring x-ray crystallography into the undergraduate curriculum at Otterbein served as the impetus for developing the site and the web apps included were engineered with this in mind. All of the apps on this site are powered by Jmol and are designed to show symmetry operations and packing diagrams in 3D. For example, those studying structural inorganic chemistry, can display various packing arrangements such as wurtzite, ice and the cubic close packed structure of nickel, to name a few. Options to highlight stacking layers or coordination environments are available. Shown here is the ccp structure of Ni with the ABC layers highlighted in different colors.



Another module breaks down the symmetry of all 32 point groups, as applied to solid objects or unit cell contents. The various elements of a given point group can be displayed and animated in order to show the actual symmetry operation. Shown here is the 2/m point group, showing the animation of the



2-fold rotation axis. The modules are powered by Jmol and will run on any operating system and web browser that supports Java. Johnston eventually plans to develop his modules into mobile apps, so you can have all this symmetry right at your fingertips!

If 2D symmetry is more your speed, the researchers at Ecole Polytechnique Fédérale de Lausanne have written an Escher sketch app for the iPhone, iPod touch and iPad, or any Java-compatible phone. The iOS app is available as a free download from the iPhone App Store, or see ***escher.epfl.ch/mobile/*** for other phone systems. The app is based on the *Escher Web Sketch* site, ***escher.epfl.ch/escher/***, which can be used to create beautifully symmetric images. With the mobile app, you can generate these images on your phone and share them via e-mail or to the *Escher Sketch Web Library*. The app has many fun features, such as "shake" to generate a new pattern, and "gravity" to let you draw just by tilting your phone. The "help" instructions include definitions of common symmetry terms, and links to websites where users can find further information. Aside from producing pretty pictures, these Escher Sketch patterns make great tools for demonstrating unit cell choices and plane symmetry operations.

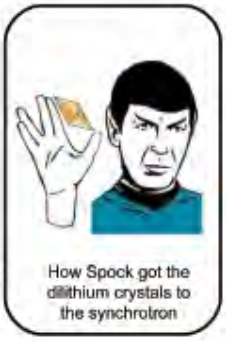
Take some time to browse over to these sites and play with their symmetry visualizations. You'll be surprised at how much more rewarding web-surfing can be!

Amy Sarjeant

DISORDERED

Synchronize these words to form an ordered solution

GINNBED	BENDING
STAGMEN	MAGNETS
AULDUTRON	UNDULATOR
TEBOSPAM	BEAMSTOP
SHRIMPEEHE	HEMISPHERE



How Spock got the dilithium crystals to the synchrotron

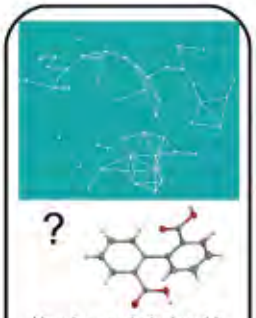
Answer:

HE BEAMED THEM UP

DISORDERED

Unscramble these words to achieve short-range order

LETSTRIP	
MOBSICYL	
IDIOTDAN	
HERTOY	
KERRAH	



How he reacted when his Emap didn't look like a molecule

Answer:

__ ____' _ "_____" ___

Fun With Refcodes

In the Spring issue, in a puzzle adapted from *BCA News*, we asked which of the following refcodes, BASSET, BULGAR, CARBON, CARNAL, CARPET, CITRUS, DOGSEX, FARMER, MUPPET, POSSUM, SURFER, WASHED, refers to the chemical name of the compound. ***CARPET is the alkaloid Cardiopetaline*** (A. G. Gonzalez, G. de la Fuente, M. Reina, V. Zabel, W. H.Watson; *Tetrahedron Lett*. (1980), **21**, 1155). In the early days of the CSD, many, perhaps most refcodes were based on the compound name. We asked whether SURFER or WASHED contained any water. ***Neither does (but DAMPEN does!).*** We also asked if any refcodes which are also English words are palindromes.

There are certainly refcodes which are palindromes (BURRUB, DALLAD, SAKKAS, etc.), ***but we are not yet aware of any which are also English words. Anyone????***

Send ideas for new puzzles /problems to Puzzle Corner Editor Frank Fronczek ***(ffroncz@lsu.edu)***.

What's on the Cover - from Eric Ortlund

The cover image depicts the evolution of steroid specificity in hormone receptors. This representation highlights the utility of ancestral gene resurrection in combination with structural biology to gain a molecular-level understanding of the forces that shaped natural protein function.

Ortlund Lab Focus: We use an array of structural and biochemical techiques to gain a molecular level understanding of transcriptional signaling - with a particular focus on lipid mediated signaling and transport. We currently pursue structural and biochemical studies of human nuclear receptors, which are lipid regulated transcription factors that play central roles in development, cancer, stress and metabolism. We have also made seminal contributions to the field of molecular evolution using nuclear receptors as a model system to study how tight molecular partnerships evolve.

Contributors to this issue: Oluwatoyin Asojo, Gerald Audette, Chris Cahill, Edward Collins, Jack Dunitz, Larry Falvello, J. A. Ferandez-Baca, Joe Ferrara, Frank Fronczek, Jane Griffin, Ilia Guzei, Michael James, Charles Lake, Peter Müller, R.M. Niclow, Eric Ortlund, Allen Orville, Chiara Pastore, Virginia Pett, S.N. Rao, David Rose, Amy Sarjeant, Cheryl Stevens, Crystal Towns, Victor Young, Christine Zardecki.

Cover: Images provided by Eric Ortlund; production by Connie Rajnak.

Cartoon: Page 40, courtesy of Randall Munro (***xkcd.com***).

Christopher L. Cahill
Vice-President

Professor of Chemistry and International Affairs, Department of Chemistry, The George Washington University, Washington, DC 20052.

Education: BS in Chemistry and Geochemistry, SUNY College at Fredonia (1993); PhD in Chemistry, SUNY Stony Brook (1999).

