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## President's Column



As this is my last ACA President's Column, I must first thank those who really make this organization work as well as it does, namely the office staff under the direction of our Director of Administrative Services, Marcia Colquhoun, and our CEO, Bill Duax. Their work on our membership services and the Annual Meeting are first rate. I also want to thank our outgoing Past-President, Marv Hackert, for mentoring me in my duties as President; he has been a tough act to follow. Our finances have been ably directed by our Treasurer, Bernie Santasiero, and our Chief Financial Officer, S. N. Rao. In fact, despite the recession and the tanking of the stock market, the ACA portfolio grew. As my predecessors reported at the close of their terms, the ACA is in sound financial condition. Bernie will continue as Treasurer for another three years. In addition, I want to thank our Secretary, Carrie Wilmot, whose excellent minutes of our Council meetings are invaluable; she will continue next year when our very able Vice President, Judy Kelly, takes over the reins.

You are all reading this in the 2009 Winter edition of *ACA RefleXions* which is edited by Connie (Chidester) Rajnak and Judy Flippen-Anderson. They are to be congratulated for their excellent work; it is always a really great read. By the way they are looking for folks to help out and act as "Guest Editors" and "Section Editors"; please contact either Connie ([conniechidester@earthlink.net](mailto:conniechidester@earthlink.net)) or Judy ([flippen@rcsb.rutgers.edu](mailto:flippen@rcsb.rutgers.edu)) for details if you are interested.

As this issue of *RefleXions* goes to press, the results of our most recent election are in. Our new Vice President is Tom Koetzle; Bernie Santasiero will serve another 3 year term as Treasurer, Carrie Wilmot continues for two years more as Secretary and Michael Murphy was elected as Canadian Representative. I'm still around next year as Past President. We also elected Ross Angel to the Communications Committee, Cora Lind to the Data, Standards and Computing Committee and Frank Fronzak to the Education Committee. Chairs for each of the Special Interest Groups were also selected (see full election results on pages 38-40). I congratulate everyone on their election and hope they have productive terms serving the ACA, and I thank all of you who voted either electronically (wasn't that easy?) or by snail mail. Your participation in this way is really appreciated by the candidates.

We also voted on the proposal to establish the designation of certain of our members as ACA Fellows for their exemplary service to both the science of crystallography and to the ACA. This proposal passed. We will now be working out the details for nominations, selection, etc. so we can begin to honor folks as ACA Fellows.

Our next Annual Meeting is July 24-29, 2010 in Chicago. The program for this meeting is being finalized as I write these notes. We will be presenting the Trueblood Award to Ton Spek, the

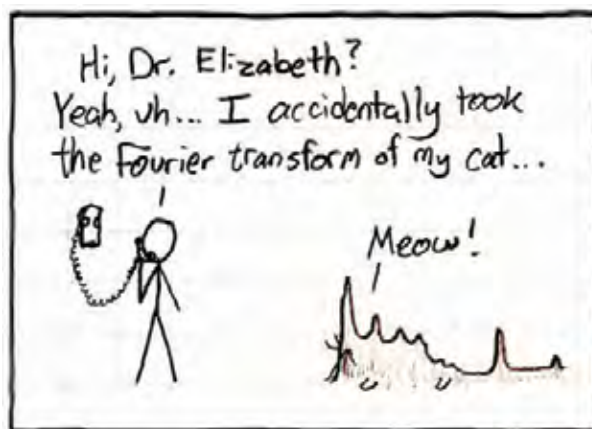
Fankuchen Award to David Watkin and the Etter Early Career Award to Ray Triebel. The program assembled by the SIG representatives and put into final form by Ross Angel, Program Chair, looks to be very exciting with something for everyone. I hope to see you all next year. Chicago is a great city to visit with many museums close at hand and nearby Millennium Park has open air evening concerts on Wednesday, Friday & Saturday. Plan on staying a few extra days to enjoy it.

What is interesting about both the Fankuchen and Trueblood Awards for Chicago is that they are both are being given to people who have developed very influential crystallographic computing systems, PLATON (Spek) and CRYSTALS (Watkin). Modern crystallography is very heavily dependent on software; it is the "lens" that we use to refocus the scattered x-rays or neutrons and create the stunning crystal structure images we use to visualize our results. Moreover, it allows us to probe into these structures and extract the most exacting details of their atomic arrangement. When well done, these programs are more than just "black boxes" having a seemingly magical property of converting diffraction data into crystal structures. The best codes also teach us something about crystallography as we work our way through some difficult problems. As most of you know well crafting this code is in the hands of a very small number of us and that computer code is not like a journal article or a book; it is far more ephemeral and completely dependent on the continued attention of someone (usually the original author) to keep it up to date with new methods, operating system changes and bug fixes. Without this attention, the software rapidly goes out of use and vanishes from the crystallographic landscape. Consequently, we could lose all of the intellectual effort that was expended to create the code, some of which is irreplaceable.

Since my last column we have sadly lost a number of esteemed friends and colleagues; Louis Delbaere, Clara Brink Shoemaker and Lisolette Templeton and we were shocked to learn of the loss of Warren DeLano (37 years old), author of pyMol, a program used by many of us to display protein and molecular structures. In addition, our two award winners

On a happier note, I wish you all the best for the holidays and I hope to see you in Chicago.

Bob Von Dreele



**Notes From the Fall Council Meeting**

**1. Membership Dues.** 2010 membership dues will remain essentially unchanged: regular \$100, postdoc/retirees from \$39 to \$40 and students from \$24 to \$25. Postdocs who moved into a tenure-track position or industry can remain at the postdoc rate until 10 years after the award of their PhD (increased from 5 years).

**2. Annual Meetings.**

**2009: Toronto.** The Meeting was a tremendous success. Attendance was just over 900 (4th largest meeting), and there were more abstracts than ever. Council wishes to thank David Rose and Jim Britten (Local and Program Chairs) and Marcia Colquhoun, Patti Coley, Jennifer Shepard and Crystal Towns for organizing and running the meeting so smoothly. Plenary lectures at the start of each day were well received, and will be continued at the 2010 Chicago ACA Meeting.

**2010: Chicago - 2011: New Orleans - 2012: Boston**

**2013.** The possibility of a joint ACA/ Denver Diffraction Conference (DXC) was extensively researched. Ultimately the meeting logistics of the DXC and ACA were too far apart to enable a joint meeting to be organized. However, it was agreed that Denver would be a great site for a future ACA Meeting.

**2014.** This will be a spring meeting, either in the southwest or west, because of the IUCr Congress in Montreal.

**3. Awards.** The 2010 Etter Early Career (*Raymond C. Triefel*), Fankuchen (*David Watkins*) and Trueblood (*Ton Spek*) award recipients have been selected (*see pages 6-7*). Special sessions at the 2010 meeting will be organized around all three awards. Nominations are due by May 1, 2010 for the 2011 ACA award (*see page 47*).

**4. ACA Website.** This will change between now and the end of year (2009) Updates to the website will be made by ACA office staff rather than by a third party as is currently done. This will enable control over the website and lead to faster posting of material. Minutes of Council meetings (including all the lunchtime meetings that take place during the annual meeting) will be posted on the new ACA website (*see page 36*).

**5. Fellows Program.** The ACA will vote on the possible introduction of a Fellows Program, which would be in-line with other societies, such as the ACS. If it passes the program would not be just for prize winners, but also for service, education and political involvement (*note added at proofing: it did pass*).

**6. ACASIGs.** There has been discussion on how to encourage ACA members to become active participants in the Special Interest Groups (SIGs). This is particularly important as the SIGs effectively organize the annual meeting sessions. The possibility of new ACA SIGs was also discussed. For example the Europeans have a SIG on aperiodic crystals. There is also an IUCr Commission and European SIG on electron diffraction. Council would welcome ideas about developing new SIGs, and ways to strengthen the ones we already have. The JANA 2-day workshop on incommensurate crystal structures at the 2009 annual meeting was very popular, so this could be a potential new SIG. It was decided to encourage attendance at SIG business meetings by using the final 20 minutes of a session organized by the SIG to start the meeting. This will be implemented at the 2011 Annual Meeting.

**7. ACA Summer Schools.** It was decided to broaden the possible summer schools supported by the ACA beyond the current small molecule and macromolecular schools. The Continuing Education Committee has rewritten the Guidelines, which were published in the fall 2008 issue of *Reflexions*. A call for summer school proposals will be announced soon.

**8. IUCr.** A very fruitful dialogue between the ACA and the IUCr was conducted during the 2009 annual meeting. IUCr President Sine Larsen feels the ACA and USNCCr (which currently represent ~50% of crystallographers worldwide) are underrepresented in the IUCr governance. The IUCr is thinking of changing their by-laws concerning the composition of the Executive Committee, which after the General Assembly in Osaka was made up of 3 Asians, 1 Canadian & 6 Europeans. The Executive Committee of the IUCr has officially confirmed that Montreal will be the site of the 2014 IUCr Congress and General Assembly.

*Carrie Wilmot*



*Back row: Jennifer Shepard, Jim Britten, Louis Delbaere, Bill Duax, Bernie Santarsiero, Marv Hackert, Marcia Colquhoun. Front row: Carrie Wilmot, Bob Von Dreele, Judy Kelly, S.N. Rao.,*



## From the Editor's Desk

**Erratum:** - Fall issue of *RefleXions* - page 21: The legend for the speaker photo for Session 1.06 (Carbohydrate Recognition) was wrong. The legend should have read: **Stephen Evans, Jeff Abramson, David Rose, Lyann Sim, Eugene Masters, Anne Imberty, Mark Currie, Ian Schoenhofen, Ken Ng. Xiaoqiang Wang is not pictured.**

**RefleXions staff:** Bomina Yu did a great job on collecting and assembling information for the awards pages in this issue (6-7). She also authored the historical article on Ken Trueblood as part of our series to acquaint younger members with the people for whom the major ACA awards are named. If you hear of an award to an ACA member please send the information to Bomina ([bomina@gmail.com](mailto:bomina@gmail.com)) so she can include it in an upcoming issue. Self-notifications are allowed - please let us know.



**Focus articles:** As part of our continuing series on the environment and evolution we have an article from Jeff Deschamps on the 'Hazards of Water' (see below) and an article from Cele Abad-Zapatero on "The Molecular Structure of Evolutionary Theory" (page 14) and two of the books reviewed by Joe Ferrera deal with evolution (pages 15-16). We also have an update on AIP activities in the area of education policy (page 20) If you do plan to make a visit to the Hill to discuss education or any issues affecting our scientific lives the AIP could be very helpful in setting it up.

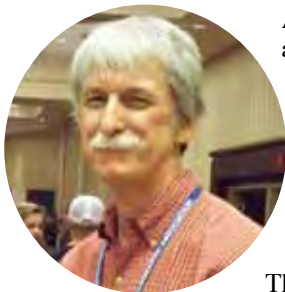
**Cartoons:** The cartoons (pages 2, and 4) in this issue were taken from [xkcd.com](http://xkcd.com) - A webcomic of romance, sarcasm, math, and language.

**Breaking news:** As we went to press we received the sad news that we have lost another noted crystallographer and friend; Liselotte Templeton. Her obituary will appear in the spring issue of *RefleXions*.

**Isn't it ironic department:** We offer this as a timely footnote to the Fall '08 *RefleXions* article "Advice to the New President", - the person that the McCain people finally listed as "Science Advisor" to their campaign, Douglas Holz-Eakin, is now jobless, and his medical insurance company refused to renew his coverage because of a pre-existing condition.

Judy Flippen-Anderson

## The Hazards of Water



As an undergraduate I remember reading an editorial on the hazards of water. It was meant to poke fun at how hazards can be exaggerated based on how they are viewed. After all water is a strong oxidizer (just look at what it can do to a piece of steel), and immersion in water can cause death! Makes you wonder if we should let just anybody handle it.

The editorial was a joke, the ACS journal it appeared in is no longer in print and my attempts to find any trace of this amusing piece on the ACS web site failed, but there are hazards with water... not with the water itself, but the packaging.

In 2004 bottled water usage was 26 BILLION liters. This is more than 28 billion bottles and according to most sources about 85% of these bottles end up as trash. From many *Adopt-A-Road* clean ups I have participated in I can say that a large fraction of the bottles you find by the roadside are from bottled water. These are outnumbered only by bottles from alcoholic beverages. It is ironic that when a local conservation group runs an *Adopt-A-Road* or *Watershed clean up* they distribute bottles of water. To help reduce the number of bottles out there this group has started distributing re-usable aluminum water bottles to their volunteers.

Why the fascination with bottled water? It isn't cheap; bottled water costs > \$1.50 per bottle -- approximately 1,900 times the cost of tap water! Is bottled water better? Many of the folks that drink bottled water think it is safer than tap water. The sad fact is that at least some bottled water is just re-packaged tap water.

Have you looked carefully at that bottled water you drink? Does the label provide an analysis of the water? The Safe Drinking Water Act, passed in 1974, was the first federal law mandating drinking-water standards for all public water systems. Many municipal water supplies, such as for New York City, boast water that is as tasty and pure as the most expensive bottled varieties. By law, municipal water supplies must provide their customers a chemical analysis of their water composition. The same is not true for those expensive bottles.

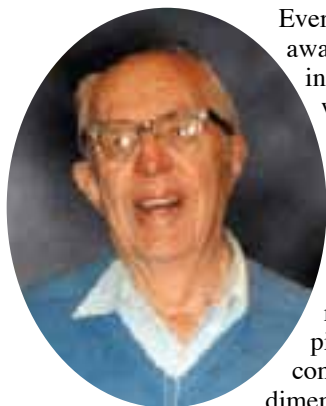
Setting aside safety, producing and distributing all those bottles of water consumes huge amounts of resources. One source estimates that manufacturing the nearly 28 billion plastic bottles used to package water in the United States requires 17 million barrels of oil. The energy required to haul one billion bottles of water every two weeks from bottling plants to supermarkets or convenience stores for sale, and the energy needed for refrigeration consumes additional oil. Depending on who you believe estimates are in the range of 50 million barrels of oil per year to almost 0.85 kg of oil per kg of water (i.e. that a 1 liter bottle of water accounts for ~ 1 liter of oil used in production and distribution)! (See Jennifer Gitlitz et al., *Water, Water Everywhere: The Growth of Non-carbonated Beverages in the United States* (Washington, DC: Container Recycling Institute, February 2007); Pacific Institute, "Bottled Water and Energy," fact sheet, (Oakland, CA: 2007); or [www.treehugger.com/files/2007/02/pablo\\_calculate.php](http://www.treehugger.com/files/2007/02/pablo_calculate.php)).

It costs more, consumes huge quantities of resources, and is likely no better than the water coming out of your tap. What next? According to Reuters, Canberra has banned bottled water, claiming to be the first in Australia to revert to the tap for the sake of the environment. Residents of Bundanoon voted to rid the town of bottled water to combat their carbon footprint. So get a re-useable bottle and start saving money and the environment.

Jeff Deschamps



## ACA Award History - Kenneth N. Trueblood



Every year the ACA presents various awards to honor researchers excelling in different areas of crystallography, whether it be teaching, early career achievements, methods development or science communication. To honor exceptional achievements in computational or chemical crystallography, the ACA founded the *Trueblood Award* in 2001 in memory of Kenneth N. Trueblood, a pioneer in the development and use of computer programs to determine three-dimensional electron-density maps from crystallographic data.

Born on April 24, 1920, Kenneth Nyitray Trueblood was a native of Dobbs Ferry, New York. He moved to Boston to study chemistry at Harvard (AB 1941), and in 1947 he obtained a PhD at Caltech in the lab of Howard Lucas. His PhD research emphasized chromatography and spectrophotometry, but this was not to be his true calling. Inspired instead by the work of Linus Pauling, Trueblood continued on at Caltech as a postdoc and thus began his brilliant career as a crystallographer.

After the two years spent with Pauling, Trueblood moved from Caltech to UCLA as a temporary instructor, replacing James McCullough who was on leave. There he quickly made his mark teaching freshman chemistry and became an assistant professor within a year, full professor in 1960, and professor emeritus after his retirement in 1989. He was also a visiting professor at the University of Ibadan, Nigeria (1964-1965) and a visiting scientist in Moscow at The Institute of Elemento-Organic Compounds (1965-1966). Throughout this time, he remained an exceptional scientist, excelling in all three areas of academic life: teaching, research, and administration, until his passing from melanoma in Los Angeles on May 7, 1998.

He stood out as a teacher. He continued to teach large freshman chemistry classes throughout his UCLA career and taught at many ACA- and IUCr-sponsored teaching schools, always providing his students with clear and relevant presentations. Additionally, he coauthored two books, *Crystal Structure Analysis* (1972) with Jenny Glusker, and the freshman chemistry text *Chem One* (1976

and 1980) with Jurg Waser and Charles Knobler. Both texts have influenced several generations of students.

A one-time graduate student, Bob Sparks, organized a memorial session in his honor at the ACA meeting in Washington, July 1998. There, some of Trueblood's former students described him as a thorough and attentive teacher. He expected them to be precise and innovative in their studies, but also worked hard to ensure that they understood the basic principles of the science. In addition, to their surprise and delight, he knew each of them by name, no matter how large the class. He was always available for them to talk to and often worked alongside his research students all night on the early computers used to help solve crystal structures.

Besides the praise of his students, Trueblood was repeatedly recognized for his exceptional teaching. He was a member of the IUCr Commission on Crystallographic Teaching and received the first UCLA Distinguished Teaching Award in 1961, the National Award for Excellence in Teaching from the Manufacturing Chemists Association in 1978, a Letters and Science Faculty Award from UCLA in 1982 and the Fankuchen Memorial Award for teaching from the ACA in 1995. Shortly after his death the large lecture room where he had taught thousands of students was named the Kenneth N. Trueblood Lecture Hall in his honor.

He also served with distinction in various administrative positions at UCLA, first as Chair of the Department of Chemistry (1965 to 1970), and then Dean of the UCLA College of Letters and Science (1971 to 1974), a position he resigned in order to return to teaching and research. He chaired the UCLA Academic Senate (1983-84). Although he retired and was considered professor emeritus (1989), he was recalled (1990 - 1991) to serve as Chair of the department (now Chemistry and Biochemistry). He also served as President of the ACA (1961), and as a member of the US National Committee for Crystallography (1960 to 1965; Vice-Chair 1963-1965). His success in these positions was rooted in his combination of modesty and interest in the well being of others that conveyed a feeling of integrity to all those who met him. He seemed always to see the best in others, and they responded to his expectations.

In the early 1970's he organized a departmental x-ray crystallography lab used by organic and inorganic chemists, as well as crystallographers, to solve chemical structural problems.

This "departmental crystallographic lab" was a huge success and copied by many chemistry departments throughout the world.

Apart from his success as a teacher and administrator, what he is really recognized for is his scientific achievements. He was a pioneer in the



Back row: Verner Schomaker, Ken Trueblood, Don Glusker, S. Ramaseshan, David Sayre, Jim Ibers, Dick Marsh; Seated: Anne Sayre, ?, Jean Trueblood, Jenny Glusker, Diana Rowley (Dorothy's sister, Mrs. Ramaseshan), Eleanor Dodson, Elizabeth Hodgkin (Dorothy's daughter), Judy Schomaker, Carol Huber, ?.



development of the use of computers for the determination and refinement of crystal structures and in the analysis of molecular motion in the solid state. Few crystallographers at that time were working with three-dimensional data because the calculations involved were unbelievably tedious and time-consuming. The NBS Western Automatic Computer had been installed at UCLA in the early 1950's and he set about using it for crystallographic work to help others.

The development of suitable programs for calculating electron-density maps and, later, for refining structures determined by Trueblood and his students Stan Mayer, Dick Prosen, F. Kruse and Bob Sparks led to his collaboration in 1954 with Dorothy Hodgkin on the crystal structure of vitamin B12. His electron-density maps determined larger and larger parts of the molecule and led to the chemical formula reported in 1955. This was the largest unknown chemical structure determined at that time. In those days information about each cycle of refinement was exchanged by snail mail and telegraph between LA and Oxford, England. Fortunately, he received a Fulbright Award (1956-57) and was able to go to Oxford to continue working with Hodgkin in person.

He continued to develop better computer programs for determining structures and contributed to fundamental interpretations of molecular motions in crystals. With Robert Long, he developed some of the very first programs for use in direct methods of structure determination. His computational expertise and collaborations resulted in the determination of more than 130 structures and 140 research papers, and contributed to the Nobel Prizes awarded to Dorothy Hodgkin (1964) and to his UCLA colleague Donald Cram (1987).

Trueblood was also awarded a Guggenheim fellowship (1976-1977) that allowed him to go to the Swiss Federal Institute of Technology and work with Jack Dunitz. He continued to collaborate with Dunitz and Verner Schomaker (University of Washington) on the computational analysis of molecular motion. When he heard the dismal prognosis of his final illness, he is said to have put the completion of an article with Schomaker (who died the previous year) at the top of his "to-do" list. Their study of the correlation of internal torsional motion with overall motion in crystals was finished in good order prior to his death and published in *Acta Cryst.* (1998). **B54**, 507-514.



