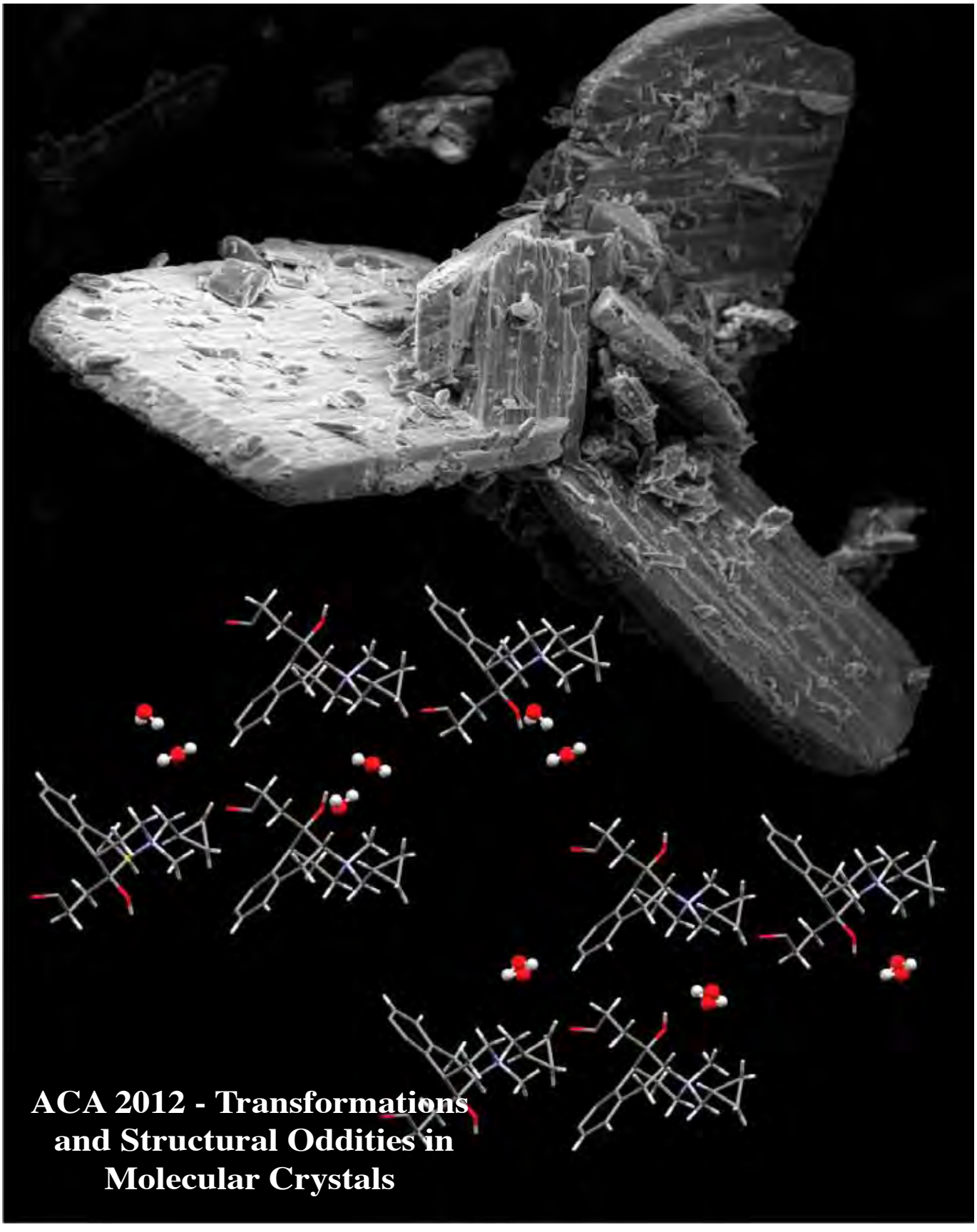
ACA RefleXions

American Crystallographic Association

Number 4

Winter 2011



# ACA 2012 - Transformations and Structural Oddities in Molecular Crystals

BRUKER

# Intense Impact...


## The New D8 VENTURE for Structural Biology

Bring the synchrotron to your home lab with a compact system that has proven high performance, easy operation, quick alignment, and the brightest and most stable microfocus rotating anode. These eye-popping features make the D8 VENTURE the choice that delivers impact. In addition, the D8 VENTURE offers low maintenance, fantastic service support, and maximum uptime.

**Contact us for a personal system demonstration – seeing is believing!** **www.bruker.com/d8venture**

ACA RefleXions

American Crystallographic Association

www.AmerCrystalAssn.org

## *Table of Contents*



*On the cover- see page16*

*ACA 2012 Award Winners*

*Election Results*

Contributions to ***ACA RefleXions*** may be sent to either of the Editors:

Connie (Chidester) Rajnak
4210 Old Field Trail
Kalamazoo, MI 49008
tel. 269-342-1600
conniechidester@earthlink.net

Judith L. Flippen-Anderson
3521 Launcelot Way
Annandale, VA 22003
tel. 703-346-2441
acareflexions@gmail.com

Photographer: Peter Müller
Historian: Virginia Pett
Puzzle Corner: Frank Fronczek
Book Reviews: Joe Ferrara

Please address questions pertaining to advertisements, membership inquiries, or use of the ACA mailing list to:

Marcia J. Colquhoun, Director of Administrative Services
American Crystallographic Association
P.O. Box 96, Ellicott Station
Buffalo, NY 14205
tel: 716-898-8692; fax: 716-898-8695
marcia@hwi.buffalo.edu

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

***ACA RefleXions*** (ISSN 1058-9945) Number 4 2011. Published four times per year in the spring, summer, fall and winter for the membership of the American Crystallographic Association, P.O. Box 96, Ellicott Station, Buffalo, NY 14205-0096. Membership in the ACA includes a non-deductible charge of $1.75 from membership dues to be applied to a subscription to the *ACA RefleXions*. Periodicals postage paid at Buffalo, New York. POSTMASTER: Send address changes to ACA, P.O.Box 96, Ellicott Station, Buffalo, NY, 14205-0096.

It hardly seems possible, but the year has just sped by and this is my final column for *RefleXions*. It's been a very rewarding year for me, highlighted by a number of important milestones including our extremely successful meeting in New Orleans and the selection of the inaugural class of ACA Fellows. I have heard back from a number of our Fellows, and they have emphasized how much they appreciate receiving this honor from their ACA colleagues. At its fall meeting the Council finalized procedures for selecting future ACA Fellows (see next column), and we look forward to welcoming a new class of Fellows each year beginning in 2012.

Plans are progressing for our 2012 meeting, which will be held in Boston July 28 – August 1, 2012. Program Chairs Bruce Foxman and Bruce Noll are well along in their endeavors, they are planning an outstanding scientific program that will kick off with a full schedule of workshops before the opening reception on Saturday, July 28. Local chair Peter Müller is hard at work behind the scenes to make sure that everything runs like clockwork . The ACA's major award winners for 2012 – John Spence (Buerger), Emmanuel Skordalakes (Etter), Ron Hamlin (Supper), and Paul Fenter (Warren), will be present in Boston to deliver their award lectures. *Please note that Boston will be our first meeting using the newly adopted Sunday – Wednesday format for the main scientific program.*

Breaking News: We will be going back to Hawaii for ACA 2013. As we did in 2006 we will be using the Sheraton Waikiki as the headquarters hotel and rooms for students and postdocs will be available at the Princess Kaiulani ***(www.sheraton-waikiki.com),*** The dates will be Saturday July 20 – Wednesday July 24, 2013. Mark your calendars now!

ACA Secretary Carrie Wilmot, *RefleXions* co-editor Judy Flippen Anderson, and I recently had the pleasure of attending the PDB40 Symposium, which was held at Cold Spring Harbor Laboratory from October 28 – 30 to commemorate the 40th anniversary of the Protein Data Bank. Many leading figures in structural biology attended the meeting and presented fascinating perspectives on the past, present, and future of the PDB. I extended hearty congratulations on behalf of the ACA and our members to the symposium organizers and to the entire Worldwide PDB team.

In closing I would like to thank the ACA's fabulous headquarters staff, Marcia Colquhoun, Crystal Towns, and Kristina Vitale for their tireless work throughout the year on our behalf. We also owe a great debt of gratitude to Bill Duax, S.N. Rao, and especially all the super volunteers (see page 1) who make *RefleXions* the premier publication that it has become.

Best wishes to you and to your families for a wonderful holiday season!

*Tom Koetzle*

## *Nomination Procedure for ACA Fellows*

1. A call for nominations for ACA Fellows will be published in the winter edition of *RefleXions* and on the ACA website. Nominations are solicited from any member (including retired members) of the ACA.

2. Nominations can be submitted at any time to the Buffalo office. The closing date for any given year is February 28th.

3. After February 28th, current Fellows will be polled for their evaluations of all nominations submitted since March 1st of the preceding year. The new class of Fellows will be appointed by Council based on the compiled results.

4. Self-nominations will not be accepted.

5. Nominations must include the following information about the nominee:

   a. Name, contact information (address, telephone number, email address), and professional affiliation.
   b. Nominees are expected to be members of ACA in good standing. Under exceptional circumstances Council may waive this requirement.
   c. Brief educational background.
   d. Professional history (positions, appointments, awards, honors).
   e. Membership in other scientific organizations.
   f. Service to the ACA and crystallography.

6. Nominations must include the following information about the sponsor:

   a. Name, contact information (address, telephone number, email address), and professional affiliation.
   b. Must be a current ACA member in good standing. The ACA office will confirm the sponsor's membership status.

7. In addition to that of the sponsor, two further letters of support must be included. The letters must clearly state how the nominee's research over a sustained period of time has had a significant impact on his/her field and detail how the nominee has contributed to the ACA.

***Announcement from the Editors:*** Our volunteer News & Awards Editor, Bomina Yu has resigned to take a new job. Consequently, Judy and Connie find themselves without a volunteer for this job. Anyone wishing to apply for this position should contact either Judy: ***acareflexions@gmail.com*** or Connie: ***conniechidester@earthlink.net.***

***Eratta***: on page 44 of the Fall issue, Brad Fulfer's name is misspelled twice, once in the figure caption and also in the text. It's Fulfer (with an F), not Fuller.

## News From Canada

How do you decide which meetings to attend? In Canada, as elsewhere, research funding is becoming more and more precious. Given the choices we have to make, travel is probably the first area that gets cut in difficult times, and what travel we do has to be cost-effective in enhancing our research and teaching.

The way I think about it, there are two main types of meetings, those that focus on methodology and techniques, and those that are focused on an area of science, whether it be biology, chemistry, materials, etc. While there is overlap between them, these types of meetings serve different purposes and constituencies. There is also the question of size. Many of us prefer intimate meetings of 100-200 people whereas others feel that larger meetings give more bang-for-the-buck, as there is more choice of scientific sessions and the opportunity to meet more colleagues. Like others, I like to mix it up and attend all types, as much as budget allows.

While a column in *RefleXions* is ceertainly preaching to the converted, I recommend that the ACA meeting be included on my colleagues' schedules on a regular basis. Those of us in the macromolecular field, and surely this is also true in other fields, are finding that more and more automation and pre-packaged laboratory practices and reagents, to say nothing of remote data collection and structure solution, has resulted in a growing generation of scientists "doing structures" with little or no appreciation of the technique. As we move further from our crystallographic community and focus more on "the Biology" (or "the Chemistry"), guided no doubt by grant review committees and institutional pressures, we lose not just the excitement and "Eureka moment" that comes with determining a brand new structure, but also the unusual level of cohesion and collegiality that has characterized the field of crystallography. There is certainly a persuasive argument that most structures can be done nowadays with the press of a button and with our sophisticated quality control software, most of these are "right". But it sure takes a lot of the fun out of it.

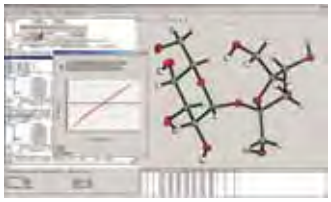
We in Canada do not have a national meeting devoted to diffraction techniques; the ACA is our home. Canadians have been represented on Council for many years, starting with ***I. David Brown*** in 1992, and we have our own Division of the ACA. Several Canadians have served as ACA President (***Louis Delbaere***, ***Penny Codding*** and ***Carol Huber***). Nevertheless, with the exception of the Toronto and Montreal meetings, attendance by Canadians has hovered between 30-50 (4-6% of attendees) since the early 1990's, despite a vastly increased crystallographic community.

Although a high quality scientific program is important, many of us get as much out of informal chats in the hallways, the exhibitor/poster area plus, of course, the bar. Science is a social activity; personal interactions are critical to disseminating our own results, learning about those of others, and maximizing our effectiveness by keeping current with the latest techniques and instruments. That's why I find ACA meetings well worth the time and money, even when both are in short supply. I hope to see you there!

Note: an update on Canadian politics since my last column in the summer 2011 *RefleXions*: the leader of the official opposition New Democratic Party, Jack Layton, unfortunately succumbed to cancer on August 22nd. The NDP made major gains in the election, particularly in Quebec, largely fuelled by Layton's personality and charisma. The NDP has few MPs with Parliamentary experience, and now both main opposition parties, the Liberals and NDP, have Interim Leaders. How this vacuum is filled will be a very interesting story to follow in the coming months.

*David Rose*

## The Future of CRYSTALS



The CRYSTALS program is widely used by chemical crystallographers involved with running analytical services, research and teaching. It has been under continuous development since the first FORTRAN versions were created by ***John Rollett*** and ***Bob Carruthers*** during the 1970's. A large number of people have contributed code or concepts for dealing with specific crystallographic problems, leading to a richness of procedures. A small number of people, in particular ***Paul Betteridge***, ***Lisa Pearce*** and ***Richard Cooper*** have made substantial changes to the infra-structure to ensure that the program remains suitable for modern users. As well as the monolithic code in CRYSTALS, the program also acts as a convenient interface to programs dealing with cifs and several diffractometer data files. It also links smoothly with checkCIF, PLATON, SIR92, SIR2011, Superflip, SHELXS, Mercury, Mogul, and MCE (an electron density visualiser). My own role has been to generally look after the code, to respond to users requests and comments and run an e-mail help desk. Following my retirement in September 2011, I hope to continue to be involved with CRYSTALS.

After a period working with Oxford Diffraction and carrying out research into small-molecule docking with macromolecules at InhibOx, ***Richard Cooper*** (***richard.cooper@chem.ox.ac.uk***) has returned to Oxford to be my successor as head of The Chemical Crystallography Laboratory. In addition to all his other responsibilities, he plans to continue to look after CRYSTALS, and when time permits re-develop and extend it. Existing CRYSTALS users can be confident that it will be maintained into the foreseeable future, and non-users looking for a single integrated work environment might like to try the program. Oxford University has made the installation kit available for commercial and non-commercial uses without cost from our website: w***ww.xtl.ox.ac.uk***. Contact Richard for more details.

*David Watkin*

***International School on Fundamental Crystallography followed by a one-day Workshop on Representation Theory of Space Groups (ISFC2010). Facultad de Química, Universidad de la República, Montevideo, Uruguay, November 29 to December 4, 2010***

ISFC2010 was co-organized by the MaThCryst Commission of the IUCr and the Crystallography, Solid State and Materials Laboratory of the Facultad de Química (Cryssmat-Lab/FQ), University of Uruguay. The School was sponsored by the University of Uruguay (Facultad de Química, CSIC and CINQUIFIMA), the IUCr, PEDECIBA and ANII (Uruguay), the ACA and the ICDD. Sixty five percent of the funds available were used to directly support students and young scientists.

***School organizers Leopoldo Suescun, Mois Aroyo and Massimo Nespolo.***

The purpose of the school was to introduce participants to crystallography and, therefore, focused mainly on basic mathematical aspects of crystallography. The participants were instructed in the derivation of all the information contained in the *International Tables for Crystallography Volume A* by ***Massimo Nespolo*** (Nancy University, France) and ***Mois Ilia Aroyo*** (University of the Basque Country, Spain); an introduction to crystallography in reciprocal space by ***Ernesto Estévez-Rams*** (Havana University, Cuba) and ***Eduardo Granado*** (UNICAMP, Brasil); and structure determination from single crystal x-ray diffraction data by ***Alberto Echeverría*** (Universidad Nacional de La Plata, Argentina). A session on the crystallographic tools included in the Bilbao Crystallography Server was presented by ***Mois Ilia Aroyo***. It was preceded by a one day preparatory session on matrix algebra and Fourier transform taught by ***Ricardo Faccio, Leopoldo Suescun*** (University of Uruguay), ***Ernesto Estévez-Rams*** and ***Mois Ilia Aroyo*** that was intended as a refresher of basic concepts for advanced participants and an introduction to new tools for undergraduate and masters students. The school was followed by a one-day workshop on representation theory of space groups, organized by Aroyo, that introduced this complex topic to advanced participants.

Five poster awards donated by the ACA (consisting of a complimentary student membership for 2011) were given to the best posters as judged by the school lecturers to (shown from top to bottom in the photos on the next page) ***Luciana Fernández Werner*** (University of Uruguay, Montevideo); ***Nicolás Ignacio Neuman*** (Universidad Nacional del Litoral, Santa Fe, Argentina); ***Rodrigo Correa*** (Universidade Federal de São Carlos, São Carlos, Brazil), ***Hugo Javier Serrano Posada*** (Instituto de Biotecnología, UNAM, Cuernavaca, Morelos, Mexico) and ***Lorraine Andrade Malaspina*** (Universidade Federal de Goiás, Goiania, Brazil). A special poster prize was awarded to ***Eduardo Bittar*** (Laboratorio Nacional de Luz Síncrotron, Campinas, Brazil).

A total of 50 participants, from Argentina, Brazil, Chile, Colombia, México and Uruguay, with backgrounds in structural biology, mathematics, chemistry, physics, materials science and mineralogy attended the week-long event that also included 30 poster presentations from all the mentioned countries. There was significant interaction among attendees as they shared intense 8 hour days of lectures, coffee, lunch and two social events where the typical "candombe" music was played and danced by local artists and participants and enjoyed by everyone.

The event has been deemed a success by the organizers, lecturers and participants. Undergraduate students in biology, chemistry and physics were introduced to symmetry and PhD students and post-docs acquired insight into the foundations





of crystallography. The lecturers praised the students will to solve all the exercises presented during the lectures and students appreciated the didactical ability and strength of the professors who lectured for hours without losing the attention of the participants.

The full results of the anonymous evaluation filled out by participants at the end of the course can be found at the ISFC2010 web site (***cryssmat.fq.edu.uy/ISFC2010***); the following excerpts have been extracted from participants' replies to the question **Please, give your general impression about the event.**

*"The ISFC-2010 exceeded greatly my expectations. The speakers were renowned specialists and were clear and made sure that the students were understanding their lecture. From my past participation on other schools on other physics subjects I can affirm that the ISFC-2010 was the best I have attended. I think that the success of this school is due to the fact it has been going on all over the world for many years and it should go on for many years to come."*

*"I think it was very good. Both from the academic and the organizational points of view."*

*"The event was perfect. The themes discussed on ISFC2010 are very important in crystallography. There were some hard concepts on these fundamental themes and the professors chosen for these are very professional. The city chosen for the event had many tourist attractions and the people were very enjoyable."*

Pictures of the event can be found at: ***picasaweb.google.com/isfc2010/Isfc2010#***

The next school (ISFC2012) is planned in Uberlandia, Brazil, in October 2012. For up-to-date information, ***www.crystallography.fr/mathcryst/***

*Leopoldo Suescun and Massimo Nespolo*

*Jenny Pickworth Glusker's work on the hexacarboxylic acid derivative of vitamin $B_{12}$ in Dorothy Hodgin's laboratory at Oxford revealed the structure of the corrin ring. At the Institute for Cancer Research in Philadelphia where she was first a member of Lindo Patterson's lab and later a principal investigator, she continued her interest in $B_{12}$ structures. Her research focus has included small-molecule compounds related to cancer, the structural aspects of the Krebs cycle and citrates, metal-ion coordination in proteins, the interaction of ligands with metal ions, and the enzymes aconitase and xylose isomerase. She is the recipient of many awards, notably the Fankuchen Award of the ACA and the Garvan Medal of the American Chemical Society. Her many professional contributions include serving as President of the ACA in 1979 and as editor of* Acta Crystallographica D *(macromolecules). One of Jenny's major interests is crystallography education; the 3rd edition of the popular textbook* Crystal Structure Analysis: A Primer *by Glusker & Trueblood appeared in 2010. She is the co-author or co-editor of a number of books on crystallography and the history of crystallography.*

As a child I lived in England in the industrial city of Birmingham. Both of my parents were medical doctors and encouraged me in my studies. My mother had wanted to study foreign languages, but she was in high school in the middle of World War I and there was, by then, a great shortage of young men available to go to medical school because so many of them were already at war. So, it was decided to send girls in high school with good grades to medical school. My mother became a medical student at Glasgow University in 1916. The university had been granting medical degrees to women since the 1890s, but was not used to such large numbers of women students in their medical school classes — about half of her graduating class in 1920 was female. She told me that the professors had to change the mnemonics so that they would be more suitable for such mixed classes. By the time that she graduated the war was over, and she went to Dublin, Ireland, and worked there during the social unrest in the early 1920s. Finally she accepted a medical post in Birmingham, England, where she met and, after a few years, married my father. From then on she stayed at home to raise her children — my sister who studied history (not a science, said my father), a brother who became a general practitioner and me. Although she was not allowed by the medical community to compete with other doctors in the area, my mother would substitute for local doctors if they had to be away from their practice for any reason. She was very frustrated that she could not continue with a career that she had put so much energy into. For this reason I decided that I would find a way to continue working, even if I had children. So, in my background, many of my parents' friends were women doctors and it was assumed that I would become one.

But I had other ideas. The school that I went to, a public school in the American sense of the word, was newly built, and had excellent scientific laboratories and a chemistry teacher (Yvonne Way) who inspired me. She had a PhD, but decided that she wanted to teach rather than do research, and it was a joy to go to her classes. I still write to her; she is in her 90s. My interest in chemistry had started when I found a book on incompatible medications among my mother's medical textbooks. It explained the chemical processes that resulted when two pills interact unfavorably for the patient. I then acquired a chemistry set that was stored under my bed and was able to mix chemicals and make wonderfully colored solutions and evil-smelling products. Thank goodness I survived that hobby. However, it made me sure that I wanted to be a chemist.