Professional Activities: ACA: Member of Standing Committee for Continuing Education (2006 to 2009); Program Chair of the 2011 Annual Meeting in New Orleans. Member of US National Committee for Crystallography (2005 to 2012).

Research Interests: Broadly speaking, I am a solid state and inorganic chemist. with a keen interest in hybrid materials, hydrothermal systems, mineral structures, f-element chemistry, the nuclear fuel cycle and the intersection of science and policy.

My scientific career began as a chemistry/geochemistry major at the SUNY Fredonia. My experience there initiated a deep appreciation for minerals and natural systems. Moving to SUNY-Stony Brook allowed me to pursue a mixed bag of natural and synthetic materials using small molecule single crystal XRD as well as synchrotron based *in situ* techniques. A post-doc at Notre Dame in the Environmental Mineralogy group (with Peter Burns) provided a much more applied foundation for directly coupling mineral structures to long-term environmental issues- in this case, the stewardship of spent nuclear fuel in geologic repositories. I began my independent career at George Washington University in 2000 and have established a research group focused heavily on the synthesis and structure/property relationships of hybrid materials. Crystallography has been at the core of our efforts and remains our primary technique for structure elucidation.

Statement: I am delighted and flattered by the nomination for ACA Vice President. The prospect of serving a community that has been my scientific home over the years is indeed humbling. I have held several positions within the community including membership on the ACA Standing Committee for Continuing Education and on the US National Committee for Crystallography. I have also served as Program Chair for the 2011 ACA Meeting in New Orleans. As such, I have worked closely with Council in the past and have a sound appreciation for what the position of Vice President entails. Moreover, this nomination comes at a time in my career where I am able to give back to an organization that has provided me with invaluable inspiration and support over the years. Having established a sustainable and well-funded research program, I am excited by the prospect of a leadership position where I can leverage my experiences thus far to help guide and shape an organization about which I am passionate.

One of the more intriguing aspects of the VP position of ACA is that this organization is vibrant and thriving. This might have prompt an eye roll or two from some readers, but think about it: here is a relatively lean organization dedicated to its members and that operates on their input and service. This is not typical for a number of other scientific organizations. Not only would I be delighted to serve, but my 'campaign' for election would emphasize my intent to enhance an already strong foundation and explore opportunities for improvement.. With respect to the latter, I see opportunities (and challenges!) for broadening participation across the Americas. We need to remember that the first 'A' in ACA includes North, Central and South America and accordingly, we should make sure we are doing our best to be inclusive and supportive. Further, my 13 years in Washington, DC have made me keenly aware of how intricately linked science and policy have become. How policy influences science and vice-versa is not only fascinating, but is also often grossly misunderstood from within the respective camps. My own interests in this arena have led to a recent promotion to Full Professor with a secondary appointment in the Elliot School of International Affairs at GW. This

Candidates for ACA Offices in 2014

The Nominating Committee (Saeed Kahn, Tom Koetzle and Carrie Wilmot) proposes the following candidates for the 2013 elections for ACA offices in 2014.

Officers:

Vice-President: **Chris Cahill & Larry Falvello**

Canadian Division Representative*: **Gerald Audette & Mike James**

***Committees*:**

Communicatons: **Oluwatoyin Asojo & Ilia Guzei**

Data, Standards & Computing: **Peter Müller & Victor Young**

Continuing Education: **Ed Collins & Allen Orville**

To nominate write-in candidates for any office, write to the ACA Secretary: **Patrick Loll, Dept. of Biochem & Molecular Biol., College of Medicine, Drexel Univ., Philadelphia, PA (pat.loll@drexel.edu).** Letters must be received by September 15, 2013 and must be signed by 5 ACA members and include a signed statement by the candidate describing his or her qualifications. Voting will be by electronic ballot. Statements from all candidates will be available on the election site. The voting window will be open in ***October 2013***.

*Only members residing in Canada can vote for the Canadian Representative

appointment speaks to an emerging awareness of the global impact of our science and specifically the disconnect between technical and non-technical communities. I see opportunities for organizations like the ACA to participate in outreach to the policy community who (believe it or not) are hungry for education and technical enlightenment. The ACA membership is full of dynamic and articulate scientists and as a consequence, I would like to see us take on a greater role and engage the policy community in interactions beyond our typical forums and 'comfort zones.'

Returning to the local level, I would hope to be able to chip away at the divide between the small-molecule and macromolecular communities within the ACA. While this is certainly not a lethal compartmentalization, anyone reading this is likely aware of the minimal overlap. Looking back at a number of ACA meetings, opportunities to have both camps in the same room at the same time often emerged around symposia based on education, best-practices and diverse keynote speakers. It is definitely not the VP's job to take over a meeting program, but I would certainly be supportive of events targeting both communities simultaneously. Moreover, our common interests in the development, support and use of national facilities can provide even more of a forum for working together across disciplines not only at meetings, but year-round.

In closing, I would be honored to serve as the next Vice President of the ACA. This is an intellectually rich organization with a sound infrastructure. Consequently, opportunities for enhancement (as opposed to repair) are all the more intriguing.

Larry Falvello
Vice-President

Professor of Inorganic Chemistry, Department of Inorganic Chemistry and Aragón Materials Science Institute, University of Zaragoza, Spain.

Education: BS, Duke University (1976). Cambridge University (Churchill College): Certificate of Post-Graduate Studies, (1997 - Olga Kennard); PhD, (1979 - Malcolm Gerloch). Post-doc, (1979-1981) Cambridge University (Malcolm Gerloch); (1981-1982) Texas A&M University (F. A. Cotton).