His dedication to his university, to chemistry, and to crystallography is made evident in all that is said and known about him. To be selected for the **ACA Kenneth N. Trueblood Award** is truly a great honor. The 2010 recipient, announced in the fall 2009 issue of *RefleXions*, is **Anthony L. Spek**, professor in chemical and computational crystallography at Utrecht University Bijvoet Center for Biomolecular Research in the Netherlands.

Previous winners are Richard E. Marsh (Caltech - 2004) and Angelo Gavezzotti (University of Milan - 2007).

*Bomina Yu*

*The author acknowledges the following for the materials used in this article: Memorials written by Charles M. Knobler and Robert L. Scott for the University of California, David Eisenberg, Jenny Glusker and Robert Sparks for the IUCr Newsletter, and Jenny Glusker for the IUCr and the ACA Newsletters.*

## Other 2010 ACA Awards

Also announced in the fall issue of *RefleXions* was the **2010 Etter Early Career Award** which will go to **Raymond Trievel**. Ray is currently an associate professor at the University of Michigan. He is being recognized for the considerable progress he has made in solving multiple crystal structures of histone methyltransferases and for developing a coupled fluorescent assay widely applicable for monitoring methylation reactions.



## 2010 Fankuchen Award to David Watkin

**David Watkin** (Oxford University) is the recipient of the **2010 Isidor Fankuchen Award**. Watkin is most famous for his stewardship of the crystallographic software package "CRYSTALS" for x-ray structure refinement and analysis. The worldwide success of CRYSTALS, used by students, academics and industrial users alike, can be attributed to its ease of use and to Watkin's unceasing support of the software and its users.



He continues to conduct numerous training workshops, counsel users via e-mail, and is regularly invited to give lectures on this software at institutes and scientific meetings worldwide.

In 1987, Watkin also co-founded the biennial BCA "Intensive Course in X-ray Structure Analysis". Over eight days of lectures and tutorials, graduate students and postdoctoral researchers learn the fundamentals of crystallographic analysis. He has also organized similar week-long computing schools and workshops around the world. All who have studied with him name his approachability, enthusiasm and ability to easily communicate difficult concepts as factors contributing to his success as a teacher and an inspiration for a whole generation of crystallographers.

Most impressive is the forethought with which Watkin embarked on the "Age Concern" project with Judith Howard (Durham University) to fill the hole that would be soon left when the current crystallographic software designers worldwide retire and stop working. The project aims to re-vitalize training in crystallographic software and innovative methods development and to foster a new generation of scientists as software developers.

David Watkin's sincere and reputed concern for the future of crystallography and the new generation of crystallographers make him a worthy recipient of the Fankuchen Award, which recognizes contributions to crystallographic research by one who is known to be an effective teacher of crystallography. Watkin will be presented with the award and he will give a plenary lecture at the 2010 ACA Meeting in Chicago.

The Fankuchen Award was established in 1971 in memory of Isidor Fankuchen (1904-1964), professor of physics at the Polytechnic Institute of Brooklyn and the first president of the ACA (1950). Coined "the Apostle of X-ray Diffraction" by Paul Ewald, Fankuchen was an active and exceptional educator. A biographical sketch of Frankuchen was written by Frank Herbstein, the 2007 recipient (published in the spring 2007 issue



of *Reflexions*). Previous winners are: Alexander McPherson (2004); James Stewart (2001); Eleanor Dodson (1998); Jenny Glusker and Kenneth Trueblood (1995); Donald Casper (1992); David Sayre (1989); Michael Rossmann (1986); Lyle Jensen (1983); David Harker (1980); Dorothy Hodgkin (1977); Andre Guinier (1974); Martin Buerger (1971).

### *The 2009 Nobel Prize in Chemistry to Ada Yonath, Thomas Steitz and Venkatraman Ramakrishnan*



Ada Yonath, Thomas Steitz and Venkatraman Ramakrishnan were born over a decade apart in different parts of the world. They had different

childhoods and role models, but over the years, their lives moved closer and closer together. The direction of their movement was toward structurally mapping the ribosome at the atomic level. This was no small feat. The ribosome is one of the cell's most complex machineries, consisting of dozens of proteins and RNA molecules several hundred nucleotides in length.

Ada Yonath (Weizmann Institute of Science) pioneered ribosome crystallography in the late 1970s. By 1990, through the application of cryo-crystallography, she was able to produce detailed diffraction maps from her crystals. Others joined the pursuit in the mid-90s, including ACA member Thomas Steitz (Yale) and Venkatraman Ramakrishnan (MRC Laboratory of Molecular Biology). In 1998, Steitz, with Yale colleagues Peter Moore and Joachim Frank (Columbia University) used electron microscopy studies to interpret the diffraction maps and produce a low-resolution 9-angstrom structure of the larger 50S ribosomal subunit.

In the year 2000, their paths converged. In August of that year Steitz published a high-resolution structure of the 50S subunit. This was followed by structures of the smaller 30S subunit published independently by Yonath and Ramakrishnan the following month. At the same time, in a second paper by Ramakrishnan's group, the structures of the 30S subunit in complex with three antibiotics that target different regions of the subunit and the structural basis for the action of each was revealed. The first crystal structure of the complete ribosome was reported a year later by Harry Noller (UC Santa Cruz). Both Steitz's and Yonath's groups have since published antibiotic-bound structures.

This year, the names of Ada Yonath, Thomas Steitz and Venkatraman Ramakrishnan will be forever tied together in history as co-recipients of the 2009 Nobel Prize in Chemistry. From diverse origins and following different routes, their paths have reached what some describe as the highest honor for scientific achievement. However, many, including the winners, have noted that the Nobel Committee's self-imposed rule limiting each prize to no more than three recipients is a shortcoming. They have stated that the work of many others, especially those named above, in contributing to "the studies of the structure and function of the ribosome" for which the prize was granted should not go unnoticed.

### *Lynne McCusker Relinquishes 4th ECA Max Perutz Award*



The European Crystallographic Association's Max Perutz Prize is awarded to recognize meritorious achievements in any branch of crystallography by a crystallographer having a clear affiliation with the ECA region. In 2009, the 4<sup>th</sup> Perutz Prize was awarded to Lynne McCusker (Laboratory of Crystallography at the ETH in Zurich, Switzerland) for her outstanding contributions to structure determination methodologies for polycrystalline materials. She presented her award lecture "The Trouble with Powders..." at the 2009 ECA meeting in Istanbul. She then felt it necessary to relinquish the prize when her requests to formally share it with longtime collaborator Christian Bärlocher, without whom she felt that the scientific achievements honored by the award would not have been possible, were denied by the ECA. Eligibility for the Perutz Prize had been exclusively limited to single researchers, with two or more person teams being excluded from nominations. More information can be found on the ECA website ([www.ecanews.org/ecaprizeweb](http://www.ecanews.org/ecaprizeweb)) and in Lynne's letter to the Editors of the *IUCr Newsletter* (Issue 17#4).

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## Clara Brink Shoemaker (1921-2009)



Clara Brink Shoemaker, senior research professor emeritus at Oregon State University, died peacefully in her sleep of liver cancer at home in Corvallis, OR September 30, 2009. Born in Rolde, Netherlands in 1921, she entered the University of Leiden in 1938 planning to major in chemistry with a minor in physics. The occupation of Holland in 1940 by armies of the Third Reich had relatively little initial

effect on student life. The following year, however, her university was shut down after a student strike although not before she was able to complete her Candidate's degree after three years of academic study. Utrecht University remained open and she was able to enroll there while resuming her academic studies with Anton Eduard van Arkel in Delft, receiving her doctorate in chemical crystallography in 1950. She also worked one day each week with Caroline MacGillavry in Amsterdam where she learned crystallography. This led to the solution and publication of the crystal structures of  $K_2AgI_3$  and  $K_2CuCl_3$ .

Clara left Holland in 1950 to work with Dorothy Hodgkin on Vitamin B12 in Oxford where her contributions resulted in three papers coauthored by Dorothy and others. After her return to Leiden in 1951, she was encouraged both by Caroline MacGillavry and Dorothy Hodgkin to consider further postdoctoral experience. Their top choices for her were CalTech or MIT. Each wrote letters of recommendation both to Linus Pauling and David Shoemaker. Possibly influenced by having a niece living in Boston who was married to Nicholaas Bloembergen, a faculty member in Harvard's Physics Department and a subsequent 1981 Nobel Prizewinner, she chose MIT. One of us (sca) was a staff member at that time in Arthur von Hippel's MIT Laboratory for Insulation Research and first met her shortly after her arrival in 1953. Crystallography was then well represented at MIT, by such major figures as Martin Buerger and Bertram Warren, both of whom warmly welcomed Clara.

Her collaboration with David, who had earlier recognized the importance of intermetallic compounds containing transition elements such as the  $\sigma$ -phase in both the iron-chromium and other systems that he had investigated while at CalTech and had reported in *Acta Cryst.* 1954, led to their first joint study. The resulting paper, published in *Acta Cryst.* the following year, established the  $\sigma$ -phase as typifying a promising new field. In August of that year, Clara and David's growing friendship culminated in marriage. The wedding ceremony took place in the MIT chapel, with her niece as Matron of Honor and Nicholaas giving the bride away. Their son Robert was born the following year.

Clara and David were the first to recognize that interstices in tetrahedrally close-packed metal crystals are exclusively tetrahedral, with coordination types restricted to a set of four having coordination numbers 16, 15, 14 and 12. They also noted that half the hexagonal holes present in  $\sigma$ -phase materials become

distorted pentagons in the  $P$ -phase, resulting in a coordination number reduction from 14 to 12 in half the atoms of the subsidiary layers. They also discerned a further difference between  $P$ - and  $\sigma$ -phase structures, namely the larger proportion (1/2) in the former vs. 3/7 with 12-fold coordination in the latter, resulting in slight distortions from regular icosahedra.

Many contributions to this new field of intermetallic structure followed in consequence, including a major paper by Linus Pauling in 1988 on icosahedral cluster  $\sigma$ -phase packing that acknowledged their early work. Among them are numerous x-ray and neutron diffraction studies by others together with some very recent modeling using *ab initio* and Calphad (Calculation of Phase Diagrams) techniques. The  $\sigma$  and  $P$  phases, now among the most intensively studied intermetallics due to their tendency to precipitate from stainless steels in the form of austenitic, ferritic or austenitic-ferritic phases, has given rise to a large literature in which the pioneering work of Clara and David is often referenced. Their later work included a wide range of such other intermetallic phases as  $\delta$ -Mo-Ni,  $\mu$ -MnAl<sub>4</sub>,  $E$ -TiNiSi,  $M$ -NbNiAl and  $\nu$ -Mn<sub>81.5</sub>Si<sub>18.5</sub>.

Clara's breadth of interests is hinted at by her four studies published with other colleagues, together with a fifth as sole author. The first, in 1959, was undertaken jointly with Barbara Low, a crystallographer then associated with Harvard Medical School. The second, in 1961, also with Barbara and one of her colleagues, had the bold objective of outlining the gross molecular structure of crystalline Type A insulin sulfate. Their analysis of the three-dimensional Patterson function revealed two independent insulin molecules in the asymmetric unit but gave no evidence of extensive parallel  $\alpha$ -helices, a result now well confirmed. The third, a contrasting small-molecule study in 1965 of  $(CH_3)_2SO$  in collaboration with Klass Eriks of Boston University and one of his students, was undertaken to resolve a controversy then current concerning the nature of the S-O bond. Some authors described it as semipolar, others as a double covalent bond. On correction for librational motion, Clara and colleagues determined  $d_{S-O} = 1.531(5) \text{ \AA}$ , significantly shorter than expected if it were semipolar, *i.e.* with both binding electrons originating at one atom. The fourth collaborative study, with Bill Pearson at the NRC in Ottawa, was undertaken in 1969 to form a coding system applicable to a wide range of layered, tetrahedrally close-packed structures forming  $\beta$ -tungsten,  $\sigma$ -,  $P$ - and related phases that subsequently enjoyed wide use. In 1983, Clara was sole author of a paper concerned with a hypothetical tetrahedrally close-packed  $\sigma$ -phase structure proposed by Erwin Parthé and collaborators in their structural study of TiMnSi<sub>2</sub>; she was able to identify an earlier study of the Fe-Si-W system that clearly demonstrated the existence of such a 'pentagon- $\sigma$ ' structure with composition FeSiW<sub>2</sub>.

Clara jointly published over two dozen papers in *Acta Cryst.* with David in the years that followed. One was an organic complex precursor to the anti-tumor agent verrucarol and related antibiotic substances, isolated from a soil fungus. Its structural determination provided a class project in a graduate course they ran jointly at Oregon State University following their move to Oregon. Their publications were not entirely confined to *Acta Cryst.*; they discussed the structure of the V-Ni-Si  $I$ -phase and the Mn-Co-Si  $S$ -phase in *Trans. Met. Soc.* in the sixties, also three-dimensional Euclidean space filling by irregular tetrahedra in *Phys. Rev. B* twenty years later.

In 1970, David accepted both the Chairmanship of the Chemistry Department at Oregon State University and the presidency of



the American Crystallographic Association. Clara and David remained fully engaged in ACA and IUCr activities following their move, including attendance at all IUCr Congresses from the 4<sup>th</sup> (Montreal, 1957) to the 13<sup>th</sup> (Hamburg, 1984). Clara, of course, anticipated an appointment in the OSU department similar to that she held at MIT but a hurdle existed in the form of state regulations concerning nepotism. These regulations prohibited close family members from holding faculty positions at the same time, not only at the same university, but anywhere within the state system of higher education. These regulations had been enacted during the Great Depression but had mostly been ignored in later years; they could, however, be invoked at any time by an administrator who so wished. (Lise Hedberg, wife of one of the present authors, had encountered this problem after working several years in the OSU Chemistry Department). Responding to David's concern, the potential impediment to Clara's appointment was examined by the president of the university, Dr. Robert MacVicar, who discovered that the law prohibiting joint family appointments contained the modifying phrase: "...except under exceptional circumstances." President MacVicar thereupon announced that any husband and wife scientific team qualified as an exceptional circumstance and Clara's appointment, as well as Lise's reinstatement, went forward. There was a small caveat: in order to preserve the appearance of propriety, neither lady could be supervised by her husband. Instead it was determined that each husband would take responsibility for the scientific effort of the other's wife. This arrangement required that each husband assure the other that his wife was doing a good job. The process was certainly easy to carry out, but seems a bit comical in retrospect.

In the years following Clara's retirement, both she and David continued their joint research each day. She gave hers up after David's death in 1995, the last of her publications appearing about ten years after she retired. However, she maintained her department contacts, joining a luncheon discussion group each Friday and participating in morning coffee-break sessions. She enjoyed both chamber and orchestral music and regularly spent several days in Ashland attending the renowned Oregon Shakespeare Festival theater twice yearly. Her declining health and dislike of night driving forced her later to terminate attendance at concerts, but she continued travelling to the Festival each spring in the company of friends.

Erudite and cultured, Clara was also kind, gentle and characteristically reserved. She loved her family and was proud of her son Robert, Professor of 18th-Century British History and Co-Director, Old Bailey Online, Plebeian Lives and the Making of Modern London at the University of Sheffield in the UK. She was delighted that her grandson Roland is presently a third-generation Shoemaker undergraduate at Reed College. Clara Brink Shoemaker was a fine person in every respect, and her friends and colleagues will miss her greatly.

We gratefully acknowledge the biographical notes on Clara compiled by Mary F. Singleton. They are available at [osulibrary.oregonstate.edu/specialcollections/coll/shoemaker/singleton/page1.html](http://osulibrary.oregonstate.edu/specialcollections/coll/shoemaker/singleton/page1.html)

Sidney C. Abrahams - Kenneth Hedberg

### Louis T.J. Delbaere (1943-2009)



We were all deeply saddened to hear that Louis T.J. Delbaere passed away suddenly on October 5 in Mississauga. Louis will be remembered by all of us for his winning and ever-present smile and his enthusiastic passion for his chosen science - x-ray crystallography. Below are the recollections of a number of us who knew Louis well, highlighting his science, mentorship and dedication to his family and the crystallographic community.

#### Louis' Early History: Manitoba, Oxford and Alberta (Michael James)

Louis was born and raised in St. Boniface, Manitoba. He attended the University of Manitoba where he received his BSc. in Honors Chemistry and his PhD. also in Chemistry. Louis began his enthusiasm for x-ray crystallography by working in the laboratory of Bob Ferguson, a mineralogist who infected many students from honours chemistry with his passion for x-ray crystallography. After receiving his PhD, Louis traveled with his wife Carol to Oxford for a post-doctoral fellowship in chemical crystallography where he worked with Keith Prout, Boris Kamenar and Louise Johnson from the Laboratory of Molecular Biophysics. Louis' major contribution from those days was the determination of the structures of two carbohydrate-amino acid structures, N-acetylglucosaminyl asparagine and glucosylasparagine. These two structures definitively characterized the covalent linkage between carbohydrates and proteins. Louis and Carol then moved to Edmonton where Louis took up a postdoctoral fellowship with Ray Lemieux in the Chemistry Department at the University of Alberta. Louis did some outstanding crystallographic work in Ray's lab and made a major contribution to understanding the structural features of the human Lewis blood-group determinants. He also collaborated with S. Masamune in the Chemistry Department on the structure of methyl-tri-*tert*-butyl [4] annulene carboxylate. This structure proved definitively that the [4] annulene ring was not square as suggested by several other influential chemists but that it was rectangular. I had the pleasure of working closely with Louis while he was with Ray Lemieux and was very pleased that he too got excited by protein crystallography. Louis was a key figure in our successful determination of the first protein structure to be done in Canada, that of *Streptomyces griseus* protease B (SGPB). Louis worked with Gary Brayer on the structure of the related enzyme SGPA and together they determined many structures of enzyme-product complexes with SGPA. Gary and Louis collaborated on the structure of  $\alpha$ -lytic protease the enzyme that started it all off when Larry Smillie of the Biochemistry Department sequenced  $\alpha$ -lytic protease and we managed to crystallize it. Last but not least Louis collaborated with I-Nan Hsu on the structure of penicillopepsin an aspartic peptidase from a fungus. The pair of them were the first to determine the



structure of an aspartic peptidase in a field with three competing groups hotly on “our tails”.

It must sound like all that Louis did was to work hard. He also had other interests and pastimes. In Edmonton, we had a squash club that would get together every Thursday evening for co-ed squash. We were not very good but we did enjoy the relaxation in the Faculty Club after this “hard” physical exercise. Louis had a passion for attending horse races that almost matched his passion for science. He was often found at the track with the racing sheets, going over the best bets of the day. Louis and Carol lived in suburban Duggan while they were in Edmonton. Their two children, Christian and Michelle were born in Edmonton and there were many family gatherings at the Delbaere home celebrating varied occasions. Louis and Carol had a very closely-knit family and their friendship and happiness was shared with all.

### *Louis in Oxford (Stanley Cameron)*

It will be 40 years next year since Liz and I first met Louis and Carol; indeed Louis and I shared, very harmoniously, a tiny railway carriage of an office as postdocs in chem-cryst with Keith Prout in the inorganic labs in Oxford. Louis and Carol were the first Canadian couple we had ever met and we marveled at their amazement that in Oxford you could see to the end of nearly every street – something of a rarity apparently in their home town of Winnipeg. We were in and out of each other’s homes quite a lot and have many happy memories of those times. On one occasion, in the night, their little Mini was hoisted up on its axles, and while somewhat precariously balanced on four birdhouses, its four wheels were stolen. Carol was, what we later came to recognize as, “Canadian polite incandescent.” Louis however, though far from pleased, could see the humor as he viewed their little Mini hoisted in the air, with four thoroughly cheesed-off families of Chickadees fluttering around their displaced homes: “Bird houses for crying out loud!” was his comment, repeated with increasing emphasis but never quite expletive. Some days later he cheerfully reported that he had a “great deal” on some replacement wheels. These, to my rather jaundiced eye, looked the exact replica of the stolen ones and I was tactless enough to say so. “You mean, I bought my own wheels back?” Louis said with a wry chuckle!

That was Louis, straight forward, honest, fair and uncomplicated, looking for and expecting the best from people. Only a few years after Louis and Carol returned to Canada, Liz and I followed. He and I met on various crystallographic occasions and committees. As a committee chair he was a dream: open, direct, no hidden agendas, and incorruptible. After a reasonable length of discussion, he would sum up: This is the way we see the problem, this is what needs doing, this is how we feel it should be done and I will do this part. Quietly and efficiently whatever bit he said he would do, got done. As a friend and colleague, I deeply miss Louis; Canadian crystallography has lost a great ambassador.

### *Louis in the Biochemistry Department, University of Saskatchewan (Wilson Quail)*

In 1979, Louis moved to the Biochemistry Department of the University of Saskatchewan in Saskatoon as an associate professor with a Medical Research Council of Canada Development Grant to start the first protein crystallography lab at the University. I was in the Chemistry Department at the time and was very interested in the possibilities of setting up a crystallography lab. Louis and I ultimately ended up sharing some students and facilities. Lata

Prasad came to work for Louis in 1986 as a research associate and has continued in the lab until the present. Her knowledge and experience as a crystallographer was and continues to be a valuable asset for the lab.