Chance then played a role in my life. Every day, before classes, the entire school of about 700 students (girls only, in those days high schools were generally not coeducational) met in a large hall. One day, in 1947, the principal announced that she had finally received her full PhD degree from Cambridge University. She explained that, until that date, women students who passed all the requirements for an academic degree did not receive the full recognition that men did. Now the university would finally accept them as members of the university with degrees, as for men. The principal wanted us to celebrate with her. I, however, was puzzled. Why should it matter whether you were a woman or a man if you did the same work? I looked up the situation for Oxford University and found they gave degrees and full university membership to women from 1920 on, so I announced I would try to go to Oxford. But my high school teachers all said that they sent science students to Cambridge and did not know too much about chemistry at Oxford. In addition my parents stepped in and said I should go to medical school (which I could do directly from high school). To deal

with these problems I made a pact with my father that if I could get into Oxford University that year I would study chemistry. If not I would go to medical school (and not complain).

Mindful of my aims, I set off for Oxford to take the entrance exams at Somerville College, the most academic of the women's colleges in Oxford University. It was necessary to take a practical chemistry examination in a laboratory, and the test was to identify an unknown material (in the days of hydrogen sulfide which invariably caused a splitting headache). This "unknown material" consisted of beautiful crystals, but, because I had spent many hours helping my father, an amateur photographer, in his dark room, I knew immediately what they were. They were crystals of sodium thiosulfate or "hypo," used in fixing solutions in photography. During this practical entrance examination every chemical I added to the "unknown material" caused sulfur to precipitate. What a mess! The person at Somerville who supervised me during the exam and then interviewed me for college was Dorothy Hodgkin, a crystallographer and future Nobel Prize winner. During my interview with her I explained about the pact with my father. Well, I was accepted by Oxford University. Many years later I asked Dorothy Hodgkin if I got accepted to Oxford because I correctly guessed the identity of the unknown material. She said that was not the case, but that she had noted that I knew how to deal with the sulfur that precipitated every time any new chemical was added.

The chemistry course at Oxford took three years, and if one wanted a classified degree, one did an additional year's research. I had a marvelous time. Dorothy Hodgkin was my tutor and we spent many hours in one-on-one weekly tutorials. She was an ideal role model with three children and a supportive husband who was at Balliol College. Her home was a haven for many visiting scientists and it was always interesting to visit her there. For my tutorials Dorothy would insist that I read and comment on all the original papers relevant to the subject she had chosen for my essay that week, so I spent much time in the Radcliffe Science Library. The laboratory experiences were good, but some of the buildings seemed antique compared with those that we had at high school. The design for the 100-year-old octagonal inorganic chemistry laboratory (later replaced) came from the Abbot's Kitchen in Glastonbury Abbey and it had a high ceiling with wooden rafters. For my research year I chose to work with Harold W. Thompson, an infrared spectroscopist who was interested in details of molecular structure. Under his tutelage I determined the interatomic distance in deuterium chloride, for comparison with that of hydrogen chloride being studied by another member of the laboratory. Then I worked on some more complicated molecules, methyl halides, but could only measure moments of inertia and not distances between atoms. However I also met my future husband, Donald Glusker, a Rhodes scholar from the University of California, Berkeley, who was working in the same lab on the spectroscopy of charge-transfer complexes.

High-resolution infrared spectroscopy was not, at that time, giving me the information that I wanted. So I started my graduate work in the laboratory of Dorothy Hodgkin, with the aim of learning how to determine molecular structure by x-ray diffraction. Dorothy was already well-known for her structural work on cholesterol while working with J. D. Bernal. She was the first to show that it is possible for protein crystals to give good diffraction patterns, and, particularly, she determined the chemical formula of penicillin by x-ray diffraction studies in the days when structure determination was very difficult. Dorothy's laboratory and workrooms were in the Oxford University Museum of Natural History that had been built with the help of the artist John Ruskin. We had desks in the very room in which, as commemorated by a plaque on the walls, Thomas Henry Huxley defended Darwin's recently published theory of evolution by natural selection against the Right Reverend Samuel Wilberforce, the then Bishop of Oxford. This took place at a meeting of the British Association in 1860. Dorothy's lab was a busy one and she shared it with Herbert ("Tiny") Powell who was famous for his work on clathrate structures. Jack Dunitz, who, in 1948, had determined the crystal structure of a calciferol derivative, at that time the most complex structure determined by x-ray crystallography, was there when I first started research. Jack was working in an elevated area in the lab that contained the microscopes for crystal viewing, but he was about to go to Caltech. David Sayre had recently left the lab, but everyone was excited about his squaring method for solving structures. Most of the other people in the lab were working on the structure of insulin or vitamin $B_{12}$. Work on this vitamin, the antipernicious anemia factor, and some of its derivatives, had been in progress in Dorothy's lab for a few years, particularly by John H. Robertson, June Broomhead (later Lindsey), Maureen Mackay and Clara Brink (later Shoemaker). John White at Princeton University was working independently on the same structure, and he collaborated with Dorothy on this throughout the years. Dorothy had decided at that time that no one should work on the much larger insulin molecule for a graduate degree because there was no guarantee that good results could be obtained for it at that time.

***Jenny in her laboratory at ICR about 1980. The DNA model was built by Ann Geale Diamond (Bob Diamond's wife). Ann grew up in the next street to Jenny in England and they went through the same schools and college. After the model arrived, Jenny learned that Ann had made model when she worked for a model-building company in Cambridge, England.***

Shortly after I had started graduate work some deep red crystals arrived in the lab from Cambridge University. They were of a degradation product of vitamin $B_{12}$ for which the

5:6-benzimidazole, D-ribofuranoside, 1-amino-2-propanol, phosphate and cyanide groups of the vitamin had been removed and the amide groups had been converted to carboxylic acid groups. The central part of the molecule, containing a cobalt atom, was still present, and that was the part of the chemical formula that was unknown and that we needed to find. Jack Cannon, an Australian, had been trying for some time to crystallize this degradation product that he had made, and finally, in despair, threw into its solution every liquid organic material he had access to, and went to Europe for a holiday. When he came back there were beautiful crystals, never grown again. So I started to work on them. The molecule was large and spectroscopic studies had shown that, like the vitamin itself, its degradation product contained a ring structure similar to (but not the same as) that found in porphyrins. Both the vitamin and Cannon's degradation product contained cobalt atoms which were useful as heavy atoms. I collected three-dimensional x-ray diffraction data on the $B_{12}$ degradation product (referred to as the hexacarboxylic acid) with a Weissenberg camera and estimated intensities by eye. Dorothy thought that anyone new working on the problem (that was me) should not be given information on what had been guessed so far from crystallographic studies on the vitamin itself. Unlike many x-ray crystallographers, she liked to work in three (rather than two) dimensions. This greatly increased the number of diffraction data to be measured and the time that had to be spent, particularly in calculating electron-density maps. But the results were much clearer.

The computational analysis of the hexacarboxylic acid was started with Patterson projections, and, to the surprise of everyone, they showed the position of the cobalt atom (saving us from the need for a three-dimensional Patterson map and thereby much computing time). One great asset of these crystals, unlike the situation for the complete vitamin crystals, was that the heavy metal, cobalt, did not lie in the unit cell near zero for two of the atomic coordinates (space group $P2_12_12_1$). This helped reduce some ambiguities in heavy-atom electron-density maps. The first map that I calculated and drew, phased only on the cobalt position just found, took six weeks (day and night) to produce (compared with seconds nowadays). The calculations were done in a room in the basement of a building at the corner of South Parks Road in Oxford on a Hollerith adding machine (used for population censuses). This calculator could only add, and we had to fool it to make it subtract numbers. The calculations were essentially those previously done with Beevers-Lipson strips. The IBM cards that were used lay in filled boxes throughout this room; they were painted different colors to show if they represented sine or cosine functions, even or odd, but they swelled when the weather became hot and humid and could not then be used. Often a policeman, bored with his beat, would escort me home in the middle of the night after a long computing session. From this cobalt-phased map John Robertson and I, late one night, found a ring structure around the cobalt. It is now called a corrin ring and consisted, like a porphyrin, of four five-membered heterocyclic rings, but had only three bridging atoms; two of the rings were directly connected.

I obtained my D. Phil. degree with J. Monteath Robertson as the external examiner, and then went to Caltech in Pasadena to work in the laboratory of Robert Corey. There, with Dick Marsh as a mentor, I studied simple peptides for a year as a postdoc. Linus Pauling kept an eye on all of us and greatly increased our interests in protein structure.

Don and I, now married, then looked for two chemistry jobs in one city. There were many companies with anti-nepotism rules, and many thought women with doctorates in chemistry should work in libraries, and then not at all if they had children. I had written to Dorothy Hodgkin for a letter of recommendation. She wrote back a letter which begins "You silly girl," telling me to go and work with Lindo Patterson (of the Patterson function) who was at the Institute for Cancer Research (ICR) in Philadelphia. That is how I came to the ICR laboratory in Philadelphia where I have worked ever since.

I had again come to a wonderful lab. Structure determination in Lindo Patterson's laboratory was then focused on molecules, such as citrates, in the biochemical Krebs cycle. Our crystallographic studies that have been carried out through the years after Lindo died in 1966 continued his studies of substrates and inhibitors of the Krebs cycle enzyme aconitase, which binds ferrous iron and interconverts citrate, isocitrate and *cis*-aconitate. Other work concentrated on the conformations and absolute configurations of biochemical ligands and how they

bound metal ions. Our studies of citrates and their derivatives led to a proposal for the three-dimensional mechanism of action of aconitase (the "ferrous-wheel mechanism"). It involved all the stereochemistries (including those of cation binding) and absolute configurations of the structures that we had determined.

Some of the compounds involved in cancer, both chemical carcinogens and antitumor agents, captured our attention. A major class of compounds that we studied were the "ICR compounds." These are acridine derivatives some of which showed antitumor and/or mutagenic activity. ICR compounds were presumed to interact with DNA, intercalating, as does acridine, between the bases of DNA; the side chains of these agents could then provide further action, such as alkylation of DNA. We determined the conformations and extents of overlap of their ring systems in packing in the crystalline state for several of these compounds.

We also tackled chemical carcinogens, starting with polycyclic aromatic hydrocarbons (PAHs) such as benzo[*a*]pyrene and 7,12-dimethylbenz[*a*]anthracene (DMBA). Such carcinogenic PAHs are oxidized in the body and the active agent is an alkylating agent such as a diol epoxide. We wanted to see if we could contribute to an understanding of their reactions in the body. Several PAHs become more carcinogenic when they are methylated at certain positions in the chemical formula. Such methylation may make it impossible, for steric reasons, for the substituted PAH molecule to remain totally planar. We wondered whether the twisting that results from this methylation enhances their possibility of interaction in the helical structure of DNA and what the effect was on the charge distribution in the molecule, that is, the ability of a metabolite to act as an alkylating agent, which is believed to be its function in cancer. Crystal structures of several metabolic products of carcinogenic PAHs that we determined included a diol epoxide of 5-methylchrysene, a presumed activated metabolite of a PAH more carcinogenic than chrysene itself. A detailed electron-density study of DMBA with Cheryl Klein and Ed Stevens resulted from high-resolution x-ray data collection and multipole refinement of the structure. Assuming that the action of a carcinogenic PAH involves interaction of a PAH metabolite (presumably formed by an interaction with cytochrome P-450), we synthesized and studied the structures of some adducts of PAHs with nucleoside portions of DNA. We measured the extent to which the PAH

*Jenny in her laboratory at ICR in 2011*

ring system lay between the bases of the nucleoside.

This led to a general interest in intermolecular interactions since structural studies reveal not only what a molecule looks like, but also how it interacts with other molecules (generally in a crystal of the same kind). Our investigations of these were greatly helped when Peter Murray-Rust came to our lab on a sabbatical. We investigated the three-dimensional geometry of the manner by which oxygen and nitrogen atoms in molecules bind to atoms in other molecules. We represented the results of our analyses in probability plots (looking like electron-density maps). Such analyses required the use of crystallographic databases, such as the Cambridge Crystallographic Data Base in England and the Protein Data Bank in the USA. We then examined, in a similar manner, several other types of intermolecular interactions, including the locations of metal ions around carboxylate ions and near heterocyclic ring systems. Each relevant published crystal structure was examined in detail to ensure that we knew the coordination number of the metal ion and its geometry; results of such investigations were provided to the appropriate database staff. Results were then used in theoretical density functional calculations in order to obtain the energies of various states. Of particular interest to date were the surroundings of divalent Mg, Mn, Ca, Zn, and Pb (which has an interesting lone pair of electrons), and trivalent aluminum. We were able to show how different $Zn^{2+}$ and $Mg^{2+}$ are when they bind ligands such as water. The binding capacities of metal ions in various ionization states and coordination numbers were represented in triangular plots with oxygen, nitrogen and sulfur at the three corners of the triangle. They showed where the metal ion lay with respect to these three most likely binding atoms in proteins. These plots serve as useful signatures of each metal ion in each of its possible valence states. For example, $Mg^{2+}$ binds the oxygen atoms of six water molecules in an octahedral arrangement, whereas $Zn^{2+}$ can have a coordination number of 4, 5 or 6 and will bind nitrogen or sulphur as well as oxygen. Theoretical studies showed that divalent and trivalent cations will bind water molecules with their hydrogen atoms pointing away from the positive charge of the metal ion. Monovalent cations do not have the full extent of this power, while quadrivalent cations may tend to initiate a chemical reaction between water and the metal ion. This suggests why so many enzymes utilize divalent metal ions to bind their substrates and, often, to aid in the catalytic mechanism.

*Jenny and Penny Codding - ACA 2003*

The enzyme structure that we have been studying through the years is D-xylose isomerase which converts D-xylose to D-xylulose and D-glucose to D-fructose. It is used industrially for the conversion of glucose to fructose to obtain high-fructose corn syrup for soft drinks and so is also referred to as "glucose isomerase." The mechanism of action of D-xylose isomerase involves binding of the sugar substrate, opening of the sugar ring system, isomerization of the sugar and possibly cyclization, and then ejection of the sugar from the active site. Time-of-flight neutron diffraction studies of this enzyme (in collaboration with Gerry Bunick and Paul Langan at Los Alamos National Laboratory) showed the ionization states of the various side chains. In one structure a deprotonated water (that is, a hydroxyl group) is located near the site of sugar isomerization, suggesting how a hydrogen atom might be transferred from one carbon of the substrate to its neighbor. By varying the metal ions and ligand it was found to be possible to view various stages of the catalytic mechanism. So, if by chance one can obtain large enough crystals, the combination of neutron and high-resolution x-ray studies will contribute greatly to the elucidation of an enzyme mechanism.

*The Glusker group at ICR in 1990: Dave Zacharias, Trixie Wagner, Carol Afsher, Liat Shimoni Livny, Jenny, Amy Katz, Bud Carrell, Chuck Bock and Eileen Pytko.*

I have greatly enjoyed my career as a crystallographer and a member of the ACA and thank all of you for the honors and tasks that have been bestowed on me through the years. I also thank the many people in my laboratory at Fox Chase, Philadelphia, who have helped make all of this possible. I have been interested in the teaching of crystallography and served as Chairman of the Teaching Commission of IUCr for several years and organized schools in Egypt, Thailand, the Chinese University of Hong Kong, Tianjin (China), Madras (India) and recently spoke at a crystallographic meeting in Turkey. Ken Trueblood and I wrote a text on x-ray diffraction of crystals and it was expanded in a later text with Miriam Rossi and Mitch Lewis. Finally, I still teach in the ACA Summer School for Small Molecules run, through summer 2011, by Charles Lake and Bryan Craven.

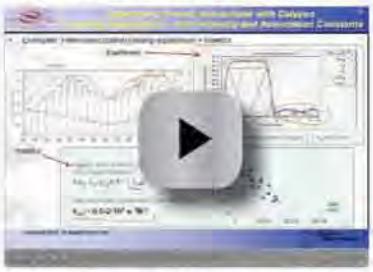
*Jenny Glusker*


# For characterizing protein-protein interactions, only the Calypso™ does it all.

Calypso. Label-free, immobilization-free macromolecular interactions.

No other biophysical method for quantifying macromolecular interactions provides as broad a range of analyses as Wyatt's Calypso. Using Composition-Gradient Multi-Angle Light Scattering (CG-MALS), Calypso gives you label-free, in-solution characterization of equilibrium and kinetic properties, hetero- and homo-association, binding affinity from picomolars to millimolars, stoichiometries of associating complexes, aggregation and self-assembly, and also measures non-specific interactions. So whether you're conducting formulation studies, developing drugs, or performing fundamental biomolecular research, the tools you need can be found in one handy place: Wyatt.com/Calypso.

**WATCH THE CALYPSO WEBINAR NOW**



Learn about CG-MALS theory and applications at: Wyatt.com/Calypso

Wyatt Technology CORPORATION

## 2011 Kyoto Prize to John Cahn

***John Cahn***, an emeritus senior fellow and materials scientist at the US Commerce Department's National Institute of Standards and Technology (NIST), was selected to receive the prestigious ***Kyoto Prize in Advanced Technology***. Cahn's numerous contributions to materials science include developing a fundamental theory that describes the behavior of mixtures of different materials and how they tend to separate at the microscale. This theory established an entire branch of materials research and is particularly important to the rational design of new alloys. Awarded annually since 1985 by the nonprofit Inamori Foundation, the ***Kyoto Prize*** is Japan's highest private award for global achievement, and honors significant contributions to the betterment of society. A diploma, the Kyoto Prize medal and a cash gift were awarded during a week of ceremonies that began Nov. 9, 2011, in Kyoto, Japan.

Practically all metals in use today are alloys; mixtures of two or more pure metals that, combined, have properties superior to either alone. The world's first known alloy, bronze, (after which an entire historical era was named) is significantly harder than either the copper or tin that are melted together to form it. Alloys are not always uniform, homogeneous mixtures. At the microscopic scale in some alloys the different elements tend spontaneously to separate slightly in twisty, random clumps, a phenomenon called phase separation. Unlike crystallization, in which one component of a solution separates out to solidify at discrete starting points (think of making rock candy), this separation happens simultaneously throughout the mixture. The phase separation and related changes in microstructure play a key role in determining the physical engineering properties of the bulk composite alloy, -*e.g.* strength, toughness, ductility, magnetic strength and thermal conductance. However, before the work of Cahn and his collaborator John Hilliard, then at General Electric, there was no good mathematical description of how this separation occurred. Developing a new alloy to meet specific material requirements was a painfully long and expensive process of trial and error. The Cahn-Hilliard equation quantitatively describes how the components of a binary mixture that becomes unstable when cooled will separate through a process called spinodal decomposition. Cahn proceeded to elaborate the theory, showing how basic thermodynamic principles could be used to design alloys that, under spinodal decomposition, would form desired microstructures. The Cahn-Hilliard equation has been applied in a wide variety of cases including the description of how galaxies began forming out of the primal material of the Big Bang in the early stages of the universe.

Born in Cologne, Germany in 1928, John Werner Cahn received his doctorate in physical chemistry from UC Berkeley in 1953. He taught at U Chicago before joining General Electric in 1954. In 1964 he became a professor in the Dept of Materials Science, MIT. In 1977 he joined NIST, then called the National Bureau of Standards, where he served in various senior positions. He is now an emeritus senior fellow in NIST's Material Measurement Laboratory, as well as an affiliate professor at U Washington. Among many other honors, he received the Materials Research Society Von Hippel Award in 1985, the Japan Inst. of Metals Gold Medal in 1994, the US National Medal of Science in1998 and the Franklin Institute's Bower Award in 2002 and is a member of the American Academy of Arts & Sciences and the National Academy of Sciences.

## 2011 Nobel Prize in Chemistry to Danny Shechtman

***Daniel Shechtman*** is Philip Tobias Professor of Materials Science at Technion (Haifa, Israel), with a BSc (1966), MSc (1968) and PhD (1972), all from Technion. After receiving his doctorate, Shechtman was an NRC fellow at the Aerospace Res. Lab. at Wright Patterson AFB, Ohio, where he studied the microstructure and physical metallurgy of titanium aluminides. In 1975 he joined the Dept. of Materials Engineering at Technion. During 1981-l983 he was on sabbatical at Johns Hopkins where he studied rapidly solidified aluminum transition metal alloys in a joint venture with John Cahn at NIST. During this study he discovered the icosahedral phase which inaugurated the new field of quasiperiodic crystals. During 1992-1994, while on sabbatical at NIST, he studied the effect of the defect structure of CVD diamond on its growth and properties. The major thrusts in the field of quasiperiodic crystals are: 1) theoretical aspects of the quasi-periodic structure and 2) experimental evidence for understanding their structure and properties. Shectman's group studies the crystallography and properties of the icosahedral phase in several binary and ternary alloy systems. Among many other awards and honors he has also won the 1990 Rothschild Prize in Engineering, the 1993 Weizmann Science Award, and the 2000 Gregori Aminoff Prize of the Swedish Academy of Sciences.

*cont'd, next page*

The 1982 discovery at NBS of the icosahedral phase, the first structure in the field of quasiperiodic crystals, was a big surprise. The solid made by rapid solidification of an aluminum transition metal alloy had long range orientational order but no translational symmetry. Indeed, it had icosahedral point group symmetry, and it is a mathematical fact that periodicity and icosahedra don't mix. All crystallographers "knew" that icosahedral symmetry was impossible for a crystal, because they "knew" that crystals have periodic structures. Most also believed that only periodic structures produce sharp diffraction patterns, another unexamined assumption that Shechtman's alloys disproved. If crystals need not be periodic, what point symmetries can they have? In principle, any of the infinite set of point group symmetries listed as noncrystallographic in the International Tables -- those with a single rotation axis of order 5 or greater than 7, or icosahedral symmetry with six intersecting 5-fold axes. (Chemistry and physics constrain these possibilities, but it is not yet known just how.) And which aperiodic atomic patterns give sharp diffraction diagrams? In 1992 the IUCr *Ad Interim* Commission on Aperiodic Crystals turned the question around: they took the diffraction pattern to be the hallmark of crystallinity, and redefined a crystal to be "any solid having an essentially discrete diffraction pattern." That left it up to crystallographers and mathematicians to figure out which solids, real and theoretical, those might be. The answers are coming in: structures have been solved, and "long range aperiodic order" is a growing field of mathematics. ***Editor's note: the above section was revised by Marjorie Senechal.***

On the morning of 8th April 1982, while on sabbatical and working at the invitation of John Cahn at NBS (now NIST), he observed in the transmission electron microscope a diffraction pattern counter to the laws of nature. This diffraction pattern had 10-fold rotational symmetry (5-fold as it turned out later) indicating that the atoms in his crystal were packed in a pattern that could not be repeated. Such a pattern was considered just as impossible as creating a football using only six-cornered polygons, when a sphere needs both five- and six-cornered polygons. This discovery was controversial, and in the course of defending his findings, he was asked to leave his research group. However, with the support of Ilan Blech of the Technion, John Cahn and Denis Gratias of Vitry, France, the work was published (*Phys. Rev. Lett.* (1984) **53**, 1951-53). The ensuing battle eventually forced scientists to reconsider their conception of the very nature of matter. In quasiperiodic crystals, the atoms are ordered and follow mathematical rules, but never repeat themselves; there is no periodicity in quasiperiodic materials. Following Shechtman's discovery, scientists have produced other kinds of quasicrystals in the lab and discovered naturally occurring quasicrystals in mineral samples from a Russian river. A Swedish company has also found quasicrystals in a certain form of steel, where the crystals reinforce the material like armor. Scientists are currently experimenting with using quasicrystals in products from frying pans to diesel engines. ***Editor's note: see also www.nobelprize.org/nobel_prizes/chemistry/laureates/2011/***

***Editor's note: We are planning a historical article on quasicrystals which will be published in the spring RefleXions. Judy and Connie invite all who remember ACA meeting sessions on quasicrystals before 2002; the IUCr meeting in Perth in 1987; or indeed anything about the controversy between Linus Pauling and Danny Shechtman to send email to either of us: conniechidester@earthlink.net or acareflexions@gmail.com.***

## *ACA Early Career Award to Emmanuel Skordalakes*

***Emmanuel Skordalakes*** (Wistar Insitute Cancer Center) has been selected to receive the ***2012 Etter Early Career Award***. Telomerase is a specialized RNA-dependent DNA polymerase that extends the ends of chromosomes to promote genome stability. It is commonly over-expressed in human cancers and other age-associated disorders. A molecular understanding of telomerase function has been significantly hampered by the difficulty of determining its high-resolution structure. Skordalakes succeeded in determining the high-resolution crystal structure of the full-length protein component of telomerase (TERT) as well as its complex bound to an RNADNA hybrid. Together with associated biochemical experiments, these studies have provided significant and novel insights into telomerase function, regulation and telomere replication. These studies also provide the first molecular framework for the design of telomerase inhibitors for therapy of cancer and other age-associated disorders.