Professional Activities: Before moving to the Department of Inorganic Chemistry at the University of Zaragoza in 1991, I was Staff Scientist at the Laboratory for Molecular Structure and Bonding at Texas A&M (1982-1991). I have participated in extramural activities, including: ACA (session organizer, 9 to date). *Acta Cryst., Section C* (Co-Editor, 2002 – present; Deputy Section Editor, 2013 – present). *Comments on Inorganic Chemistry* (Associate Editor, 2002 – present). Member of the IUCr Commission on Journals. Peer review for various journals. ISIS Facility Access Panel (Diffraction) (2006 – 2009). Institut Laue-Langevin Scientific Subcommittee 5a (diffraction) (2010 – present). Participation in NSF Site Visit Panels. Member: Governing Council of the Aragón Materials Science Institute, (2002-2007), organizing committee for the International Summer School on Neutron Techniques in Molecular Magnetism, Jaca, Spainm (2006) and the instrument development team for the TOPAZ neutron diffractometer at the Spallation Neutron Source.

Research Interests: Crystal structure, solid-state reactions, single-crystal-to-single-crystal transformations and other dynamic processes in molecular solids, coordination chemistry and neutron scattering. My in-house laboratory devotes considerable effort to the preparation of new molecular solids. In recent years this has involved transition-metal cubanes, complexes of orotate, and mixed-metal (transition metal / lanthanoid) complexes. We explore the resulting solids using diffraction – single-crystal diffraction if possible – and characterize their structures and the structural transitions that can be provoked by effects such as dehydration. When needed, we collaborate with others, principally in magnetism and neutron diffraction. I am acutely aware of the changing landscape in research organization, with funding agencies emphasizing collaborative efforts aimed at problems of broad scope. At the same time, I am also conscious of the need to provide our research students with a solid grounding in fundamental techniques; and this is where diffraction methods need special attention in today's academic research environment.

Statement: It is an honor to have been nominated as a candidate for Vice-President of the American Crystallographic Association. I have felt at home in the ACA ever since attending my first ACA meeting at College Station, Texas, in 1981, on the campus of Texas A&M. There I heard some talks about how the ACA is special, with genuinely shared interests and common purpose. More than thirty years later, I can add that I have accumulated plenty of experience to support that sentiment. The special treatment of younger scientists is particularly important, and our practice of facilitating their participation in meetings is still one of our most beneficial activities.

There are several things that the ACA already does well, and I think that Council and the association officers should do everything possible to see that these continue:

The annual meeting: Beyond the function of general scientific interchange, the meeting provides important exposure and early-career experience to young scientists. In the past their participation was facilitated by the relatively inexpensive venues of that era. More recently attendance has been aided by travel grants and hotel bargains for students. By whatever means, this help

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ISNS Article: ***Multiple Groups Claim to Create First Atom-Thick Silicon Sheets-*** Silicon-based material might prove useful in electronics, but multiple teams are claiming credit for creating it first.

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should continue and should be expanded.

The other critical aspect of the meeting is the scientific program. Mindful that each SIG has to present its own proposals, I would look for opportunities to promote crosstalk among the SIG's before they propose their session topics, with the aim of a more comprehensive program and as little overlap as possible.

The ACA web presence: The ACA web site is, in my opinion, one of the best among organizations of similar size and scope, with a good balance between material for members and outward-facing content. We should aim to keep the content of our website current and we also need to be aware of new developments in the world of mass communication in order to maintain a presence that is as modern as possible without sacrificing stability.

In addition to continuing what we are doing well, other areas in which the ACA should be active, or more active, include:

Science advocacy: Science advocacy has two main components – the first is an active defense of science in general terms, making sure that science-based information on topics important to the general public is always present in freely available media. The second important area of science advocacy is that directed at funding agencies. I think it is important that there be institutional and individual voices to make the case for science funding, including funding for crystallography in its broadest definition.

Crystallographic education: Our first role in education is as an advocate, and we can do this both through our web presence and by communicating with other interested groups. One issue that is especially important is the level of education in structural science, including diffraction, in curricula in chemistry and physics. We, as an organization, can and should comment about such issues.

There are presently some important activities underway in the ACA about which the next Council will have to be aware – the strategic planning study, the new journal and the start-up of the Latin American Division.

Much of what the ACA does well, such as the scientific program at our annual meeting, is achieved through the efforts of individual members. As for Council and the ACA officers, in addition to the functions specified for them in the ACA by-laws, I see their role as one of promoting the success of the efforts of all of those who serve as organizers, committee members, and participants. If chosen to serve as Vice-President / President / Past President, I will maintain that principle as a guide while conducting the duties of those offices.

Gerald F. Audette
Canadian Representative

Associate Professor, Center for Research on Biomolecular Interactions, Department of Chemistry, York University.

Education: BSc, University of Alberta; PhD, University of Saskatchewan (L.T.J. Delbaere & J.W. Quail); Postdoc, U. Alberta (B. Hazes).

Professional Activities: Chair, Canadian Division of the ACA (2012-13); Session Co-Chair - Structural Enzymology (I), 2013 ACA Honolulu Meeting (2013); American Crystallographic Association (1996-2013); Canadian Society for Molecular Biosciences (1998-2013); Canadian Institute of Chemistry (2007-2013); Canadian Institute for Synchrotron Radiation (1997-2009); Canadian Light Source User Advisory Committee (2002-2004); Co-Editor in Chief, Journal of Bionanoscience (2006-2010); Organizing Committee, Canada-India Frontiers 2011 Symposium, York U. (2011); Co-Organizer, Protein Crystallography Workshop, CLS Annual Users' Meeting (2004); Organizer, Applications of Synchrotron Radiation in the Life Sciences Workshop, CLS User's Meeting (2002); Co-Organizer, CLS Annual Users Meeting (2002-2004).

Research Interests: The application of x-ray crystallography and other methods to understand how microorganisms utilize multi-protein complexes for transferring genetic material and effector molecules across membranes, and facilitate adherence to a variety of surfaces. I am interested in how these systems are assembled from their component proteins, as well as their effects on infection and the development of multi-drug resistance, using the conjugative type 4 secretion system of the F plasmid of *E. coli* as a model system. I am also interested in how these secretion systems assemble fiber-like pili for surface and cellular adherence, motility etc. In particular, we are examining how the relatively simple structure of an engineered pilin can direct protein nanotube assembly in the absence of the hydrophobic helix which is used to drive native pilus assembly. We are also exploring the development of pilin-derived protein nanotubes for biosensor applications.