In 1988, Louis and I obtained our first synchrotron data set at the EMBL outstation at DESY in Hamburg, thanks to the help of Keith Wilson and Zbigniew Dauter. The candidate crystal was one of *Griffonia simplicifolia* lectin IV complexed with a synthetic Lewis b blood group determinant. The compounds were supplied by Ray Lemieux. Previous data on this crystal form obtained on a lab x-ray source could not be solved, but the synchrotron data gave a publishable structure. Subsequently, synchrotron data from other crystals were obtained at the Photon Factory in Tsukuba, Japan, NSLS at Brookhaven, the APS at Argonne National Lab and on return visits to Hamburg. Louis became interested in growing protein crystals in zero gravity. An experiment that he set up resulted in crystals of the Jel42 Fab fragment that were superior to earth grown crystals. This was the first successful crystallization of a protein in space by a Canadian lab. Good data resulted in better structures and papers. Papers on the structures of *Griffonia simplicifolia* lectin IV complexed with a synthetic Lewis b blood group determinant, *Ulex europaeus* lectin I complexed with a synthetic O(H) blood group determinant, the histidine-containing phosphocarrier protein HPr from *Enterococcus faecalis*, the trifluoperazine complex with calmodulin, phosphoenolpyruvate carboxykinase and the V8 Protease from *Staphylococcus aureus* were published.

In the mid 1990’s, Saskatoon was selected as the site to build a Canadian synchrotron. Because he was one of the few scientists in Saskatoon with experience at a synchrotron, Louis took on the job of getting the Canadian scientific community behind the idea. He organized mini-symposia on synchrotron applications for protein crystallography around the country. He spoke with members of the granting agencies. He lobbied scientists in other areas that might use synchrotron radiation. Others worked on getting the University to support the idea and then getting politicians at both the provincial and federal levels behind the idea. Amazingly, it all came together and the Canadian Light Source (CLS) is now in Saskatoon. Louis didn’t do it all by himself. Many were involved, but his contribution was critical. Louis continued his involvement with the CLS as it was constructed, brought into operation, and then expanded. He was the project leader for the first protein crystallography beamline at the CLS.

Louis was in the second year of a seven-year term of a prestigious Tier 1 Canada Research Chair in Structural Biochemistry when he died. Louis worked on many committees to advance science at all levels. He had been the Chair of the Canadian National Committee for the IUCr since 2005. He was President of the ACA in 2005. At the Osaka IUCr meeting in 2008, he successfully led the committee promoting Montreal as the site for the IUCr meeting in 2014 and he had recently been elected for a six-year term to the executive (EC) of the IUCr.

The welfare of his students was always important for Louis. He took great efforts to get good positions for his students. Their successes were his successes.

Louis’ family had high priority in his life. His fourth grandchild had just been born in Ottawa. Louis had stopped over for a day in Toronto to visit a cousin on his way from Buffalo to Ottawa to meet his new grandson. He collapsed on Saturday, October 3 and died on October 5, 2009. He will be greatly missed by his many friends and colleagues.



*Top - left: Louis presenting the Etter Early Career Award to Jennifer Swift (ACA 2005); right: Louis and Carol at the opening reception (ACA 2005). Bottom - left: One of the many hats he wore during his remarks opening the banquet in Orlando (2005), right: Louis, Mike James and Bob VonDreele at the banquet (ACA 2009)*

### ***Louis as Supervisor and Mentor (Gerald F. Audette)***

The development and progress of his students was a central priority of Louis throughout his career. By the numbers, Louis supervised or co-supervised seven PhD students, eight Masters, five postdoctoral fellows and research associates, a number of technicians and countless undergraduate honors projects and summer students. Louis' group at the University of Saskatchewan was never so large that students got lost in the crowd, and he took great pains to help his students secure good positions for themselves following the receipt of their degrees. Of the PhD students Louis supervised, four are now professors in their own right (Osama El-Kabbani, 1987; Zongchao Jia, 1992; Scott Napper, 1999; Gerald F. Audette, 2002), one is a research officer at the NRC in Montreal (Allan Matte, 1996); one has just joined the CLS (Shaunivan Labiuk, 2003) and one is currently a postdoctoral fellow at the National Microbiology Laboratory in Winnipeg (Julien Côtélesage, 2007). Louis' group at the time of his passing included a post-doctoral fellow, two PhD students and his long-time research associate Lata Prasad.

To his students, Louis was more than just a supervisor – he was a mentor and a friend. Louis' style was one of quiet enthusiasm and encouragement. He was always available to discuss problems, directions and the latest crazy ideas that we'd come up with. He taught us to follow the data, be open to various viewpoints and methods, be patient and to "trust the electron density ... it

doesn't lie". Things like that apply not only to crystallography, but also to our view of the world as a whole. He instilled a passion to make sure that the correctness of the analysis and the crystallography, rather than the flash of the story, was what was critically important. He taught us not to over-interpret the data, but to make sure it was correct, and from there to move forward confidently in addressing our hypotheses. He also felt that an important part of his students training was their participation in the community. He encouraged everyone to be a member of the ACA, and to present posters at least once a year at a conference. These conferences were primarily the annual ACA meeting, but also included the IUCr congress, various Canadian meetings and the Erice meetings. This was something that we all took advantage of; they had an unspoken and often unappreciated (by us at the time) value. Louis would make a point of introducing all his students to his colleagues during poster sessions and other formal and informal situations; we've all ended up with international networks of professional contacts and colleagues. I remember Louis' enthusiastic support of my attending the Erice meeting in 2000 over the 1999 IUCr congress; his thoughts were simple – the smaller setting of Erice would result in more productive interactions for me. He was right; being one of 4 Canadians at the meeting (including Louis and Carol) of about 90 delegates provided me with a fantastic opportunity to interact with and discuss the science with all the presenters, to put faces to names and to develop my own international network of colleagues.



Louis actively fostered our professional development, in addition to our development as independent crystallographers, through the example of his active and enthusiastic involvement in the community.

It was not all work with Louis. During my time at the University of Saskatchewan, Louis and Carol started ballroom dancing at the same time as we (my wife Shelagh and I) did. It was a wonderful time, and through it our friendship deepened beyond the supervisor-student role. Louis and Carol continued dancing after we left in late 2001, saying it was their weekly “date night”, and several colleagues have enjoyed dancing with Louis and Carol over the last several years. They also never missed an opportunity to celebrate the successes of the group. They brought the lab together for Christmas and any parties at their home were wonderful events filled with laughter, wonderful food and the inevitable Trivial Pursuit. When Louis was Chair of the Biochemistry Department, he extended these events to the department during the annual student evaluations. I remember seeing Louis on his deck in front of his barbeque flipping hamburgers and hot dogs with a smile on his face and ready laugh. It was the personal touch that made people want to follow where he led, which sums up Louis’ style as a mentor. His sudden passing came as a great shock; we will miss him.

### *Louis and the IUCr (Sine Larson)*

Louis’s scientific career is an excellent demonstration of the science that can be achieved by the advanced application of crystallographic methods, and his colleagues recognize him as a prime representative of the crystallographers in Canada and of crystallographers worldwide. He was a leading figure in the Canadian crystallographic community. He chaired the Canadian delegation at the IUCr Congress in Osaka 2008, where Canada’s successful bid for the IUCr Congress in 2014 was presented. The participants in Osaka remember well Louis’ happiness when Montreal was selected. It was clear that he looked forward to welcoming crystallographers from all over the world to Montreal in 2014. Another important election that took place at the Osaka Congress was the one that made Louis a member of the IUCr EC. After a few months he took on the important task of chairing the IUCr Sub-committee on the Union Calendar, which handles applications for support for international crystallographic meetings. Louis chaired the Committee efficiently and with great understanding for the importance of distributing the 150,000 US dollars in a way that promotes crystallography worldwide. He was also IUCr representative to the ACA. For the work of the IUCr it is essential that its EC possesses knowledge and insight into the way crystallography is developing worldwide. Global awareness was more than a ‘buzz word’ to Louis, he was known and respected by crystallographers all over the world and was an excellent representative of the ‘Americas’.

### *Warren L. DeLano (1972 – 2009)*



On November 3<sup>rd</sup> our community tragically lost Warren DeLano, widely known as the creator of the molecular graphics program PyMOL. Warren grew up in Palo Alto, California at a time and with a loving family that greatly valued the development

of computer technology and science. His life-long commitment to computational biosciences began when Warren was an undergraduate research student in Axel Brunger’s laboratory majoring in Molecular Biophysics and Biochemistry (MB&B) and Computer Science at Yale University. He initially worked on structure prediction of helical bundles and molecular replacement, and then made a major contribution to the Crystallography and NMR System (CNS) by implementing powerful scripting capabilities for the new system. He also started to work on what would eventually become the Open Source molecular graphics program PyMOL.

As a graduate student at UCSF in Jim Wells’ laboratory at Genentech, he worked on the use of peptide-phage display to see if naïve peptides would seek out a well-known promiscuous epitope at the Fc region of antibodies. Remarkably his phage selected peptide, shown by the x-ray structure to be a simple  $\beta$ -hairpin, bound exactly over the promiscuous epitope! Importantly he revealed the highly adaptive nature of these interfaces. To visualize this adaptive property he began to further develop the software for PyMol in his spare time. In particular he developed a special application he called RigiMol: one of the first molecular movie programs which allows one to morph between static structures.

Warren’s impact on crystallographic software spreads beyond PyMOL and CNS, spanning almost two decades. Paul Adams retained him as a consultant in the very early days of the Phenix project. There ensued many lively and passionate discussions about how to develop a new crystallographic software system with the current computational tools. Warren’s insight and experience developing PyMOL were major contributors to the decision to use Python as the scripting language in PHENIX. This choice also made it easy for the Phenix developers to integrate PyMOL with PHENIX.

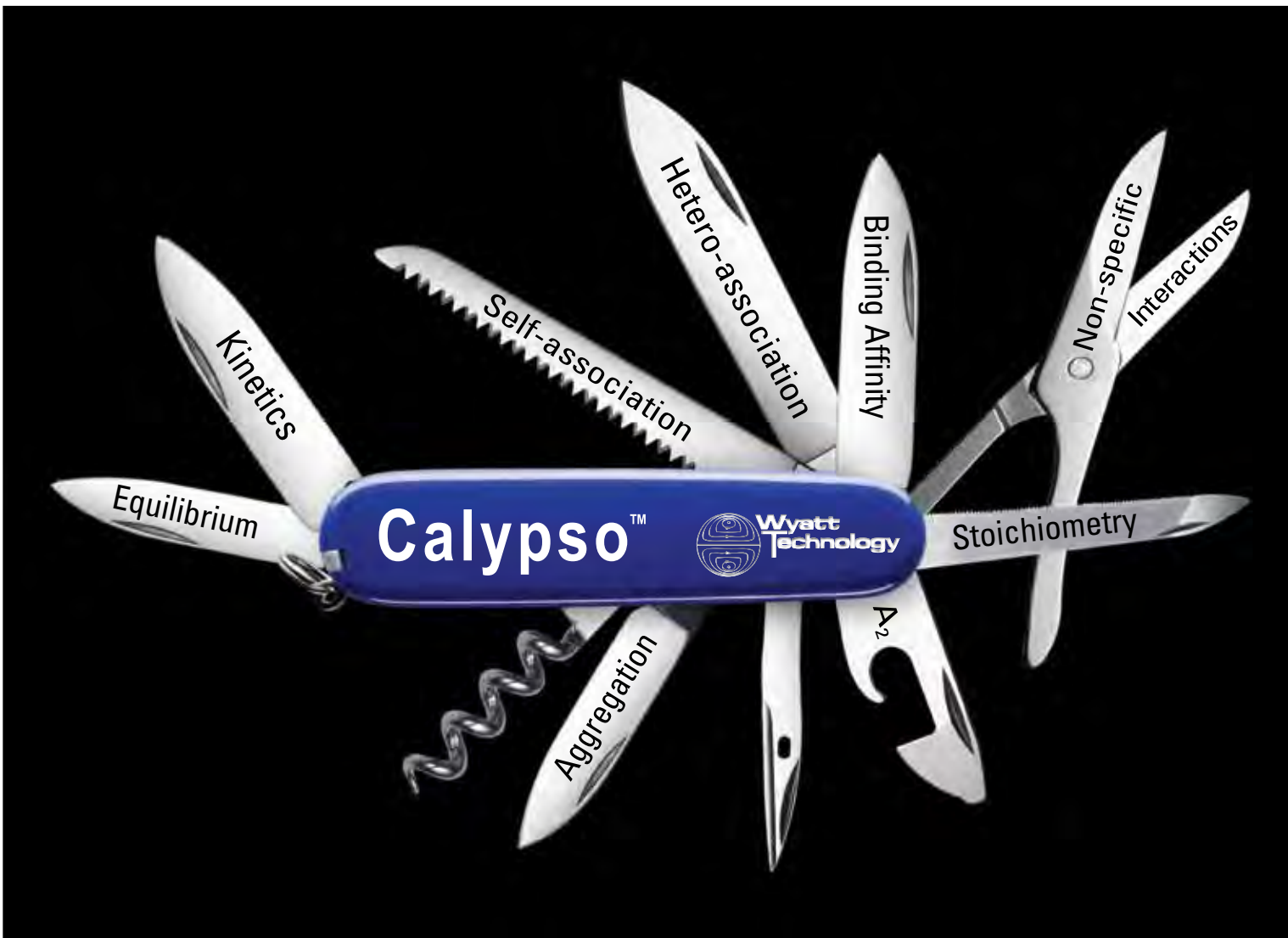
He left us with much undone that he wanted to do. Warren was a truly visionary thinker and to be deprived of his future work is a huge blow to the scientific community.

To honor Warren’s memory we have put together a mission statement for the Warren L. DeLano Memorial Award for Computational Biosciences, with the approval of Warren’s family. This award shall be given to a top computational bioscientist in recognition of the contributions made by Warren L. DeLano to creating powerful visualization tools for three dimensional structures and making them freely accessible. The award, accompanying lecture, and a honorarium will be given annually in the context of a national bioscience meeting or a Bay Area gathering of computational bioscientists at Stanford, UCSF or UC Berkeley. In selecting recipients of the award special emphasis will be given for Open Source developments and service to the bioscience community.

The award selection committee, consisting of experts in the computational and biological sciences, will accept nominations from anyone. Further information can be found at [www.jmdelano.com](http://www.jmdelano.com).

*Axel T. Brunger and James A. Wells*





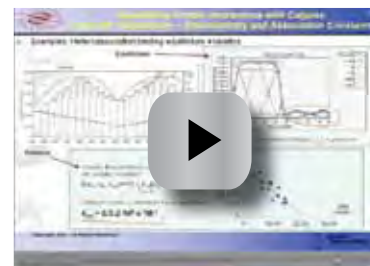
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## The Molecular Structure of Evolutionary Theory: Notes of a Protein Crystallographer

All over the world, there have been celebrations dedicated to the work and life of Charles R. Darwin (1809-1882) on the 200<sup>th</sup> anniversary of his birth. Coincidentally, this year also marks the 150<sup>th</sup> anniversary of the publication of *On the Origin of Species* (Darwin, 1859). Several threads converged in my mind to convince me that it was worth writing an essay for *Acta Cryst. D*\*. First, celebrating within our scientific field of enquiry Darwin's anniversary; its connection to the publication of the *Origin of Species* and the desire to pay homage to the 'old man'. Second, the need to clarify the key tenets of Darwin's ideas and how our discoveries and those of many others in related (molecular) and unrelated (cell or more traditionally biological) domains are being used to refine, revise and extend the original concepts of Darwin. Finally, briefly reviewing the importance and subtlety of those evolutionary concepts in structural biology; this is something that I thought needed to be addressed so that we can establish a bridge with the evolutionary biologists speaking in their own terms. The two groups, 'molecular' and 'evolutionary' biologists, can learn something from each other.

What is the Structure of Evolutionary Theory? The five pillars are well documented in the book thus giving credence and making a compelling case for the overall mechanism:

1. Within a given environment, all organisms produce more offspring than can survive to reproduce themselves.
2. All organisms naturally vary, typically by small differences from one another.
3. Offspring inherit characteristics from their parents and tend to be more like their parents than others.
4. At least some of the variations in an organism lead to a greater number of its offspring surviving and reproducing relative to the offspring of others.
5. This 'natural selection' means that these particular variations will become more prevalent in the population (as a consequence of the differential survival and laws of inheritance) as they are passed on to future generations. This translates to an adaptation of the organism to the environment.

Darwin, being a child of Victorian and conservative England, could only conceive these processes acting in a very slow and incremental way, by 'graduated steps' (*Natura non facit saltum*). Thus the notion of small, gradual, changes is an inherent part of classical Darwinism. Those five processes, operating gradually for long periods of time, are the fundamental tenets of 'Darwinism'.

What about the current views on evolutionary theory? Before his untimely death, S. J. Gould (1941-2002), one of the most eloquent writers of evolutionary biology, published a *magna opus* entitled *The Structure of Evolutionary Biology* that can arguably be considered the current synthesis of evolutionary thought. This is a voluminous book (~1,400 pages) in Gould's inimitable prose. It will be a tough read at the beginning but the intellectual insights will overcome the initial pain, especially if we are to create a durable bridge with the evolutionary biologists. The *Acta D* article \* reviews its content and attempts to put the discoveries of structural biology in the context of current evolutionary thought.

The personal perspective is that the doors are open for the full and detailed analysis of macromolecular structure in the

explanation of the molecular mechanisms of evolution. Most current evolutionary studies overemphasize the role of genes and replication as the dominant forces shaping evolution at the molecular level (i.e. 'selfish genes'), but in my view underestimate the power and subtlety of the forces operating at the protein level (catalysis, regulation, chemistry and other). By being able to dissect at the atomic level the separate contributions of 'physicochemical constraints' versus 'selection forces' in the evolution of proteins and biological systems, we can make our strong future mark in the field of evolutionary biology.



*Darwin's home (Down House) in the outskirts of London*

Darwin's home was a study, a laboratory and a home where he and his wife Emma Wedgwood (of Wedgwood pottery fame) raised a large family. Photo courtesy of Beth Weller taken during our recent visit to celebrate Darwin's birthday.

I do encourage macromolecular crystallographers and structural biologists to read the article to understand better what the 'structure' of the theory of evolution is and what macromolecular structure has contributed and will continue to contribute towards the better understanding of its content. There is still much to be done for new generations. Gould's *magna opus* probably represents the conceptual synthesis and the current status of the biological, developmental and possibly genetic structure of evolutionary theory. The *Molecular Structure of Evolutionary Theory* is still to be written.

*Cele Abad-Zapatero*

\*Excerpted from C. Abad-Zapatero, (2009) *Acta Cryst. D* **65**, 1341-1349. (see *Acta* paper for a full list of references). The support and friendship of Alicia Guasch during the preparation of the *Acta* essay and this brief note are greatly appreciated by the author.

*Editors note: See book review of Origin of the Species on page 16*

*Small-Angle Scattering of X-rays by André Guinier and Gérard Fournet; translated by Christopher B. Walker*



Published in 1955, this book is long out of print and quite difficult to find. Fortunately, Angela Criswell located a copy for this retrospective review. Given that SAXS is such a “hot topic” these days, it was remarkable to find that this old tome is still a relevant and useful reference for researchers today.

To frame the perspective of the authors, it is notable that they opined (in chapter 6) that “These remarks explain why the study of proteins [dilute

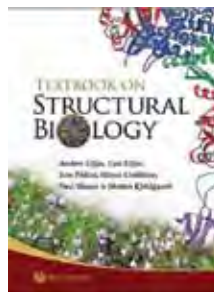
solutions] offers one of the best applications of this method. As a matter of fact, a large number of investigations have already been carried out on proteins, as is shown in the bibliography at the end of the text. We believe that it is in this field small-angle scattering can give the most valuable and important results from a general point of view.”

We are coming up on the 50th anniversary of the publication of “Structure of Hæmoglobin: A Three-Dimensional Fourier Synthesis at 5.5 Å. Resolution, Obtained by X-Ray Analysis” [*Nature* **185**, 416-422 (1960)] by Perutz, Rossmann, Cullis, Muirhead, Will and North. Guinier and Fournet did not foresee the explosion in protein structure that would start five years later. Yet, it is quite interesting that, 55 years after publication, structural biologists have come back to SAXS as a tool for understanding the solution structure of proteins - that stage before crystallography takes over.

Chapter 1 provides a very basic introduction to the scattering process, while Chapter 2 explains the theory in detail. Readers should be forewarned: Chapter 2 provides an in depth overview of the mathematical background behind the calculation of the radius of gyration, pair distribution function and even the second virial coefficient. Chapter 3 provides a detailed discussion of the three pinhole SAXS camera. The only detectors available then were Geiger counters and film so the reader must keep in mind that there has been 55 years of instrument development in the interim. Nevertheless, the discussion is useful in understanding modern SAXS cameras. Chapter 4 introduces readers to the interpretation of results. Chapter 5 compares the SAXS method with other then state-of-the-art techniques to validate the results from Chapter 4. Chapter 6 goes through a number of applications, with the first part of the chapter devoted to the study of proteins in dilute solutions. Finally, an extensive bibliography is provided, that is obviously only current to 1955.

There are more modern textbooks and reviews on this subject, and the tools for collecting data and generating results have changed in the intervening 55 years, but anyone who is seriously interested in learning about SAXS would benefit from reading this classic text.