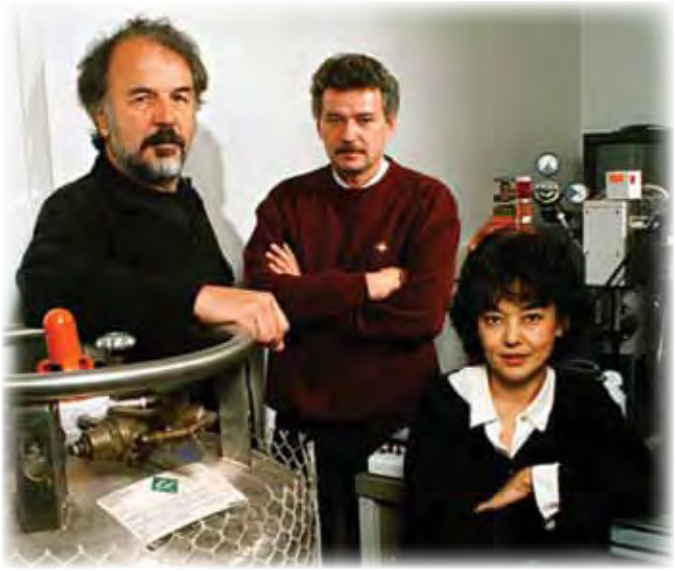
## *Marvin Hackert Elected to IUCr Executive Committee*

Election results from the ***IUCr General Assembly in Madrid***, August 2011:

**Gautam Desiraju** - **President of the IUCr** for the triennium 2011-2014.
**Claude Lecomte** - **Vice-President** for the same period.
**Luc Van Meervelt** - **General Secretary and Treasurer**.
**Marvin Hackert** - **Ordinary Member**

J. M. Guss and H. Dabkowska were also elected for six-year terms, and W. Depmeier for a three-year term. Sine Larsen (as Immediate Past President); E. Boldyreva and J. M. Perez-Mato (as Ordinary Members) continue on the Executive Committee.

## 2012 Gregori Aminoff Prize to Marat Yusupov and Gulnara Yusupova, and Harry Noller



*Harry Noller, Marat Yusupov and Gulnara Yusupova at UC Santa Cruz in 1999. Photo from the UCSC website.*

The Royal Swedish Academy of Sciences has awarded the ***2012 Gregori Aminoff Prize in Crystallography*** to ***Marat Yusupov*** and ***Gulnara Yusupova*** (Institut de Génétique et de Biologie Moléculaire et Cellulaire, France) and ***Harry F. Noller*** (UC Santa Cruz) for their crystallographic studies on ribosomes. They succeeded in mapping the ribosome structure at the atomic level, providing a basis for the development of targeted antibiotics. Ribosomes are long chains of RNA and proteins interlaced together in complicated foldings. They are fragile complexes of different size entities, which only assemble when a new protein has to be put together and they change shape constantly to ensure that only the correct amino acid is allowed to attach to the nascent protein chain.

Gulnara Yusupova and Marat Yusupov, aided by their collaborators in the former Soviet Union, managed to crystallize parts of ribosomes from bacteria in the late 1980s, and eventually started collaborating with the doyen of ribosome biochemistry, Harry Noller in the US. In 2001, two decades after their initial success, clean crystals of whole ribosomes were obtained. Mapping the structure of ribosomes from cells with a cell nucleus (e.g. human cells) took more time and milestone results were published in *Nature* and *Science* by Noller and by Yusupov and Yusupova, now in France. Finally, in 2010, the Yusupov couple managed to map the entire gigantic structure, an important first step towards understanding and producing targeted antibiotics.

The prize will be awarded at the Royal Swedish Academy of Sciences' annual meeting on 31st March 2012. (2011 Laureates Lia Addadi and Stephen Weiner were announced in the winter 2010 issue of *RefleXions*.)

## 2012 ASBMB Awards

The American Society for Biochemistry and Molecular Biology announced their 2012 awards, to be presented at their annual meeting that begins April 21st. The awardees will be giving lectures during the meeting.

***Judith Voet*** (prof. emeritus, Swarthmore College), and ACA member ***Donald Voet*** (assoc. professor at U Pennsylvania), won the ***ASBMB Award for Exemplary Contributions to Education.*** The Voets have made significant contributions to the teaching of biochemistry and molecular biology through their writing. Together, they have authored the comprehensive textbook *Biochemistry*, and *Fundamentals of Biochemistry* and co-edited the educsational journal *Biochemistry and Molecular Biology Education*.

***David Sabatini*** (assoc. professor at MIT and an HHMI investigator), won the ***Earl and Tressa Stadtman Scholar Award***, given to a scientist with 10 years or less of post-postdoctoral experience, including medical residency and fellowship. Sabatini is a leader in the ongoing elucidation of the mTOR pathway, a master regulator of growth. He is also a member of the Whitehead Institute for Biomedical Research.

***Barry Honig*** (Columbia University professor and HHMI investigator) won the ***DeLano Award for Computational Biosciences*** for his work in macromolecular interactions in biology. The award is given to a scientist for innovative and accessible development or application of computer technology to enhance research in the life sciences at the molecular level. Honig's software tools and their underlying conceptual basis are widely used by the general biological research community to analyze the role of electrostatics in macromolecular interactions.


Most scientists regarded the new streamlined peer-review process as "quite an improvement."

*Cartoon Coutesy of Nick D. Kim (www.lab-initio.com/indexl.html*

## 2011 ICDD Awards

During their annual meeting in March the ICDD announced that ***Brian O'Connor*** (Emeritus Professor of Applied Physics, Curtin University, Australia) was selected to be the ***ICDD 2011 Distinguished Fellow.*** This award is given to a member in recognition of long and meritorious service to the ICDD. Over the years, Brian has contributed his considerable expertise to the ICDD, all the while building a distinguished career. He has been an ICDD member since 1983, and has held several positions on the Board of Directors: consultant to the Board, Member-at-Large, and Vice-Chairman. He also served as Regional Co-chair for the Indian Ocean Rim where he worked with affiliated groups and associations in Australia, Malaysia and India. He established cooperative relationships between the ICDD and other groups; the AXAA (Australian X-ray Analysis Association), the Australian Academy of Science, and the IUCr. He has frequently participated in various ICDD workshops and exhibitions. Brian has more than forty years of experience in both single crystal and powder diffraction studies. He is known for his advancements in the expansion of modern x-ray and neutron diffraction analysis, including applications of Rietveld crystallographic metrology for material characterization and development of advanced ceramic materials from Western Australian minerals. Brian has authored more than 200 publications, some of which can be found in the ICDD publications *Advances in X-ray Analysis* and the *Powder Diffraction Journal*.

The ICDD also named two new Fellows at their annual meeting. The Fellow Award recognizes individuals who have devoted their time and talent beyond what is normally expected of a member. Recognized for their leadership in a noteworthy ICDD activity, the ***2011 ICDD Fellows*** are: ***Lawrence Bernstein*** (Terrametrix, CA), below left, and at right, ***Richard Bostwick*** (SPEX SamplePrep, NJ).

Larry Bernstein became involved with the ICDD in 1992 when he was named Consulting Editor, and in 1997 became an ICDD member. He has since been working with the Minerals Task Group which meets twice a year, on a volunteer basis, to review the mineral patterns that are available for publication in the PDF, focusing on standardization, classification, and accuracy of mineral data. Larry is also an active participant on the Minerals Subcommittee. Richard Bostwick is an active participant in the ICDD Education Programs, specifically the *Specimen Preparation Workshop* within the *X-ray Fluorescence Clinic* and the stand-alone, three-day *Specimen Preparation Workshop*. Richard has taught specimen preparation for more than 30 years, also lecturing on the subject. SPEX SamplePrep has supplied equipment such as grinders, mixers, mills, and presses to ICDD programs to provide a truly hands-on experience for attendees.

## 2011 Nobel Prize in Physics to Perlmutter, Riess & Schmidt

The Swedish Royal Academy announced that the ***2011 Nobel Prize in Phyics*** would be divided: one half to ***Saul Perlmutter*** (Supernova Cosmology Proj., LBNL and UC Berkeley), and the other half jointly to ***Brian P. Schmidt*** and ***Adam G. Riess*** (The High-z Supernova Search Team, Brian at Australian Natl Univ., and Adam at Johns Hopkins Univ. and Space Telescope Science Inst.). They were cited for the discovery of the accelerating expansion of the universe through observations of distant supernovae.

***From left to right: Brian Schmidt (photo by Belina Pratten, Australian National U., Adam Riess (Homewood Photography), Saul Perlmutter (Photo: Ariel Zambelich*** 

In 1998, cosmology was shaken at its foundations as two research teams presented their findings. The team headed by Saul Perlmutter had been working for 10 years. Brian Schmidt headed another team, launched at the end of 1994, where Adam Riess played a crucial role. The research teams raced to map the universe by locating the most distant supernovae. More sophisticated telescopes on the ground and in space, as well as more powerful computers and new digital imaging sensors (CCD, Nobel Prize in Physics in 2009), opened the possibility in the 1990s to add more pieces to the cosmological puzzle.

The teams studied type 1a supernovas, which are explosions of white dwarfs, - - old compact stars that are as heavy as the sun but as small as the earth. A single such supernova can emit as much light as a whole galaxy. The teams found more than 50 distant supernovae whose light was weaker than expected, a sign that the expansion of the universe was accelerating. The potential pitfalls had been numerous, and the scientists found reassurance in the fact that both groups had reached the same conclusion. For almost a century, the universe has been known to be expanding as a consequence of the Big Bang about 14 billion years ago. However, the discovery that this expansion is accelerating is astonishing. The acceleration is thought to be driven by dark energy, but what that dark energy is remains an enigma - perhaps the greatest in physics today because dark energy constitutes three quarters of the universe.

### *Pilkington Award*


The ***Society of Glass Technology*** (SGT) is pleased to announce the ***Sir Alastair Pilkington Award*** in honor of a key figure in the development of glass technology during the twentieth century. As a young man very early in his career Pilkington invented the famous Float Glass Process which has transformed the manufacture of all flat glass products world-wide. He was a working engineer, but his invention spanned the industry / science divide. It involved the application of the fundamental understanding of the physics of fluid flow in complex geometries and complex heterogeneous high temperature chemistry at the tin-glass interface. His interest in glass went far beyond the everyday reality of multinational manufacturing which his invention made possible. --He was also sensitive to the long history of glassmaking, took delight in the beautiful artifacts made by glassmakers through the centuries, and actively encouraged young people to share his enthusiasm for all things to do with glass.

Applications are invited from any field of glass science where publication in referred journals is the norm.. There is no absolute age limit but it is expected that applicants will be under 40 years of age. Full details for the rules and criteria for the Award can be found on the Society website (***www.sgt.org***).

*Adrian Wright (**A.C.Wright@reading.ac.uk**)*

### *From Science Now, Sept 22nd, 2011: Neutrinos Travel Faster Than Light, According to One Experiment -by Adrian Cho*

The data come from a 1300-metric-ton particle detector named Oscillation Project with Emulsion-tRacking Apparatus (OPERA). Lurking in Italy's subterranean Gran Sasso National Laboratory, OPERA detects neutrinos that are fired through the earth from the European particle physics laboratory, CERN, near Geneva, Switzerland. As the particles hardly interact with other matter, they stream right through the ground, with only a very few striking the material in the detector and making a noticeable shower of particles. Over 3 years, OPERA researchers timed the roughly 16,000 neutrinos that started at CERN and registered a hit in the detector. They found that, on average, the neutrinos made the 730-kilometer, 2.43-millisecond trip roughly 60 nanoseconds faster than expected if they were traveling at light speed. "It's a straightforward time-of-flight measurement," says Antonio Ereditato, a physicist at the University of Bern and spokesperson for the 160-member OPERA collaboration. "We measure the distance and we measure the time, and we take the ratio to get the velocity, just as you learned to do in high school." Ereditato says the uncertainty in the measurement is 10 nanoseconds. However, even Ereditato says it's way too early to declare relativity wrong. "I would never say that," he says. Rather, OPERA researchers are simply presenting a curious result that they cannot explain and asking the community to scrutinize it. "We are forced to say something," he says. "We could not sweep it under the carpet because that would be dishonest."

### *What's on the cover:*

The *Transactions* symposium at ACA 2012 in Boston, *Transformations and Structural Oddities in Molecular Crystals*, will honor Bruce Foxman.

The cover image depicts single crystals of a chloride salt of a morphinan quaternary ammonium ion, which is a peripherally-restricted μ-opioid antagonist being developed for the treatment of opioid-induced constipation (OIC), a common and often limiting side effect of opiate-based pain therapy.

Crystalline hydrates of the chloride salt are chemically stable, but show dynamic exchange of water in the solid state at elevated temperatures. Physical characterization reveals that the material contains up to two equivalents of water depending on environmental conditions. Although the drug substance is isolated as a dihydrate from aqueous solution, the monohydrate is the stable form under ambient conditions. The crystal structure of the dihydrate established that the material has a bi-layer motif. Initially, a single crystal structure for the monohydrate was elusive. Recently, with the expert help of Bruce Foxman, the single crystal structure of the monohydrate has been solved. In addition, Foxman observed and captured the dynamic change from dihydrate to monohydrate. The results and depiction on the cover highlight the single crystal to single crystal dehydration of dihydrate to the stable monohydrate development form of the drug.

The cover image was generated by Magali Hickey at Alkermes, plc (***www.alkermes.com***) and they retain the right to grant permission for reuse.

## Index of Advertisers

NEW

INCOATEC
innovative coating technologies gmbh

# The IμS High-Brilliance


- for Cu, Mo & Ag
- up to 60% more intensity
- component recognition
- improved safety features
- fully compliant with Machinery Directive 2006/42/EC

www.incoatec.de

## *Herbert Aaron Hauptman (1917-2011)*

Herb Hauptman died on October 23, 2011 at the age of 94. He was a co-winner of the Nobel Prize in Chemistry in 1985 for developing mathematical methods for deducing the molecular structures of chemical compounds.

Herb was born in New York City, the oldest of three sons of Israel Hauptman – a printer - and Leah (Rosenfeld) Hauptman who was a sales clerk in the ladies' hat department of a prominent New York City department store. In later years, he fondly recalled the passionate interest and the innate understanding and appreciation of science and mathematics that arose in him at a very early age. He described how he often entertained himself as a youth by playing with mathematical calculations related to things in his home environment.

He attended Townsend Harris High School, where his interest in science and mathematics was nurtured, and then went on to the City College of New York where he graduated in 1937. He also earned a master's degree in mathematics at Columbia University in 1939.

On a blind double date in the fall of 1940, Herb found that he preferred his friend's date. Displaying the same drive that later led to his professional success, he quickly acted on his emotions and, within a matter of weeks, married his young bride, Edith Citrynell, an educator.

Shortly after he and Edith were married, he joined the legions of young American men who were sent to serve in World War II. A Navy ensign, he was stationed in the Southwest Pacific where he was trained as a weather forecaster. He was made a permanent "officer of the day" and was responsible for responding to a variety of crises. While he only had one day of firefighter training, he also served as a Fire Marshall in the Philippines – an assignment that twice nearly cost him his life. His time in the war was marred with close calls and the constant presence of death and destruction. During his war years, he spent his rare moments of spare time studying calculus (he brought the book with him to the South Pacific) and solving mathematical problems. His wartime experience was a constant memory throughout his life and led him, in future years, to protest actively against American involvement in other military actions, including the Vietnam War.

In 1947, he began working at the Naval Research Laboratory (NRL) in Washington, D.C. where he remained until 1970. During his career there, he also earned his PhD in mathematics from the University of Maryland in 1955.

During his time at NRL, he became fascinated with the problem of how to directly determine molecular structures through the methodology of x-ray crystallography, a problem that had daunted other scientists for decades. Along with Jerome Karle, he co-published a solution in 1953 in a book entitled, *Solution of the Phase Problem I: The Centrosymmetric Crystal*. However, for many years other scientists were skeptical of the work and it was largely ignored. It was finally accepted in the 1970's and received the recognition it deserved with the award, in 1985, of a Nobel Prize that he shared with Jerome.

In 1970, he joined the crystallographic group of a small, non-profit biomedical research institute, the Medical Foundation of Buffalo (MFB). In 1972, he became MFB's Research Director and later, its President. In 1994, MFB was renamed the Hauptman-Woodward Medical Research Institute (HWI) to honor him as well as Helen Woodward-Rivas, the philanthropist who provided the seed funds for the institute.

Herb also served as Professor in the Department of Structural Biology, the Department of Biophysical Sciences and as

***Herb's group in Buffalo (ca 1979): Front row left to right: Doug Rohrer, Phyllis Strong, George DeTitta, Elaine DeJarnette, Mary Erman, Vivian Cody, Steve Potter, Kay DeVine, Dave Smith, Dave Langs.***

***Back row left to right: Chuck Weeks, Bill Duax, Mary Fronckowiak, Ed Greene, Herb, Bob Blessing, Jane Griffin, Doug Dorset, Walt Pangborn.***

Distinguished Professor in the Department of Computer Science at the University at Buffalo. In the 1990's and early 2000's, he collaborated with his Buffalo colleagues to develop improvements to his methods that permitted successful application to much larger molecules.

A member of the ACA and the US National Academy of Sciences, he received many honorary degrees from colleges and universities in countries as far away as Poland, Israel and Italy. He received an honorary degree from the State University of New York at the 2009 commencement of the University at Buffalo. He received numerous other awards including the Niagara Lutheran Humanitarian award for 2009. Most recently he was named to the inaugural class of ACA Fellows. Herb continued to work on his own new research projects in addition to serving as a mentor and teacher to younger scientists and staff members. He came to work at HWI every day until he was well into his nineties.

As a hobby, he enjoyed making stained-glass artwork inspired by mathematically defined, complex geometrical shapes. A permanent collection of these beautiful creations resides at HWI.

In addition to his wife, Edith, he is survived by their daughters Barbara Hauptman and Carol Fullerton, PhD, his brother Robert, and many nieces and nephews. He was predeceased by his brother Manuel in 2009.

Adapted from the announcement posted on the HWI website ***(www.hwi.buffalo.edu).***

## *Nominations for 2013*

***ACAAwards:*** Nominations for the ***Isadore Fankuchen, Kenneth Trueblood, Bob Bau Neutron, and Etter Early Career*** awards are due by May 1, 2012.

***NOTE: Daniel Nocera (MIT), winner of the 2011 Wood Science Writing Award, will be at the meeting in Boston to receive the Award and present a talk at the banquet.***

***ACA Offices and Committees:*** In the fall of 2012 we will elect a new Vice-President and one person to each of the ACA Standing Committees (Continuing Education, Communications, and Data, Standards and Computing). Suggestions are due to by February 1, 2012 (send to ***marcia@hwi.buffalo.edu***). Two of the members of the nominating committee are Judy Kelly and Gerald Stubbs.

Full details describing the criteria for all ACA awards and offices can be found on the website (***www.AmerCrystalAssn.org***). All Nominations should be sent the ACA office (***marcia@hwi.buffalo.edu***)

## *2012 Dues are Due*

Please renew promptly and remember to support your favorite ACA Award Funds. ***NOTE: It is now possible to renew online at www.AmerCrystalAssn.org.***

## Robert (Bob) Snyder (1941-2011)

Robert L. Snyder passed away early on the morning of September 1st, 2011, from complications due to cancer. At the time of his death, Bob was Professor and Co-chair of the School of Materials Science and Engineering at the Institute of Technology (Georgia Tech), a member of the Nanoscience and Nanotechnology Faculty (NanoTECH), and Chairman of the Denver X-ray Conference Organizing Committee. Bob leaves behind his loving wife of 48 years, Sheila, his daughter Krissy, his son Robert, and their families. Many ACA members personally knew Bob, as he was an ambassador of materials science and engineering as well as all types of x-ray analysis. He made numerous friendships around the world, and was generally known for his passion for life and the intensity and excellence of his science.

Bob was born in Plattsburg, New York in 1941. He received his BA in Chemistry from Marist College and his PhD from Fordham University in 1968. He entered the field of materials through his PhD research and continued it as a post doctoral scholar at the University of Pittsburgh and National Aeronautics and Space Administration (NASA). At the University of Pittsburgh, Bob was a National Institute of Health (NIH) fellow in the crystallography laboratory. Bob began teaching at the New York State College of Ceramics at Alfred University in 1970, and rose through the academic ranks to Professor of Ceramic Science in 1982. He became Professor Emeritus in 1996. He chaired the Material Science and Engineering Department at Ohio State from 1996 through 2002. He became co-chair of the School of Materials Science and Engineering at Georgia Tech in 2002. He enjoyed extended leaves to be a visiting scientist at Lawrence Livermore Laboratory (1977), National Bureau of Standards (1980, 1981), Sandia National Laboratory (1987), Siemens Central Research Laboratories Munich (1983, 1991), and the Université de Rennes (1995). During this time, he met and collaborated with many international scientists and fellow ICDD members who also became lifelong friends.