Statement: I am honored to have this opportunity to represent the Canadian crystallographic community as a candidate for the Canadian Representative on Council. The ACA was the first association I joined as a student, and has been my professional home for close to 20 years. I have been privileged to meet many friends, from fellow students (when I started) who have since become collaborators and colleagues, to senior scientists and Nobel Laureates that I read of in my early studies, not to mention my Canadian crystallographic colleagues, through the ACA. Everyone I met at ACA meetings was willing to provide pointers and suggestions, and understood the challenges and triumphs that solving and refining a structure using crystallographic methods entailed. And I learn more about the technical advances in crystallographic hardware and software, as well as recent exciting and interesting structures, at the ACA meetings than anywhere else.

I once heard it said that the ACA was more like an extended family than an association. I believe this statement. I have always found that ACA meetings were an exceedingly welcome place for students, and remember the first one or two Mentor-Mentee dinners. The first small dinner was quickly expanded because of the interest, and these events have become an important mainstay of the ACA meeting! It is a great

way to meet more senior colleagues, share stories and a laugh, and get a sense of what to think about beyond the minute details of your own project. I started giving back to the community in this way, by becoming a mentor at an ACA meeting (even though I still felt like a mentee), and encourage my students to join the ACA. At the 2009 Toronto meeting, while I was not a member of the local organizing committee, I was happy to see many of my students volunteering their time to make the meeting a success. I have also been engaged in the promotion of crystallography to the general public with the Canadian Light Source, have been a member of the CLS User's Advisory Committee, and have organized CLS workshops at several CLS Annual Users Meetings. I am currently the Chair of the Canadian Division (2012-2103), and am a session co-chair for the upcoming Honolulu meeting.

It would be a pleasure to represent our community as Canadian Representative on Council. Crystallography in Canada is a diverse landscape and David Rose has been an excellent voice on council for the past 3 years. I hope to continue in that role, be an active voice for Canadian crystallography in the Americas, encourage more Canadian involvement in the ACA, and lend my experience and enthusiasm to the position.

Michael James
Canadian Representative

Distinguished University Professor, Department of Biochemistry, University of Alberta, Edmonton, Alberta.

***Education*:** BSc (Hons) Chemistry, Univ. of Manitoba, Winnipeg; MSc Mineralogy, Geology, Univ. of Manitoba, (R B Ferguson). DPhil., Chemical Crystallography, Oxford University, UK (D.C. Hodgkin).

Postdoctoral Fellowship, Chemistry Department, University of Alberta, Edmonton (S D. Hall).

Professional Activites: I was the program chair for the Calgary ACA Meeting. I have also been the Chair of the Canadian National Committee way back when. Probably in the late 70's or early 80's. I have been elected to fellowship in the Royal Societies in London and in Canada, and have received the Alberta Centennial Medal, the Ayerst Award in Biochemistry, the University of Alberta Faculty of Medicine and Dentistry Award for Excellence in Mentoring, and the 2009 ACA Buerger Award.

***Research Interests*:** Ever since I had the opportunity to be present at the Royal Institution in London when Sir David Phillips and his colleagues announced the successful determination of the molecular structure of the first enzyme, hen egg white lysozome, I have been fascinated by the relationship of the structure and function of enzymes. Our first studies were on the structures of the bacterial serine peptidases that, surprisingly, adopt the fold of α-chymotrypsin a member of the mammalian pancreatic serine peptidases. The structure of SGPB from *S. griseus* became the basis for our studies of enzyme-inhibitor interactions using variants of the third domain of the ovomucoid from turkey with Michael Laskowski, Jr. and his colleagues at Purdue University. Michael's work ultimately ended in the development of an algorithm that related sequence to the strength of binding between two proteins. I then moved on to the study of the structure and mechanism of pepsin-like enzymes from fungi. We were rewarded with the elucidation of the first structure of an aspartic proteinase and later with its catalytic mechanism. More recently, working with Kohei Oda in Japan and my colleagues in Alberta, we determined the structure and elucidated the catalytic mechanism of the sixth class of proteolytic enzymes, the glutamic peptidases. The structure of that enzyme allowed us to design, synthesize and determine the mode of binding of a nanomolar inhibitor of the enzyme, eqolisin. My interests range to a variety of other enzyme families, but staying within the hydrolases, our group has been active in the area of the glycoside hydrolases and we have determined the structures of two lysosomal enzymes that are associated with the genetic diseases,Tay-Sachs disease and Sandhoff. The defective enzymes involved in these two diseases are hexosminidase A and hexosminidase B. Members of my group, in particular, Brian Mark and Joanne Lemieux, solved the structures of these enzymes and showed that this family of glycoside hydrolases removes galactosamine residues from the non-reducing ends of GM2 gangliosides and mutant forms of the enzyme result in a building-up of harmful amounts of unmetabolized gangliosides and eventually cell-death. There is no known cure or treatment for Tay-Sachs disease but work on the design and synthesis of pharmacological chaperones is benefiting from knowledge of the structure and mechanism of these hexosaminidases.

But enough of my research interests. Let's turn to my statement of why you should elect me as your representative on the ACA council.

***Statement*:** I have been a member of the ACA, on and off, since my time as a graduate student working for my Master's degree at the University of Manitoba (1963). The first meeting that I attended was in Minneapolis in 1968. Over the years I have realized just how beneficial it is for us Canadians to have the opportunity to be members of the ACA, whether your interests are in mineralogy, chemistry, structural biology, diffraction physics or instrument development. The ACA provides for all of these disciplines and brings together the best people to pass their knowledge and experience on to the younger generation of crystallographers.

So far, I have not given you any reason why you should vote for me; I don't have a platform but I do have, even now, a lot of energy to tackle new projects that are and will be of importance to Canadian crystallographers.