*Textbook of Structural Biology by A. Liljas, L. Liljas, J. Piskur, G. Lindblom, P. Nissen and M. Kjeldgaard, published by World Scientific (2009), 580pp, ISBN: 978-981-277-207-7*



I started this book not knowing what level of prior experience the reader needed. After reading the first few chapters, I concluded that the reader had better have an organic chemistry, biology and crystallography course under their belts, since advanced concepts are introduced without description. I read the book and I realized that this text provides a well thought out and reasonably current survey of structural biology.

The first four chapters introduce structural biology, protein and DNA structure, as well as lipids and membrane structure. The remaining twelve chapters describe, in great detail, the current state of the art in structural biology, including: enzymes, DNA replication and recombination, transcription, protein synthesis and translation, protein folding and degradation, membrane proteins, signal transduction, cell motility and transport, cell-cell interactions, the immune system, viruses and the evolution of macromolecules. The last chapter on macromolecular evolution is particularly interesting in that this year is the 150th anniversary of the publication of “On the Origin of Species”. Each chapter is elucidated with structures from the recent literature as well as historical examples where appropriate. Each protein is provided with its PDB code so it very easy to study a given structure in depth. However, this is also my one complaint, as the reader is forced to go to the PDB to find references for the structures.

There are six appendices on diverse topics such as energetics, fold comparison, prediction of conformation, assignment of function, protein modification and a current list of Nobel laureates. The main text is 484 pages with well written prose. I enjoyed reading this book and recommend it for an advanced level class in structural biology or as a current reference text.

*Remarkable Creatures: Epic Adventures in the Search for the Origin of Species by Sean B. Carroll, published by Houghton Mifflin Harcourt (2009), 311 pages, ISBN 978-015-101485-9*



I first heard about this book in an interview with the author on *Science Friday*. I was intrigued and ordered myself a copy the same day. The book is an elucidation of our understanding of evolution. This book describes the three categories of scientists involved in this process: naturalists, paleontologists and molecular biologists. The naturalists include Alexander von Humboldt, Charles Darwin, Alfred Russel Wallace and

Henry Walter Bates. These scientists risked life and limb in pursuit of answers.

The paleontologists included Eugene Dubois, Roy Chapman Andrews, Neil Shubin and the Leakeys. Dubois is the discoverer of Java Man. Andrews began his career mopping floors at the American Museum of Natural History and became director many years later. Several character traits given to Indiana Jones came from Andrews, including the six-shooter and the fear of snakes. Shubin discovered the Tiktaalik, a sea-to-land transitional species, in 2004. The Leakeys, of course, are responsible for much of our knowledge of early hominids and how they used tools.



The last section covers the modern scientists who have helped us understand evolution including, Linus Pauling, who really needs no further introduction, and Allan Wilson. Wilson first studied the genetics of chimpanzees and humans, and provided the idea of a mitochondrial Eve. A great tribute to Charles Darwin, the book celebrates the 200th anniversary of his birth and 150th anniversary of the publication of *The Origin of Species*.

I am also pleased to report that Sean B. Carroll now has a monthly column in the *New York Times* titled "Remarkable Creatures"

***On the Origin of Species by the Means of Natural Selection* by Charles Darwin ISBN-10: 0451529065**

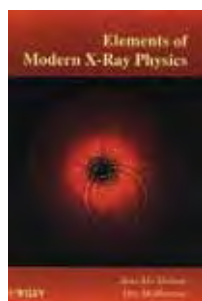


This classic was published in November 1859 (150 years ago), yet is not widely read, or at least as widely read as it should be. Paul Swebston and I thought it most appropriate to review *Species* at this time. I actually tried to read this book at about 8 years old and it was clearly too much for me then. It's embarrassing to say I waited four decades to try again.

Darwin's attention to detail and descriptive prose are superb. The theory of evolution is a classic scientific theory fully capable of discredit by evidence. The good news is that there has been no evidence to refute the principles set forth. In fact, two recent bodies of work show the theory continues to be valid: a recent report on the Framingham Heart study suggests humans are still evolving (Sean G. Byars, Douglas Ewbank, Diddahally R. Govindaraju and Stephen C. Stearns - *PNAS*). A genomic analysis of 40,000 generations of *E. Coli* (Jeffrey E. Barrick, Dong Su Yu, Sung Ho Yoon, Haeyoung Jeong, Tae Kwang Oh, Dominique Schneider, Richard E. Lenski and Jihyun F. Kim, *Nature*, 2009) further indicates evolution is an ongoing process. I find it amazing that Darwin was so well able to describe evolution using only observation - both locally with pigeons, dogs and other domestic animals and globally with all the species he encountered on the Beagle.

The *Origin of the Species* is divided into nine self-described chapters: introduction; variation under domestication and under nature; struggle for existence, natural selection, and divergence; variation and heredity; difficulties for the theory; geologic record; geographic distribution; classification, morphology, embryology, rudimentary organs; and concluding remarks. Each chapter provides a wealth of examples to support Darwin's hypotheses. In addition, each chapter provides its own introduction and conclusion, but I would not skip the middle parts because those are the best.

***Elements of Modern X-ray Physics* by Jens Als-Nielsen and Des McMorrow, published by Wiley (2001), 335 pages, ISBN: 0471498580.**



I was lamenting to Wayne Hendrickson about the difficulties in sorting out resonance scattering for a presentation I had given at an ECM because different authors use different notation for the same parameters, or worse the same notation for different parameters. Wayne told me he was using "Elements of Modern X-ray Physics" by Jens Als-Nielsen and Des McMorrow for his x-ray diffraction course so I bought a copy. I don't often read textbooks cover to cover, but the book is well written, and worth the time and effort.

The book starts with an excellent introduction to x-ray interactions and sources. Next, refraction and reflection are discussed. I should point out that the text explains clearly the relationship between absorption and  $f''$  here, useful for understanding concepts in the last chapter. The next two chapters are devoted to diffraction. The penultimate chapter reviews photoelectron absorption and EXAFS.

The final chapter on resonance scattering is a must read for young macromolecular crystallographers. This chapter provides a lucid explanation of "anomalous scattering", the phase problem, the breakdown of Friedel's law and MAD phasing.

All Reviews by Joseph D. Ferrara,

**Note: Joe's review of *Biomolecular Crystallography: Principles, Practice, and Application to Structural Biology* by Bernhard Rupp will appear in the spring issue of *Reflexions*.**

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***MX Frontiers at the One Micron Scale: Workshop Makes Case for Micro-Beams, July 23-24, 2009, Brookhaven National Laboratory***

Macromolecular crystallographic (MX) structure determination at synchrotron radiation sources has the potential to advance significantly through use of x-ray beams of one micron or smaller cross-sections. Recently, the MX Frontiers at the One Micron Scale Workshop in structural biology explored scientific opportunities made possible through the use of micro-beams, and anticipated technical challenges for developers of MX beam lines at NSLS-II. Over 100 attendees participated in the workshop, which included a day-and-a-half of lectures, discussions, and a semi-formal poster session. The workshop was particularly relevant given the development of NSLS-II, a brilliant new synchrotron facility under construction at BNL. As he welcomed participants, **Wayne Hendrickson** (Columbia U), the recently appointed Associate Project Director for Life Sciences at NSLS-II, highlighted the facility's design features and new capabilities. Regarding the future at NSLS-II, Hendrickson predicted that "what we think of as difficult today will become routine by 2015."

**David Eisenberg** (UCLA) then illustrated Hendrickson's assertions as he spoke about his adventures in microcrystallography of biological specimens, which have led to stunning breakthroughs in structure determination of proteins in the amyloid state from crystals that are 10,000 times smaller than conventional samples. Eisenberg revealed that it was the scientific problem of Alzheimer's and other amyloid-related diseases that first sparked his interest in micro-diffraction and he expects further developments to enable him to probe even smaller granules *in vivo*.

He was followed by **Gebhard Schertler** (MRC) who spoke about the structure of G protein coupled receptors and shared his work studying the structures of rhodopsin and beta adrenergic receptors, all membrane proteins yielding small variable crystallites. He highlighted the crucial role microcrystallography played in his work, requiring extensive experimentation in close collaboration with beamline scientists "on equal terms."

Tiny beams also drive the development and use of new crystallographic methods, such as that of serial crystallography pursued by **John Spence** (Arizona State U). After summarizing the state of microdroplet delivery, he addressed the problem of

solving protein structures from molecular aggregates containing only a few unit cells. Serial crystallography assumes mastery of powder diffraction analysis, a technique then reviewed by **Irene Margiolaki** (ESRF). In a lucid talk, she highlighted the experimental and analytical methods that now yield high resolution structures of modest size proteins, such as the SH3 domain of ponsin.

In the afternoon of the first workshop day, talks given by **Colin Nave** (DLS), **Robert Fischetti** (APS), **James Holton** (ALS) and **Elsbeth Garman** (Oxford U) addressed radiation damage issues and their potential mitigation using micro-beams.

In his after-dinner talk, **Christian Riek** (ESRF) traced the origins of micro-diffraction at ESRF's ID13 beamline to small-angle scattering and documented its multi-disciplinary evolution. However, crystallography dominated his program as he demonstrated remarkable results ranging from work with chromatin to spider silk, to inorganic dusts, and eventually to Eisenberg's amyloid proteins. In a bold outlook, he touched on the many optical techniques and innovative instruments that now propel micro-diffraction towards the nano-scale, a development that will require exhaustive experimental studies as well as strong, renewed collaborations between scientists in the field.

Talks continued on the second day of the workshop addressing optics and instrumentation issues, including integrated beamlines, related to micro-beams. **Clemens Schulze-Briese** (SLS), **Sean McSweeney** (ESRF), **Gwyndaf Evans** (DLS), **Masaki Yamamoto** (Spring-8), **Kenneth Evans-Lutterodt** (BNL) and **Antonio Lanzirotti** (U. Chicago) presented these new challenges.

The workshop concluded with a final discussion that considered the key question of whether or not a solid case had been made in favor of micro-beams. Participants debated the matter with enthusiasm throughout, deliberating about the appropriateness of the one micron scale, the role of submicron beams, and the usefulness of beamlines with flexible capabilities. Ultimately, the sum of lectures and discussions clearly illustrated that tiny beams will enable new science, particularly so if the beam is of sub-micron size. At this scale, structural work will be characterized by experimentation rather than routine measurements and involve many pursuits in life sciences such as MX, SAXS, and fiber diffraction, potentially borrowing from electron microscopy as well.



**Speakers and workshop organizers -listed from left to right. Front row: Dieter Schneider, Gebhard Schertler, David Eisenberg, Christian Riek, Irene Margiolaki, Colin Nave, Robert Fischetti, Masaki Yamamoto, Lonny Berman. Back row: Marc Allaire, Wayne Hendrickson, James Holton, Elsbeth Garman, John Spence, Gwyndaf Evans, Clemens Schulze-Briese, Sean McSweeney. Missing: Kenneth Evans-Lutterodt and Antonio Lanzirotti.**



The workshop was sponsored by the NSLS-II, NSLS, DOE Office of Biological and Environmental Research, DOE Office of Basic Energy Sciences, Brookhaven Science Associates, BNL Biology Department, NIH National Center for Research Resources, and the National Institute of General Medical Sciences. It was also supported commercially by FMB-Oxford Ltd, Bruker AXS, and Area Detector Systems Corporation, and organized by *Dieter Schneider, Marc Allaire, and Lonny Berman* with the great support of *Gretchen Cisco* and her NSLS team.

Please refer to the workshop website for further information. [www.nsls.bnl.gov/newsroom/events/workshops/2009/mx/](http://www.nsls.bnl.gov/newsroom/events/workshops/2009/mx/)

*Marc Allaire*

### ACA 2009 - Workshop on Incommensurate Crystal Structures

Based on the great interest expressed at the session on incommensurate and modulated structures (organized by *Lee Daniels*) at the 2008 ACA meeting, a two-day workshop, attended by ~ 40 crystallographers, was held Friday and Saturday, 24-25 July in Toronto. Because the Jana2006 program package is by far the most commonly used to solve and refine incommensurate structures, we invited *Václav Petříček, Michal Dušek, and Juan Manuel Perez-Matao* to lead the workshop. They periodically offer a three-day Jana workshop in Europe, and felt that it was impossible to do justice to the topic in only one day, hence the unusual two-day ACA workshop.



Students were required to download and install Jana2006 ([www.xray.fzu.cz/jana](http://www.xray.fzu.cz/jana)) on their own computers before the workshop. The software was packed with a demo version of Diamond for visualization, as well as data for the examples used in the workshop and a detailed “cookbook” of instructions. The software installation and configuration went remarkably smoothly, and we were able to get to work rapidly. Students were also expected to have worked through two simple examples –  $(\text{NH}_3\text{CH}_2\text{CH}_2\text{NH}_3)\text{ZnCl}_6$  and *bis*[N-(2-benzylidenepropylidene)phenyl]ether. These examples covered the mechanics of the program and data file handling, determination of symmetry, solving the structures using charge flipping, editing of atomic parameters, refinement, assigning hydrogens, finding the pseudo-merohedral twinning matrix from group-subgroup transformations, and creating a CIF for publication.

The workshop began by considering single crystal data on the disordered structure of  $[\text{Cu}(\text{CH}_3\text{NHCH}_2\text{CH}_2\text{NH}_2)_2][\text{Pt}(\text{CN})_4]$ , followed by an introduction to modulated structures. For the rest of the day, we worked on the simple (3+1)d modulated structure of  $\text{YPO}_3$  using single crystal data.



*Left to right: Michal Dušek, Carla Slebodnik, Amy Sarjeant, Qi Gao*

The second day began with an introduction to aperiodic crystals and superspace symmetry, followed by solving the modulated structure of  $\text{KSmMo}_2\text{O}_8$  using synchrotron powder data. A lecture on incommensurate tools to investigate families of commensurate compounds was followed by work on the commensurately modulated structure of ephedrine.

The workshop was intense, and we learned a lot. As always, the challenge is to keep in practice once we get home. The charge flipping program Superflip incorporated into Jana2006 was especially impressive at solving structures.

*Jim Kaduk and Olivier Gourdon*



**The 18<sup>th</sup> annual Buffalo-Hamilton-Toronto (BHT) Regional Meeting, November 6, 2009, McMaster University.**

Those of us who have been involved from the start find it hard to believe that 18 years of collegiality and science have gone by. The meeting was coordinated by **Lynne Howell** with local organization by **Murray Junop**, **Alba Guarné** and their teams.

Despite the name of the group, the constituency continues to grow and now includes, in addition to the original cities, Guelph, Kingston (Queen's), London (Western), Rochester and, for the first time this year, Waterloo. There was the usual enthusiastic turn-out of about 100 attendees.

The morning keynote workshop was given by **Philip Bourne** (UCSD and the RCSB Protein Data Bank). Phil reminded us that our structures are only the beginning, and often the most exciting and significant results can come from the use of bioinformatics analysis of structural data in areas as diverse as homology modeling, molecular replacement and evolutionary biology. The last is developing into a particularly exciting application.

In the afternoon, we had some very impressive short research talks from **Christopher Garnham** (Davies Lab, Queen's), **Lili Sampaleanu** (Howell Lab, SickKids, Toronto), **Monica Pillon** (Guarné Lab, McMaster), **Jesse Sundlov** (Gulick Lab, Hauptman-Woodward), **Thomas Grant** (Snell Lab, HWI), **Wes Errington** (Privé Lab, Toronto), **Danielle Visschedyk** (Merrill Lab, Guelph) and (Pai Lab, Toronto). Unfortunately, **Da Duan** (Allingham Lab, Queen's) could not present due to a case of 'flu. It is heartening to see that the next generation of structural biologists will continue to provide Philip Bourne and the research community with fascinating results.



**From left to right: Philip Bourne, Christopher Garnham, Lili Sampaleanu, Jesse Sundlov, Monica Pillon, Thomas Grant, Danielle Visschedyk, Wes Errington, Wing Yiu Chan (Photo by Alba Guarné).**

The BHT continues to be supported by our generous sponsors, VWR, Molecular Dimensions, Microlytic, Rigaku, Bruker, Qiagen, Hampton Research, Oxford Diffraction, Oxford Cryosystems and Art Robbins. The traditional wine and cheese reception, sponsored this year by Microlytics, Qiagen and Rigaku, was a great way to wind down the day while waiting out rush hour traffic.

Next year's meeting has been scheduled for Fireworks Day, November 5, 2010. Anyone who happens to be in the vicinity is more than welcome to join us for an inspiring and fun day.

*David Rose*

**2009 ACA Course on Small Molecule Crystallography, June 22 - July 1, Indiana U of PA.**

This year 25 students attended from the US, Uruguay, Brazil, Thailand and Scotland. The course included 8 days of instructions (lectures in the morning, workshops in the afternoon and computer tutorials at night), a day to tour Pittsburgh and a day allotted to final student presentations. On the final day, 22 of the 25 students submitted a course evaluation (using a scale of 1- 5 with 5 being excellent). This feedback has been instrumental for the continued growth and development of the course since 2003. The course was judged to be very successful with 100% of respondents stating that they would recommend the course to others. They gave a very high rating to the category "Did you enjoy the course scientifically" (4.77) and "Did you enjoy the course socially" (4.91). Unfortunately, IUP had to cut many corners due to the state of the economy resulting in building closures and reduced services for conferences (for example, IUP no longer supplies linen and pillows in the dormitories).


Our lecture series was lead by our quintessential lecturers, **David Duchamp** and **Jenny Glusker** who laid down the basic foundation of the student's crystallographic knowledge. They are outstanding lecturers who strongly contribute to the success of the course. **Cora Lind**, continued to show her enthusiasm and skill for teaching crystallography giving the students an excellent background in powder diffraction as well as contributing to the basics. She is a very dynamic lecturer. **Jim Kaduk** and **Brian Toby** continued their awe inspiring lectures and tutorials on advanced topics in powder diffraction. **Peter Müller**, our SHELX expert, organized an excellent tutorial as well as presenting very interesting lectures on "difficult structures" and "twinning". Modern instrumentation was discussed detail by **Sue Byram** and **Lee Daniels**. **Bryan Craven** presented a very informative talk on atomic displacement parameters. **Curtis Haltiwanger** returned to give an excellent lecture discussing "Single Crystal Data Processing" while spending time one-on-one with the students, teaching them to solve and refine structures. **Aina Cohen** gave a wonderful introduction to synchrotron sources and presented a tutorial on the use of the Stanford synchrotron. This is a very important addition to the course. Students should aware that the facilities at national laboratories are available and accessible to help promote good science. Students were provided with a hard copy of all lecture notes as well as a CD-ROM containing all notes, presentations, tutorials and course photographs.

A major advantage of holding the course at IUP is the tremendous IT support we receive from the IUP College of History and Social Sciences. Their superb IT staff headed by **Eric Strittmatter** provided the ACA faculty with an outstanding computer facility. They clearly take great pride in ensuring that all software was running at peak efficiency and were directly responsible for the computer facility receiving tremendous positive feedback from the students and faculty. The evening computer tutorials were given by **Jim Kaduk**, **Brian Toby**, **Peter Müller** and **John Woolcock**. This year, four diffractometers were available to the students. The x-ray facility at IUP had a Rigaku Miniflex and a Bruker D8 Advance powder diffractometer, Rigaku-Americas Inc. and


Bruker AXS Inc. continued their strong support by bringing an SCXmini benchtop X-ray Crystallography System (Supported by *Lee Daniels*) and a Smart X2S Benchtop Diffractometer (Supported by *Bruce Noll*), respectively. The students were also given access to the Bruker APEX II diffractometer at Duquesne University by *Jen Aitken* and *Tomislav Pintauer*. The experimental sessions were very successful due to the indispensable services of *Cora Lind*, *Lee Daniels*, *Bruce Noll* and *Peter Müller*. These individuals worked with students individually into the wee hours of the morning helping the students collect and process data. *Bruce Noll* and *Peter Müller* made trips between IUP and Duquesne to mount samples and operated the APEX II instrument.

The organizers and students are grateful for the direct financial support donated by the ACA, USNCCr, ICDD, PDS, Bruker-AXS and Rigaku Americas. Their generous donations supported the student scholarships and course infrastructure. The USNCCr donation also covered travel awards to scholars from South America and Thailand. The organizers would also like to thank *Pat Craven* and *Melissa Habedank* for their assistance in organizing the course picnic/pool party and *Yuan Hu*, *Andrew Kerr* and *Aaron Barns*, for operating the course van service and looking after the students. Their contributions directly influenced the success of the course. Overall, the course evaluations revealed that the 2009 ACA Course was successful in achieving its goals and we plan on holding the ACA Course at IUP summer 2010.

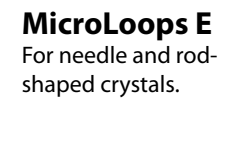
*Charles H. Lake and Bryan M. Craven*




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## ***AIP-Member Society Education Policy Objectives and Activities***

In March, the Committee on Public Policy advised the AIP to increase its efforts to influence science education policy. AIP asked Member Societies to define our education policy goals, and used their input to set the following objectives

*(1) Establish a supervisory position at the Department of Education (ED) to oversee STEM (Science, Technology, Engineering and Mathematics) programs.*

A government review in FY06 found over 100 federal STEM programs or \$3.12 billion.

The Department of Education (ED) is a major source of STEM education funding.