He was the author of two textbooks, edited nine technical books, and contributed chapters to nine books and encyclopedias. He held eight patents, and published over 265 papers on materials and materials characterization which have been cited by other authors more than 2000 times. Bob presented more than 1,000 talks around the world including more than 40 plenary and keynote lectures. His fundamental textbook, *Introduction to X-ray Powder Diffractometry,* that Bob wrote with his close friend Ron Jenkins (seen with Bob in the photo at the bottom of the left colum), has been used and distributed to hundreds of students attending ICDD workshops and clinics for more than 15 years.

Bob always had a passion for all types of x-ray analysis as applied to solid state materials. He was Chairman of the Board of the ICDD from 1996-2000, as well as a board member in consecutive terms from 1986-2004. He served as the Chair of the Marketing Committee since 2005. As board member and chairman, Bob promoted alliances with other database organizations that directly led to the dramatic growth of the Powder Diffraction File over the last 15 years.

Bob was also a champion for developing software and automated analysis programs for powder diffraction. He served as a member of the Denver X-ray Conference Organizing Committee and was the current chairman of that group. For many years, he served as an editor for the proceedings of the conference, *Advances in X-ray Analysis*. He was a Principal Editor for the journal *Materials Research* and the *Journal of the American Ceramic Society*. Bob chaired the High Resolution Neutron Powder Diffraction research team at Brookhaven National Laboratory and was on the executive committee of beamlines X3 and X7 at the Argonne National Synchrotron Light Source. He was chair of the founding committee for the International Society of X-ray Analysis. He also chaired numerous ACA committees and was a member of the IUCr Commission on Powder Diffraction. He was also a founder of the US-Japan Workshop series on Superconductivity from 1989-97.

In recognition of his many contributions, Bob received several awards which include:

*Distinguished Fellow, ICDD, 2005*
*Hanawalt Award, ICDD, 2004*
*TMS Leadership Award, 2002*
*Fellow, American Society of Metals, 1999*
*American Ceramic Society Outstanding Educator, 1999*
*Fellow, American Ceramic Society, 1993*
*Chancellors Award for excellence in teaching, Alfred Univ, 1980*

***Bob with Jim Kaduk (left) and Cam Hubbard (right)***

During his career, Bob formed many lasting relationships with members of the international community. Through his passion and friendship, he impacted the field as an innovator, teacher, administrator, and mentor. ICDD will be collecting remembrances (i.e. photos, stories) of Bob's life to present to his family. If you would like to contribute, please send them to ***shertz@icdd.com***.

*Tim Fawcett*


# Smarter, Faster, Brighter

With more than double the Cu X-ray intensity, CSD cell check tools and real-time email notifications, the Agilent SuperNova is better than ever. Find out more at **www.agilent.com/chem/smarter**



The Measure of Confidence

Agilent Technologies

## *A Celebration of the Life and Work of Hirotsugu Tsuruta (1962-2011)*

Here, on behalf of his many friends and colleagues, we mark the passing of one of the unsung heroes of structural biology, Hirotsugu (Hiro) Tsuruta, Senior Scientist at the Stanford Synchrotron Radiation Lightsource (SSRL), SLAC National Accelerator Laboratory, and the Department of Chemistry, Stanford University, who died of cancer on 25 August, 2011 at the age of 49.

Hiro was born in Sasebo, in Nagasaki Prefecture, Japan, on 18 August 1962. He received his BSc in solid state physics and MSc in materials science at the Department of Materials Science, Faculty of Science, Hiroshima University, in 1985 and 1987, respectively. He subsequently earned his DSc in biophysics from the Department of Materials Science, Faculty of Science, Hiroshima University in 1990. He spent a postdoctoral year at Hiroshima University, supported by the Japan Society for the Promotion of Science, mainly at the Jichi Medical School. His long involvement with synchrotron radiation started with his graduate thesis work, much of it done at the Photon Factory. During this time he was involved in several collaborative research projects using synchrotron radiation small-angle x-ray scattering, but his main contribution was the development of time-resolved solution scattering experiments using a stopped-flow rapid mixer specifically designed for time-resolved solution scattering experiments at sub-zero temperatures. Using this device, he studied the allosteric transition of aspartate transcarbamylase, under the mentorship of Hiroshi Kihara, Takayuki Sano and Toshiaki Ohta, as an exchange graduate student at the Department of Physics, Jichi Medical School. As a postdoctoral fellow, he continued to perform time-resolved small-angle x-ray scattering studies on biological macromolecules and also interacted extensively with Yoshiyuki Amemiya (Photon Factory; now at University of Tokyo) and Katsuzo Wakabayashi (Osaka University).

In 1991, Hiro moved to the Stanford Synchrotron Radiation Laboratory (SSRL) and the Department of Chemistry in 1991 as a Science Research Associate in the Structural Molecular Biology program. During his 20-year career since then, he led the effort to develop the structural biology SAXS beamline BL4-2 into one of the most highly performing and productive experimental facilities in the world today, enabling structure function studies for many systems of biomedical importance. Important technical accomplishments were the development of a low-angle single crystal diffraction instrument for large unit-cell crystals such as those from viruses, of an ultra-small angle scattering instrument, which can also be used for phase-contrast x-ray imaging, of instrumentation for time-resolved SAXS, and of increased automation for solution SAXS.

Despite these impressive technical accomplishments, Hiro was primarily science driven. His keen scientific interests and intellectual curiosity concerning structure–function relationships in biological macromolecular assemblies were directed to a wide variety of systems including virus particles, molecular chaperon proteins, kinases, heatshock proteins and transcription regulators. Building on his graduate work, he was involved in a number of pioneering studies of dynamical structural changes of these kinds of systems using time-resolved techniques. Over the years, he had many fruitful long-term collaborations with a number of researchers, among them Jack Johnson (Scripps Research Institute) on virus maturation, and Evan Kantrowitz (Boston College) on allosteric transitions of aspartate transcarbamoylase.

Hiro was very conscious of the need to give back to the community that had nourished him, especially towards the end of his life. These service activities included co-authoring *Volume F of International Tables for Crystallography,* serving as chair of the ACA Small Angle Scattering SIG, most recently on the Scientific Advisory Committee for Petra-III and the NIH NCRR/GM Advisory Committee for structural biology beamlines at NSLS-II. He was a consultant for the SIBYLS SAXS beamline construction at the ALS. A perhaps even greater contribution, that is easy to underestimate, is the large number of SSRL SAXS users at BL4-2 he has mentored over the years providing everything from intellectual advice to dealing with all the mundane technical problems that beamlines are prone to, more often than not at 3:00 in the morning, on a weekend.

Those of us in the doughty tribe of synchrotron scientists recognize we have lost one of our own. A modest man, Hiro epitomized what is best in a beamline scientist, not only as a facilitator of great science from the outside user community but as a scientific visionary and technological driver in his own right. His unflagging good nature, enthusiasm and optimism were an inspiration to us all. Hiro addressed his life outside of synchrotrons just as passionately. He played second bassoon and saxophone for the Peninsula Symphony Orchestra where his dedication, craftsmanship, and attention to detail informed by his deep love of classical music made him a fine musician recognized by his peers. At home, he was a gifted cook, dog trainer and athlete. Hiro will be missed. He is survived by his partner of many years, Christine Trame, and parents and siblings in Japan.

*Britt Hedman and Tom Irving*

# GeniX 3D High Brilliance X-ray Beam Delivery System

*Increase your equipment capability with a reliable low maintenance x-ray source.*


## New product features

Higher brightness source coupled to efficient multilayer FOX 3D optics
X/Y stage providing intuitive alignment
Fixed and referenced output X-ray beam

## In the tradition of the reknowned GeniX platform

Proprietary closed loop water cooling for high reliability
Control unit with smart power management
Low power and low maintenance system
Variety of beam properties and radiations (Cr, Cu, Mo…)

## Suitable for many applications

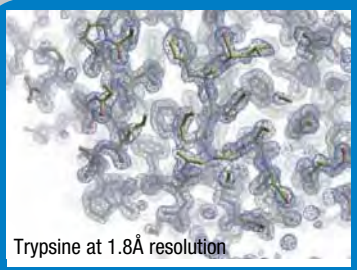
Protein crystallography
Powder diffraction
Small angle x-ray scattering
Stress measurement
Micro spot mapping: diffraction and fluorescence
High pressure diffraction

Increased brightness
for a higher useful flux
in your application

Improved ease of use

Simplified equipment
integration

## The ultimate low power beam delivery system


Trypsine at 1.8Å resolution

Improved I/σ for small crystals

Faster data collection

Designed for easy integration on every diffractometer

**SHAPE YOUR PERFORMANCE IN 3D**

Xenocs
Brighter solutions

Xenocs SA
19 Rue François Blumet
38360 Sassenage - FRANCE

*Phone: +33 (0)4 76 26 95 40*
*Fax: +33 (0)4 76 26 95 49*
sales@xenocs.com

www.xenocs.com

### *Notes of a Protein Crystallographer - Cold Spring Harbor Meeting in 1971 Revisited: A Commemoration of the Birth of the Protein Data Bank (PDB40).*

I began writing these notes at Blackford Hall within the grounds of Cold Spring Harbor Laboratory, Friday, October 28, 2011; a diaphanous morning. Looking through the window, a beautiful view of the Long Island Sound is in the horizon. For me this is a pilgrimage to the origins of the Protein Data Bank and also an occasion to experience from the inside what in 1971 was referred to as the 'Coming of Age' of Protein Crystallography[1].

How many times had I seen the volume of the proceedings of that momentous meeting on the bookshelf of my PhD mentor, Marvin L. Hackert, in his office in Patterson Laboratories at the University of Texas at Austin. I had landed at UT Austin in the fall of 1972 (just as the volume had been published) as a graduate student sponsored by a Fullbright Scholarship from the Spanish-American Binational Committee. How many times had I browsed through the black and white photographs of the icons of the field: Max Perutz, Warner Love, Dorothy Hodgkin, Lyle Jensen, Michael Rossmann and so many others, unknown at that time but now full-fledged Nobel Prize Laureates (e.g., Tom Steitz)? How many times had I looked with envy at the roster of participants in such a remarkable gathering? Sadly, some have passed away: Aaron Klug, Paul Sigler, Don Wiley, and Carl-Ivar Brändén among others but many were present this time also.

As soon as the commemorative meeting was called by the currently Worldwide PDB (wwPDB), I could not resist signing up to go to commemorate four events: i) the celebration of the spectacular trajectory of our field during these past four decades; ii) the 40th anniversary of the birth of the PDB; iii) my personal satisfaction of having been a 'real' protein crystallographer for forty-years and; iv) the pleasure of stepping on the 'sacred grounds' where so many pioneers of macromolecular crystallography and molecular biology had previously been, met and discussed the insights and advances of the field. Incidentally, after more than twenty two years at Abbott laboratories as a protein crystallographer and drug-designer, Jonathan Greer, my manager at Abbott labs and a participant in the 1971 symposium gave me his personal copy of the CSH volume that I now treasure and that I consulted as an inspiration to write these notes.

It was indeed a momentous meeting planned with loving care by the entire Protein Data Bank team to commemorate the birth of the PDB. It was a unique opportunity to see old friends and enjoy ourselves. The mood was celebratory as many of the old participants in the meeting were there to present reminiscences, anecdotes, historical vignettes and sociological insights on the events and forces that made the birth of what is now the Protein Data Bank a reality. But there was also a 'show' of the novel structures, methods and combined approaches that will maintain the macromolecular structural community as a vibrant area of research for many years to come and the PDB as a critical resource for the structural and biomedical community at large. It was refreshing to see so many young and eager crystallographers in the audience mingling and discussing their latest results with the old timers.

I have selected a few highlights to convey the excitement of the meeting. The complete details are available from the official meeting site at CSHL (***meetings.cshl.edu/meetings/pdb40.shtml)***, including also the full book of abstracts. ***Michael Rossmann*** opened the meeting with an excellent historical perspective of the early work on hemoglobin and myoglobin at Cambridge, UK, in the late fifties and early sixties and the events leading to the community effort to create a central depository of macromolecular structures. He then went on, emphatically saying that 'he was not a fossil', to present the latest results of his work on the structures of the multiple components of the T4 phage.

***Jane Richardson*** described her journey from being the master illustrator of the first protein structures with ribbons and helices to her efforts to improve the quality of new structures. ***Axel Brunger*** presented his latest efforts to enhance the structure determination and refinement of low resolution structures, using a novel refinement term based on the interatomic distances $D_{ij}$. ***Richard Henderson,*** one of the pioneers of the structure determination of rhodopsin by electron diffraction using low doses, reviewed the challenges still facing the high resolution determination of structures by electron microscopy. After a hilarious introduction by ***Gerard Kleywegt*** (PDBe), a few gentle remarks by ***Hans Deisenhofer*** reminded the audience that not everybody in the community of protein crystallographers of the seventies and eighties accepted the notion of depositing the efforts of their many years of hard labor in a common depository.

***PDB40 Speakers: Back row: Soichi Wakatsuki, Johann Deisenhofer, Michael Rossmann, Janet Thornton, Andrej Sali, Richard Henderson, Stephen Burley, Wayne Hendrickson. Front row: Susan Taylor, Jane Richardson, Ad Bax, Axel Brunger, Mei Hong, Cheryl Arrowsmith, Wah Chiu, Angela Gronenborn. Not shown: Kurt Wüthrich, David Searls and David Baker. Photo from RCSBPDB.***

*PDB Staff - Past and Present (photo by Constance Brukin)*

***John Markley*** (Chair) and ***Kurt Wüthrich*** reviewed the contributions of the methods related to NMR and ***Mei Hong*** kept the audience spellbound with her latest results using solid state NMR to study the detailed structure of proteins embedded in membranes. ***Wayne Hendrickson*** retold the story of the breakthrough of the Crambin structure at atomic resolution and described his latest work on SLAC1 and related proteins. I was particularly intrigued by the ideas and concepts expressed by ***David Searls*** reviewing the language of molecular and structural biology in relation to linguistics and the possibility of expressing the molecular biological processes in the future in a 'linguistic framework' to facility their description. Appropriately, ***Helen Berman*** closed the meeting describing the spirit of the assembly with the following words: collegiality, community and collaboration, passion and persistence.

Where will the PDB be ten years from now? This might not be as difficult to guess, but how about predictions for the PDB at the its 80th anniversary? Very shrewdly, the organizers prepared a white board in the main hallway of the meeting where attendees could put their comments, guesses and predictions for the next celebration of the PDB at fifty and eighty years old. Prompted by the white board, I intently looked at the crystal ball a few times. Within the next ten years: Will we have a sizeable number of structures obtained by single molecule diffraction? Will the promise of these methods be realized helping us to populate the PDB with structures of macromolecules obtained 'without crystals'? or with micro (nano?) crystals? I also made a guess at the longer projections: Would there be an entry (or a section) at the PDB of 'far tomorrow' for cell organelles such as mitochondria, chloroplast? You, the reader, can make your own predictions.

A more detailed account of the meeting will be presented elsewhere by the organizers. This brief note was threaded with personal notes, reminiscences, and jotted comments, combined with some scientific details of the talks presented by the prominent speakers. It is not meant to be a full report or not even a professional meeting summary. These are just the 'notes of a protein crystallographer' at the celebration of his 40th anniversary in the profession.

In closing, I do wish that the new generations of macromolecular crystallographers have the opportunity to browse the website of the meeting with the corresponding photos (***meetings.cshl.edu/galleries/pdb40/***). More importantly, I also wish that those images of the old and new protein crystallographers, together with the proceedings of the meeting, copies of the presentations and discussions, inspire them as the volume published in 1972 inspired me forty years ago. Anniversaries are to be celebrated but they are also supposed to inspire the new generations to seize the torch and continue the path of discovery: different tools but the same spirit.

**[1] D.C. Phillips, pg. 589. Structure and Function of Proteins at the Three-Dimensional Level. *Cold Spring Harbor Symposia on Quantitative Biology. Volume XXXVI.* Cold Spring Harbor Laboratory, 1972.**

*Cele Abad-Zapatero*

**Annual Statement of Ownership, Management, and Circulation**

1. Publication Title: ACA RefleXions
2. Publication Number: 1958-9945
3. Filing Date: September 15, 2011
4. Issue Frequency: Quarterly
5. Number of Issues Published Annually: 4
6. Annual Subscription Price: $1.75
7. Location of known office of Publication (s: 700 Ellicott Street, Buffalo, NY, 14203
8. Location of Headquarters or General Business Office of Publisher: PO Box 96, Ellicott Sta., Buffalo, NY, 14205
9. Full Names and Complete Mailing Addresses of Publisher, Editor and and Managing Editor: Publisher: ACA C/O 700 Ellicott Street, Buffalo, NY, 14203; Editor: Judith Flippen-Anderson, 3521 Lancelot Way, Annandale, VA 22003; Managing Editor: Connie Chidester Rajnak, 4210 Old Field Trail Dr., Kalamazoo, MI 49008
10. Owner: American Crystallographic Association, Inc.
11. Known Bondholders, Mortgagees, and Other Security Holders Owning or Holding 1 Percent or More of Total Other Securities: None
12. Tax Status: Not Changed During Preceding 12 Months

| 15. Extent and Nature of Circulation | | | Average No. Copies Each Issue During Preceding 12 Months | No. Copies of Single Issue Published Nearest to Filing Date |
|---|---|---|---|---|
| a. Total Number of Copies (Net press run) | | | 2300 | 2400 |
| b. Paid and/or Requested Circulation | (1) | Paid/Requested Outside-County Mail Subscriptions Stated on Form 3541 | 1491 | 1677 |
| | (2) | Paid In-County Subscriptions Stated on Form 3541 | 0 | 0 |
| | (3) | Sales Through Dealers and Carriers, Street Vendors, Counter Sales, and Other Non-USPS Paid Distribution | 0 | 0 |
| | (4) | Paid Distribution by Other Classes Mailed Through the USPS | 443 | 500 |
| c. Total Paid and/or Requested Circulation (Sum of 15b.(1),(2),(3),and(4)) | | | 1934 | 2177 |
| d. Free Distribution by Mail | (1) | Outside-County as Stated on Form 3541 | 52.25 | 49 |
| | (2) | In-County as Stated on Form 3541 | 0 | 0 |
| | (3) | Other Classes Mailed Through the USPS | 0 | 0 |
| e. Free Distribution Outside the Mail | | | 0 | 0 |
| f. Total Free Distribution (Sum of 15d. and 15e.) | | | 52.25 | 49 |
| g. Total Distribution (Sum of 15c. and 15f.) | | | 1986.25 | 2226 |
| h. Copies not Distributed | | | 113.75 | 74 |
| i. Total (Sum of 15g. and h.) | | | 2100 | 2300 |
| j. Percent Paid and/or Requested Circulation | | | 97.23% | 98% |

16. Publication of Statement of Ownership will be printed in the Winter 2011 issue.
17. I certify that all information furnished on this form is true and complete.
(signed) Marcia Colquhoun for American Crystallographic Association, Inc.

## Reflections on the ACA 2011 Workshop on Symmetry-Mode Analysis

The availability of reliable and user-friendly software tools has now made symmetry-mode analysis (often referred to as reprsentational analysis) accessible to the general crystallographic community. Derived from group theory, symmetry-modes are an especially simple description of the degrees of freedom that arise when a crystalline solid undergoes a transition from high to low symmetry. Symmetry modes are the degrees of freedom that "nature" uses in deciding how to distort a parent structure.

The full-day workshop was held on Saturday May 28th during the 2011 ACA meeting in New Orleans, and was attended by 26 participants from academic institutions, industrial research facilities and national and international government laboratories. The presenters included ***Branton J. Campbell*** and ***Harold T. Stokes*** (Brigham Young University, USA) and ***J. Manuel Perez-Mato*** (University of the Basque Country, Spain). Co-organizers ***John S. O. Evans*** (University of Durham, UK) and ***Juan Rodriguez-Carvajal*** (Institute Laue Langevin, France) provided many of the detailed examples presented. ***Alan Coehlo*** (Brisbane, Australia) and ***Juan Rodriguez-Carvajal*** further provided critical support through the development of direct symmetry-mode refinement capabilities within their respective TOPAS Academic and FULLPROF software packages.

The workshop provided one hour of instruction on the basic concepts and applications of symmetry-mode analysis, and five hours of hands-on training in the use of the ISODISTORT and AMPLIMODES software packages to perform such analyses. Participants learned how to generate and visually explore the symmetry modes of a distortion, to decompose a known structure into symmetry-mode amplitudes, and to directly refine a symmetry-mode model against powder diffraction data using either TOPAS Academic or FULLPROF. Displacive distortions, occupational orderings, lattice strains and magnetic orderings were each considered. The most interesting transitions often involve more than one type of order parameter, as is the case with multi-ferroic materials.

The workshop ended with a panel Q&A session that included each of the presenters and ***Andrew S. Wills*** (University College, London). Many of the questions involved the limitations and possible extensions of symmetry-mode analysis. One oft-requested feature is the ability to use symmetry modes to describe the orientational distortions of rigid-molecules or rigid-polyhedral units. Regarding incommensurate distortions, ISODISTORT can now treat one-dimensional modulations involving multiple superposed irreps. But the implementation of higher-dimensional modulations still needs work. There was also some discussion of symmetry-mode refinement as a SDPD (structure solution from powder data) approach, which led the panel to compare and contrast the requirements of displacive and magnetic distortions.

The workshop website ***(www.physics.byu.edu/faculty/campbell/smaworkshop2011)*** includes links to articles on symmetry-mode analysis and also links to all of the hands-on tutorial examples and instructions. Anyone is welcome to download and work through these examples on their own.

*Branton Campbell*

## Emilio Segrè Visual Archives 2012 Calendar

The 2012 wall calendar from the Emilio Segrè Visual Archives at the American Institute of Physics features a year's worth of physicists at work and play, with representation from each of AIP's Member Societies! Each month's image has a unique historical caption, and most months also have links to extended historical content on the web. 11"x17" ***Order it online: http://photos.aip.org/calendar/***

### *Puzzle Corner by Frank Fronczek*

### *Answers to fall issue puzzles:*

***DISORDERED word puzzle*:** TWOFOLD CRYSTAL POLYMORPH FOURIER TWINNED

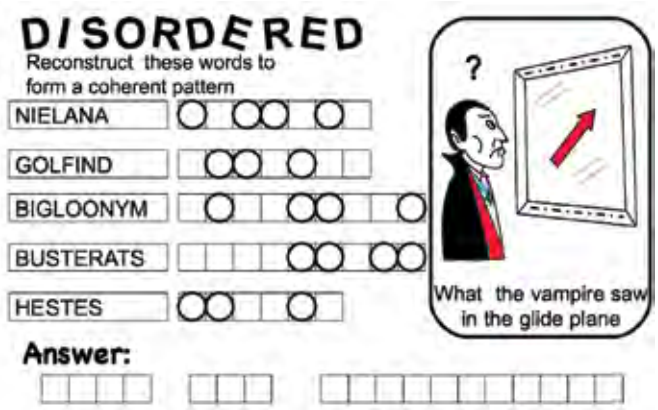
Why the crystallographer couldn't identify the chromatography fractions: *Answer:* He didn't know WHAT TO "COLUMN"

***What was "The Grand Ah-whoom"? How does it relate to disappearing polymorphs?***

"The Grand Ah-whoom" is the title of Chapter 116 of Kurt Vonnegut Jr's 1963 novel *Cat's Cradle*. It is the sound of the beginning of the end of the world, brought about by a seed crystal of the fictional polymorph Ice-Nine (melting point 114.4° F) falling into the sea, which causes the oceans to freeze. As a postscript to their classic 1995 *Acc. Chem. Res.* article "Disappearing Polymorphs" (28, 193-200), Dunitz and Bernstein quote a passage from Cat's Cradle, illustrating the seeding phenomenon, which causes once-ubiquitous polymorphs to give way to other forms. In Vonnegut's case, ordinary ice could no longer form, because higher-melting seed crystals of ice-nine were everywhere. At ordinary temperatures, liquid water - and thus life - could no longer exist either.