Speaking of Canadian crystallographers, I was surprised, and amazed to learn that only 50% of us are members of the ACA. Why is that? One possible reason may be that our efforts in meeting attendance are focused on the specialties we have chosen in crystallography. By this I mean those of us who specialize in the structural biology of membrane proteins attend those meetings that are geared specifically for that sub-discipline. Or if we are mineralogists, we attend those geology meetings to

discuss our discoveries of new minerals. While I can understand these reasons and even perhaps used them at times to rationalize my failure to pay annual dues, I don't think overall that these are good reasons. If one looks at the programs of the past few ACA meetings, I am sure that you will find topics into which your interests fit well. In addition, we all employ similar crystallographic techniques and to attend a meeting where these techniques are discussed is of paramount importance. Where else could you hear about the developments in serial femtosecond diffraction experiments? John Spence treated those of us who attended the 2012 Boston ACA meeting to the future of crystallography in his acceptance speech for the Buerger Award. The instrument manufacturers are all in attendance at these meetings and ready to discuss the next best thing for data collection since photographic film! (Just kidding) I strongly urge all of my Canadian colleagues to renew their ACA memberships. Collectively we benefit a great deal by being members of the ACA. I certainly will do whatever I can to boost the numbers of our colleagues who are members of the ACA to 100%.

Oluwatoyin (Toyin) Ajibola Asojo
Communication Committee

Associate Professor, National School of Tropical Medicine, Baylor College of Medicine Houston Texas.

Education: BSc Hons Trent University Peterborough ON Canada (1993), PhD University of Houston, Houston TX 1999, postdoc NCI Frederick MD (1999-2000).

Professional activities: Associate Professor (2011 to date), Assistant Professor Pathology and Microbiology University of Nebraska Medical Center (2005 to 2011), Research Assistant Professor Eppley Cancer Institute (2003 to 2005), NIH IATAP fellow (2001 to 2003), Staff scientist Tibotec, Rockville MD (2000-2001), Member: IUPAC, AACR, ACA, ACS, ASTMH, Reviewer for NIH and NSF, and for APS and IUCR journals.

Research Interests: I am a protein crystallographer and my current research interests include crystallographic studies of proteins from parasites, targeted inhibitor discovery for multidrug resistant cancer, bacteria, and infectious diseases. I work with an interdisciplinary group of scientists to develop vaccines and therapeutics for diseases related to poverty.

Statement: It is my privilege to accept the nomination for the ACA Communications standing committee. The dissemination of crystallographic data (their relevance as well as applications) to the broader scientific and general audience is an important task that I am excited to contribute to if elected. For many people, it is difficult to appreciate the value of something that they do not understand. There remains an ever widening divide between crystallographers, and the general public. To compete in an era of ever shrinking funding and resources, there is a need to effectively communicate the value of crystallography. Crystallography is much more than a peripheral skill set and is inherently exciting. Anyone from preschoolers to accomplished scientists, can be captivated by the beauty of crystals, electron density maps, and refined structures, even x-ray instrumentation is "awesome" according to my 5 year old. However, unless it is presented appropriately to different audiences its merits and beauty will remain hidden. I believe that a role of the ACA communication's committee is to break down the intricate science and unveil how the work of crystallographers enhance life as we know it. Additionally, effective communication of the activities and achievements of the ACA to crystallographers at all stages of their careers is vital towards achieving the missions of the ACA. I have learned over the years the difference between "dumbing down" science and effectively communicating my work to different groups and I have developed the skills required to take on the responsibilities as a member of the communications committee. Having worked as a crystallographer in government, and academia, as well as industry, I have learned how to share my scientific data with a broad audience, from preschoolers onwards. If elected, I will actively participate in enhancing the PR efforts of the ACA and work to ensure that the missions and goals of the ACA are met. Thank you.

Ilia Guzei
Communications Committee

Chemistry Department, University of Wisconsin-Madison, Madison, WI.

Education: PhD in chemistry (1996), Wayne State University, Detroit, MI, MS in chemistry (1992), Lomonosov Moscow State University, USSR.

Professional Activities: ACA Poster session chair (2011-13), ACA workshop and session organizer, Acta Cryst. C co-editor (2005- prsent), ACA summer school instructor (2012), Instructor in a short course in crystallography (2004-present), Coordinator of the Bruker users meetings (2001-prersent).

Research Interests: Small molecule single-crystal x-ray crystallography, twinning, non-routine crystallographic experiments, crystallographic software development and ligand steric properties in organometallic compounds.

Statement: As the International Year of Crystallography 2014 is approaching, I believe this position provides a unique opportunity to reiterate to the general public and scientific community the significance of crystallography, the role it has played in scientific discoveries and everyday life and the importance of teaching the graduate and especially undergraduate students symmetry and crystallography.

My professional pursuits are a good match for this committee's activities. As

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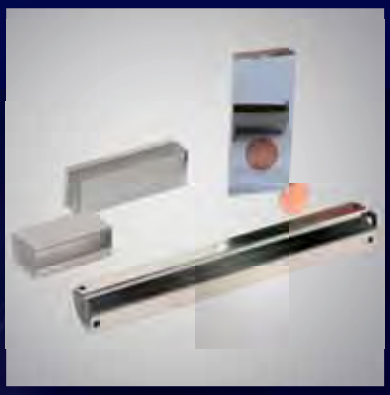

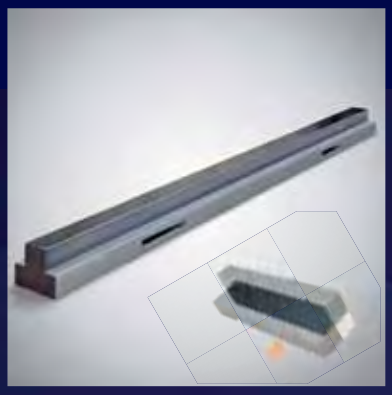

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a contributor to *Reflexions* and co-editor of *Acta Cryst. Section C*, I have experience with writing and evaluating scientific manuscripts, which goes along with the committee's coordination of the ACA publications and preparation of reviews of crystallographic research. I enjoy organizing meetings and workshops and have been the ACA meeting Poster Chair three times, thus helping with the annual ACA meetings and press conferences would be second nature to me. As an amateur photographer I possess skills in videotaping, an activity that is taken seriously at our annual meetings when recording historical and plenary lectures is necessary.