There is no person, or office to hold responsible, or advocate for STEM programs at ED.

*(2) Make science a weighted component of the Adequate Yearly Progress (AYP) measure.*

Science tests are administered to students, but the results are not counted in AYP.

NCLB (No Child Left Behind) is on its last legs, but science must have a place in whatever comes after.

If we act now we can make science a key component of the NCLB reauthorization.

*(3) Improve the use and distribution of professional development funds in Title II (A) of NCLB.*

The ultimate objective is to make the use of present funds more efficient.

We are looking for language changes that will direct more funds to train physicists.

This objective is the least well defined, but may have the greatest immediate impact.

AIP, AAPT, AAS, and APS have secured significant congressional support for objectives (1) and (2). AIP is presently scheduling meetings with pertinent congressional offices and committee staff to move two pieces of legislation - H.R. 2710 and H.R. 2511 – that would enact our objectives. Most recently, several offices indicated their intent to become cosponsors of these bills, thanks entirely to our combined efforts. We have recently provided input to the President's Council of Advisors on Science and Technology (PCAST), and hope that they will endorse the positions outlined above. It is also important to note that AIP continues to work with appropriators to ensure adequate federal funding for proven science education programs.

There are many opportunities for ACA participation. On an individual level, ACA members can participate in congressional Hill visits and ask AIP to assist in the planning, scheduling, and operation of those visits. ACA members can also stay informed on science policy news by signing up for FYI at [www.aip.org/fyi](http://www.aip.org/fyi). As an organization, ACA can choose to endorse policy letters occasionally drafted by AIP on education policy issues, which AIP staff would gladly direct to appropriate policy makers.

*Rob Boisseau AIP (301-209-3094, [RBoissea@aip.org](mailto:RBoissea@aip.org))*

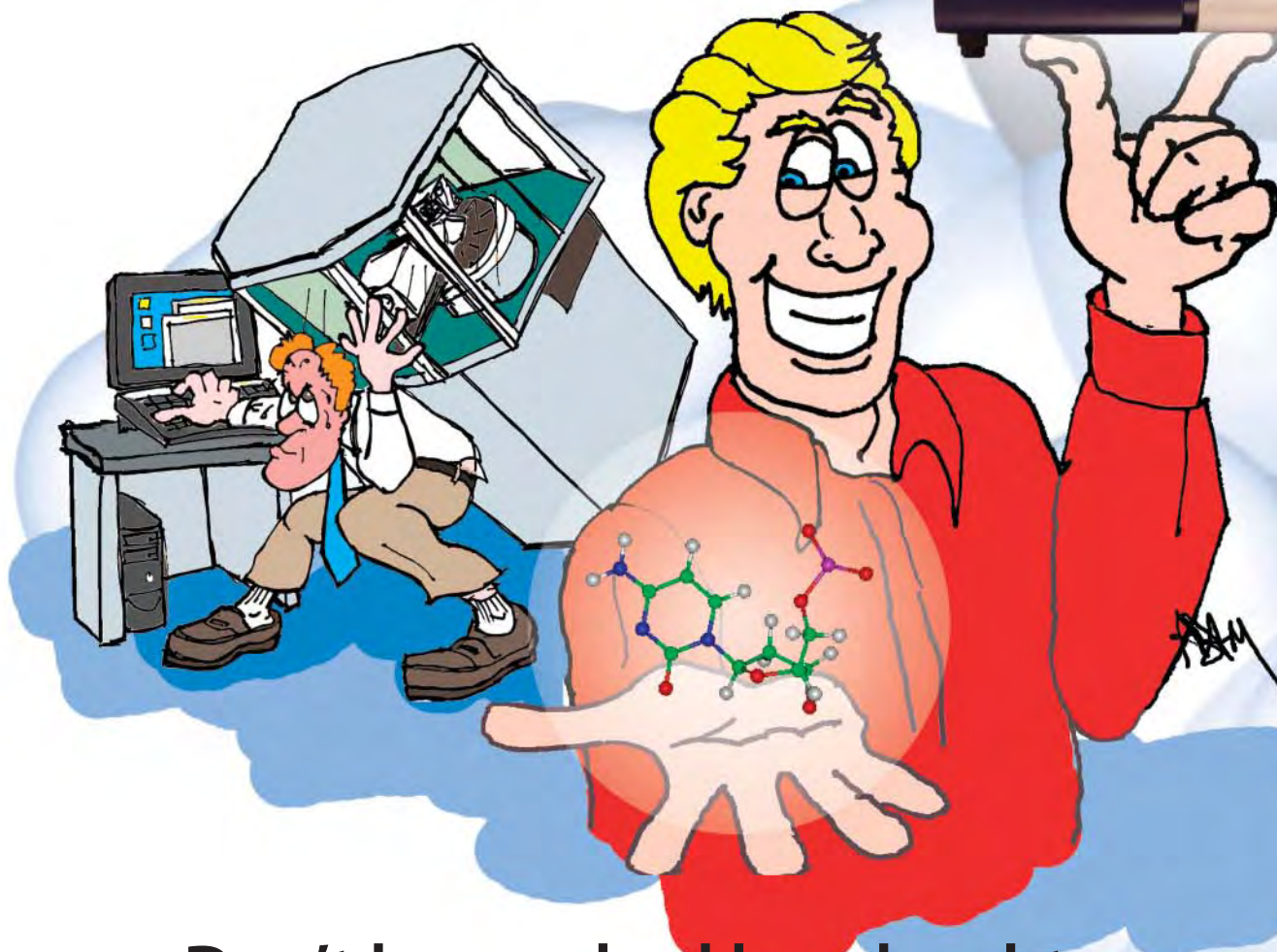


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*Due to the generosity of our community we were able to make a record number of travel grants for ACA 2009 in Toronto. Following are some of the impressions and experiences of the students who were recipients of these grants.*



**Jason Grigg**

I am very grateful to the ACA for generously providing me with a travel grant. I found the technique oriented sessions, including “Crystallization Methods”, “Tips and Tricks of the (Computing) Trade” and “Refinement (Computational)” particularly useful at this early point in my scientific development.

This was my first experience at an ACA meeting and I appreciated the obvious sense of community among the attendees. There was a focus on encouraging involvement at every level and a true collaborative atmosphere. I look forward to attending future ACA meetings and becoming a contributing member of the Association.



**Dejan-Kresimir Bucar**

ACA meetings enjoy a ‘must-go’ status on my

calendar. As a supramolecular and organic solid-state chemist-in-training, I primarily attend ACA meetings to learn about the latest advances in crystal structure determination, to meet colleagues, and to hear about the latest developments in their research. This years meeting was particularly exciting to me owing to the “Supramolecular Chemistry” sessions. They were in my opinion, without any doubt, among the best that I have attended at various ACA, ECM and ACS meetings within the last four years. Not only did the sessions cover an impressive range of topics relevant to supramolecular chemistry and crystal engineering, but the organizers managed to assemble the leading authorities in the field to present their pioneering research. It was highly educational, inspiring, and entertaining! I would also like to point out the new “Would You Publish This” session. It was the perfect environment to discuss one’s problematic crystal structures with highly qualified crystallographers. I truly hope that this session develops into an integral part of ACA meetings. Altogether, the meeting was once again a great experience for me and I would like to express my sincere thanks to the ACA and the organizers of the “Supramolecular Chemistry” session for allowing me to share the podium with all those eminent speakers.



**Jeff Lee**

I want to thank the ACA for the grant without which it would have been difficult for me to attend and I would have missed the opportunity to present my research.

Compared with other meetings I have attended, this was definitely one of my favorites. The quality and scope of the science was outstanding. I particularly enjoyed the “Structure-based vaccine design” session and the discussion on where the future in this area is headed and how we can use the existing structures of viral antigens to design molecules that are better able to elicit a particular immune response. I want to thank the organizing committee for making this meeting such a success!!

Since I did my graduate work in Toronto, it was really nice to be back in the city to see my old colleagues and mentors. It was also very easy to network during the poster sessions and receptions. I was able to meet graduate students, post-docs and faculty from around North America and the world. I enjoyed the wonderful opportunities to discuss and exchange ideas and opinions with other participants at the meeting.

Once again, many thanks to the ACA and I look forward to the 2010 ACA meeting in Chicago- see everyone there!



**V. Mitch Luna**

I would like to express my sincere thanks to the ACA for

the travel grant, as well as the support of my supervisor, C.D. Stout, and the Canadian Institutes for Health Research made my attendance possible. I would also like to thank the organizers of the *Structural Enzymology* session, Emil Pai and Felix Vajdos, for the opportunity to present a lecture. This was only my second time at an ACA meeting and it was as informative and enjoyable as the first. It was an absolute joy to be able to interact with accomplished crystallographers from all fields. I particularly enjoyed the sessions on *Membrane-associated Proteins* and *Structure based Drug Design*. The poster sessions and social events were great venues to meet the next generation of crystallographers.

Thanks again to the ACA for this great opportunity. Overall, I felt the meeting was informative and very well organized. I look forward to attending future meetings.



**Nicoleta J Economou**

I would like to thank the ACA for the travel grant. This was my first ACA experience and I am definitely looking forward to future meetings. It was fantastic to be at an international meeting and to learn about the latest news in crystallization, data collection, data processing and refinement. In between the sessions and events there was time to meet other crystallographers and talk about my project and to get their input. It is always fun to interact with people that

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are as excited as you are about crystallography such as other graduate students, people from industry, academia, beamline scientists and vendors.

I definitely would encourage all students to take part in the events designed especially for them, such as the YSSIG mixer and the Mentor/Mentee dinner. At the YSSIG mixer, I met other graduate students, with whom I have kept in contact even after Toronto. At the Mentor/Mentee dinner I had the opportunity to have one-on-one conversations with experienced crystallographers in a more relaxed environment.

Leaving the ACA meeting in Toronto, I felt that I was up to date on what is going on in our field and that I had gained new contacts and friends. I am grateful to the committee for giving me the opportunity to enjoy this experience.



**Brandon Mercado**

I am so grateful to have received a travel award. Traveling there with Christine Beavers and Marilyn Olmstead was not only fun, but also extremely educational. Robert Heuther invited me to participate in the Etter Early Career Award Symposium as a student presenter, which marked my first oral presentation at a national conference. I also enjoyed meeting Anthony Spek and George Sheldrick. I benefit almost daily from their contributions to crystallography and felt privileged to have had the opportunity to interact with them one on one. I had

sushi with Bruce Noll and Michael Ruf from Bruker and got to reconnect with Joseph Tanski, one of my professors at Vassar College, over oysters. It was also a blast getting to explore Toronto with the students from the University of Ottawa and to expand my network in the crystallography community. I would like to thank you again for providing me with the funds to travel to Toronto and participate in an academically, socially, and personally fulfilling experience. I definitely plan to attend the 2010 conference in Chicago.



**Sean Dalrymple**

I would like to extend my gratitude for the travel support. As this was my second ACA meeting, it was a pleasure to reunite with many of the crystallographers I met previously and it was a great forum for getting acquainted with the names I have read about in the literature. Academically, the mix of well established and young scientists provided for an interesting environment in which to learn about cutting edge techniques that will undoubtedly help me develop my skill set for future employment. The vendor exhibit was also an excellent resource for learning about new advances in the areas of crystal mounting, data collection, and solution refinement. As a postdoc making the jump from small molecule structure determination to the world of protein crystallography, the conference provided many

sessions of interest to me including great talks covering crystallization methods, refinement, diagnostics, instrumentation, and tips & tricks of the trade. Additionally, the professional directions panel discussion was particularly informative and I am sure many students and postdocs found that session enlightening and took from it many tidbits of information that will help in their future career development, I know I did. Given the recent passing of my supervisor, Louis Delbaere, the conference was particularly memorable for me personally as it was the venue where I really saw how special a person he was to so many people. Besides being a wonderful supervisor, he was a truly kind human being; Louis, you will be greatly missed. Finally, I would like to thank the coordinators of all the symposia for their time and efforts in organizing such an interesting series of presentations. As I am nearing the end of my current postdoc in the Delbaere laboratory, it was an excellent opportunity to meet and talk with potential employers. At future ACA meeting I hope to get the chance to continue interacting with all the great people I had the opportunity to meet.



**Navdeep Sidhu**

This was my first ACA meeting and I am grateful for the travel grant. Discussing

research issues with a great and diverse group of crystallographers helped me see alternative ways of looking at and solving problems—useful in escaping the local minima of my own thought processes. The workshop “Handling Twinning in Macromolecular Crystallography,” the poster sessions and many talks were among my favorites.

It was nice to see that the meeting was also attended by conferees from abroad, including Uruguay, New Zealand, the Czech Republic, India, and even the United States. Hopefully, meetings can also be held in the future in Latin America, which could be helpful in promoting science and education in economically less advantageous settings.

The poster sessions served as potent nucleation points. They worked squarely in the diffusion-limit regime and when they ended, withdrawal symptoms were acutely felt, with many a young crystallographer apparently requiring a further therapeutic administration of posters over a more chronic period. And, at the end of the day, it was interesting to find even small and large-molecule crystallographers finally seeing eye-to-eye in front of a microphone—a karaoke one that is.

My sincerest thanks are also due to my mentor Louis Delbaere and the University of Saskatchewan College of Graduate Studies and Research, Canada, for the rest of the much-needed financial support which made it possible for me to attend the meeting. It was a highly stimulating and memorable educational experience. I also appreciate all the great service the ACA staff provided before and during the meeting.

Just over a month after the above article was submitted, we sadly learned that Louis had suddenly become critically ill the previous day. He passed



away that evening, only weeks before he was slated to receive his earned Doctor of Science, which he has now received posthumously.

There are excellent scientists, compassionate people, and caring mentors. Louis was all of those simultaneously. He had grace and humility. A colleague of his said he had never seen him wear a frown in three decades. That would be just Louis. Hearing the good-natured Delbaere laugh often gave his presence away—an icing on the cake of his pleasant sense of humor.

At the memorial service, the priest told the congregation how, after one of his sermons, Louis came up to him and said, “Father, you should never discount the scientific method.” There are many ways one could say that. With his generous approach and convincing argument, he won Father over to the method.

In teaching crystallographic theory, Louis spoke of the work done in prison by the remarkable Kathleen Lonsdale [the first woman President of the IUCr and the first woman elected as Fellow of the Royal Society (“Lonsdale, Kathleen,” Contributions of 20th Century Women to Physics (CWP)), [www.physics.ucla.edu/~cwp](http://www.physics.ucla.edu/~cwp)] who was sentenced upon her refusal to pay a fine stemming from her decision to live by her pacifist beliefs. The crystallographer who figured out space groups seemed to defy spatial confinement if not in body then at least in human spirit. And don't the best among our species also defy their temporal confinement to one lifespan?

At his memorial service, I felt the need to talk to as many people who were close to him as I could. In his wife, Carol, children, grandchildren, and siblings, even some friends, I could see some of Louis. In the many lives he touched

around the world, Louis seems to transcend time. His grandchildren continued his legacy by making it impossible for me not to smile a bit even on such a sombre day.

As I left that day, I recalled and found some solace in what Louis' friend had said: “Science can give you answers. But who do you call when you don't have the answer?” Feigning self-importance, he had then gone on to answer his own question, “You call the priest. Not because we have all the answers. But because we can help you let it go.” Father's message had been inevitably religiously framed but, whether one shared his belief or not, I think his underlying message had been a general one: It was human.

In the weeks that have gone by since, I realized how much Louis taught through simply living the way he did, through example, rather than so many words. Such teaching demands imagination from the learner. The lesson is not always immediately clear. I am figuring it out as I go.

It was a great privilege to be his student. Louis is sadly missed, and will be affectionately remembered always.



**Chuttree Phurat**

I was very glad to be one of the travel award winners and very excited because it was my first time to an ACA meeting. At soon as I stepped up to the registration

desk, I could feel the warm greeting. I liked many events that I experienced at this meeting. Due to the excellent management in scheduling oral and poster sessions, I was able to participate in almost every seminar. I liked many sessions especially those on supramolecular chemistry, structure-based drug design, problem structure solution and refinement, and professional directions. I learned more about crystallographic study that will help me figure out what I will do after graduation and to decide on my future career. I also liked the vendor exhibit even if it was just for a few days. Furthermore, with the meeting place in the city center there were a lot of shops and restaurants within walking distance so I could enjoy my time after the seminars. Finally, I have always thought that “*Experience is the best teacher*”. The most important lessons can't be taught. We learn in life from our participation in situations.



**Jamaine Davis**

The ACA meeting was a great experience. I enjoyed meeting and talking with prominent structural biologists, as well as conversing with fellow postdocs and graduate students. Attending this meeting, with the help of the travel award has prompted me to become more involved with the YSSIG. I am excited to be a part of such a valuable group.



**Viivi Majava**

I would like to thank ACA for the travel grant. At the Sheraton, it was nice to be part of the underground network, “the Path”, in the city of Toronto.

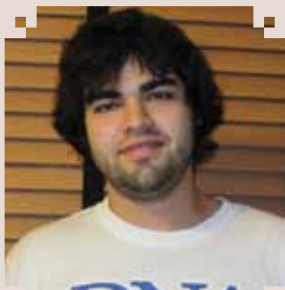
There were many interesting sessions including *Exciting Structures*, *Crystallization methods*, *Complementary Methods for Macromolecular Crystallography*, *Structure-based drug design*, etc.

As I am interested in combining different methods in my studies, I was happy to listen to lecturers presenting not only the different aspects of crystallography but also many other methods like small-angle x-ray scattering that can be combined with crystallography. The meeting also gave me a lot of new perspectives on other research areas.

Moreover, I think it was very practical that the poster sessions were organized on three different evenings, so that we had a chance to see as many posters as possible and to exchange ideas with other participants.

I attended the workshop on *Handling Twinning in Macromolecular Crystallography* organized by George Sheldrick, Garib Murshudov and Peter Zwart. I found the workshop very useful and I will try the different programs for my datasets in the future.

Finally, I would like to thank Ronan Keegan and other CCP4 staff for helping me with many CCP4i problems at the CCP4 booth.



**Colin McCrimmon**

I would like to thank both the ACA for the travel grant and my supervisor, Cameron Mura, who has served as a guide and role model in all my research aspirations and without whose help I could never have attended. This was my first academic conference and I was thoroughly delighted by the experience. While the “magic” of these conferences may wane over time, I cannot express the honor I felt simply to be present at a meeting where one could walk from room to room and hear some of the brightest and most well known scientists in the world. I thoroughly enjoyed the poster sessions which gave me a chance to talk with and meet some of these scientists. Furthermore, I have only had one class on the theory of x-ray crystallography so, to say the least, I learned many interesting things that one cannot find in a classroom. Once again I would just like to extend my sincere gratitude to the ACA for providing me with a means to attend and for all the planning and preparation which ensured that my first conference could not possibly have been better.



**Alister Gould**

I attended ACA 2009 as a newly transferred PhD student into the lab of Brian Shilton. This was my first ACA meeting, and the largest conference I have attended to date. I enjoyed the open format of the talks. With several presentations taking place simultaneously, I had the opportunity to contrast the techniques and findings of different disciplines of crystallography and find those discussions, even from disparate fields, that most interested me. I valued the chance to learn more about the practices and history of small molecules structure determination, as well as the work being done in biochemical topics as varied as pharmaceutical development, biofuels production, and structural vaccinology. Among my most valuable experiences was my exposure to the wealth of career possibilities available in all these areas.

Additionally, in presenting my own findings on the mechanisms of ATPase regulation and substrate specificity in an ABC transporter, I was able to discuss my findings with others and to share my understanding with those working in related research. These conversations assisted in my writing of a recently submitted paper.

Without the generous travel grant my attendance would have been much more difficult or even impossible. Thanks for giving me this opportunity to participate and learn.



**Haemi Chung**

I would like to thank ACA for the travel award and for giving me an opportunity to present my work. This was my first ACA meeting and also my first time in Toronto. The meeting gave me the opportunity to meet a lot of people from all over the world who are involved in crystallography. I had a great time presenting my research project, had opportunities to discuss my research with other people in this field, and even found some possible collaborators. It was a fabulous experience and I really enjoyed this meeting. Thank you again for your very generous support.



**Peter Gin**

As I descended the escalators from the bustling hotel lobby, I had no idea of what to expect entering the ACA annual meeting. Having arrived late the night before because of inclement weather, the trip did not start off as I had planned. With an approaching oral presentation on my mind, the familiar feelings of nervous excitement began to arise. However, that quickly subsided as I approached a smiling face at the registration desk. I was greeted warmly and told that they were expecting me. I was promptly presented with my materials and to my delight, a travel award. After thanking the courteous staff, I made my way towards the presentation areas. Having a few minutes before my session began, I briefly looked over some poster presentations while enjoying the refreshments made available to us. I couldn't help but recognize how

everything was planned out in such a professional manner. I began to relax. I knew that I had nothing to worry about. This level of professionalism carried on throughout the day, and my state of mind allowed me to confidently present my research to a room full of distinguished scientists. I was also honored to receive the Margaret C. Etter Student Lecturer Award from the Small Angle SIG. To say the least, I was extremely impressed by and thankful to attend my first ACA meeting.