### *Winter Puzzles:*

***Question:*** What poem ends with the Law of Constancy of Interfacial Angles (Steno's Law)?




### *Contributors to this Issue:*

*Cele Abad-Zapatero, Mayank Aggarwal, Ana Bianchi, Branton Campbell, Christopher Davies, Kevin Eccles, Tim Fawcett, Joe Ferrara, Ana Ferraras, Frank Fronczek, Jenny Glusker, Shimelis Hailu, Lauren Hatcher, Brit Hedman, Magali Hickey, Orassa In-Noi, Tom Irving, Christopher Kane, Melanie Kirkham, Tom Koetzle, Vishal Koparde, Anna Kowalska, Pankaj Kumar Giri, Patrick Loll, Melissa Menard, Massimo Nespolo, Allen Oliver, Mary Parker, Connie Rajnak, Eric Reinheimer, David Rose, John Roudebush, Clare Rowland, Amy Sarjeant, Eddie Snell, Charlotte Stern, Cheryl Stevens, Ian Stokes-Rees, Leopoldo Suescun, Courtnie Vogelsberg, Hsiu-Wen Wang, David Watkin, John Westbrook, Adrian Wright, Briony Yorke, Erik Yukl*


***The Age of Entanglement: When Quantum Physics was Reborn*** by Louisa Gilder. (2009) Random House ISB:978-1-4000-9526-1

This book came highly recommended to me by Charlie Carter. The book sounded fascinating so I ordered a copy right away. The author has done an excellent job of researching all the personalities of the greats of quantum theory...from Einstein and Bohr to Feynman and Bell and beyond, while describing the concepts of entanglement in easy-to-understand language. One feature of the author's writing that makes the book enjoyable is that interspersed throughout are details about the lives of the players and their interactions.

The book starts off with a chapter about John Bell, a scientist at CERN. Bell himself provides a nice example of entanglement: Bertlmann's socks. What Bell did is to take Einstein's "spooky action at a distance" and make it understandable and, more importantly, provide the impetus to test it.

Next, the book follows the greats of quantum theory through the development of the basic concepts to what we recognize today as modern quantum theory. This starts in 1909 and ends in 1935, with the Einstein, Podolsky and Rosen paper on what we now call entanglement.

Part two covers the period 1940 to 1952, where we are told how quantum theory was tweaked by the second generation of theorists. Part 3 starts with Bell and follows his rediscovery of entanglement. We also learn about the first experiments in the 1970s to prove entanglement is measurable. Part 4 reviews the modern aspects of entanglement from 1981 to 2005.

Entanglement is a big deal. Quantum computing has the potential to change the way we do computing and cryptography. While our comprehension is perhaps still in its infancy, this "spooky action" certainly has the potential to change our lives, if not our children's. A basic understanding will go long way toward understanding the future ... and maybe even the past.


***Speeches by Martin Luther King, Jr.: The Ultimate Collection*** (2011) Audiobook ASIN: B004NT1AGW.

April 12, 2011 marked the 150th anniversary of the American Civil War. May marks the 50th anniversary of the start of the Freedom Rides - a significant step in the American Civil Rights Movement. These are very important turning points in American history, fresh in my mind because of reports on NPR. I saw this book in the audible.com catalog and downloaded a copy.

I was disappointed in two aspects of this anthology. First, the speeches, interviews and rallies are anachronistic. The listener does not get the benefit of the evolution of King's works, let alone that the Central Park Rally in 1968, after his death, precedes his final speech in Memphis. This was disorienting for me. The other complaint I have is that there was no introduction to the audio. Some speeches are easy to identify, for example, the "I Have a Dream" speech and his Nobel lecture, but others are not.

Having said this, make no mistake that the words of Martin Luther King, Jr. are powerful and stirring. He was right about civil disobedience, as was Ghandi. The process may be slow and difficult but the results are astounding - just look at the last American presidential election.

***The Information: A History, A Theory, A Flood*** by James Gleick (2011) Pantheon Books, New York ISBN: 0375423729

I've always enjoyed James Gleick's writing and picked up a copy of *The Information* as soon it came out. I will admit it was stuck in the queue as I finished a couple of other books.

This is a great summer read. Gleick starts off with a brief introduction to Claude Shannon, the Bell Labs' scientist who coined the phrase "bit" at nearly the same time his colleagues invented the transistor. Gleick then takes a step and introduces us to the first method of long distance communication - African drums - and how redundancy was built into the code to provide error correction. While numerous methods of long distance communication were developed, it was the telegraph and Morse code that was next great leap. But, we learn it wasn't the telegraph that was important but the coding method, which provided for the shortest messages within 25% of ideal for English. Next comes the telephone and the needs for switching circuits and amplifiers. Interspersed is a discussion of Babbage's engines, which were decades ahead of their time.

Claude Shannon reappears as a student of Vannevar Bush at MIT and during WWII as a cryptographer and analog programmer. Shannon's coup de grace is The *Mathematical Theory of Communication*, which it could be argued represents the initiation of Information Theory. (I was so intrigued by this that I bought a copy and the review is on page 30). Gleick then takes the reader through a modern description of entropy and the relationship between energy, entropy and information.

We ourselves store information and Gleick describes the verification of the central dogma of molecular biology. Gleick next weaves in the concept of memes first proposed by Dawkins in the *Selfish Gene*. At this time we learn how memes have affected society as Gleick smoothly segues into the modern digital communication age.

***Crystals, X-rays and Proteins - Comprehensive Protein Crystallography*** by D. Sherwood and J. Cooper (2010) Oxford University Press. ISBN: 978-0-19-955904-6

Tf (crystal) = Tf (motif) × [Tf (infinite lattice)] * Tf (shape function)].

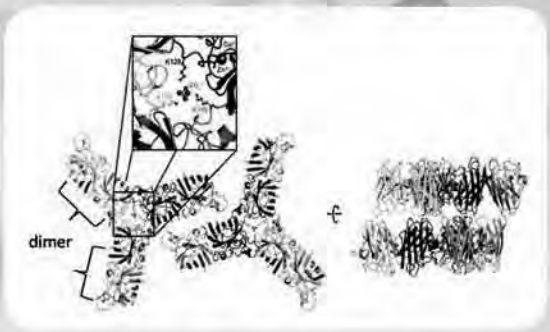
The Fourier transform of the crystal is equivalent to the FT of the motif (molecule) times the convolution of the FT of the lattice, a

Jena Bioscience

# What's new in Crystallography?

## LEXSY in Structural Biology

- Structure determination of the new $P2_12_12_1$ crystal form of recombinant human Cu/Zn superoxide dismutase (SOD1) expressed in our proprietary eukaryotic expression system LEXSY[1]




## Screens

- Pi-minimal/Pi-PEG Screen[2]
- JBScreen Pentaerythritol – a modern screen based on 4 alternative polymeric precipitants

## Plates

- 20% Price Cut on MRC Plates
- Lipidic Cubic Phase Screening Kit

## Phasing

- JBS Tungsten Cluster Derivatization Kits

[1]Gazdag *et al.* (2010) Purification and crystallization of human Cu/Zn superoxide dismutase recombinantly produced in the protozoan *Leishmania tarentolae*. *Acta Cryst.* **F66**:871.
[2]Gorrec *et al.* (2011) Pi sampling: a methodical and flexible approach to initial macromolecular crystallization screening. *Acta Cryst.* **D67**:463.

Jena Bioscience GmbH
Loebstedter Str. 80
07749 Jena
Germany

Phone +49 (0)3641-62 85 000
Fax +49 (0)3641-62 85 100
www.jenabioscience.com
info@jenabioscience.com

Jena Bioscience

series of Dirac delta functions and the FT of the shape function, is all you need to know. Well not really, but if you truly understand this equation then you are a long way toward understanding the principles of x-ray diffraction.

The first two-thirds of this book was like a thriller to me. Even though I knew the answer, I wanted to see how the author would address the next topic and I could not put it down. The last third did not have the same grip on me and I kept asking myself what happened - did someone else write Part III? The book is divided into three parts, but you know that already: Part I is *Fundamentals*, Part II is *Diffraction Theory* and Part III is *Structure Solution*.

Parts I and II provide an integrated approach to teaching diffraction theory. The authors take the reader through crystal basics and the wave theory of electromagnetic radiation along with the mathematical tools to understand them. In Part II the authors painstakingly develop diffraction theory by analyzing one dimensional lattices then three dimensional lattices. Next the authors explore the concept of lattices with motifs and develop all the details from first principles. The latter includes the derivation of the Laue equations and Bragg's law. I found the step wise description of the Fourier transform and the effect of applying it to various functions and objects something that would help students immensely in understanding the relationship between direct space and reciprocal space.

Part III provides a description of the modern methods for protein crystallography. Much attention is spent on Patterson methods and the phase problem, with the same attention to detail as the first two parts. There is a good description of least squares refinement and the adaptions for constraints and restraints. Maximum likelihood and simulated annealing are also described. However very little about statistics is discussed. This is a very important topic in crystallography and deserves more space. I found Part III lacking in the practical aspects of modern protein crystallography although it is very well referenced.

***The Mathematical Theory of Communication*** by Claude E. Shannon and Warren Weaver (1949) Library of Congress Card Catalog Number: 49-11922

A couple of months ago I read *The Information* by James Gleick (see review on page 28), which talked in detail about *The Mathematical Theory of Communication* by Claude E. Shannon. Gleick's concepts intrigued me so I thought I would read his book for myself. It was originally published as a pair of papers in the *Bell System Technical Journal* in 1948. I found a 1998 paperback edition on Amazon, but I probably could have found a much early version on the Barnes and Noble used bookstore.

Gleick does a much better job of summarizing the content than I could hope to do. TMTOC is a masterpiece. There is a forward by Richard E. Blahut and Bruce Hajek. The section by Weaver is titled *Some Recent Additions to the Mathematical Theory*.Unless you remember your statistical mechanics, it is a good idea to read these introductory sections. Shannon's work is math, plain and simple. What is so interesting is how he distilled modern communication into a few simple theorems that seem obvious.

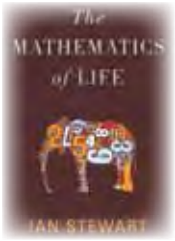
Instead of trying to review the book, I will tell what I relearned. First, if you want to get your point across you need five things: a message, a transmitter, a channel (which is likely to have noise), a receiver and finally an object to acknowledge the content.

This applies to every form of communication. I have a colleague whose accent I cannot understand and who claims I am going deaf. In order to understand each other we have to repeat messages at the appropriate level of redundancy to ensure they are communicated. After reading the book and thinking about it, I realize that some of the redundancy condition is fulfilled by body language and facial expression. His lips don't move. Maybe I am doing some sort of primitive lip reading to fill in the blanks and when I can't see him I don't understand him. Taking this further, the best way to make sure your message is received properly is to have the receiver repeat the message in his own words. Of course, there is little one can do if the receiver has a memory problem and promptly forgets the message.

Let's think about email. How often do we feel inundated by the number of messages we receive in a day? The point at which we stop responding is perhaps the point at which the bandwidth of the receiver is exceeded.

The theory behind CDs and MP3s is described in the book; that is, sampling digitally at twice the highest frequency to capture all the information in a signal. Note, that this is not an original idea of Shannon's. Efficient compression is also described.

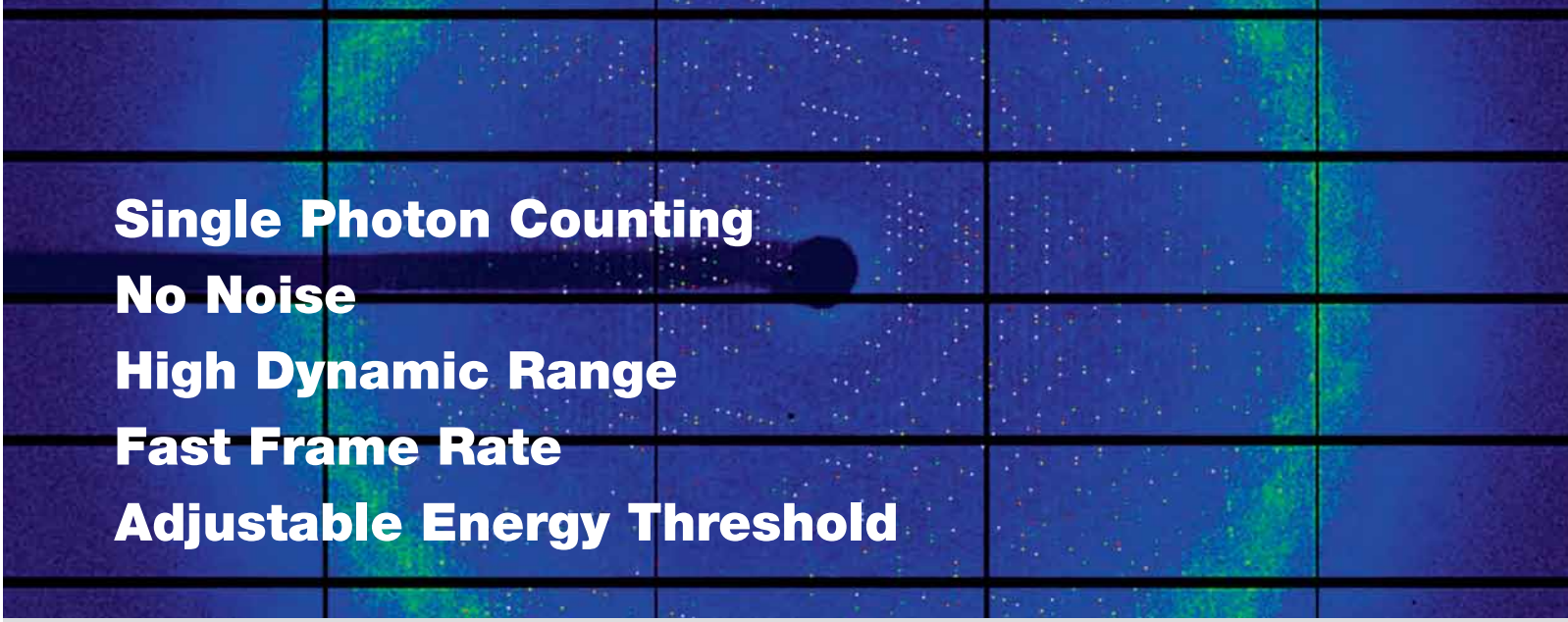
This is a very short book but, looking back, it is probably one of the most important books of the modern era.




***The Mathematics of Life*** by Ian Stewart (2011) Basic Books, ISBN: 978-0-4650-2238-0

Ian Stewart suggests that there have been five revolutions in biology and that we are experiencing a sixth one now. He first lays out the five revolutions: invention of the microscope, the classification of life, the theory of evolution, the discovery of genetics, and the determination of the structure of DNA. The current revolution is then the mathematical interpretation of biological information. As the book follows the timeline of discovery, chapters elaborating on Stewart's position are interspersed with chapters describing the first five revolutions. Chapter 2 provides a brief history of the technology that led to the invention of the microscope by Leeuwenhoek and information that the microscope revealed - small creatures and cell structures - and how it impacted science. The next chapter explores Linnaeus' classification scheme.

Chapter 4 is the first chapter to look at the impact of mathematics on understanding biology. Here we see the use of the Fibonacci series to describe plant growth and an explanation of why it works. The next chapter is devoted to evolution and nicely summarizes the Wallace-Darwin theory. Chapter 6 introduces the reader to Mendelian genetics and chapter 7 reviews the determination of the structure of DNA.



**Single Photon Counting**
**No Noise**
**High Dynamic Range**
**Fast Frame Rate**
**Adjustable Energy Threshold**

# DECTRIS X-ray detector systems

DECTRIS offers a wide variety of detector systems for a broad range of applications

## PILATUS 2-D detector systems

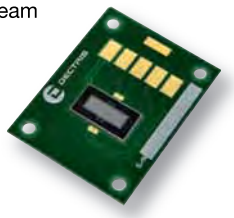
PILATUS detector systems are based on CMOS hybrid-pixel technology and deliver outstanding results in various applications. A wide range of models ensures that a suitable PILATUS detector can be chosen for every measurement.


## MYTHEN 1-D detector systems

MYTHEN is a one dimensional silicon strip detector system, which can be combined to form multi-detector arrays covering large angles (MYTHEN 6K).


## XBPM Beam Position Monitors

XBPM4 is a 4-quadrant x-ray beam position monitor based on CVD diamond technology, suitable for hard x-ray synchrotron beam lines.



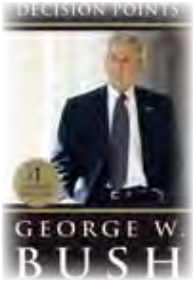
DECTRIS
Next Generation X-Ray Detectors

DECTRIS Ltd. | Neuenhoferstrasse 107 | 5400 Baden | Switzerland | info@dectris.com | www.dectris.com

The remaining chapters support the author's thesis that the sixth revolution is mathematics. A description of the Human Genome Project, and how it was realized and the results (not very useful yet), is followed by reclassification of life *via* heuristics and associated calculations to best define the tree of life. I found chapter 10 particularly interesting in the way that Stewart describes the packing of virus particles in 3 and 4 dimensions. The latter representation allows for a lattice representation of icosahedra. We only see the non-lattice representation in three dimensions.

Chapter 11 covers neural processing which includes a discussion about signal transmission, walking and image processing in the visual cortex. Stewart next looks at knots and folds, important for understanding DNA and proteins. In chapter 13, the author looks at stripes and spots and how we model their generation. Game theory and how it impacts evolution is described in chapter 14. Chapter 15 takes a look at networks while Chapter 16 reviews population dynamics. The next two chapters ask the questions "what is life?" and "are we alone?" These interrogatories are intimately related since we may not be alone and we might not recognize life unless it looks a lot like us. The last chapter summarizes the author's proposition regarding the sixth revolution of biology.

The book is well written and well referenced. The author has a grasp of the literature and uses it well. It is a book I would recommend for a good history of the integration of biology and mathematics targeting the average reader. The author does take a few jabs at American philosophy but I think readers of the book would understand.




***Decision Points*** by George W. Bush (2011) Crown Publishing, ISBN: 978-0-307-59061-9

I bought this book because I felt that, in order to properly discuss what happened during the years 2000-2008, I needed to know what President Bush was thinking and why. When I told my mother I had bought a copy she admonished me for paying full price and I told her I got my copy for 80% off. My colleague Mark Benson heard me talk about the book and dared me to review it, so here it is.

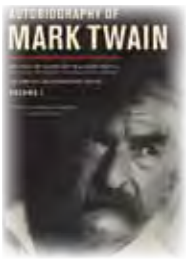
The book is organized around various episodes in Bush's life. The result is that topics are fully explored from start to finish, so there are overlapping timelines. I don't think I have to say this but please make sure to read other books that cover this period. I recommend *Twilight of the Bombs* by Richard Rhodes for a different perspective on the issue of WMD in Iraq as well the 9/11 Commission Report (for obvious reasons).

The book starts off with a brief description of why he wrote it. The first chapter addresses his decision to quit drinking the day after his 40th birthday and his subsequent return to his faith. It also describes his childhood and the story of the loss of his little sister to leukemia. Chapter 3 covers the decision to run first for Governor of Texas in 1994, and then President in 1999, and include details about how he ran the campaigns. The next chapter covers decisions regarding personnel, including the selection of Cheney for VP, and the Cabinet and Supreme Court after the election.

The remainder of the book covered a variety of disparate topics, including his decision to limit stem cell research, 911 and the immediate aftermath, the wars in Afghanistan and Iraq, Katrina, aid to Africa to combat AIDS, the Surge, bringing democracy to Iraq and Afghanistan and, finally, the current financial crisis.

I believe that the book does in fact answer the two questions of what and why. Is he telling the truth? I believe that he is telling the truth (as he sees it). I have disagreed with many of his decisions, but history tells us he had bad information. Did he adequately question the information? History also tells us that he did not. To paraphrase Bush, "I will be long gone before history decides if I made right decisions." I thought the book was well written, but Bush did have the help of speechwriter Christopher Michel. Finally, I did have to laugh when he concludes with a description of cleaning up after his Scottish terrier on a morning walk after leaving the White House. He says it was ironic that he was picking up that which he had been avoiding for the last 8 years.

***Autobiography of Mark Twain, Vol. 1*** by Mark Twain (2010), University of California Press 2010 ISBN: 978-0520267190




My mother gave me a copy of this for my birthday last year. I let it sit on the nightstand before cracking it open because I had heard some less than stellar reviews and, frankly, it was heavy and I was afraid it would hurt the dog if I fell asleep and it tumbled off the bed. Reviewers should not read reviews.

The introduction, by editors from the *Mark Twain Project*, describes Clemens' strict rules for the publication of this book: nothing for 100 years after his death, a second edition 25 years after the first edition, and a third and final edition another 25 years later, each disclosing a little more. The reason for this is that Clemens wanted to be honest but not offend anyone nearly or recently deceased.

It turns out that, although this is a long book, it is by no means tedious. Clemens' philosophy on autobiography is to write about what you want when you want. Herein lies a problem: if you expect the autobiography to follow chronological order then you will be disappointed. However, if you treat this book as a series of short biographical sketches and essays (after the introduction) you will be treated to the gift of Clemens' prose and a time capsule of American politics, religion, business, home life and war. What I found most fascinating is that little has changed in the past 100-plus years. For example, I found the story of Clemens' threat to sue the phone company for breach of contract for failure to install a line humorous yet contemporary.

I enjoyed reading this and look forward to Volumes 2 and 3.