As a US IUPAC Young Observer at the 2013 IUPAC Congress in Istanbul I am excited to represent the USA as a crystallographer. There are many ideas about coordinating IUCr, ACA, and IUPAC activities during the IYCr 2014, one of which – crystallographic education in undergraduate colleges – is particularly appealing. I will actively work with these three organizations to disseminate information about the role that crystallography plays in our lives and why it is important to continue funding fundamental and applied science.

Edward J Collins
Continuing Education

The University of North Carolina at Chapel Hill, Department of Microbiology and Immunology, Chapel Hill, NC.

Education: Ph.D. The University of Texas at Austin 1990.

Professional Activities: ACA member since 1986. Biomac and Synchrotron SIG session chair for ACA sessions 2006-2013. Program Chair Orlando ACA meeting 2005.

Research Interests: Host Pathogen interactions. MHC:TCR interactions. Evolution of TCR recognition of peptide/MHC complexes. Bacterial heme uptake by gram-negative bacteria.

Statement: It is an honor to be nominated to the Continuing Education Committee of the ACA. It is critical to provide quality resources to both novice and experienced crystallographers.

I have seen an alarming trend on NIH study sections demonstrating that protein crystallography, like small-molecule crystallography not too long ago, has been relegated to a necessary, but routine technique. We must continue to educate all of our people that that they are valuable voices to the greater scientific community. Everyone values the information that we provide, but they appear to be uninformed. They do not understand the real problems associated with this scientific discipline.

I have a long standing interest in crystallographic education. I am the course director for a macromolecular crystallography course at the University of North Carolina. I have chaired or co-chaired "education" centric sessions at the annual ACA meetings for the past seven years.

Andy Torelli, Peter Horton and I have put together a website that has images that may be used for data processing and phasing. These datasets have common pathologies that can be used by crystallographers or educators to learn how to either avoid or work around these pathologies. What is particularly valuable is that the software developers were gracious enough to provide tutorials for how they thought data processing and refinement should work for these pathologies. This approach has received excellent feedback, but should be expanded to include small angle and small molecule data so that our larger community can be served as has the macromolecular community. If elected, I plan to work closely with members of the Communications Committee to make resources such as this readily available to better serve our entire constituency.

Allen Orville
Continuing Education

Biophysicist, Photon Sciences Directorate and Biosciences Dept, Brookhaven National Laboratory, (BNL) Upton, NY.

Education: BS, Biology (1983) and PhD, Biochemistry, Univ of Minnesota (1997), postdoc - Howard Hughes Medical Institute, Univ of Oregon (1997-2000).

Professional Activities: ACA member since 2003. Chair or Co-Chair: Structural Enzymology (ACA 2008 Knoxville); Structural Enzymology: Mechanistic session (ACA 2010 Chicago); Structural Enzymology I – Spectroscopy & Complementary Methods (ACA 2011 New Orleans); instructor and beamline scientist at "RapiData - Collection and Structure Solving at the NSLS: A Practical Course in Macromolecular X-Ray Diffraction Measurement" (2007 – 2013); organized, "Removing the mystery from mystery density: A workbench for correlated single-crystal spectroscopy and x-ray crystallography" at BNL (2011); Spokesperson for NSLS-II beamline "SM3: Single-Crystal Spectroscopy & Macromolecular Crystallography at a Three Pole Wiggler Beamline," (2010 – present); State of Georgia voting board member for the South East Regional Collaborative Access Team (SER-CAT), Argonne National Laboratory, Argonne, IL (2004 - 2006).

Research Interests: Structural basis of enzyme reaction mechanisms; macromolecular crystallography, especially at synchrotron and free electron laser x-ray sources; spectroscopy; systems biology at the microbe-plant interface, especially symbiotic N_2-fixation by rhizobia within root nodules of leguminous plants; serial

micro-crystallography with acoustic droplet ejection methods; oxygen activation and enzyme reactivity in solution, and in low temperature crystals; methods for poising and promoting enzyme reactions in crystals; single-crystal spectroscopy correlated with x-ray crystallography from the same sample.

Statement: Which is better, 16 or 84,000? If it were lashes with a wet noodle, then we are likely to answer "16"; whereas, if it were diffracted x-ray photons, then we are most likely to reply "84,000 please!" And yet, with every 10,000 x-ray photons that pass through our samples we crave the 16 x-ray photons that give rise to a diffraction pattern (hopefully to high resolution), and try to ignore the 84,000 electrons liberated in our samples via the photoelectric effect. Indeed, many of us build careers, in part, on the atomic structures revealed by those rare, diffracted x-rays. That other number is significantly bigger and it can be a problem; but, it is also an opportunity.

I think that a hallmark of education (or enlightenment) is the ability to learn and grow gracefully from difficult situations. My life to date has taught me that "teachable moments" are not relegated to the early developmental deadlines I negotiated in South Dakota or the Big Ten environment at the University of Minnesota. I am grateful for all my past experiences because they each prepared me in unique and complex ways. Formal training is by no means the end of anyone's education. Rather, our training and background provide us with the confidence, as well as the necessary courage, to stand on the precipice at the frontiers of our fields. This gets more and more terrifying during times of increasing competition for declining resources; a current and pressing challenge before us.