**Peder Cedervall**

The twinning workshop was a perfect start to the week in Toronto. It was great to learn from the research software developers what tools and programs are available to deal with twinning issues. There were a lot of stimulating talks throughout the week. I found it very interesting to listen and talk to other researchers about their work. Another valuable part of the conference was talking to the vendors and people from the beamlines about the latest and greatest. I feel very privileged to have received a travel grant and for the opportunity to give a talk, as well as present a poster.



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**Zhen Xu**

I am grateful for the travel grant. As a young investigator in the field of protein crystallography, I was very interested in the exciting sessions on macromolecular structures and the development of new methods for structural determination. There were so many great presentations on the above topics and I greatly benefited from all of them. First, I would like to thank all the speakers for their wonderful talks on complicated structures and crystallization methods in the sections sponsored by the BioMac group. Second, I was particularly thankful for the informative panel discussion on professional directions sponsored by the YSSIG and I really appreciated it for their valuable suggestions on our future careers. Third, I would like to thank all the session organizers, speakers and the poster presenters who made this meeting colorful and successful. Finally, I would like to thank the IUCr, Bristol-Myers Squibb, ICDD, Rayonix, Art Robbins Instruments and the ACA for providing me the travel funds which were really helpful to me. I hope that more young scientists will benefit from this program in future.


**Mayasree Oottil**

I would like to thank ACA for the travel award. The conference provided a wonderful learning opportunity in many different areas of crystallography. As a newcomer to the discipline of crystallography, it was fascinating to see the wide range of crystallographic techniques and methods of data analysis.

The workshop on using JANA was really impressive and informative. Among the conference sessions, I particularly enjoyed "Energy Related Materials" and "Problem Structures". The quality of posters was also very impressive. I am thankful to ACA for giving me an opportunity to present my research work and it helped me to discuss my research with various researchers from around the globe. As a graduate student this conference also provided me an excellent opportunity to network with other students. Thanks again!


**Safiyah Forbes**

I am very thankful to the ACA for the travel award. I would also like to thank the organizers

of the supramolecular session, Christer Aakerøy and Gary Enright, for giving me the opportunity to present a lecture on improving the thermal stability and solubility of active pharmaceutical ingredients.

I also had the opportunity to speak with a lot of interesting people after my talk providing me with great feedback to take back to the laboratory and apply. Overall the highlight of this year's conference for me was having the opportunity to listen to Gautam Desiraju, Joel Bernstein, Pierangelo Metrangolo, and James Wuest along with many others, whose talks were very informative and educational.

Finally, I wish to thank the ACA again for providing me with a travel grant that provided access to other great scientists.


**Catherine Tupper**

This was my first ACA conference. As I work closer to the engineering/metallurgy side of materials science, there were many sessions that were not directly applicable to my specific research. However, some were in similar fields and increased my understanding, while others exposed me to completely new, interesting topics. The format and atmosphere of the conference were both encouraging and valuable for me as a young graduate student, very early in my career. The "Professional Directions" panel discussion was particularly helpful. It raised many issues that I had not previously considered,

but have been thinking about since. The diverse background and career paths of the panelists illustrated a measure of diversity within crystallography of which I had been unaware.


**Prashant Chopade**

This was my first ACA meeting and I am greatly honored by the ACA Travel Award without which it would have been really difficult for me to attend and for having my abstract selected for an oral presentation in the *Supramolecular Symposium*. I was able to meet many people eager to provide suggestions on my research and many who were interested in where the research was heading. I particularly enjoyed the sessions on *Supramolecular Chemistry*. I was fortunate to attend talks given by superstars in the field such as Joel Bernstein, Gautam Desiraju, Pierangelo Metrangolo.

I also enjoyed the atmosphere of the meeting, as well as Toronto itself. Thank you again for this great opportunity and I look forward to future ACA meetings.


**Harkewal Singh**

As a graduate student majoring in protein crystallography, I always want to listen to the experts in the field and the ACA provided me this opportunity. I had a very good experience at ACA 2009. Not only was listening to the talks of the pioneers of this field of great benefit to me, the opportunity to present my own work was terrific. In science it is important to carry out quality research but equally important is the presentation. This becomes essential when you are in graduate school. I am grateful to the ACA since they gave me this opportunity and awarded me a travel grant to support my trip. Several people stopped by my poster and I had some good discussions. I now feel more motivated and excited about working in protein crystallography. Besides being among the best of crystallographers I also enjoyed the nice weather of Toronto. Thank you ACA and I look forward to being at the ACA meeting in 2010.



**Kristopher White**

My trip to Toronto for ACA 2009 and my presentation represented the culmination of a great deal of hard work from two summers at SSRL, and, perhaps more importantly, I feel that the impressions I took away from the conference will play an important role in guiding my interests as I prepare for graduate study in biophysics. Never having attended a scientific conference before, my expectations for the ACA meeting were somewhat limited; by the end of the week,

however, I was pleasantly surprised by both the quality of the material and the affability of the attendees time and time again.

In terms of subject matter, I certainly enjoyed hearing about exciting new macromolecular structures, but I was particularly interested in the developments outlined in the sessions on diagnostics during data collection and computational refinement. As a student with limited prior exposure to the many of the topics discussed throughout the week, the theory-rich presentations given during those sessions provided me with the requisite background needed to understand the new ideas that were presented. I particularly enjoyed James Holton's talk on using simulated diffraction images to learn more about the assumptions made by protein crystallographers during data collection.

These types of problems relate in some ways to my own work, and getting to learn from someone interested in addressing similar issues, albeit in a much more rigorous manner, was a thoroughly rewarding experience. Indeed, my time in Toronto was full of similar experiences, and I was a new member before the week was even half over. See you in Chicago!



**Haiyan Chen**

I am very grateful for the travel award. My main goal for the ACA Meeting was to attend the JANA workshop and learn the software. The workshop turned out to be

great. The instructors were very patient and very helpful. I also got help from more experienced attendees. After the workshop, Dr. Petříček personally helped me and another student from my group in the analysis of our data using JANA software. We were very excited that our data could be successfully processed with the software. At the ACA meeting itself, I got the chance to meet and interact with many people. It was very delightful to talk with one of the professors from my graduate school, whom I haven't seen for quite a few years. I got advice from the respectable James Kaduk on powder diffraction. As a first time attendee, I really like the meeting very much.

Thanks again for your organizational efforts!



**Daniel Pohl**

The 2009 ACA meeting was the first conference I have ever attended so without a basis for comparison I can only give my opinion of it. The Sheraton hotel in downtown Toronto was an ideal location because there was no need to travel to and from the conference and hotel each day and it provided access to whatever other needs a person might have via the underground mall. The organization of the conference itself was done well and I refer specifically to the schedule provided to all attendees that listed all the talks so that one could decide where to be at what time depending on his/her interests. I also found the grouping of talks into sessions with common themes a good idea because it allowed me to attend a string of interesting talks all together

in one session while avoiding others entirely! Unfortunately I missed the opening night but the YSSIG mixer that followed was enjoyable. One unfortunate thing for me in the field of high pressure small molecule crystallography was that the vast majority of talks and posters were about macromolecular crystallography. Still there were some talks relevant to my field including a session on Phase Transitions. Overall I think the conference was a success and I hope to attend the next meeting in Chicago.



**Adrian S. Wibowo**

The 2009 ACA meeting was the first conference I attended during my graduate career. Although there was plenty of excitement in attending the meeting, for the most part it was overshadowed by nervousness. I did not know what to expect out of a national conference such as the ACA. I knew that the majority of the conference consisted of seminars involving advances and new discoveries with the field. However, even with that knowledge, my first reaction when I finally experienced the meeting first hand was a sense of being overwhelmed with its many aspects such as the industrial exhibition, seminars, poster sessions and meeting new colleagues.

I looked at the conference as a chance to learn more about the field, specifically to understand the progress that has taken place in the methods of experimentation



with new techniques and instrumentation. What surprised me the most was the extraordinary advancement of microfocus x-ray beams that have been developed and are now available at synchrotrons. It is amazing how they can be manipulated to diffract even the tiniest of crystals. Having experienced formation of micro-crystals of my own target protein, I could immediately see how such a tool could be used to help solve structures where only micro-crystals can be grown. This development showcased how far the field has come and it seems that more advancements are in store. Throughout the conference, I was able to find new colleagues that shared my experiences. Getting to know those in my field is invaluable and I have met a number that I hope to keep in contact with and speak to again at future ACA meetings.

In all, there were a number of highlights that made the meeting a good experience, however the most important thing that I gained was a better understanding of where I am in my own knowledge of the field of crystallography. I saw where my experience in a research lab was fairly strong but more profoundly where I needed to improve. I found myself understanding talks where I had first hand experience more readily than those where I had no experience. Self reflection was the biggest benefit I gained from the conference. It became clear to me that crystallography is a vast field that is ever growing and advancing, and that keeping up with all these aspects is important when it comes to furthering my own career.



**Jason Benedict**

I would like to thank the ACA for their generous travel award. Once again, I had the opportunity to speak before a receptive audience and thoroughly enjoyed engaging with individuals curious about my presentation. From the Q&A to the poster sessions to the socials, it was great reconnecting with old friends and making new acquaintances. Was there anything I didn't like? With so many excellent speakers, I was forced to choose between overlapping talks on several occasions. Despite a few missed talks, I generally considered myself lucky to have this problem. Thanks again to the ACA for your generous support and for organizing another great meeting.



**Mark Hunter**

First, I would like to thank the ACA and all of the sponsors for the travel award. The 2009 ACA meeting in Toronto was the first ACA meeting that I have attended and, additionally, it was the first conference at which I gave a presentation. I did not know what to expect, but I was still surprised to see how much information I was able to gather and learn. I was

introduced to experiments that were similar, as well as very different, to mine, and the combination of talks and poster presentations led to a very enjoyable experience.

The sessions on complimentary methods to macromolecular crystallography and membrane proteins were particularly exciting. These talks were very much related to my areas of research and provided me the opportunity to interact with some of the experts in the fields.

I received a lot of feedback on my talk that opened up new avenues of experiments, furthering me along in my scientific studies. Some of the discussions led to information sharing and potential collaborations, also helping my research. As a fourth-year graduate student, these types of interactions with the broader community are invaluable.

Overall, the experience was memorable, and as such, I look forward to attending the 2010 edition of the conference.



**Nicholas Deifel**

I wish to thank the ACA for the travel grant. I also wish to thank the organizers of the supramolecular chemistry section, Christer Aakeröy and Gary Enright, for affording me the opportunity to present a lecture at the meeting. The feedback I received after my talk was invaluable and is helping to shape some of my current research efforts. Additionally, I was excited

to meet several prominent scientists presenting in the same section including Gautam R. Desiraju.

The quality and relevance of the talks I saw far exceeded any other professional conference I have attended. As a young crystallographer, I found the *Would You Publish This?* session, and the heated conversation it spawned, particularly interesting. I certainly hope this session is organized in future meetings.

Though this was only the 2nd ACA meeting I have attended, it annealed my love for this organization and the greater crystallographic community. Thank you for this opportunity, I look forward to attending many more ACA meetings in the future.



**Miha Andrejasic**

When my boss Dusan Turk asked me in January if I wanted to go to the ACA meeting this year I was thrilled. Although there was a little disappointment when I found out it was going to be in Canada, particularly in Toronto, which I have already had an opportunity to visit. The next thing that raised my excitement and expectations was the acceptance of my abstract for an oral presentation. Even though it was in the General Interest section it was a great opportunity.

I joined my visit to ACA09 meeting with a short visit to my family near Toronto, so when I arrived at Sheraton Hotel the jet lag was already off. I enjoyed working late hours preparing my speech in the lobby since the atmosphere there was incredible

with lot of participants working and surfing the net. Probably many new friendships were made and many new ideas were born there.

The organization and care which was taken for speakers was excellent. With all that support nothing could go wrong. As for my presentation, well, there was still a lot to be learned about how, when and even if I could answer questions. Otherwise the presentation went smoothly, to my satisfaction.

The poster sessions were a little bit crowded but joyful. The social part was indeed a little bit disappointing. The youth mixer was excellent but for the rest of the days there were less organized events. I must give a big plus to Rigaku for organizing the Fun Run, which should also come to European meetings and become a permanent event here.

There was only one thing that bothered me. Since I came from Europe it was difficult to tell where I came from so I had to 'upgrade' my nametag. It was a big surprise to me that people recognized each other based on university names. This was the weirdest thing since just based on a university name everyone knew where you were from. So for the next ACA meeting I will have to work a little bit on learning the locations of of universities in the US and Canada. Otherwise a big cheers for organizers.



**Anna Gardberg**

I would like to thank the ACA for the travel award. My travel budget had been eaten up by traveling to synchrotrons and reactors for data collection, so this award enabled me to attend the meeting. The meeting was very valuable both for the scientific content and for the networking opportunities. I spoke with professional colleagues in neutron diffraction and obtained useful advice. I met with representatives from crystallographic programming consortia, pharmaceutical firms, and crystallographic instrumentation companies.

My primary goals in attending the meeting were to learn about the latest advances in instrumentation, software, crystallization technology, and neutron crystallography, and to learn more about opportunities for crystallographers in industry. Thus, I particularly enjoyed the poster sessions and the oral sessions on structure-based drug design, crystallization, and computational aspects of refinement. I was also flattered to be asked to speak in the "Large Small Molecules" session.

Thank you, ACA, for helping me attend this very productive and enjoyable meeting.



**Katherine Sippel**

I would first like to express sincere appreciation to the ACA for the travel grant. While this was not the first time I have attended an ACA conference, it was the first time I felt I had a sufficient knowledge base to

fully appreciate the material being presented. Particularly I was amazed at the advances in computation which not only make structure solution simpler but also more accurate. I was also encouraged by the degree of integration between x-ray crystallography and other techniques, demonstrating this field's capacity to adapt to any question that needs answering. The poster sessions were quite exciting and allowed me to test the extent of my knowledge from the biological to the crystallographic and everything in between. I also had the pleasure of interacting with the experts in my field and gaining unique insights and perspectives on my projects. The "Professional Directions" panel was informative and I appreciated the frankness and candor with which the questions were answered. Overall the meeting in Toronto was a pleasurable experience and I look forward to next year's meeting.



**Peter Horanyi**

It was wonderful to visit Toronto in July. This was my first time in Canada and I felt very lucky to be in such a beautiful place! I was amazed with the richness of the architecture and the history of the city. The ACA meeting was excellent as always! I really enjoyed seeing the most recent accomplishments in crystallography as well as meeting fellow crystallographers at the social events. I am partial to the single crystal, macromolecular part of

the field and I found something new and exciting throughout the meeting and at each of the Poster Sessions. I am very thankful to the ACA for the Travel Award! It is fantastic that both the ACA and Rigaku corporation, both offer travel bursaries for postdocs and I was lucky enough to receive travel support from Rigaku also this year. It has benefited me immensely to interact with these wonderful organizations and I advise everyone to explore multiple avenues when looking for travel awards. The awards allowed me to showcase my recent structural findings in outer membrane transport of vitamin B12 and I received some very useful comments. I was also able to Co-Chair the refinement (computational) session as a YSSIG representative only because of the financial help from both the ACA and Rigaku. Again I would like to thank both organizations for giving me this excellent opportunity



**Janeth Presores**

Participation in the ACA meeting greatly enriched my experience as a graduate student, as I was able to present my research and broaden my knowledge in crystallography. I'm grateful to the ACA for providing a venue for graduate students to get acquainted with an array of topics pertaining to *Solid state Chemistry*. I particularly enjoyed the discussions in *Supramolecular Chemistry*, *Green Biochemistry*, *x-ray*



*diffraction instrumentation and Crystallization Methods*, and the many advances in structural techniques complementary to x-ray crystallography. The opportunity to attend lectures and to interact with professors whose papers I have read was a very valuable experience. As a new user of SHELX, I especially benefited from lectures on the determination of problem structures, from George Sheldrick, no less! Also unforgettable was the engaging exchange of ideas and sharing of joys and challenges of research through interactions with other graduate students. I would like to thank the ACA organizing committee for a very pleasant meeting, for the travel grant, and the opportunity to present my first talk at an international meeting.



**Paulo Carvalho, Jr.**

I would like to thank the ACA for the generous travel grant. I found the meeting to be extremely enjoyable. For me, it was a privilege presenting my research at a poster session and I am honored to have won the AIP Undergraduate Research prize. When I was notified that I was selected to have a grant I was surprised and pleased and I was also very pleased to visit Toronto. It was both my first ACA Meeting and my first time in Canada. As an undergraduate, I found the information presented to be very interesting the informative.

The ACA meeting is always a great event. Many famous

scientists not only from the USA, but from many other countries present different aspects of crystallography. For a young person it is a great opportunity to listen to interesting discussions and to learn about the direction of their future investigations. I visited the poster session and the products show, met many fellow scientists and had very stimulating conversations. It was a great to present my work on *Hydrogen-bond Patterns in the 1,3,6-cyclohexanopentol*. There were various topics at high levels of research on display, and ample opportunity to interact with a wide variety of researchers from various parts of the world. This experience allowed me to gain a better understanding of the dedication it takes to be a successful.

The organizers did a wonderful job. The meeting blended many things that made this young scientist happy: I was exposed to great scientific discoveries and techniques. I see my participation in ACA meeting as an incentive to continue in this area of research. It was and always will be a pleasure to have this experience and I am grateful to the ACA for making it possible for me to be at this wonderful meeting.



**Troy Johnson**

I would like to start by thanking the ACA for the travel grant. This was my first opportunity to attend an ACA meeting and I thoroughly enjoyed the experience. The

sessions were well planned with many informative talks. I especially enjoyed the structural enzymology sections, since these talks directly relate to my research interests. I presented my research at the first poster session and received enthusiastic comments and feedback on my work. The most beneficial aspect of attending this meeting was the opportunity to meet and network with established experts in the field of crystallography. Once again I would like to thank the organizers for giving me the opportunity to attend and for putting on a wonderful meeting. I am looking forward to attending many more ACA meetings in the future.



**Arbin Rajbanshi**

My sincere appreciation to ACA for providing me with the travel grant. This was my first talk at ACA and it was an honor for me to be given the opportunity to share my research with national and international intellectuals. It was a great opportunity and a fascinating experience for me to attend the lectures and poster sessions to learn about recent developments in the diverse fields encompassing crystallography. Especially the supramolecular session was of much interest, as it related more to my own research. It helped me to gain innovative ideas and broadened my views. I was able to discuss my project with senior scientists, professors and fellow researchers, who gave me valuable comments and suggestions. The opening reception and young scientists

mixer let me meet with many other fellow graduate students and discuss our projects and future goals. In addition, the range of exhibitors helped to keep us informed about the latest technologies, instruments, and software available for our research. I am looking forward to attending more ACA meetings in the future.



**Samroeng Krachodnok**

I had a great time both at the conference and in Toronto. I would like to thank everybody for their kindness and openness during the meeting, especially the organizing committee that brought together, expert crystallographers for discussions and suggestions regarding my work and also the exhibitors for eye-opening new innovations, especially for mounted single crystal equipments.

I was especially interested in the evening session on "Would You Publish This?", for example, a porphyrin structure with an R-factor higher than 10% and the weakly diffracting chiral organic molecule and so on. For first or related structures, we believe their structures should be published because the structural model is correct and significant but it gets rejected because of the high R-factor.

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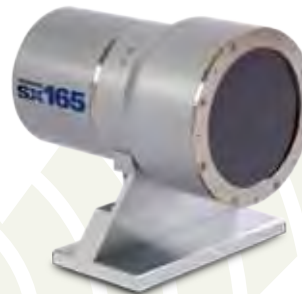
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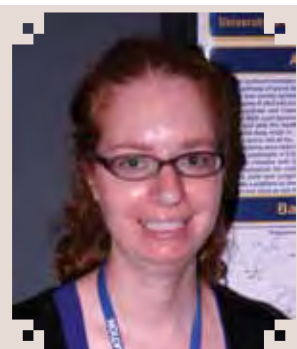




**Ainsley McFarlane**

This was my first ACA meeting and I had a wonderful time. I found the sessions to be very interesting and I learned a great deal. In particular, I enjoyed the sessions relating to macromolecular crystallography. I thought that the "Professional Directions" session was a good chance for young scientists to learn about future career prospects in crystallography.

I presented a poster and I enjoyed discussing my work with other scientists. I appreciate all of the good comments which I received. I also really enjoyed the social events at the meeting. It was really nice to meet other students and researchers in the field. I would like to thank the ACA for their generous support, without which I would not have been able to attend



**Stacie Bulfer**

First of all, I would like to thank the ACA for the travel grant. As this was my first ACA meeting, I wasn't sure what to expect, but found it to be a great experience. I liked that there was a wide

variety of session topics and especially found the sessions on "Crystallization Methods and Refinement (Computational)" interesting and informative. Additionally, I liked presenting and participating in the poster sessions. I was able to discuss my work with several people and also learned more about topics that were unfamiliar to me.

I also liked the social aspects of the conference. I ran in the 5K Fun Run sponsored by Rigaku. They organized a beautiful course along Lake Ontario that I'm sure was enjoyed by everyone who participated. I also had a great time at the Rayonix Jazz Night, which had an incredibly talented band. Again, I would like to thank the ACA for the travel award. I really valued the opportunity to attend the conference in Toronto and am looking forward to Chicago in 2010.