*Joseph D. Ferrara*

## ACA Election Results

*Council Officers*

**Vice President**
*Cheryl Stevens*
**Secretary**
*Patrick Loll*

*Standing Committees*

**Communications**
*Eddie Snell*
**Continuing Education**
*Amy Sarjeant*
**Data and Standards**
*John Westbrook*

*SIGS*

**Biological Macromolecules**
*Chair-elect: Fred Dyda*
**General Interest**
*Chair-elect: Jeanette Krause*
**Industrial**
*Chair-elect: Magali Hickey*
*Secretary: Mark Oliveira*
**Materials Science**
*Chair-elect: Peter Khalifah*
**Neutron Scattering**
*Chair-elect: Katherine Page*
**Powder Diffraction**
*Chair-elect: Antonio Dos Santos Moreira*
**Service Crystallography**
*Chair-elect: Christine Beavers*
**Small Angle Scattering**
*Chair-elect: Richard Gillilan*
*Secretary: Volker Urban*
*Member-at-large: Ken Littrell*
**Small Molecules**
*Chair-elect: Louise Dawe*
*Secretary: Carla Slebodnick*
**Synchrotron Radiation**
*Chair-elect: Graeme Card*
**Young Scientist**
*Chair-elect: Albert Reger*

*Canadian Division*

*Chair-elect: Gerald Audette*

## *Cheryl Stevens -Vice-President*

Office of the Dean, Ogden College of Science and Engineering, Western Kentucky Univ., Bowling Green, KY.

***Research Interests:*** My research focuses on the use of x-ray crystallography for determination of the structures and charge densities of inhibitors of cancer growth and initiation (P450 and tyrosine kinase). I am also interested in QSAR, substrate docking, and database mining of these enzymes/substrate systems. My research projects have been funded by the NIH, Department of Defense, Board of Regents, and the Petroleum Research Fund.

***Statement:*** It is an honor to have been elected Vice-President of the ACA. I attended my first ACA meeting in Columbia, Missouri (spring, 1983) when the ACA had two meetings each year and hosted them on college campuses. I was fortunate enough to be able to serve as a local co-chair for the annual meeting in New Orleans in 1990. It was the first meeting that the ACA held entirely at a hotel. We certainly have grown in both membership and diversity of scientific interest since my early days. I was impressed then by the tight knit community of crystallographers and still believe that type of community exists. I look forward to being involved, as Vice-President and then President, as the ACA plans for the future of our organization and community.

I believe that as a professional society, it is our responsibility to:

*Organize* intellectually stimulating and relevant conferences. This is especially important for engaging young crystallographers as they develop their research programs and their careers.

*Advocate* for the ACA in the larger scientific community, especially with respect to the importance of x-ray diffraction in an expanding group of scientific disciplines.

*Educate* crystallographers, other scientists, and the general public about crystallographic concepts, tools, and applications.

*Provide* leadership to the Special Interest Groups as they determine programming for annual meetings.

*Secure* funding for our programs and initiatives so that we can be as strong as possible.

My positions as chair of a large and diverse department at a small liberal arts college, Associate Dean for Research, member of the Advisory Committee of the Louisiana Cancer Research Consortium, Director of the Molecular Structure and Modeling Core facility, researcher in crystallography, and teacher have given me the experience necessary to serve on the ACA Council. I am confident that my past accomplishments, experiences, and suite of transferrable skills will serve me well during my tenure on Council.

## *Patrick J. Loll - Secretary*

Professor of Biochemistry and Molecular Biology, Drexel University College of Medicine, Philadelphia, PA.

***Research Interests:*** Structural basis of antibiotic activity; anesthetic recognition by proteins; deubiquitinating enzymes; macromolecular crystallization.

***Statement:*** The ACA has been a fantastic resource for me over the last two decades, and I am delighted to be able to support its continued success by discharging the duties of the Secretary. In addition to acting in an organizational support role, the Secretary is a member of Council, and as such can influence the ACA's future direction. I feel prepared for this role, since: 1) my own research places me within the burgeoning structural biology "wing" of the ACA, and I have developed a keen appreciation for the tremendous new challenges facing structural biology in the post-genomic era; and 2) during my career I have also been lucky enough to be exposed to many other aspects of diffraction, including chemical crystallography, methods development, solution scattering, and crystallographic education. These experiences have given me an appreciation for the extraordinary diversity and scope of the disciplines falling under the ACA's umbrella, and I believe it is critical that the ACA continue to represent the broadest possible spectrum of interests. As Secretary, I will work conscientiously toward this goal

.

## *Edward Snell - Communications*

Hauptman-Woodward Medical Research Institute, Buffalo NY.

***Research Interests:*** Macromolecular crystallization, metalloproteins and complexes, radiation damage, technique development and complementary structural methods, e.g. small angle solution scattering.

***Statement:*** Beware of Greeks bearing gifts (especially if they are large and wooden). I was reminded of that saying on receiving a phone call with a polite query on whether I might consider running for the ACA Communications Standing Committee. After putting the coffee cup down the first question I asked was what do they do? After some further conversation and a little research on the ACA website, I found that they "*meet annually to plan the work of the Committee, coordinate electronic and printed publications of the ACA, organize a press conference at the annual meetings and prepare reviews of crystallographic research*". I'm probably the worst person to be involved with this as I still have lapses putting the 'u' in color and talk about aluminium quite a lot. However, I noted that the description of the committee used a capital 'C' therefore it must be important. Sometimes it's easy to make decisions with an appropriate coffee deficit in the morning. I said yes and found I had to write a description of what I'd do should anyone be foolish enough to elect me. I'm a physicist who took a right instead of a left and ended up looking at proteins instead of particles. I found many of them to be difficult to crystallize (both the proteins and particles) so I've gradually drifted toward resolving this and in cases where I can't, staying with the solutions. This has given me a background in many of the areas that the ACA represents. I'm equally capable of communicating with a biologist or beamline scientist and of stepping outside my comfort zone in protein crystallography to look at a broader view of the field.

Jesting aside, I'm fascinated by crystallography - the ability to see the world on an atomic scale. At every level it offers richness to those who take a closer glance - the key for the Communications Committee is encouraging that more detailed glance. Beyond the science that each of us is interested in, we see crystals produced that are as beautiful as the most precious gemstones (and to their growers just as valuable). From the biological perspective the structures that result reveal fascinating images of life and these images provide the landmarks for a landscape that reveals the very living process.

I'd like to use the Communications Committee to bring this perspective to the general public, the decision makers and our colleagues in other disciplines. I'd like to raise the awareness of the diversity of research encompassed by the ACA and the importance of that research in advancing our knowledge of the world around us. My area of interest is biological crystallography but it's important that the Communications Committee encompass all the areas exemplified by the membership and show the importance of crystallographic research and why it should be strongly supported. I've been a member of the ACA since crossing the pond in 1996 and have been to every ACA meeting since then. The ACA has helped me by bringing together a scientific family (and the uncle you don't talk about in the cupboard) with common interests. I feel it's important to give something back to the ACA. My way of doing it is by serving on this committee.

## *Amy Sarjeant Continuing Education*

Department of Chemistry, Northwestern University, Evanston IL.

***Research Interests:*** Structure elucidation and compound identification of complex network materials *via* single crystal and powder diffraction.

***Statement:*** As single crystal x-ray diffraction becomes a widespread tool for chemical analysis it is our job as crystallographers to ensure that each new generation of chemists understands the fundamentals of this technique. Modern instrumentation and advancements in software have allowed crystallographic experiments to become routine such that even those who have no formal training can solve structures. Consequently, the casual user may lack a full understanding of both the power and the limitations of the technique. It is imperative that those who use crystallography to support their research are able to do so wisely. To this end, the foundation of crystallographic education

should begin within the undergraduate curriculum. In much the same way that techniques such as mass spectrometry and NMR are introduced and continually reinforced throughout undergraduate education, so should crystallography be an integral part of basic chemistry.

It has been noted that there is a lack of young crystallographers entering the field to pick up where retiring developers are leaving off. By demystifying crystallography for young chemists, we can spark an interest in the discipline that will carry over into graduate and post-graduate careers and help to fill this gap. By developing educational programs such as the ACA Summer School, we can reach scientists of all levels and encourage them not only to use crystallography to support their research, but also to continue to develop the technique.

In my current position at Northwestern, I have the opportunity to participate in undergraduate and graduate level classes where crystallography is incorporated in the coursework. It is inspiring to see undergraduate students elect to pursue crystallography for their independent research projects, and equally inspiring to help graduate students solve their own structures. I will bring this same enthusiasm for crystallography to the Continuing Education Committee

## *John Westbrook – Data, Standards, and Computing*

RCSB PDB - Rutgers University, Piscataway, NJ.

***Research Interests:*** Developing new tools and infrastructure to support technical challenges in data acquisition, data validation and standardization, and data mining in the structural biology and life sciences domains. Current projects include: The RCSB PDB (***rcsb.pdb.org***), the Protein Structure Initiative Structural Biology Knowledgebase (***sbkb.org***), the Nucleic Acid Database (***ndbserver.rutgers.edu***), the 3D Electron Microscopy Database (***EMDatabank.org***), the mmCIF & PDBML Resource sites (***mmcif.pdb.org & pdbml.pdb.org***), and Ligand Expo (***ligand-expo.rutgers.edu***).

***Statement:*** The crystallographic community has a distinguished history in developing standards for data representation and data quality. I believe the ACA Data Committee should continue to play an important role in supporting these activities as it is uniquely positioned to promote a broader understanding of existing and emerging data standards.

This could could be done in various ways. The committee can identify new ways to support and promote the activities of the public data repositories and open source software projects on which our community depends. For commercial database resources and software applications the committee could negotiate licensing incentives for ACA members, facilitate access to these resources for academic users, and promote the adoption of community data standards.

The committee can also sponsor educational outreach activities that take advantage of ACA resources such as *RefleXions*, annual meetings, and the ACA website. Some high priority educational activities include: introductory or tutorial programs for new and young investigators, programs focused on data integration, and programs targeting data issues with new and leading edge technologies.

Data standardization can also extend to providing unambiguous digital identifiers for individuals. A number of open standards are emerging which aim to provide this functionality. By selecting an open identifier standard and facilitating its adoption by the ACA, the DSC committee can help members establish secure and portable digital identities linked to their professional profiles and publication data.

## *We gratefully acknowledge the continued support of* ACA CORPORATE MEMBERS *and welcome new members*

*Agilent Technologies*
**www.agilent.com**

*Area Detector Systems Corp.*
**www.adsc-xray.com**

*Art Robbins Instruments*
**www.artrobbinstrumentscom**

*ATPS Inc.*
**www.atpsinc.com**

*Axxora LLC*
**www.axxxora.com**

*Blake Industries, Inc.*
**blake4xray@worldnet.att.net**

*Bruker/AXS*
**www.bruker-axs.com**

*Cambridge Crystallographic Data Centre*
**www.ccdc.cam.ac.uk**

*Charles Supper Company, Inc.*
**www.charles-supper.com**

*Cryo Industries of America, Inc.*
**www.cryoindustries.com**

*Dectris Ltd.*
**www.dectris.com**

*Douglas Instruments Limited*
**www.douglas.co.uk**

*Int'l Center for Diffraction Data*
**ww.icdd.com**

*Incoatec GmbH*
**www.incoatec.de**

*Jena Bioscience GmbH*
**www.jenabioscience.com**

*MiTeGen LLC*
**www.mitegen.com**

*Molecular Dimensions, Inc.*
**www.moleculardimensions.com**

*Nexus Biosystems*
**www.iori.com**

*Oxford Cryosystems*
**www.oxfordcryosystems.com**

*Rayonix/MAR USA*
**www.mar-usa.com**

*RCSB-Protein Data Bank*
**www.rcsb.org/pdb**

*Rigaku Americas, Inc.*
**www.Rigaku.com**

*TTP LabTech Ltd*
**www.ttplabtech.com**

*Wyatt Technology*
**www.wyatt.com**

*Xenocs* **SA**
**www.xenocs.com**

Sponsorship Opportunities are Available for the 2012 ACA Meeting in Boston

*QUARTZ* *($100 - 499)*

*SAPPHIRE* *($500 - 999)*
Avanti, Inc.

*EMERALD* *($1000 - 2499)*

*RUBY* *($2500 - 4999)*
Dectris, Inc.

*DIAMOND* *$5000+*
International Union of Crystallography

***The following notes were written by recipients of 2011 ACA travel grants. They were asked to comment on their personal experiences at the ACA meeting: what they thought of the venue, the events for young scientists, the overall program and their own presentation, were they first timers and whether or not they are ACA members. They were unanimous in giving thanks for the award and many indicated that they would not have been able to attend without the additional support provided by the student travel fund. These 'kids' are our future – please keep this in mind when you are asked to contribute to the travel fund.***

***Vishal N Koparde***

The organization of the meeting created a perfect environment for interaction with experts in the field and gave me the opportunity to meet other researchers like myself. I particularly enjoyed the presentations in the *Protein Structure Initiative* sessions and believe that it would be great if, after the meeting, the talks were available for download as PowerPoint files for attendees. I would also like to point out that the food at the opening ceremony and the YSSIG mixer was really delicious and provided a good taste of Cajun hospitality. I was extremely honored to present my research to some of the best protein crystallographers in the world. Their feedback has been the most valuable for me and I am sure will help me propel my research in the right direction.

I would also like to thank my mentor, Glen Kellogg, for supporting me in every way possible. I look forward to attending more ACA meetings in the future.

***Hsiu-Wen Wang***

Science is not only about discovery, but it is also about communication. Thanks for giving me an opportunity to experience a conference focusing on a wide variety of crystallographic studies. I am now an ACA member and this was my first ACA meeting and it was a great pleasure to meet and talk to so many different people. I was very excited to talk to those who share the same ideas that I do and to listen to those who are passionate about the world of symmetry in different subjects. Lots of what I learned during the meeting will be valuable in my future research and I plan to rejoin the ACA next year.

***Ian Stokes-Rees***

New Orleans was my first ACA experience. As a computational biologist it was interesting to spend several days speaking with industry scientists, visiting the booths, and seeing some of the latest and greatest equipment on display. As an engineer by training, scientific instrumentation always fascinates me. My own research focuses mostly on novel computational techniques for protein structure determination, so I collaborate with crystallographers. During the past year some of the tools and techniques I've worked on have had wider use in the community, so attending the meeting allowed me to present a poster on this work and to speak with people who had tried the web-based service we host at Harvard Medical School. People who hadn't used the service also took time to talk about how it could help them solve difficult structures, and many people provided valuable suggestions on how to improve the technique.

I was able to catch up with people from the RCSB, CCP4, Phenix, Global Phasing, and HKL. Speaking with beam line scientists also allowed me to discuss some promising collaborations in person rather than by phone or email, and some of these collaborations are now moving forward. There were many interesting talks even for a non-crystallographer such as myself, and I was impressed to see how many sessions were standing-room only.

The engagement of the YSSIG was also great -- a group of early career researchers who want to make connections and contribute to the effectiveness of the ACA itself and add to the value of the meetings by helping develop the field and growing the membership.

Finally, what a great city New Orleans is! It was great enjoying the food and atmosphere with colleagues and we look forward to hosting the ACA here in Boston this time next year.

***Briony Yorke***

I was extremely excited when I first saw the program for the meeting as a number of sessions were extremely relevant to my area of research. Without the travel grant it would have been difficult for me to fund the trip from the United Kingdom and so I am grateful for the opportunities presented to me by the ACA both before and during the conference.

As a new PhD student starting my research in time-resolved crystallography I was particularly excited by the opportunity to see both Keith Moffat and Philip Coppens present their work. As a first time attendee I was a little apprehensive about attending without other members of my group or PI but found the atmosphere welcoming and supportive. It was easy to approach people to discuss their work and I found that even the most distinguished

scientists were happy to take the time to share their thoughts regarding my poster. I was honored to receive the RSCB PDB poster prize and found the awards banquet provided an opportunity to socialize with people working in diverse fields.

The location of the meeting was fantastic, everyone seemed to appreciate being so close to the cultural center of New Orleans and there were many opportunities to sample the local cuisine and culture. I would like to extend my thanks to the many people who went out of their way to help make my trip both productive and enjoyable.

*Anna Kowalska*

I am a graduate student at Technical University of Lodz, Poland and a visiting student at University of Virginia. I was excited to have an opportunity to present results of my scientific work at the meeting in New Orleans.

The whole time I spent in New Orleans was really interesting and fruitful. This was my first chance to attend such a prestigious world class conference. The excellent presentations lived up to my expectations.

I am excited about my scientific work, and I feel grateful to have been able to share and discuss my results with outstanding professionals in the field. This was an excellent platform to establish myself and gain new insight into possible areas of research. I attended numerous lectures and some of them broadened my knowledge in areas I am already familiar with, but there was also a whole list of subjects that were still an enigma for me. That reminds me of a quote of Isaac Newton "What we know is a drop, what we don't know is an ocean". I am sure that attending the conference helped to fill a little bit of this ocean of my ignorance. Also as a graduate student at Polish and American universities this international conference was a perfect place to build a scientific network between not only two continents but worldwide.

I have only one suggestion for future meetings which might be helpful. It would be excellent if the chairs of parallel sessions would kindly request from speakers to keep their talks within the allocated time limit. This would allow the participants to move from one session to another during the breaks between speakers without disturbing anybody's talk.

I am looking forward to Boston!

*John Roudebush*

This was my first ACA meeting as well as my first visit to New Orleans. It was also the first time I had presented my work to an audience of crystallographers and I really did not know what to expect.

My first impression of the meeting was in regards to its size: larger then a Gordon conference but smaller then ACS or MRS. Even smaller considering that I belong to the subgroups of small molecule and solid state crystallographers. I missed the new attendee orientation session due to a preexisting conflict, so I felt a bit confused when I first arrived. Fortunately some collaborator friends were happy to show me around and soon enough I felt welcome.

The conference attendees and events all gave the impression of a small community, and a nice event to see your friends at, year after year. The *Would you Publish this* session was both informative and entertaining. I learned and laughed a lot. The award dinner was a bit of a mystery to me. I didn't buy a ticket, but in hindsight I feel like I should have, because most people did, although I didn't really feel "in the know" enough to go. The city of New Orleans was a fantastic experience: architecture, culture, waterfront, wine bar and music are just a few words that describe my memorable experiences.

When it came time to prepare my talk "knowing your audience" was a challenge. My area, solid state chemistry, begs to have some background presented to give the audience a connection between the crystallography and the properties of the materials. I also felt obliged to give some background on the crystal structure and the techniques I used for the refinement. But after doing all this, I felt like my talk "fell flat". I think it was just too much information at once for a general audience. It was an experience to learn from, and I'm happy for it. I hope to attend and present at ACA again!

*Melanie Kirkham*

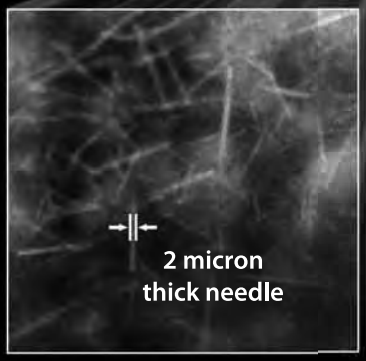
This was my first ACA conference, and it was very enjoyable. The smaller size and tighter focus was a nice contrast to larger general-interest meetings. The smaller size also facilitated meeting new people, and the tighter focus meant there were many engaging presentations close enough to my field to be of interest, but far enough away to introduce me to new ideas and research areas.

I started the ACA experience by attending the *Symmetry-Mode Analysis* workshop taught by Branton Campbell, Harold Stokes and Manuel Perez-Mato. The workshop was an excellent introduction to a newer technique with lots of potential for extracting meaning from crystal structure distortions and for looking at the relationships between structures. My only wish is that we would have had more time to go into the details of the technique.

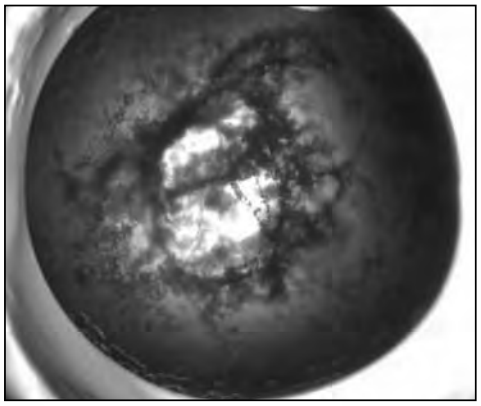
During the conference itself, I attended primarily the materials science-oriented sessions. These sessions contained a lot of interesting talks, including in the areas of pair distribution function analysis, magnetic structures and many reports of distinctive crystal structures, superlattice structures, etc. I was honored to be asked to present in the *Materials for a Sustainable Future* session, chaired by Ashfia Huq and Claudia Rawn. The other speakers in the session presented many insightful talks in areas such as batteries, thermoelectrics and metal-organic framework materials.

# 2 µm

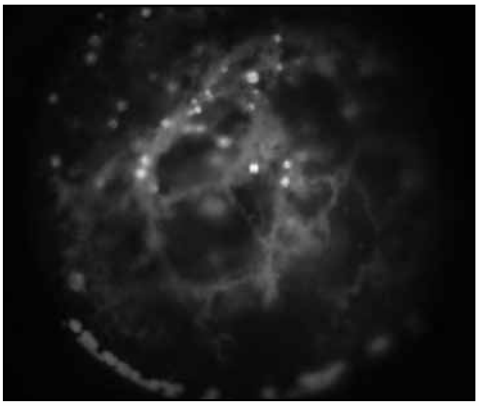
Leading With Innovation




## Minstrel™ DT UV



Visible image of microcrystals in precipitate



UV image of microcrystals in precipitate


## Ultra high resolution optics. Benchtop affordability.

Rigaku is dedicated to delivering the highest image quality possible on the market. This is evidenced with the previous release of our Minstrel HT UV optics. In continuation of this discipline, we are pleased to announce the delivery of our highest image resolution capability in an affordable bench top format. We proudly introduce the new Minstrel DT UV system.

Our optics are not "off the shelf", but custom designed specifically for the imaging of protein drops with both visible and UV light. With this system, you will be able to detect features below 2 µm, as with the needle crystal shown above.

**Which leaves one question:**
**What will you see with your new Minstrel DT UV?**

Rigaku

Rigaku Corporation and its Global Subsidiaries
website: www.Rigaku.com | email: info@Rigaku.com

I was not previously an ACA member, joining specifically for this meeting and I have also enjoyed the *Physics Today* magazine. The ACA's commitment to supporting upcoming and early-career crystallographers is also very helpful and encouraging. Continuing to be an ACA member is definitely in my plans.