So, what is the role of continuing education within the ACA? I think the answer is multidimensional; much like the research strategy I promote now at beamline X26-C at the National Synchrotron Light Source and plan to continue at beamline SM3 at the NSLS-II. My philosophy is to extract as much information as possible from every sample and thus we collect x-ray diffraction, electronic absorption and Raman vibration spectroscopic data from almost every crystal. This takes more education and training than typically anticipated by nearly every scientist that uses our facility. This challenges us to make the facility more accessible. But, it also yields expanded capabilities and transforms the thinking of the research groups that take advantage of the beamline. This strategy is not difficult, nor is it common. Similarly, we have to be creative and expansive in our scientific education and training, now more than ever. We need to listen to the needs, be aware of the possibilities and offer relevant educational opportunities to an ACA membership that spans decades of experiences.

I talked with numerous colleagues at meetings last summer and wondered aloud how was it possible that politicians and special interest groups had succeeded in exploiting the scientific method and language to their benefit. I was astounded to hear a congressional leader label a scientific result as "opinion." A major political party member even suggested eliminating the largest scientific funding agency in the US government as a cost saving measure. Therefore, I suggest that continuing education must also include the general public and impact our political system too. After all, tax payers pay the salaries of most of us. Don't they deserve to know what it is that they bought? An educated public will not likely tolerate political folly indefinitely.

I think we should each take every opportunity we are given to describe what we do in language that the public will understand. We as crystallographers are lucky because our results are often beautiful and readily accessible by the public. For example, I prepared an artistic image and presented it as a framed gift to my Bikram Hot Yoga instructor. It was of the protein dermcidin (an antimicrobial peptide secreted in human sweat, PDB code 2ymk) embedded in a simulation of *E. coli* lipid bilayer as recently proposed by Song et al (1). My wife calls these types of images "cosmic spaghetti," but she and my Yoga instructor both resonated immediately to the image and the concepts it conveyed. Without opportunities to be educated, humanity will not move forward. Teachable moments are probably more prevalent than many of us realize.

1. Song, C., Weichbrodt, C., Salnikov, E. S., Dynowski, M., Forsberg, B. O., Bechinger, B., Steinem, C., de Groot, B. L., Zachariae, U., and Zeth, K. (2013) Crystal structure and functional mechanism of a human antimicrobial membrane channel, *Proc Natl Acad Sci* **110**, 4586-4591. (3607029)

Peter Müller
Data, Standards & Computing

Director X-Ray Diffraction Facility, Massachusetts Institute of Technology, Cambridge, MA.

Education: Vordiplom (BA equivalent) Chemistry, Univ of Kaiserslautern, Germany (1994); PhD Inorganic Chemistry/ Crystallography with George Sheldrick, Univ of Göttingen, Germany (2001); postdoctoral work in Molecular Biology with David Eisenberg, University of California Los Angeles (2001-2004).

Professional Activities: Regular reviewer for *J. Appl. Cryst.*, *Acta Cryst.*, *J. Am. Chem. Soc.*, *Organometallics*, *J. Phys. Chem.*, *Crystal Growth & Design* and other journals; Co-Editor of *Acta Cryst. Section C* (since 2008); Chair: ACA GIG (2007, 2010 and 2014); Service SIG (2008 and 2014); Secretary: Service, Small Molecule and General Interest SIGs (several times since 2003); Session Chair and organizer of ACA meeting sessions on Teaching Advanced Crystallography (2004), Data Collection Strategies (2005), Whole Molecule Disorder (2006), Teaching Gadgets (2007), General Interest (2008, 2011), Cool Structures (2009), Blast from the Past (2010), Reviewer Practices (2013); Local Chair of the 2012 ACA Meeting in Boston; Organizer of the SHELX workshop (ACA 2007); Unofficial ACA Photographer (Duax style) and volunteer staff photographer of ACA *Reflexions* (since 2008 if I remember right); Member: ACA Standing Committee on Continuing Education (2008-2011; Chair 2011); IUCr Commissions on Chemical Crystallography and Teaching (currently); IUCr/Oxford Univ Press Advisory Committee (currently). Faculty - ACA Small Molecule Summer

Schools (2006 - 2013); Organizer of an annual crystallographic symposium at MIT (2005 - 2014); Teacher at Structure Refinement and Data Reduction workshops in Göttingen, Germany (1997 and 2003), College Station, TX (2000), Madison, WI (2003 and 2005), Beijing (2009), Nanjing (2011), and Syracuse (2012). Main author and editor of "Crystal Structure Refinement" (IUCr Texts on Crystallography number 8, Oxford University Press 2006).

Research Interests: Data Collection Strategies, Refinement Methods, Whole Molecule Disorder.

Statement: I have been an active ACA member for some time now and have held various offices over the years. Serving the crystallographic community through the ACA SIGs and committees is important to me and when the Nominating Committee asked whether I'd run for the Standing Committee on Data, Standards, and Computing I agreed.

As a Co-Editor of *Acta Cryst*. and as reviewer for many non-crystallographic journals, I have been involved in discussions about which data should be submitted to whom at what time and in which format. It would be interesting for me to experience similar discussions from a different perspective, that is as a member of the Data, Standards, and Computing Committee.

Several years ago, I was part of a group of crystallographers working on a white paper on data safety and archiving to ensure availability of current diffraction data for future generations. Among other things, we were discussing a CIF-like open format for raw diffraction data where the header of every image would explain exactly how the data should be interpreted. That would allow anybody to write their own integration even a few hundred years from now when our beautiful methods may only be of historical interest and the current proprietary software may no longer run on the then available computer systems. Having all pertinent information properly included in the raw data files could make it possible to understand what "a frame" is even if diffractometers are largely unknown to the person discovering such files. This is an idea comparable to Adobe's digital negative (DNG) format for images from digital photo-cameras (which are not so different from modern area detectors). According to Adobe, DNG is "a publicly available archival format for the raw files generated by digital cameras. By addressing the lack of an open standard for the raw files created by individual camera models, DNG helps ensure that photographers will be able to access their files in the future." As a member of the Data, Standards, and Computing Committee I will push for a renewed effort towards preservation of crystallographic data for future generations.

Victor G. Young, Jr.

Data, Standards and Computing

Senior Research Associate, LeClaire-Dow Instrumentation Facility, University of Minnesota.