**Richard Dowling**

In attending this conference I hoped to receive useful input that would stimulate and inspire progress in my present area of research and also increase the scope of my knowledge and experience to broaden my perspective. In my research I examine the effects of additives on polymorphism, to try and relate the crystal structure to the kinetic effects of nucleation and growth. Therefore I gave priority to talks concerning small molecules, particularly those by researchers seeking to address the occurrence of co-crystals and polymorphs through crystal engineering.

I found the talks by Gautam

Desiraju, Simon Parsons and Joel Bernstein particularly interesting on the subject of polymorphism and the talks by Christer Aakeröy and Daniel Adsmond interesting on the subject of co-crystals. I also sought out talks whose subjects were peripheral to my research. John Holyoake's presentation on a SAXS study of SDS co-solvent solution was relevant to me as I have examined micellar additives in my own work, and it was interesting to observe his approach. The session on 'Energy Related Materials' was of interest to me because I think it is an important area for future research.

The opportunity to present my work to an expert, critical audience enabled me to further refine my scientific communication and discursive skills. My poster on crystal growth rather than crystallography generated significant interest. Most observers were interested in the dramatic change in the growth rates of different polymorphs due to certain additives, particularly where the growth rate was observed to increase. Questions mostly concerned the application of my methodology to other more complicated systems. I believe that this demonstrates the value in understanding simpler systems of small molecules more thoroughly so that crystal structures of larger molecules such as active pharmaceutical ingredients and even proteins may begin to be analyzed in terms of their nucleation and growth.

In attending this conference I also hoped to gain exposure to leading academics and industrialists, providing me with an early opportunity to become actively involved in the crystallographic community, and therefore increasing the likelihood of successful future collaborations. I was drawn to the poster of Garth Simpson,

by his observations of the crystallization of amino acids. I also met and had an interesting discussion with Simon Parsons about his observations of glycine polymorphs at high pressure.

At this conference I was given an introduction into the field of crystallography. I now have a much better knowledge of the techniques available to crystallographers studying the solid state. I also gained insight into general crystallographic phenomena that can only come from those who are established in their field.



**Ankit Gupta**

I would like to thank the ACA organizing committee for the travel award and offering me an excellent opportunity to present my work in the Etter Award symposium. This was my first ACA meeting and it was a pleasant experience. I attended many sessions and especially enjoyed the ones on drug design, green chemistry and SAS modeling. I was glad that this meeting had a good blend of attendees from academia and industry. The YSSIG mixer and the Rayonix Jazz night were great to attend. Throughout the meeting, there were ample opportunities to meet fellow students and scientists in the field and discuss with them their research. This meeting broadened my knowledge about the field and gave me a preview of the diverse areas of research available to me.

Overall, it was a great experience and I look forward to attend many more in the years to come.



**Jason Porta**

This year I was really looking forward to the talks on aperiodic crystallography, and I was very pleased that there were so many. The workshop on JANA2006 was also very enjoyable and informative. It was particularly fun to work through the sample problems and have tutors right there to answer any questions.

I thought the location of the meeting was great as well. Having the exhibition hall and lecture rooms in one centralized location made the meeting seem more cohesive. Being in the center of Toronto was also very nice. I really enjoyed visiting Toronto, and am looking forward to Chicago next year.



**Jae-Hyuk Her**

It is truly my honor to have received an ACA travel grant. I want to take this opportunity to express my gratitude to the organizing committee, my collaborators and my mentors, Terrence J. Udovic and Craig M. Brown at the NIST Center for Neutron Research. Although I have attended several ACA meetings over the last several years, I am always interested in the science

and technology on display and never disappointed. The newest and brightest ideas in the crystallographic field have always been presented initially at an ACA meeting and I believe that such a tradition will continue. I should also mention the efforts of the organizing committee to create timely discussion sessions, reflecting the most bleeding edge research topics and also the efforts of the individual session chairs who do great jobs of inviting the best talks and posters, making the whole meeting successful. The satellite workshop program I attended this time, *Jana – Incommensurate Crystal Structures*, was impressively well prepared and the speakers were very professional as well.

It was also a great pleasure to share my current research results with other bright minds who came from not only America, but from all over the world. I am a powder diffractionist and new-structure hunter; the ACA meeting will unquestionably be the first location I will respectfully present my humble contributions to the scientific society when I achieve them, as I have done so far.



**Andreas Lemmerer**

I am currently a postdoc doing a two-year stint in Joel Benrstein's Lab at Ben-Gurion University of the Negev. I am hoping to pursue an academic career in the future. To this end, the conference provided good exposure to the type of crystallographic research

being done around the world and particularly in the United States. Being more familiar with the European crystallographic community, having attended the Erice Summer School and two European Crystallographic Meetings, it was enlightening hearing more about the research done at American institutions. Especially the sessions on Supramolecular Chemistry which were enthusiastically attended and followed by me.

The main benefit and advantage I gained out of this meeting was the talk I was able to give. Previously, I have been limited to poster presentations of my work. This talk was my first at an international conference and thus a major milestone in my career has been achieved, as well as being able to present my research on a more direct and personal level. For this, I am very grateful to the organizers and the session chair for allowing me to speak.

A second benefit, and one that is at the heart of such common interest meetings, is making future contacts for collaborations and this I was able to do as well.



**Ping-Yen Hsieh**

Attending ACA2009 in Toronto was very valuable to me. I went to the JANA workshop where I learned how to use superspace theory and supercells to identify modulated structures. The conference itself, honestly, it was the most wonderful meeting I have ever seen. The schedules and sessions were clear and well organized. In addition, the location was

so comfortable because I did not need to walk a long way. Even though I am not really a crystallographer, I still found many topics of interest. My research focuses on hydrogen storage materials especially on metal-organic framework materials (MOFs). There were some interesting presentations about hydrogen-bonding connected MOFs, and surprisingly, they are stable at high temperature and with good hydrogen adsorption ability. These behaviors are definitely related to their crystal structures. Furthermore, solid oxide fuel cell (SOFC) materials also attracted my attention. There were many amazing talks about how to identify the crystal structures of solid electrolytes and modify them as "superionic conductors" to improve the performance of the SOFC. I really enjoyed having the time to talk and discuss problems with those researchers who are the leaders in these fields and I received many useful suggestions for my future research. I really appreciated this travel award which supported my attendance at this nice meeting.

Thank you very much!!



**Misty Balcewich**

I would like to thank the ACA for the travel. This meeting was of particular importance for me. Having been born and raised in Winnipeg, Manitoba, Canada I wanted to be a part of a meeting which so well showcased the large and growing crystallographic community within Canada. It was also a chance to participate in the recognition of some



highly regarded Canadian researchers. Travel within Canada is not always the most economical, therefore this award ensured my participation in the meeting and for that I am grateful. This was my second ACA meeting (the first being in Salt Lake City in 2007) and in my opinion these are great meetings, especially for students to attend to not only educate themselves about the work being done in North America but all over the world. There are a large variety of research topics presented and it is important, as a student, to see all of the different areas and ways that a tool such as crystallography can be applied to enhance the field of structural biology in particular. This meeting is a great opportunity to meet your peers and develop professional connections and relationships with other students, many of whom will most likely be your colleagues for the remainder of your

career. It also gives students the ability to gain knowledge and insight from those who have been using crystallography for the entirety of their careers, especially enhanced by the large number of social events that are organized throughout the conference. In short, this meeting gave me the opportunity to learn new techniques, learn new applications, expand my research interests and meet new people who share my passion for crystallography.



**Robert Gruninger**

I would like to thank the ACA for the travel grant.

This was my second meeting and I thoroughly enjoyed myself. Not only did I receive excellent comments on the work I presented but I also learned a great deal from the many excellent sessions. I am venturing into the exciting world of membrane proteins and I learned a great deal about how to work with these difficult proteins. It was also very reassuring to see that many people have successfully determined the structures of several integral membrane proteins. Thanks again to the for both the travel award and all of the hard work that went into putting together this meeting.

**Mike Hast**

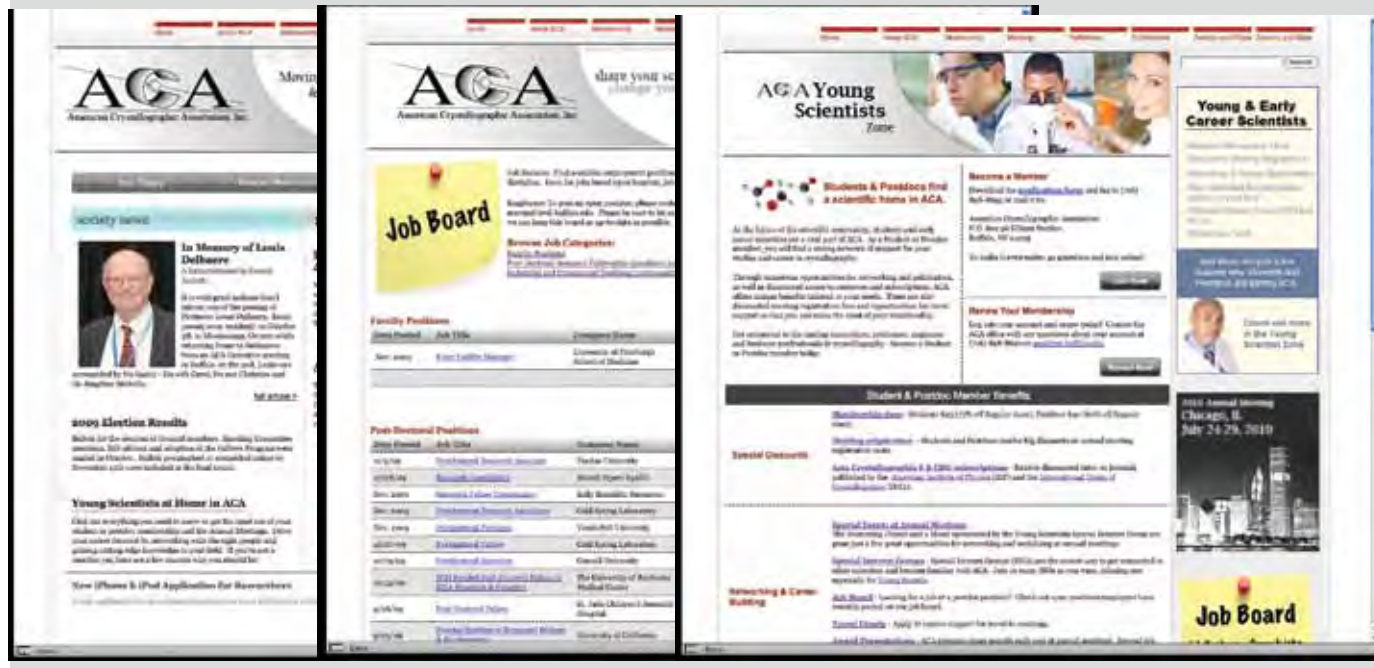
As a senior graduate student, it is always gratifying to be able to present the results of years of hard work to my peers. The ACA meeting was my first opportunity to do this at a large national/

international meeting, and it was terrific that the attendees were unified by experimental techniques that I have held dear since beginning graduate school. Previously, I had attended conferences which were smaller and not focused on a particular technique, but rather on the biology of the system I study. Interest in the token macromolecular crystallography poster at these meetings is marginal at best-- what a nice change at ACA! The poster sessions, as I had hoped, were engaging, and I had a number of positive interactions. I was surprised at how much I actually got out of the lectures. Many of the technique- and software-driven talks were full of information that I could apply immediately upon returning to my lab. I appreciate the efforts of the ACA to facilitate such positive experiences for its student and postdoc members. I look forward to attending next year in Chicago

**New ACA Websites**

The ACA is proud to announce the launch of two new websites. The homepage has been redesigned with simplicity in mind to offer a more user-friendly experience. All the information you need to know about SIGs, membership, summer schools, job postings and more is readily available at [www.AmerCrystalAssn.org](http://www.AmerCrystalAssn.org)

The Meeting website has also undergone some changes in design. You can visit [meeting2010.amerCrystalAssn.org/](http://meeting2010.amerCrystalAssn.org/) to find out everything you need to know about the 2010 Chicago Meeting.



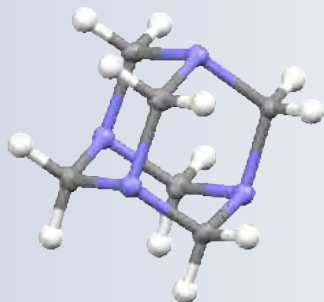
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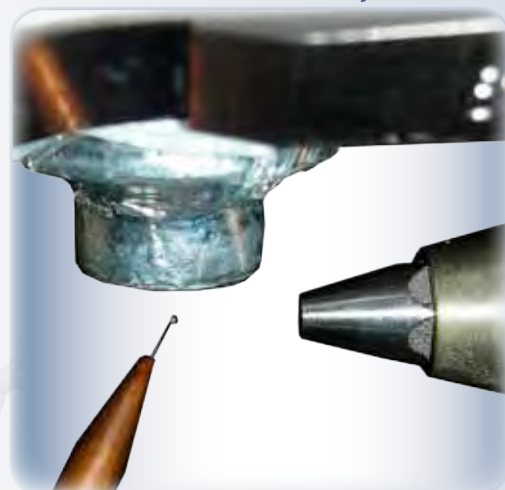


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**ACA Election Results**

**Council Officers**

**Vice President**  
Tom Koetzle

**Treasurer**  
Bernie Santarsiero

**Standing Committees**

**Communications**  
Ross Angel

**Continuing Education**  
Frank Fronczek

**Data and Standards**  
Cora Lind

**SIGS**

**Biological Macromolecules**  
Chair-elect: John Rose  
**General Interest**

Chair-elect: Marilyn Olmstead  
**Fiber Diffraction**  
Chair-elect: Paul Langan  
**Industrial**

Chair-elect: Paul Swepston  
**Materials Science**  
Chair: Jim Kaduk  
**Neutron Scattering**

Chair: Christina Hoffman  
**Powder Diffraction**

Chair-elect: Peter Stephens  
**Service Crystallography**

Chair-elect: Amy Sarjeant  
**Small Angle Scattering**  
Chair: Byeongdu Lee

Secretary: Kenneth Littrell  
Member: Gregory Beaucage  
**Small Molecules**

Chair-elect: Gary Nichol  
**Synchrotron Radiation**

Chair-elect: Henry Bellamy  
**Young Scientist**

Chair-elect: Jamaine Davis

**Canadian Division**

Chair: Michael Murphy

**Should the ACA institute a fellows program**  
Yes

**Thomas F. Koetzle - Vice-President**



Senior Chemist, Brookhaven National Laboratory (Retired); Special Term Appointee, Argonne National Laboratory; Scientific Secretary, Instrument Development Team for the TOPAZ Single-Crystal Diffractometer at Oak Ridge National Laboratory's Spallation Neutron Source (SNS).

**Statement:** Ever since I joined the ACA as a fresh postdoc, I have thought of the ACA as my professional home. I have received so much from the ACA during my career and I consider it a privilege to have the opportunity to serve and to give back a small measure of what I have received.

Many times over the years I have heard members express their feelings for the ACA as a unique community. Looking back to the first meeting I attended, in 1970 in New Orleans, I can still remember the warmth and friendliness of a number of eminent, senior crystallographers

in attendance who showed genuine interest in me and in answering my questions. As the ACA has grown, I feel it is truly remarkable that this community atmosphere has endured and, indeed, has strengthened. It is a testament to the efforts of our many colleagues who have served on the ACA Council, and of our incredible dedicated staff in the Buffalo Office, that each year when we convene at our annual meeting we can enjoy the unique 'small town' atmosphere that is the ACA. We can, and indeed we must, leverage our strength as a cohesive community to maximize our effectiveness going forward.

This is a time of exciting opportunities with the significant new support for science in the Federal Government's economic stimulus package. From the perspective of the crystallographic community, a significant portion of new funding is likely to be channeled through user facilities and shared resources. The ACA should continue to play a central role in informing the community on the resources that are available, and in coordinating education and outreach activities with those of the user facilities. For example, we should foster increased interaction of the ACA Small Molecule and Macromolecular Summer Schools with schools and workshops sponsored by the neutron and synchrotron radiation facilities. I feel that it also would be useful for the ACA to establish a formal presence at the facilities' annual user meetings so that, in particular, young scientists who are users of crystallography at the facilities will be encouraged to join the ACA. Years back, the formation of Special Interest Groups helped the ACA meetings attract those who may identify themselves primarily as biologists, chemists, or materials scientists. Today, by reaching out to the synchrotron and neutron user facilities and other shared resources, the ACA can participate fully in the growth stimulated by these facilities. Outreach activities such as this will help ensure that the ACA retains its place at the center of gravity of our community. At our own annual meetings, I would encourage the program chairs to arrange more sessions with joint sponsorships in order to further our interactions with societies having shared interests with the ACA.

The person elected to serve as ACA Vice-President, and then as President, has the responsibility to be a spokesperson for our community. I believe that my varied background working at user facilities and at the PDB, where I have had the privilege of interacting with a broad cross-section of the ACA membership, together with my experience serving as President of the Pittsburgh Diffraction Society will be valuable in this role. The relationships that I have formed through the ACA have always been a source of tremendous satisfaction to me, and I welcome the chance to be of service to our community.

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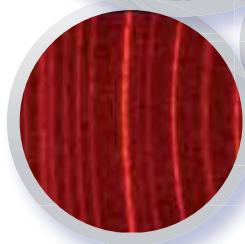
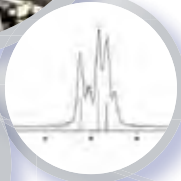


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**Bernard D. Santarsiero - Treasurer**



The ACA is in currently in excellent financial shape. We continue to keep membership dues and conference costs low while still providing the resources necessary to host interesting annual meetings by choosing wisely in meeting sites and organizing excellent scientific programs. I have been a member of the ACA for nearly thirty years and I continue to marvel at the continuing improvement and expansive use of our craft, and thoroughly enjoy attending the annual meetings with old colleagues and new acquaintances. It will be an honor to serve again as your Treasurer I hope that you will seek me out to voice concerns and offer suggestions about the ACA: [bds@uic.edu](mailto:bds@uic.edu).

**Ross J. Angel - Communications**



Within the ACA it is important not to let the great breadth of crystallography become a barrier to communication and exchange of ideas; all of us would benefit from greater integration of the scientific program at our annual meetings by the promotion of more inter-

disciplinary sessions. Outside of our organization, we should take the opportunity of our annual meetings to advertise our science to the general public. We must also work with our scientific colleagues to overcome the common impression that crystallography now only has a service role. We must regain the respect that the profession of crystallography used to receive. Perhaps the ACA could take one step towards this goal by initiating an ACA lecture tour to universities and colleges.

**Cora Lind - Data Committee**



Crystallography has been transformed from an “experts only” field to a tool open to many researchers. With this increase in user base comes the responsibility for our community to provide databases and standards that allow users of crystallography to ensure the soundness of their data even if they are not “experts in crystallography” in the traditional sense.

Databases play an important role both in user education and evaluation of experiments. Knowledge of and access to databases is therefore crucial. This should include agreements about frameworks for educational use like granting short-term educational licenses for crystallography classes or summer schools. At the same time, these opportunities will need to be advertised to the community so that instructors are aware of these options, which are already considered by some companies.

In addition to databases, standards are often necessary to properly evaluate experimental conditions, instruments and thus data quality. Diffraction standards for diffractometer alignment under ambient conditions are readily available through NIST and other vendors. However, standards for non-ambient experiments are little explored, and knowledge about standards and appropriate calibration procedures is less widespread. Many users of variable temperature options on in-house diffractometers rely on thermocouple readout for their non-ambient experiments, which can lead to significant errors in temperature estimates. “Standard procedures” are rare to non-existent. Users would benefit from suggestions for standardized procedures (including *in situ* temperature standards) for non-ambient experiments for different types of variable temperature stages.

**Frank Fronczek - Continuing Ed**



Continuing education is arguably the most important function of the ACA. This is because, despite the central importance of crystal structure determination in so many fields of science, there is currently little formal teaching of crystallography in many (most?) departments, as compared to a generation ago. ACA summer courses and workshops have become critically important should be supported, encouraged, and expanded. We should also be paying more attention

to what happens *after* summer courses and workshops. Having someone more experienced to talk to is invaluable. The ACA should assist by continuing to encourage the mentor-mentee concept, helping to pair young people with more seasoned crystallographers with whom they can feel comfortable in asking for regular guidance. Much more can be learned from such encounters than from textbooks and websites. The ACA should also actively encourage universities with a wealth of data-collection resources to provide help to those who are at institutions without diffractometers. It is an excellent way of continuing crystallographic education, puts instruments to good use at times when they might otherwise lie idle, and embodies the cooperative spirit of our association.