***Eric Reinheimer***

I continue to marvel at the new and amazing scientific discoveries being reported each year. One of the first talks I attended, *Massively Parallel Geometric Calculations of Small Molecule Crystal Structures*, was presented by Jason Mercer during the first GIG. I found this talk fascinating as these methods could be used to find candidate void spaces in metal-organic frameworks and to design small molecules for host-guest interactions. This talk was followed by a talk by Olga Smirnova where she outlined her work on new models in mathematical crystallography. In the session covering practices useful in the publication of crystallographic data, I especially enjoyed the talk presented by Jerry Jasinski in which he outlined the crystallographic publication toolbox he has used successfully with his undergraduate researchers. As a young crystallographer, I found his instruction very worthwhile and informative.

I also attended the series of lectures dedicated to Philip Coppens. The talk given by Eric Collet was excellent and summarized how time resolved x-ray diffraction techniques can be used to study materials capable of undergoing a phase transition, such as the famous TTF-chloranil. Later talks during the same symposium by Yu Wan and Sebastien Pillet summarized how the methods pioneered by Coppens have been extended to spin crossover materials. Later, I was given the extreme pleasure of filling in for Katherine Kantardjieff as the session chair for the *Undergraduate Research Symposium*. Awards for outstanding research presentations were given to Stephanie Cowin of the University of Missouri-St. Louis for her presentation, *Steric Effects of Metal Halide Layers and Clusters* and to Mary Elizabeth Parker of the University of Tennessee-Knoxville for her presentation titled *Single Crystal Growth, Crystallography and Magnetic Properties of Maus' Salt*. To see the poise each of these young ladies displayed during the course of their presentations was very rewarding.

As always, the *Cool Structures* session was very interesting. The results reported by Nathan Schley on his water-soluble iridium half sandwich complexes for catalytic water oxidation were quite fascinating. I later marveled at the presentation by Peter Müller in which he outlined the course of actions he took to solve and refine a tricky crystal structure. Later, the structure and disorder in $K_4V(NCS)_6(OCMe_2)_x$ was described in great detail by Saul Lapidus.

The session I found most beneficial highlighted crystallographic teaching techniques and how ingredients from your local grocery store can help to teach how the proper screening of conditions can be streamlined to accentuate teaching of high throughput methodologies. Later in this session, Nigam Roth highlighted some crystallography experiments using amino acids, useful for an undergraduate laboratory because of their ease in crystallization due to hydrogen bonding effects.

The poster sessions always represent a wonderful opportunity to peruse examples of diverse research topics presented by researchers from around the globe. During the course of my poster session, I had the chance to meet and discuss the formation of a potential collaboration with a researcher from UC Davis. Poster sessions such as these not only highlight the great work by each researcher, but also provide the backdrop for critical thinking and idea exchange. One cannot discount the camaraderie that exists among crystallographers. The poster sessions gave me the opportunity to interact with many great crystallographers whose careers and successes I hope to someday mirror.

The first professional conference I attended as a young MS student was the 2001 ACA meeting in Los Angeles. Ever since that first interaction with ACA and with those whom compose its membership, I have been a member. As my scientific career has progressed, I still feel that the passion displayed by its members and staff can serve as an example to all scientific societies. Again, I sincerely thank the American Crystallographic Society for their generous award of the travel grant. The annual meeting of the ACA was an extremely rewarding experience, one that I plan on continuing in the many years to come.

***Kevin Eccles***

This was my first international conference and I traveled from Cork in the Republic of Ireland to attend. As a PhD student involved in crystal engineering and cocrystallization, the amount of crystallography I do is focused towards small molecule crystallography. For me the ACA meeting was both enjoyable and educational bringing together a large variety of disciplines that showcased the broad range and challenges of crystallographic research. The meeting showed me the limitless potential of crystallography, and the importance it has on everyday research.

The friendly atmosphere and helpful nature of both the ACA committee and the attendees made the meeting a pleasant experience for me. I thought the research presented was outstanding which reflects the tremendous job the program committee did in selecting the speakers. I enjoyed meeting researchers who were as passionate about crystallography as I am.

The conference was different than what I was expecting. The atmosphere was relaxed and I received many positive suggestions and comments on some problems that had come up in my research. The new student orientation on the first day was particularly important. It allowed me to meet and talk with other new students close to my own age that helped remove some of my nervousness. The session was

# GRYPHON LCP

## Mix And Dispense LCP With The Gryphon LCP


### Fastest Setups

The Gryphon LCP sets up plates fast, reducing evaporation and providing reproducible results. A 96 reaction plate is ready to seal in less than 2 minutes.

### Best In Class Dispensing

Dispense LCP down to 25 nL with less than 5% CVs. Dispense 96 buffer solutions at one time.

### Versatility

- Membrane Proteins
- Soluble Proteins
- GPCR
- Microseeding
- Sitting Drop
- Hanging Drop
- Bicelles
- Sponge Phase
- Mix LCP

ARI
Art Robbins Instruments

*Superior performance and reliabilty... Superior results.*

www.artrobbins.com

chaired by a student that also helped me adjust to the conference lifestyle and plan my schedule for attending talks. The meeting was so vast, with numerous sessions occurring at once, so it was very good to able to plan in advance which sessions to attend.

The speakers in the sessions I attended were well prepared and jumped straight into the topic. Most speakers talked about the topic at hand, and did not over sell a long introduction. A key session for anyone interested in an academic career was the one on *Scholarly and Pragmatic Aspects of Crystallographic Publications Practices*. This session proved insightful with current editors of top journals discussing common errors and problems that arise during publishing. All the poster sessions were very enjoyable and allowed for a more active discussion in an informal setting. The posters on display varied across a broad scope.

Certain areas of the conference were weak such as professional odysseys, which was an informal discussion about career paths and life choices. I could relate to the discussion about the uncertainty in choosing between academia or an industrial career, however I did not really feel that it gave me any insights into my own personal choices. A major disadvantage was that presentations by undergrads and PhD students were competing against more well known speakers. I tended to attend the talks by the more well known speakers and, as a result, did not attend as many undergrad and young PhD students presentations as I would have liked. A comment for future planning would be to have undergrad and young PhD students talks all on the same day.

I am currently an ACA member and I plan on continuing to be a part of the ACA. I hope that my experience in the ACA will help convince fellow academics at my university to become a part of the ACA. One of the major aspects of an academic lifestyle is publishing in journals. Workshops and tutorials on publishing would be of great interest to undergraduate and postgraduate students. *ACS Publications* has a similar idea using e-mail and video links called publishing your research 101 series, which I have found very useful.

***Shimelis Hailu***

This was my first ACA meeting and it was a very good experience. The presentations were informative and showed me the current frontier research in the field, especially in protein crystallography. The presentations were on the exact scheduled time and the way the meeting was organized as a whole was perfect. I noticed that almost all of the posters I saw were on large molecules or proteins and very few were on small molecule structures. I learned (if this meeting was any indication) that this field is among those that are lacking in diversity.

***Erik Yukl***

This was my first ACA meeting as I am new to the field. Having begun a postdoc in a protein crystallography lab about one year ago, I particularly enjoyed the inclusive atmosphere which provided graduate students and postdocs the opportunity to engage with more senior scientists. Despite my novice status, I was even invited to present my research which was an exciting, albeit somewhat nerve-wracking, opportunity.

The quality and impact level of the science presented at the meeting was exceptional. I had the pleasure of hearing about some very exciting research in protein crystallography and was also introduced to some tools and techniques with which I was not familiar. This is the essence of a successful meeting, the introduction of new and stimulating ideas. The meeting was a wonderful introduction to crystallography and I hope to continue attending for many years to come.

***Christopher Davies***

This was my first ACA meeting and my first reaction upon arrival was the small size of meeting, which is very different from the annual meetings of larger professional societies. I thoroughly enjoyed the smaller group because I could navigate around to the different sessions with ease. Also, I especially enjoyed my time at the meeting because it was my first specialized meeting. Being around other individuals that shared a similar interest in using crystallography gave me a greater appreciation for the technique. This was evident during the poster sessions. In discussing my research, everyone I spoke to understood the complexity and work that goes into our research making the discussions more meaningful for me compared to those I have had at meetings where the attendees do not understand or use crystallography. Lastly, this meeting allowed me to connect with professors and students from around the country that provided a wonderful networking opportunity for the future in terms of potential reviewers, colleagues, and employers. Overall, I thought the meeting was productive and well organized. This being my first meeting, I did not really notice anything that I would change for future meetings. I plan on attending the ACA Meeting annually throughout my career.

***Ana E Bianchi.***

The ACA meeting had a special significance for me. I am Argentine and this was both my first international conference outside Latin America and my first stay in the US.

I was impressed by the diverse topics presented, by the quality of the oral presentations and by the huge number of posters, which provided me a wonderful opportunity for interacting with other researchers on subjects related to my own studies . The meeting was really nice and positive for me. My English is not fluent. Therefore, I really appreciated the patience and efforts made by both my peers and the experts to understand me when I explained my work. I also value the suggestions I received on ways to improve my research results with other techniques.

For my first trip to the US I found New Orleans to be an attractive city with fascinating history. I was able to visit two of its plantations and they were certainly impressive.

I would like to conclude this short letter saying that I shall have very nice recollections of the days I spent there.

***Melissa C. Menard***

This was my first ACA meeting and I became a member just prior to attending the meeting. I consider myself a budding crystallographer, and ACA membership has provided me with an opportunity to connect with other crystallographers through the member directory and to look for jobs in the field through the jobs board.

The meeting was very beneficial to my research. The poster session provided a menagerie of different research and a unique opportunity to ask all my burning questions in close contact with prominent members and even some legends of the crystallography community. I presented a poster on my research and serendipitously met someone interested in doing theoretical calculations on my materials. I also took advantage of the exhibition hall to learn about all the latest instrumentation from the no-liquid-nitrogen-necessary cyro system to the new solid-state detectors to the latest dual anode sources. From shaking hands with George Sheldrick and taking a picture with Ton Spek, I had more fun than when I went to Comic Con.

There was a wonderful diversity of talks. My biggest problem was deciding which talks to go to and which to subsequently miss. The most interesting sessions for me were *Crystallography and the Search for New Materials, Materials for a Sustainable Future*, and, my favorite, *Would You Publish This?* Due to a last minute cancellation, I was also given an opportunity to speak about my research in the general session and met with wonderful support and probing questions.

By providing an informal and welcoming atmosphere, the ACA provides a unique opportunity to make connections and learn about new research. I plan on continuing as a member of and hopefully attend the Boston meeting.

***Mary Parker***

Attending ACA 2011 was a rewarding experience for me. Not only did I meet top scientists in my field, but I also met other students interested in crystallography and gave my first talk at a professional conference. Preparing for my talk was an experience in itself. Turning the research I had been working on for the past year into a concise presentation helped me understand the broader impact of my work in the scientific community. I enjoyed attending other talks and was encouraged that I could understand and learn from them even as an undergraduate student. I enjoyed interacting with my mentor, my academic advisor and graduate students from my school who attended the conference, and it was exciting to meet new scientists and students in the field. I was even able to talk to several scientists about opportunities for graduate school. Some fun aspects of the conference included exploring New Orleans, eating Jambalaya, and going to the conference social events. Overall, it was a positive experience and a wonderful trip!

***Pankaj Kumar Giri***

The ACA meeting provided me with a much broader perspective about current advances in x-ray crystallography than you find at most conferences. This will enable me to develop avenues for my research and expand my scope to include areas I hadn't thought of, now and throughout my professional career. The PHENIX workshop was very useful. It provided a good starting point for the remainder of my meeting experience. Most of all, I would say that this experience has brought me a renewed passion and interest in the work that I do as I now see how it fits in and relates to work done by others.

Many of my own research ideas have been born out of my interactions with other scientists (or hearing their presentations) at conferences. Although I have attended other academic conferences and meetings none of them compare to the discussions I had with my peers and great scientists on such a broad range of interesting scientific topics in New Orleans. The entire experience will be quite memorable to me. Although there was time for socializing and relaxing, science was intertwined with everything we did. The injection of mentors into many of the lunches and dinners (especially the mentor and mentee session), and the opportunity to spend time with other young scientists certainly made this an experience I will remember.

Meeting people on both a professional and personal level will have a tremendous impact on my career as a scientist. The conference opened many doors for collaboration and learning. It was a unique opportunity to be able to discuss science with such a diverse group of students.

My presentation provided me with the opportunity to demonstrate my knowledge and potential. It also enabled me to network with renowned experts in the field at this early stage of my career. It was therefore an important milestone for my future working life in research.

***Courtnie Vogelsberg***

Attending the ACA meeting in New Orleans was a great experience. In particular, I especially enjoyed attending the *Fast Science, Modern Aspects of Crystal Engineering*, and *Small Molecule Molecular Machines* sessions. The work that was presented on nano- and pico- second time-resolved x-ray diffraction was beautiful! Additionally, presenting my talk at the *Small Molecule Molecular Machines* session was a great experience. I really enjoyed interacting with the audience members and listening to their feedback. I look forward to attending ACA meetings in the future.

***Clare Rowland***

I applied for a travel grant to attend the ACA meeting in New Orleans knowing that I would be unable to go without one. If I got one, great; if not, no big deal. I'm glad I felt this way at the time: If I had had any sense of what I would have missed by not attending, I would have been a bundle of nerves waiting to hear back. I had previously attended two national ACS meetings but had never been to a smaller conference, and I had no idea what a difference there would be. For one thing, most of the sessions were pertinent to me, and as a result most of the talks I attended were right up my alley. A lot of people must have felt that way because the sessions were all (remarkably) well-attended. In fact, I had anticipated a small turnout for my talk, as it fell on the last day of the conference, but I was surprised to find the room just as full as it had been mid-meeting. Arguably more valuable than attending talks, however, was the ability to broaden and deepen my ties to the crystallographic community. I knew a handful of people in attendance prior to the meeting, and I had a chance not only to catch up with them but also to meet many more. In fact, I met more people and had more in-depth conversations with them than at larger (and 'less intimate') meetings, and many of them will likely remain important contacts throughout my professional career. On a less academic note, the location was phenomenal. Having never been to New Orleans, I was eager to see the city; and it was just a short walk to explore the French Quarter and Garden District, ride the ferry and the streetcar, and eat beignets, po' boys, gumbo, and oysters. In short, anything I could want to do in the Big Easy was practically around the corner (except pet alligators, but I got to do that, too).

***Lauren Hatcher***

I would like to thank the Synchrotron Radiation SIG for the honor of receiving their Etter Award and for the opportunity to be part of such a diverse meeting program. I found the *Transactions* symposium in honor of Philip Coppens particularly enjoyable, with a wonderful selection of interesting speakers. We were spoiled by a wealth of exciting plenary speakers, whose inspiring lectures made it worthwhile braving an early 8 am start! Those early starts were made particularly challenging by the temptation to enjoy the fabulous entertainment on offer in New Orleans both day and night, and particular thanks must go to the local organizers for hosting such a great conference in this vibrant and fascinating city. I really enjoyed my first experience at an ACA meeting and look forward to hopefully having the opportunity to attend more meetings in the future.

***Christopher Kane***

The 2011 ACA meeting was one of the best I've been to. I had the ability to interact with esteemed professors in the field and was provided a very comfortable environment to share my [naïve] opinions among well-respected professionals. I thought the attendance by graduate/undergraduate students my age was appealing. The meeting sessions were well attended and well scheduled. At times I had difficulty figuring out which sessions to attend since there were so many quality presentations scheduled. Most importantly, the number of attendees was excellent; an ACS meeting boasts thousands of chemists, making it difficult to converse with professionals in the field. The size of this meeting, as well as the atmosphere, made interactions more relaxed and enjoyable. Perhaps the only shortcoming with the conference was the price; on top of the $200 registration fee, tickets to the banquet and other events were extra. I feel privileged to have presented at this conference, let alone receive a travel award and look forward to attending next year in Boston, MA.

***Mayank Aggarwal***

Having now been actively involved in protein crystallography for a year, the ACA meeting provided me with a great platform to expand my understanding of frontier studies in the development of both protein and small molecules. It was the first conference I had been to since starting graduate school and I'm happy to say I wasn't disappointed. Meeting with some of the leaders in the field, listening to some excellent talks and looking at how fast the technology is changing by visiting the vendors exhibiting their latest products was fascinating. It is meetings like these that bring students, post docs, professors, vendors and employers together and give them an opportunity to interact in both a professional and social setting.

The poster session was another great way of getting to know what others are doing around the world. My poster was well attended and at no point of time during my session was I without an audience. I won one of the best poster awards and it instilled in me great confidence for public speaking.

I believe the meeting was very successful and I applaud the organizers for doing a great job.

no liquid...

no dewar...

no compressor...

...what a breath of fresh air

## Allow us to introduce the DTC.

**For uncomplicated sample cooling, the Desktop Cooler (DTC) is hard to beat. The DTC refrigeration unit and a dry air source; that is all that's required to deliver a cold gas stream with a temperature range of 170 Kelvin to room temperature.**

The mechanical cooler does not require a separate helium compressor, which means that cooling water is not required and maintenance is reduced to virtually zero. The DTC is simple to set up and control and can be left running for weeks at a time.

Certainly, for those working within this temperature range, the DTC offers convenient and simple cooling at an attractive price.

Now isn't that a breath of fresh air?

Oxford Cryosystems

**For further information on the DTC visit www.oxcryo.com**

*Orrassa In-Noi*

I am a graduate student from Suranaree University of Technology in Thailand. This was the first time I ever attended an ACA meeting and everything about the meeting impressed me and makes me want to come again. The meeting provided me with many opportunities to interact with experts in the overall field of crystallography and applied materials chemistry.

The experience of seeing another country and talking with internationally known scientists will certainly be beneficial for my professional growth. I learned about research trends and updated myself on technology from the exhibit booths. I also had a great experience sightseeing around New Orleans.

### *USNCCr Travel Grants to the Madrid Congress*

This summer, the US National Committee for Crystallography (USNCCr) in conjunction with the ACA organized a travel fellowship grant for US early career scientists involved in crystallography research to present their work at the XXII Congress of the International Union for Crystallography (IUCr), held in Madrid, Spain, on August 22 – 30, 2011. The funding for the program was generously provided by the National Science Foundation, CHE-1118370.

Fourteen fellowships were granted to the following early career scientists: Heba Abourahma (The College of New Jersey), Breann Brown (Brown University), Weiming Bu (University of Pennsylvania), Benjamin Frandsen (Brigham Young University), Tara Michels-Clark (University of Tennessee), Gregory Halder (Argonne National Laboratory), Kathryn Hastie (The Scripps Research Institute), Lyndal Jensen (University of Minnesota), Melissa Menard (Louisiana State University), Gary Nichol (University of Arizona), Silvina Pagola (College of William and Mary), Jason Porta (University of Nebraska), Stacey Smith (Brigham Young University), and Alex Vecchio (The State University of New York, Buffalo & The Hauptman). Furthermore, a one-on-one mentoring experience was also provided (pre, during, and after the Congress) to the early career crystallographers. All the mentors were current or past UNSCCr members such as Miriam Rossi, Marvin Hackert, Joseph Ng, Peter Stephens, Victor G. Young, Chris Cahill, Gloria Borgstahl, Angus Wilkinson, Brian Toby, Katherine Kantardjieff, Jim Kaduk, Bernhard Rupp, Amy Sarjeant, and George Phillips.

On August 23rd, the USNCCr organized a mentoring dinner where Lesia Crumpton-Young, who received in 2009 the prestigious Presidential Award for Excellence in Science, Mathematics, and Engineering Mentoring, gave a presentation entitled *You've Got the Power: Being the Best Mentor*. In addition, on August 24th, the USNCCr in cooperation with the Spanish crystallography community organized a US-Spain reception that was attended by 140 crystallographers from the US, Spain, and Latin-America. The goal of the event was to foster collaborations between crystallographers in these regions, with many major professors and their respective graduate students invited, including mentors and mentees.

Finally, an IUCr Young Observers experience was also provided to our travel fellows.The US awardees were the first early career cohort attending the General Assembly as observers. The USNCCr hopes this science policy experience facilitated the development of a future generation of crystallography leaders.

Some of the many highlights the awardees listed when describing their impressions after the Congress were: meeting foreign colleagues and potential collaborators, discussing their research with distinguished members of the international community, exposure to current international research, unique international perspectives on similar research topics, as well as networking for collaborative opportunities and career development.

*"Attending international meetings is very important from my point of view because it allows one to see what others are doing in other parts of the world in one's specific area of research. This is key for advancement and research progress. The cost of travel to such international meetings is prohibitive most of the time, so having a travel fellowship helps tremendously in making the trip happen."*

All awardees reflected on the importance of financial support received from NSF that made this travel fellowship program possible, noting that they would not have been able to attend the Congress otherwise.