Education: PhD, Inorganic Chemistry, (1985) and Postdoc (1985 – 1988), Arizona State University.

Professional Activities: Manager, X-Ray Crystallographic Lab, LeClaire-Dow Instrumentation Facility, Univ of Minnesota (1995 – present); Crystallographer, Chem Dept, Iowa State (1990 – 1995), Consultant, WX-5 group, LANL (1988 – 1990); ACA member since 1988; USNCCr: Member (2006 – 2011); US representative to IUCr Congress (XXII in Osaka, Japan and XXIII in Madrid, Spain); Local Co-Chair for the ACA meeting in St. Paul, MN (2000); Chair: Service SIG (1999); Member: Apparatus & Standards Standing Committee (2000 – 2002: *renamed the Data, Standards & Computing Standing Committee in 2001*); ACA Nominating Committee (2003-2004), ACA Poster Prize Chairman (2009 – 2010); Faculty, ACA Summer Course in Crystallography (2012 – 2013).

Research Interests: I have a keen interest in using all crystallographic methods at my disposal to assist in the structural elucidation of materials, single crystal or otherwise. My primary crystallographic method is single crystal diffraction using the instrumentation in our state-of-the-art laboratory. These tools provide a great deal of publishable data, but quite often serve to inspire us to pursue complementary methods at our national laboratories using synchrotron radiation or neutron diffraction. Twinning continues to be of research interest since these problem structures appear more frequently as we employ more powerful sources both at home and at synchrotrons. More recently we have employed MAD single crystal diffraction experiments to distinguish the fractional occupancies of first-row transition metals in several heterobimetallic model systems.

Statement: I am honored to be nominated for the Data, Standards & Computing Standing Committee for a *second* time. Many things have changed since I served over a decade ago. My fellow crystallographers are using brighter sources in their home laboratories as well as traveling to the national labs. Area detectors have replaced nearly every serial diffractometer. Computers are fast and inexpensive. Trusted computer code is being ported onto new architectures. All of these activities are of interest to the Data, Standards & Computing Standing Committee. In preparation to write this statement, I read the annual reports of the committee's activities for the three previous years. The committee is actively involved with numerous issues regarding our crystallographic databases, collaborating with IUCr commissions having a similar mission, and organizing topical sessions at our annual ACA meetings, amongst many other activities.

All of the members of this committee bring some crystallographic issues of interest to pursue while in office. My particular interest is to see definitions for twinning adopted for the CIF dictionary. This has been no small task. I have collaborated with a number of crystallographers worldwide to help in this endeavor. At this time a set of definitions is being prepared for submission to COMCIFS. It is my hope the actions of this committee would assist this project. I look forward to working with the committee in all their activities if elected.

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Stanford PULSE Institute at SLAC
Emmanuel Smith
University of South Florida
Hilary Stevenson
University of Pittsburgh
Qi Sun
Vanderbilt University
Dazhi Tan
Columbia University
Sonia Thangavelu
The George Washington University
Michael Thompson
University of California Los Angeles
Jennifer Wierman
Cornell University
Qiang Zhu
SUNY - Stony Brook
Christina Zimanyi
Massachusetts Institute of Technology

2013 Etter Early Career Award

Eric Ortlund
Emory University

Etter Student Lecturers

Bio-Mac SIG
Adam Roberts
UNC - Chapel Hill
General Interest SIG
Colleen Lopez
California State Univ San Marcos
Powder Diffraction SIG
Xiaohao Yang
Columbia University
Small Angle Scattering SIG
Donghyuk Shin
Sungkyunkwan Univ., Korea
Materials SIG
Mirijam Zobel
University Erlangen, Germany
Synchrotron SIG
Jennifer Wierman
Cornell University
Neutron SIG
Rebecca Beadling
Indiana University of Pennsylvania
Small Molecule SIG
Andre Cairns
University of Oxford, UK
Service SIG
Christopher Rackauckas
Oberlin
Young Scientists SIG
Karim Sutton
University of Oxford, UK

IUCr Interregional Awards

Sebastian Suarez – Argentina
Julian Puszkiel – Argentina
Jaime Rincon Cardona – Argentina
Kaavya Krishna Kumar – Australia
Tatyana Kardash – Russia
Andrew Cairns - UK

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ACA 2013 July 20-24, 2013

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

Awards:

Trueblood	Tom Terwilliger
Fankuchen	Richard Dickerson
Bau Neutron	Tom Koetzle
Etter Early Career	Eric Ortlund

Program Chairs:

Jeanette Krause

Allen Oliver

Poster Chair

Ilia Guzei

Session Photos

Victor Young

Photos: Hawaii Tourism Authority
Tor Johnson

JULY 2013

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

AUGUST 2013

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

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

11-16 **17th Int'l Conf. on Crystal Growth and Epitaxy (ICCGE-17),** Warsaw, Poland: *science24.copm/event/iccge17/.*

SEPTEMBER 2013

1-6 **12th Int'l Conf. Quasicrystals,** Krakow, Poland: *www.icq12.fis.agh.edu.pl/.*

18-20 **71st Annual Pittsburgh Diffraction Conference**, HWI Medical Res. Inst., Buffalo, NY. ***Organizers: Eddie Snell and Joe Luft***: *pdiffraction@hwi.buffalo.edu*.

OCTOBER 2013

14-29 **X-ray Methods in Structural Biology,** Cold Spring Harbor, NY: *meetings.cshl.edu/courses/2013/c-crys13.shtml.*

DECEMBER 2013

7-10 **AsCA 2013,** Hong Kong: *asca2013.org.*

MAY 2014

24-28 **ACA2014, Albquerque, NM.** Convention center and Hyatt Regency. ***Local Chairs: Zoe Fisher and Kate Page. Program Chairs: Christine Beavers and Petrus Zwart.***

AUGUST 2014

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

SEPTEMBER 2014

14-20 **15th Int'l Conf on the Crystallization of Biological Macromolecules,** Hamburg, Germany: *www.iccbm15.org.*

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

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

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