**Contributors to this Issue:**

- Sidney Abrahams, Marc Allaire, Miha Andrejasic, Ross Angel, Gerald Audette, Misty Balcewich, Jason Benedict, Rob Boisseau, Axel Brunger, Dejan-Kresimir Bucar, Stacie Bulfer, Stanley Cameron, Paulo Carvalho, Jr., Peder Cedervall, Haiyan Chen, Prashant Chopade, Haemi Chung, Sean Dalrymple, Jamaine Davis, Nicholas Deifel, Jeff Deschamps, Richard Dowling, Larry Falvello, Nicoleta Economou, Joe Ferrera, Safiyah Forbes, Anna Gardberg, Peter Gin, Alister Gould, Olivier Gourdon, Jason Grigg, Robert Gruninger, Ankit Gupta, Marl Hast, Kenneth Hedberg, Peter Horanyi, Mark Hunter, Jae-Hyuk Her, Ping-Yen Hsieh, Michael James, Troy Johnson, James Kaduk, Tom Koetzle, Samroeng Krachodnok, Sine Larsen, Jeff Lee, Andreas Lemmerer, Cora Lind, V. Mitch Luna, Viivi Majava, Colin McCrimmon, Ainsley McFarlane, Brandon Mercado, Mayasree Oottil, Chuttree Phurat, Daniel Pohl, Jason Porta, Janeth Presores, Wilson Quail, Arbin Rajbanshi, David Rose, Bernard Santarsiero, Navdeep Sidhu, Harkewal Singh, Katherine Sippel, Catherine Tupper, Bob Von Dreele, James Wells, Kristopher White, Adrian Wibowo, Carrie Wilmot, Zhen Xu, Bomina Yu

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July 24-29, 2010

Sheraton Chicago Hotel & Towers  
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**Deadlines:**

Abstracts: March 31, 2010

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**Workshops**

**GLOBAL Phasing Software Suite for Macromolecular Crystallography**

Organizer: Gerard Bricogne

**PLATON**

Organizer: Lee Daniels

**Sulfur-SAD Data Collection and Phasing**

Organizers: B.C. Wang, Albert Fu, John Rose

**Getting the Most out of the CCP4 Suite**

Organizer: Charles Ballard

**Crystallography: World of Wonders**

Organizers: Cora Lind, Christine Zardecki, David Goodsell, Claudia Rawn

**Award Symposia**

**Trueblood Award in honor of Anthony Spek**

**Fankuchen Award in honor of David Watkin**

**Margaret C. Etter Early Career Award in honor of Ray Trievel \***

**Transactions Symposium**

**The First Element : in Memory of Bob Bau**

Organizers: Christine Hoffman, Larry Falvello, Thomas Proffen, Nibuo Nimura

**Plenary Lectures**

Jim Ibers

**Nobel Laureates: Ada Yonath, Thomas Steitz and Venkatraman Ramkrishnan**



*Local Chair*

**Bernie Santarsiero**

University of Illinois at Chicago

[bds@uic.edu](mailto:bds@uic.edu)



*Program Chair*

**Ross Angel**

Virginia Tech

[rangel@vt.edu](mailto:rangel@vt.edu)

\*Etter Award Symposium: This symposium is exclusively for young scientists to present their research to a general audience. Young scientists are encouraged to submit their abstract, in any field of crystallography, directly to this symposium. Questions about submissions to this symposium should be sent to Ryan Jackson (YS-SIG chair) at [ryjacks@gmail.com](mailto:ryjacks@gmail.com)

*Microsymposia*

*Biological Macromolecules*

**Lighting the Way: in Memory of Louis Delbaere - Chair: John Allingham**

**Structural Enzymology: Mechanistic - Chair: Allen Orville**

**Biological Impacts of Structural Enzymology - Chair: Charles Carter**

**Molecular Motors - Chair: Francis Tsai**

**Longer Wavelength Phasing - Chairs: BC Wang & Manfred Weiss**

*Fiber*

**New Development in Fiber Diffraction: Cryo- Micro-diffraction and Complementary Techniques**

**- Chairs: Paul Langan & Joseph Orgel**

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**Functional Materials - Chair: Jason Hodges**

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**Weird Materials - Chair: Cora Lind**

**Mechanisms of Phase Transitions - Chair: Branton Campbell**

*Service, General Interest & Small Molecules*

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**My First Modulated Structure - Chair: Victor Young**

**Would you Publish This ? - Chairs: Carla Slebodnick & Danielle Gray**

**Crystal Structures Made Difficult by Solvent Molecules - Chairs: Tom Emge & Saeed Khan**

**Absolute Structure Determination; Where are we Now? - Chair: Joe Reibenspies**

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**Pushing the Envelope on SAS - Chair: Ed Lattman**

**Membrane & Associated Proteins - Chair: L. Yang**

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**Professional Odysseys - Chairs: Anna Gardberg & Megan Barker**

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**Structural Insights into the Cause and Treatment of Cardiovascular Disease - Chairs: Holly Soutter & Barry Finzel**

*Small Angle Scattering & BioMac*

**Macromolecules, Complexes & Assemblies - Chairs: Hiro Tsurata & Ed Lattman**

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**Precipitates and Voids in Advanced Materials - Chair: Ken Littrell**

*Materials, Powder*

**Energy Related Materials - Chairs: Ashfia Huq & Taner Yildirim**

*BioMac, Young Scientists & Canadian Division*

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**Radiation Damage - Chairs: Janet Smith & James Holton**

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**Automation and Data Collection - Chairs: Annie Heroux & Rick Walter**

*Fiber, Small Angle Scattering & Synchrotron*

**Fibril Forming Pathological Peptides: Prions, Amyloids & Friends - Chair: Joseph Orgel**

*Powder, Small Molecules & Materials*

**Non-ambient Environments for Specialized Experiments - Chairs: Angus Wilkinson & Christine Beavers**

*BioMac & YSSSIG*

**Software Integration and Databases - Chairs: Ed Collins & Peter Horanyi**

*General Interest, Small Molecules & YSSIG*

**Blast from the Past: What was Old is New Again- Chair: Peter Müller**



**ACA Chicago - July 24-29, 2010**

**Staying Green:** We will once again be distributing the full set of abstracts only on CDs with a hardcopy Program Schedule. We will not have a new meeting bag so if you would like one you should remember to bring your favorite from an earlier meeting. In addition to 'greening' the meeting these measures have proven both popular and cost effective allowing us to continue offering morning and afternoon coffee breaks as well as food at the opening reception and snacks at the poster sessions without a major increase in registration costs.

**Nobel Laureates:** All three 2009 Chemistry Nobel Prize Laureates, Ada E. Yonath, Thomas A. Steitz and Venkatraman Ramakrishnan, will attend and give presentations at the 2010 ACA meeting in Chicago. They were jointly awarded the Nobel prize for their work leading to the detailed mapping of the atomic structure of the ribosome - one of the cell's most complex machineries that translates information in mRNA and produces proteins - by diffraction methods. The high resolution structures reveal not only the basic translation mechanisms but, as important, the check mechanisms that greatly reduce the errors of translating RNA information in to protein structures. This work therefore not only provides great insights in to the basic machinery of living cells, but also opens up opportunities to develop novel drugs targeted directly at the ribosome level.

**Financial support** for young scientists will be available through the sponsorship of the IUCr. Applications for this support should be made by the abstract deadline on the meeting web site.

The Organizing Committee will observe the basic policy of non-discrimination and affirms the right and freedom of scientists to associate in international scientific activity without regard to such factors as ethnic origin, religion, citizenship, language, political stance, gender, sex or age, in accordance with the Statutes of the International Union.

**Registration fees**

Fee	Advance (before May 31)	Late (after May 31)
Regular Member	\$450	\$650
Retired Member	\$175	\$265
Post doc Member	\$220	\$330
Student Member	\$175	\$265
Nonmember*	\$650	\$950
Post doc Nonmember*	\$330	\$495
Student Nonmember*	\$265	\$396
Guest**	\$ 50	\$ 50

WK.01 GLOBAL	\$135
WK.02 PLATON	\$140
WK03 - SAD	\$120
WK04..CCP4	\$120
Outreach Workshop	Free to CPS teachers

**Mentoring Dinner Sponsored by the YSSIG**

Mentor	\$35
Mentee	\$25
Banquet	\$60 (\$30 students)
YSSIG Mixer	Free for students and post-docs \$20 for all others

\* 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, Exhibit Show and Get Together on Sunday morning.

Register on-line or download forms to register by fax or mail

Questions: [aca@hwi.buffalo.edu](mailto:aca@hwi.buffalo.edu)

[meeting2010.amerocrystalassn.org](http://meeting2010.amerocrystalassn.org)

**Exhibit Show 2010**

An exhibition of the latest instruments and techniques for sample isolation, purification and preparation, crystal growth and data collection, computer software for data storage, retrieval analysis, graphics systems, databases, and books, journals and other materials essential to modern crystallographery is scheduled to begin on the evening of Saturday, July 24 in conjunction with the Opening Reception. The 2010 Show will run through Tuesday evening July 27th. The exhibit show will be closed on Wednesday July 28th but posters will remain accessible. The Advertising and Exhibits Div. of the American Inst. of Physics is managing the show. For further information contact Bob Finnegan, AIP, 2 Huntington Quadrangle, Suite 1N01, Melville, NY 11747, [rfinneg@aip.org](mailto:rfinneg@aip.org), ph. (516) 576-2433; fax (516) 576-2481. ACA Corporate Members will receive 10% off one booth fee. Not a member? Join now!

Not-for-profits groups are eligible for a discounted booth fee of \$450 for one booth. Booth rental is \$1,600 for all others. Register online at [www.AmerCrystalAssn.org](http://www.AmerCrystalAssn.org)



## 2010 Art in Crystallography Prize

ACA *RefleXions* Editors are accepting entries to the **2010 Art in Crystallography** contest in the form of images emailed to either Editor ([conniechidester@earthlink.net](mailto:conniechidester@earthlink.net) or [flippen@rcsb.rutgers.edu](mailto:flippen@rcsb.rutgers.edu)). Entries should be accompanied by a paragraph explaining the science and the method of producing the image. A photo of the artist would be appreciated but is not required. Prizes consist of a small monetary award and a banquet ticket at the annual meeting. Winning entries will be posted on the web and will be displayed at the ACA Meeting. (Winners are not required to attend the meeting). We will also feature images in *ACA RefleXions* from time to time. Please let us know if you are interested in being a judge.

## Nominations for 2011 ACA Awards

The **Elizabeth A. Wood Science Writing Award**, established in 1997, is given periodically to authors of books or articles that bring science to the attention of a general audience. Nominations are due by May 1, 2010.

Nominations for the **A. L. Patterson Award** are due by May 1, 2010.

Nominations for the **Margaret C. Etter Early Career Award** are due by May 1, 2010. The members of the selection committee for 2010 are Radu Custelcean, Svilen Bobev and Ryan Jackson.

Full details describing the criteria for all ACA awards can be found on the website ([www.AmerCrystalAssn.org](http://www.AmerCrystalAssn.org)). All Nominations should be sent the ACA office ([marcia@hwi.buffalo.edu](mailto:marcia@hwi.buffalo.edu))

## 2010 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](http://www.AmerCrystalAssn.org)**

## Nominations for ACA Offices for 2011

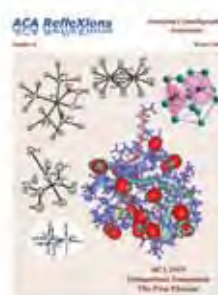
In the fall of 2010 we will elect a new Vice-President and one person to each of the ACA Standing Committees (Continuing Education, Communications, and Data, Standards and Computing). Suggestions (due by February 1, 2010) should be sent to **Alan Pinkerton** ([apinker@uoft02.utoledo.edu](mailto:apinker@uoft02.utoledo.edu)), **Marv Hackert** ([m.hackert@mail.utexas.edu](mailto:m.hackert@mail.utexas.edu)) or **Steve Ginell** ([ginell@anl.gov](mailto:ginell@anl.gov)).

## Summer 2010 Travel Funds Available



Rigaku Americas Corporation will award summer travel bursaries (to be used for travel to a scientific conference) in the amount of US \$500 each to the five (10) post-doctoral fellows who provide the most compelling explanation as to how they intend to pursue a career in structural biology. Applications must be received by February 28, 2010 and winners will be announced in early April. To apply go to: [www.rigaku.com/protein/postdoc.html](http://www.rigaku.com/protein/postdoc.html).

## What's on the Cover



The cover of this issue highlights Bob Bau's work with the First Element (Hydrogen). The 2010 ACA *Transactions* Symposium is dedicated to Bob's memory. The images used on the cover were selected and produced by **Larry Falvello**. Starting at the lower left and proceeding clockwise the images are:

**Bau-1 – Early rhenium carbonyl hydride.** Characterization of an anionic rhenium carbonyl hydride [ $H_2Re_3(CO)_{12}^-$ ], Churchill, M. R., Bird, P. H., Kaesz, H. D., Bau, R., & Fontal, B., *JACS* (1968), **90**, 7135-6.

**Bau-2 – Neutron structure of Zeise's salt – eta-2 pi complex and one of the first ever organometallic compounds.** Neutron diffraction study of the structure of Zeise's salt,  $KPtCl_3(C_2H_4) \cdot H_2O$ , Love, R. A., Koetzle, T. F., Williams, G. J. B., Andrews, L. C. & Bau, R. *Inorg. Chem.* (1975), **14**, 2653-7.

**Bau-3 – Hydrogen bond with hydrogen as acceptor.** Concept of the hydrogen ( $\delta^+$ )...hydrogen ( $\delta^-$ ) interaction. A low-temperature neutron diffraction study of cis-hydridohydroxotetrakis(trimethylphosphine)iridium(III) hexafluorophosphate, Stevens, R.C., Bau, R., Milstein, D., Blum, O., & Koetzle, T. F., *J. Chem. Soc., Dalton Trans: Inorg. Chem.* (1990), 1429-32.

**Bau-4 – Metal-metal bond with four bridging hydrogens.** A quadruply hydrogen-bridged metal-metal bond. The neutron diffraction analysis of octahydridotetrakis(diethylphenylphosphine)dirhenium(IV), Bau, R., Carroll, W. E., Teller, R. G. & Koetzle, T. F., *JACS* (1977), **99**, 3872-4.

**Bau-5 – Five-coordinate hydrogen.** Five-coordinate hydrogen: neutron diffraction analysis of the hydrido cluster complex [ $H_2Rh_{13}(CO)_{24}]_3^-$ ; Bau, R., Drabnis, M. H., Garlaschelli, L., Klooster, W. T., Xie Z., Koetzle, T. F. & Martinengo, S., *Science* (1997), **275**, 1099-1102.

**Bau-6 – Rubredoxin by neutron diffraction.** Neutron crystallographic study on rubredoxin from *Pyrococcus furiosus* by BIX-3, a single-crystal diffractometer for biomacromolecules, Kurihara K., Tanaka I., Chatake T., Adams M. W. W., Jenney F. E. Jr, Moiseeva N., Bau R. & Niimura N., *PNAS* (2004), **101**, 11215-20.

## L'ORÉAL USA Fellowships for Women in Science

Now in its seventh year, the L'Oréal USA Fellowships announces the 2010 call for applications by exceptional female postdoctoral researchers. Since its launch in 2003, L'Oréal USA's Fellowship program has recognized and rewarded 30 extraordinarily talented young women scientists engaged in breakthrough research projects at leading universities and research institutions across the country. This year L'Oréal USA will award five more women with grants of up to \$60,000 each. Applicants are welcome from a variety of fields, including the life and physical/material sciences, computer science, engineering and mathematics. In addition, the application process has moved online. Applicants may apply at: [www.lorealusa.com/forwomeninscience/](http://www.lorealusa.com/forwomeninscience/).



**MARCH 2010**

- 11-13 **Sixth International Workshop on X-ray Radiation Damage to Biological Crystalline Samples**, Stanford Synchrotron Radiation Laboratory (SSRL), Stanford, CA. [smb.slac.stanford.edu/news/workshops/rd6/index.shtml](http://smb.slac.stanford.edu/news/workshops/rd6/index.shtml)

**APRIL 2010**

- 12-16 **MaThCryst School on fundamental Crystallography**. Bloemfontein, South Africa ([www.crystallography.fr/mathcryst/SouthAfrica2010.php](http://www.crystallography.fr/mathcryst/SouthAfrica2010.php)).

**JUNE 2010**

- 3-13 **Structure and Function from Macromolecular Crystallography: Organization in Space and Time** Erice, Italy. *Directors: Tom Blundell and M. Armenia Carrondo* [www.crystalerice.org/erice2010/2010.htm](http://www.crystalerice.org/erice2010/2010.htm).

**JULY 2010**

- 18-23 **Gordon Research Conference in "Diffraction Methods in Structural Biology"** Bates College, Lewiston, Maine  
Chair: Andrew Leslie, Vice-chair: Ana Gonzales. [www.grc.org/programs.aspx?year=2010&program=diffrac](http://www.grc.org/programs.aspx?year=2010&program=diffrac)  
*(It would be an easy trip from Lewiston to Chicago for ACA 2010)*
- 24-25 **ACA Annual Meeting - Chicago, Illinois** *Local Chair: Bernie Santarsiero (bds@uic.edu), Program Chair: Ross Angel (rangel@vtech.edu)*

**AUGUST 2010**

- 29-2 **ECM 26**, Darmstadt, Germany. Conference Chair: Hartmut Fuess ([hfuess@tu-darmstadt.de](mailto:hfuess@tu-darmstadt.de)). [www.ecm26.org](http://www.ecm26.org).

**SEPTEMBER 2010**

- 12-16 **13th ICCBM**, Crystallization Workshop, Trinity College, Dublin, Ireland, [www.iccbm13.ie](http://www.iccbm13.ie).
- 20-23 **XTOP2010, The International Conference on High-resolution X-ray Diffraction and Imaging**, University of Warwick, UK, [www2.warwick.ac.uk/go/XTOP2010](http://www2.warwick.ac.uk/go/XTOP2010)

**OCTOBER 2010**

- 1-3 **AsCA2010**, Busan, Korea. [www.asca2010.org](http://www.asca2010.org)

**MAY 2011**

- 21-26 **ACA 2011 - Sheraton New Orleans**

**AUGUST 2011**

- 22-29 **XXII IUCr Congress - Madrid, Spain**

**JULY 2012**

- 28-2 **ACA 2012 - Westin Boston Waterfront**

**2010 ACA Summer Small Molecule Course**

The 10-day intensive course will be offered tentatively June 21<sup>st</sup> through June 30<sup>th</sup>, 2010 at the Indiana University of Pennsylvania, located in the town of Indiana about 80 miles east of Pittsburgh, PA. The course will cover both single crystal and powder diffraction and each day will consist of lectures in the morning, hands-on workshops in the afternoon and computer tutorials at night. While some advanced topics will be introduced (Structure solution from powder data, advanced probability methods, solving difficult structures), the curriculum will mostly emphasize fundamental crystallography and no prior crystallographic experience will be assumed. Attendees are encouraged to bring their own single crystal or powder samples for x-ray data collection and are expected to have completed at least undergraduate courses in chemistry, physics and mathematics and are advised to read in advance "Crystal Structure Analysis: A Primer", by Jenny P. Glusker and Kenneth N. Trueblood, Oxford Univ. Press (1985).

The organizers aim for a total of 24 attendees, who in past years have come from the U.S. and abroad from academia (students and faculty), government and corporate institutions. There will be at least 12 experienced teaching faculty present. Tuition will be \$300 (or \$800 for applicants from corporate labs). Student apartment housing at IUP (including breakfast and lunch) is available for an additional \$450 (\$750 or \$1,250 for corporate labs). Approximately 12 student scholarships will be offered (exceptional undergraduate students will be considered) and will consist of a waiver of tuition and living costs. The scholarships will be awarded based on the student's (1) scientific ability, (2) expected benefits from the course and (3) skills in English. We encourage applications from Latin America.

Instruments at IUP will include two Bruker-Nonius CAD4 single crystal diffractometers, a Bruker D8 Advance and a Rigaku Miniflex powder diffractometer. In the past, Rigaku-Americas brought a SCXmini X-ray Crystallographic System and Bruker AXS brought a Smart X2S Benchtop Diffractometer to the IUP laboratory. Students will also have access to the Duquesne University X-ray Facility which has a Bruker APEX II single crystal diffractometer and a PANalytical X'Pert Pro powder diffractometer. The IUP computer facilities are excellent and each student will have access to an individual computer during the nightly tutorials. Access will also be available to the Cambridge structural data base and the ICDD powder diffraction data base. The software used in the course will be Bruker-Nonius SHELXTL, Rigaku Americas CrystalClear, GSAS/EXPGUI, FullProf, CRYSFIRE and CRYSTMOL.

The Course registration form can be obtained from the ACA web site at [www.hwi.buffalo.edu/ACA/](http://www.hwi.buffalo.edu/ACA/). Completed forms must be received before May 14<sup>th</sup>, 2010 by Charles H. Lake, Chemistry Department, Indiana University of Pennsylvania, Indiana, PA 15705, USA or electronically [lake@iup.edu](mailto:lake@iup.edu) for full consideration. Further information will be updated on the web site or can be obtained from [lake@iup.edu](mailto:lake@iup.edu) or [craven@icubed.com](mailto:craven@icubed.com) Foreign students may be accepted early to provide extra time to process visas

*Charles H. Lake and Bryan M. Craven, Organizers.*



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The image displays three different models of Rigaku X-ray generators. The MicroMax-007 HF is a large, blue and white cabinet with a rotating anode assembly. The FR-E+ SuperBright is a smaller, white and blue cabinet. The MicroMax-002+ is a compact, black and white unit on a stand. The background features abstract blue and green molecular structures and arrows.

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