*Ana Ferraras*


***US Delegates to the IUCr Congress in Madrid from left to right: Victor Young (University of Minnesota), Chris Cahill (George Washington University), Katherine Kantardjieff (Chair, California State Polytechnic University), Brian Toby (Argonne National Laboratory) and Joseph Ng (University of Alabama, Huntsville).***

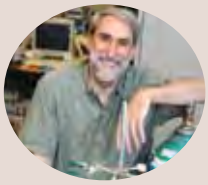
## 2012 Award Winners

Etter Early Career
Emmanuel Skordalakes

Buerger
John Spence

Supper
Ron Hamlin

Warren
Paul Fenter



Wood
Daniel Nocera

The ACA gratefully acknowledges contributors to the various award funds

### M J. BUERGER

Rudolf Allmann
Helen M Berman
Abraham Clearfield
Philip Coppens
Karl F Fischer
Theodor Hahn
Andrew Howard
Heinz Jagodzinski
Michael James
Carroll Johnson
Judith Kelly
James Knox
William C Stallings
Hugo Steinfink
Robert M Sweet
Thomas C Terwilliger
Thomas R. Webb
Bernhardt J Wunsch

### M C. ETTER EARLY CAREER

Christer Aakeroy
J Michael Bennett
Helen M Berman
Joel Bernstein
Doyle Britton
Carolyn Brock
William R Busing
Abraham Clearfield
William L Duax
Paula Fitzgerald
Judith C Gallucci
Richard Gilardi
Jane F Griffin
Lyndal Jensen
Clara Kielkopf
Cheryl Klein Stevens
Mariusz Krawiec
Roger Lalancette
James H Loehlin
Edgar F Meyer
Bruce Noll
William H Ojala
Pius S Padayatti
Connie Rajnak
Timothy Rydel
Carl H Schwalbe
Dmitriy Soldatov
Leonard J Soltzberg
Vukica Srajer
William C Stallings
Edwin Stevens
Robert M Sweet
Thomas C Terwilliger
Raymond C Trievel Jr.
Thomas R. Webb
Mark Whitener
Victor Young

### LATIN AMERICAN INITIATIVE

Edward Collins
Jose Miguel Delgado
Mary DeLucia
Graciela Diaz de Delgado
William L Duax
Frode Mo
Robert M Sweet
Doletha Szebenyi
Thomas C Terwilliger
Brian H Toby
Iris Torriani

### I. FANKUCHEN

Helen M Berman
Robert H Bragg
Bruce W Brown
Donald Caspar
Abraham Clearfield
Philip Coppens
Hellmut J Juretschke
J Lawrence Katz
Eaton E Lattman
Frank Milillo
Connie Rajnak
Michael G Rossmann
Timothy Rydel
William C Stallings
Hugo Steinfink
Robert M Sweet
Doletha Szebenyi
Thomas C Terwilliger
Dale Tronrud
Thomas R. Webb
Winnie Wong-Ng

### A. L. PATTERSON

Andrew J Allen
Helen M Berman
Horace Carrell
Abraham Clearfield
Philip Coppens
Fred Dyda
Paula Fitzgerald
Frank Fronczek
Richard Gilardi
Jenny Glusker
Philip W Hemily
W G J Hol
Xinhua Ji
Alan D Mighell
M. Gary Newton
Bruce Noll
C E Nordman
Edward Prince
Connie Rajnak
W Robert Scheidt
Nadrian C Seeman
George M Sheldrick
Vukica Srajer
William C Stallings
Robert Stewart
Robert M Sweet
Thomas C Terwilliger
Dale Tronrud
Thomas R. Webb

### L. PAULING

Helen M Berman
Abraham Clearfield
David E Cox
David R Davies
Robert Degeilh
William L Duax
David J Duchamp
Paula Fitzgerald
Frank Fronczek
Judith C Gallucci
Richard Gilardi
Kenneth Hardcastle
Hakon Hope
Andrew Howard
Carol P Huber
Thomas Hurley
Steven Jordan
Pavol Juhas
Hellmut J Juretschke

*Pavel Karen*
*Clara Kielkopf*
*James Knox*
*Matt Larson*
*Catherine L Lawson*
*Mark Mashuta*
*Bruce Noll*
*Richard Norwood*
*Connie Rajnak*
*David Rose*
*Frank J Rotella*
*John Roudebush*
*Timothy Rydel*
*Michael R Sawaya*
*Leroy W Schroeder*
*Brahama D Sharma*
*George M Sheldrick*
*Harold G Smith*
*William C Stallings*
*Robert M Sweet*
*Thomas C Terwilliger*
*Diana R Tomchick*
*Mark Whitener*
*Angus Wilkinson*
*David Worcester*
*Guangteng Wu*

### STUDENT TRAVEL

*Sourav Adak*
*Ueli Aebi*
*Christine Beavers*
*Brad Bennett*
*Helen M Berman*
*Jeffrey T Bolin*
*Richard G Brennan*
*Roger Burnett*
*Charles W Carter*
*Abraham Clearfield*
*Edward Collins*
*David E Cox*
*Douglas Davies*
*Nicholas Deifel*
*Jeffrey Deschamps*
*William L Duax*
*Drake S Eggleston*
*Ulrich Englich*
*Klaus Fleischmann*
*J. Flippen-Anderson*
*Frank Fronczek*
*Judith C Gallucci*
*Nick Gerasimchuk*
*Richard Gilardi*
*John Helliwell*
*Thomas Hurley*
*Semra Ide*
*T Iverson*
*Michael James*
*Steven Jordan*
*Pavol Juhas*
*Judith Kelly*
*James Knox*
*Thomas Laube*
*Youli Li*
*Frode Mo*
*Bruce Noll*
*Richard Norwood*
*Pius S Padayatti*
*Erich F. Paulus*
*Marc Pusey*
*Connie Rajnak*
*David Rose*
*Michael G Rossmann*
*Frank J Rotella*
*John Roudebush*
*Timothy Rydel*
*Mark A Saper*
*Arthur Schultz*
*Brahama D Sharma*
*George M Sheldrick*
*M Mercedes Silva*
*Edward Snell*
*Vukica Srajer*
*William C Stallings*
*Hugo Steinfink*
*Peter Stephens*
*Robert M Sweet*
*Thomas C Terwilliger*
*Brian H Toby*
*Diana R Tomchick*
*Marie-Claire McKenna*
*Joseph Wedekind*
*Mark Whitener*
*Carrie Wilmot*
*Amanuel Zellelow*

### SUPPER

*Abraham Clearfield*
*Andrew Howard*
*Carol P Huber*
*James Knox*
*Masahi Miyano*
*Bruce Noll*
*Robert M Sweet*
*Thomas C Terwilliger*
*Thomas R. Webb*

### B. E. WARREN

*John Barnes*
*Michael Bedzyk*
*Robert H Bragg*
*Abraham Clearfield*
*Philip Coppens*
*David E Cox*
*Takeshi Egami*
*Heinz Jagodzinski*
*Youli Li*
*Leroy W Schroeder*
*Lester Siegel (in memoriam)*
*Robert M Sweet*
*Thomas C Terwilliger*
*Thomas R. Webb*
*Winnie Wong-Ng*

### E. A. WOOD

*S C Abrahams*
*Lawrence S Bartell*
*Helen M Berman*
*Abraham Clearfield*
*Melinda Dixon*
*Richard Gilardi*
*Ethan A Merritt*
*Bruce Noll*
*Edward Prince*
*Connie Rajnak*
*Timothy Rydel*
*James L Smith*
*William C Stallings*
*Robert M Sweet*
*Thomas C Terwilliger*

### HISTORY

*J. Flippen-Anderson*

### K. N. TRUEBLOOD

*Lawrence S Bartell*
*Helen M Berman*
*Joel Bernstein*
*Horst Borrmann*
*Doyle Britton*
*Carolyn Brock*
*Horace Carrell*
*Abraham Clearfield*
*Charles L Coulter*
*Robert Degeilh*
*David J Duchamp*
*Frank Fronczek*
*Judith C Gallucci*
*Jenny Glusker*
*Elizabeth J Goldsmith*
*James A Golen*
*Kenneth Hardcastle*
*Hakon Hope*
*Carol P Huber*
*Lyndal Jensen*
*Lisa A Johnson*
*Richard E Marsh*
*Emily Maverick*
*Bruce Noll*
*Connie Rajnak*
*Brahama D Sharma*
*George M Sheldrick*
*Anthony Spek*
*William C Stallings*
*Robert M Sweet*
*Thomas C Terwilliger*
*Ivan Vorontsov*
*Thomas R. Webb*
*Mark Whitener*

### BOB BAU

*Abraham Clearfield*
*William L Duax*
*Douglas M Ho*
*Judith Kelly*
*Bruce Noll*
*John Roudebush*
*Carl H Schwalbe*
*George M Sheldrick*
*Robert M Sweet*
*Thomas C Terwilliger*
*Thomas R. Webb*
*Winnie Wong-Ng*

### Silver Honor Roll

*(donations of 500-1000)*

**The estate of Lester Siegel**

*Local Chair - Peter Müller*
*pmueller@mit.edu*

*Program Chair - Bruce Foxman*
*foxman1@brandeis.edu*

*Program Chair - Bruce Noll*
*bruce.noll@bruker-axs.com*

*Poster Chair - Ilia Guzei*
*iguzei@chem.wisc.edu*

*Session Photos - Jeff Deschampdes-champs@nrl.navy.mil*

Boston 2012
AMERICAN CRYSTALLOGRAPHIC ASSOCIATION

***July 28 - August 1, 2012***
***Westin Waterfront Hotel***
***Boston, Massachusetts***
***Deadlines:***
***Abstracts: March 31, 2012***
***Travel Grant Applications: March 31, 2012***
***Advance Registration: May 31, 2012***
***Hotel Reservations: July 5, 2012***
***Abstracts accepted online only***
***40% of all talks will be from contributed abstracts***
***Submit abstracts - Register - Full call for papers***
***www.amercrystalassn.org/2012-meeting-homepage***
***Sponsorship Opportunities***
***www.amercrystallasssn.org/2012-sponsorship***
***Information for Exhibitors***
***www.amercrystallasssn.org/2012-exhibits***

## *Workshops*

***Refmac and Coot***
**Organizers: Paul Emsley & Garib Murshudov**

***Structure Refinement and Disorder Modeling with OLEX2***
**Organizer: Ilia Guzei**

***Modeling Refinement of Nanoparticle Structures from Diffraction Data***
**Organizers: Thomas Proffen, Katherine Page & Reinhard Neder**

***Crystallography - World of Wonders (K-12 teachers)***
**Organizers: Cora Lind & Claudia Rawn**

## *Award Symposia*

***Buerger Award in honor of John Spence***
***Warren Award in honor of Paul Fenter***
***Suppper Instrumentaion Award in honor of Ron Hamlin***
***Margaret C. Etter Early Career Award in honor of Emmanuel Skordalakes***

## *Transactions Symposium*

***Transformations and Structural Oddities in Molceulcar Crystals***
***In Honor of Bruce M. Foxman***
**Organizers: Kraig wheeler, Magali Hickey & Gracia Diaz de Delgado**

## *Plenary Lecture*

***Don Caspar - The History of Structural Biology***

## *Banquet Speaker*

***Daniel Nocera - 2011 Wood Award Recepient***

## *Microsymposia*

*SAS*
**Macromolecular Science with Scattering Methods – Chair: Xiaobing Zuo**
**Functional Nanomaterials – Chairs: Kevin Yager & Tad Koga**
**Precipitates and Voids in Advanced Materials – Chair: Ken Littrell**
**Complementary Techniques in Structural Biology – Chairs: Eddie Snell & Arwen Pearson**
*BioMac*
**Structural Genomics for the Home Lab – Chair: Ward Smith**
**Structural Approaches to Enzyme Mechanisms – Chairs: Karen Allen**
*BioMac and YSSIG*
**Exciting Sructures – Chairs: Eric Armstrong & Graeme Conn**
**Data Collection with the Pros – Chairs: Ed Collins & Andrew Torelli**
**Structural Enzymology – Biology: Chairs: Zac Wood & Cynthia Stauffacher**
*BioMac and Synchrotron*
**Radiation Damage – Chairs: Stephan Ginell &Ana Gonzalez**
**Membrane Proteins from Start to Finish – Chair: Vadim Cherezov**
**Extended Wavelength X-ray Crystallography – Chairs: B.C. Wang & Bob Fischetti**
*Service & Small Molecule*
**25 Years of Service Crystallography: Past and Future – Chairs: Ken Haller & Curt Haltiwanger**
*YSSSIG*
**Etter Early Career Award Symposium – Chairs: Eric Montemayor & Yulia Sevryugina**
*Small Molecule*
**Important Science From Small Molecule Structures – Chairs: Larry Falvello & Alberto Albinati**
**Cool Structures – Chairs: Xiaoping Wang & Jeanette Krause**
*GIG, Small Molecule and Continuing Education*
**Protein and Small Molecule Crystallography at Undergraduate Institutions: Research, Pedagogy and Professional Development – Chairs: Kraig Wheeler & Roger Rowlett**
*Service*
**Would you Publish This? – Chair: Carla Slebodnick**
*Synchrotron*
**Advanced Hardware and Applications – Chair: John Rose**
*SAS & Synchrotron*
**Emerging Sources: Theory and Practice (3 sessions) – Chairs: Marius Schmidt, Yun-Xing Wang, Byeongdu Lee, Lin Yang, Volker Urban & Keith Moffat**
*GIG*
**General Interest – Chairs: Allen Oliver, Jeanette Krause**
*Fiber, SAS, BioMac, Synchrotron and Neutron*
**Fibril-Forming Pathological Peptides: Prions, Amyloids, and "Friends" – Chairs: Olga Antipova & Joseph Orgel**
*Materials, Neutron, Powder and SAS*
**Materials For a Sustainable Future (2 sessions) – Chairs: Greg Halder, Andrey Yakovenko &Venkatesh Pignali**
*Materials, Neutron, and Powder*
**Local Structure/Partially Ordered Systems – Chairs: Thomas Proffen & Katherine Page**
***In Operando/In Situ/* Parametric Studies – Chair: Antonio Dos Santos Moreira**
**Functional and Emerging Materials and Technology (2 sessions) – Chairs: Jim Kaduk & Xiaoping Wang**
**Phase Transitions in Inorganic Systems – Chair: Branton Campbell**
**Magnetic Materials – Chair: Ashfia Huq**
*Industrial and Small Molecule*
**Crystallographic Information in Pharmaceutical Res and Dev (2 sessions) – Chairs: Magali Hickey & Matt Peterson**
*Industrial and BioMac*
**Protein Structure Determination in Industry – Chairs: Stephen Burley & Paul Swepston**
*Service and GIG*
**Public Domain Software – Chairs: Xiaoping Wang & Nigam Rath**
*BioMac, Synchrotron and Canadian Division*
**Complementary Methods – Chair: Michel Fodje**
*Fiber, SAS, Synchrotorn, Neutron, Service, and Canadian Division*
**Flesh and Blood: Intact and In Situ Connective Tissue Diffraction Studies - Chairs: Joseph Orgel & Olga Antipova**

## ACA Boston - July 28 - August 1, 2012

***Who Needs to Register :*** Everyone must submit a registration form (including invited speakers) with the appropriate fee.

***New Schedule:*** The 2012 Meeting will have a 4-day, 5 concurrent session pattern such that there will still be as many talks as during a 5 day meeting. The meeting will start with workshops on Saturday, July 28, and scientific sessions on Sunday, July 29 and will end on Wednesday, August 1, after the Awards Banquet.

***YSSIG Activities:*** Following a series of well-received events and sessions at the meeting in New Orleans, the YSSIG is planning several events for Boston. ***The most popular elements of the YSSIG Mixer and the Mentor/Mentee Dinner will be combined into a single event designed to promote professional networking and communication between younger and more established ACA members. Details on the exact time and venue will be posted to the meeting website.*** For those interested in professional development, we hope to fit in a 'Professional Odysseys' panel that will comprise 3-4 crystallographers who have pursued different career paths. They will discuss their experiences, give advice and answer questions. Several sessions at the upcoming meeting are being co-sponsored by YSSIG including a follow-up to the popular "Blackboard Session" held in New Orleans (hybrid workshop/lecture session) that will focus on practical aspects of data collection and maximizing data quality at the beamline with the crystals you've got. Finally, we will host another "Insider's Guide" to the meeting, complete with tips to maximize the impact of your attendance and interests in getting involved as a young scientist or mentor in the ACA.

***Obtaining a VISA:*** Advanced planning by foreign travelers is critical. Not all foreign attendees will need a VISA, however if one is needed: ***Applications should be made 90 days in advance of the travel date. For further information contact: the US Department of State (travel.state.gov/visa/visa_1750.html) .***

***Staying Green:*** As in New Orleans the full set of abstracts will be distributed only on CDs with a hardcopy Program Schedule.

***Hotel Update:*** In an effort to reduce housing costs we have renogiated the contract with the Sheraton to include ***FREE WI-FI*** in the sleeping rooms. The rates at the Sheraton are competetive with other properties in the vicinity. We are able to offer these rates by committing to fill a certain number of rooms. Staying in the conference hotel helps us meet our room block which also brings with it the free meeting space that helps keep registration fees in line and allows us to offer the many 'extras' you have come to know and love.

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

***As further incentive to stay in the conference hotel a number of lucky attendees will be selected at random to receive one nights accommodation free!***

***Financial support:*** Young scientists will able to apply for travel support. Applications should be made by the abstract deadline on the meeting web site.

The Organizing Committee will observe the basic policy of non-discrimination that is in accordance with the statutes of the International Union.

## Registration fees

| Category | Early (before May 31) | Late (after May 31) |
|---|---|---|
| Regular Member | $500 | $700 |
| Retired Member | $195 | $295 |
| Post doc Member | $250 | $350 |
| Student Member | $195 | $295 |
| Nonmember* | $700 | $950 |
| Post doc Nonmember* | $350 | $450 |
| Student Nonmember* | $285 | $385 |
| Guest** | $ 65 | $ 65 |

| | Students / Others |
|---|---|
| WK.01 Refmac and Coot | $100 / $140 |
| WK.02 Structure Refinement and Disorder Modeling with OLEX2 (fee includes lunch) | $130 / 170 |
| WK.03 Modeling and Refinement of Nonoparticle Structures from Diffraction Data | $100 / 140 |
| WK.04 Crystallography - World of Wonders (free for High School Teachers) | |

**Workshop fees will increase after May 31, 2012**

**Social events**

| | |
|---|---|
| Opening Mixer | included in reg. fee |
| Banquet | $70 ($35 students) |
| YSSIG Event | TBD |

* The nonmember registration fee includes a complimentary one year ACA membership. Those registering as nonmember post docs or nonmember students must include documentation of this status with the registration form.
**Guest registration includes Opening Reception and Exhibit Show.
Register on-line or download forms to register by fax or mail.

***www.amercrystalassn.org/content/pages/2011-homepage***
***Questions: aca@hwi.buffalo.edu***

### Meeting Sponsors (as of 12/1/2011)

| | |
|---|---|
| *Diamond* | *IUCr* |
| *Ruby* | *Dectris* |
| *Sapphire* | *Avanti* |

***NOTE: Daniel Nocera (MIT, winner of the 2011 Wood Science Writing Award, will be at the meeting in Boston to receive the Award and present a talk at the banquet.***

### MARCH 2012

8-16 **32nd Berlin School on Neutron Scattering**. Lise Meitner Campus/Helmholtz-Zentrum Berlin fur Materialien und Energie. ***nschool@helmholtz-berlin.de***

19-23 **ICDD Spring Meeting,** ICDD Headquarters, Newtown Square, PA.

26-27 **Small Molecule Interactions Internat'l Symposium,** Ruhr Universität Bochum, Germany ***www.rub.de/smi*** Contact Vera Vasylyeva: ***vv-smi@rub.de*** or Sebastian Marquardt: ***sm-smi@rub.de***

### JULY 2012

28-2 **ACA2012, Westin Boston Waterfront Hotel, Boston, MA. See pp51-53** ***www.amercrystalassn.org***

### AUGUST 2012

7-11 **ECM27 27th European Crystallography Meeting**, Bergen, Norway. ***ecm27.ecanews.org/***

### SEPTEMBER 2012

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

### DECEMBER 2012

20-24 **AsCA'12.** Adelaide, Australia. ***www.asiancrysassn.org***

### JANUARY 2013

8-13 **10th NCCR Pratical Course & 3rd Winter School: Introduction to Biomolecular Modelling,** Kandersteg, Switzerland. Contact Sraboni Ghose, U Zurich Winterthurerstrasse 190 CH - 8057 Zurich.

### JULY 2013

20-24 **ACA 2013 will be back in Hawaii at the Sheraton Waikiki**

### AUGUST 2014

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

## 2012 ACA Summer Chemical Crystallography Course has a New Home

The 10-day course will be offered from June 18 through June 27, 2012 at the University of Notre Dame in South Bend, Indiana, USA. South Bend is about 80 miles east of Chicago, IL and 100 miles north of Indianapolis, IN. The course will emphasize both theoretical and practical aspects of chemical crystallography; diffraction theory, symmetry operations, structure solution and refinement, powder diffraction techniques and high energy sources are some of the topics that will be discussed. No prior knowledge of crystallography is expected from attendees. However, a good understanding of undergraduate level chemistry, physics and mathematics is desirable. Attendees are advised to read either: "*Crystal Structure Analysis: A Primer*, 3rd Ed." by Jenny P. Glusker and Kenneth N. Trueblood (Oxford Univ. Press, 2010) or "*Crystal Structure Determination,* 2nd Ed." by Werner Massa (Springer, 2004) as prefaces for the course.

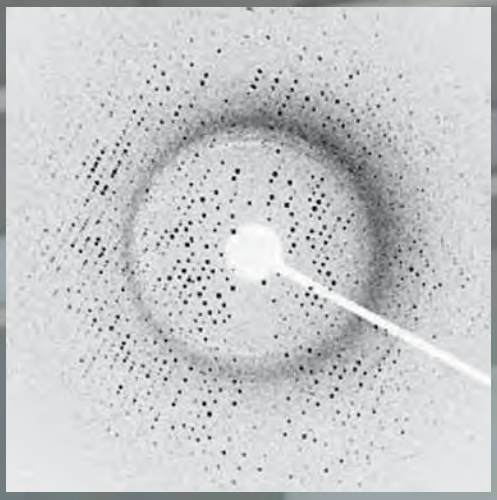
The organizers are aiming for a total of 25 attendees. In previous years there has been a broad demographic of students from both the US and abroad with affiliations in academia, government and industry. Anyone interested in the course is encouraged to apply. The faculty will consist of at least 10 experienced crystallographers with backgrounds spanning corporate to industrial to academia. Tuition will be set at $350 (or $850 for attendees with an industrial affiliation). Housing will be available on-site at Notre Dame for approximately $500 for the entire course for double occupancy. A wide variety of dining options are available on campus.

Scholarships will be available to approximately 12 eligible attendees based on the student's scientific ability and expected benefits obtained from the course. Primarily the course is a graduate level course, however, applications from strong undergraduates will be considered. The organizers wish to encourage international students to apply.

Instrumentation at the University of Notre Dame that will be available for the course includes three single crystal diffractometers operating both molybdenum and copper radiation and two powder diffractometers (one bench-top and one full-size floor mount). Computer support will be provided by the university with computing resources allocated to each student. All commonly used crystallographic software (SHELXTL, GSAS/EXPGUI, FullProf, CRYSFIRE, CRYSTMOL, OLEX-2, shelxLe, TOPOS) and databases (CSD and ICDD) will be available for use.

The course registration form and additional information regarding the course are available at the course website: ***www.acasummercourse.net.*** Completed application forms must be received by one of the organizers: Allen Oliver, Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN 46556, USA; Amy Sarjeant or Charlotte Stern, Department of Chemistry, Northwestern University, Evanstown, IL 60208, USA either by post, or electronically *via*: ***info@acasummercourse.org.*** International students may be accepted early to assist in preparation time for travel visa applications.

*Allen Oliver, Amy Sarjeant and Charlotte Stern*



# Spot the difference?

Two protein crystals grow in the same drop. One diffracts, one doesn't. You have one chance of success, as disturbing the drop means the second crystal dies. Which would you choose?

TAKE THE AGILENT PX SCANNER CRYSTAL CHALLENGE AT
**www.agilent.com/chem/crystalchallenge**



The Measure of Confidence

Agilent Technologies

BRUKER

# Brightest...all air-cooled


## The Exciting New D8 VENTURE with PHOTON 100

Why wouldn't you be excited about a system that has proven high performance, whisper-quiet operation, the brightest microfocus and all air-cooled components that run without the need for water cooling. All these features make the D8 VENTURE a natural choice for your lab and the environment. In addition the D8 VENTURE offers minimal installation requirements, fantastic service support and thousands of dollars of energy savings per year.

**Contact us for more details and system demonstration!** **www.bruker.com/d8venture**

Innovation with Integrity

Crystallography