

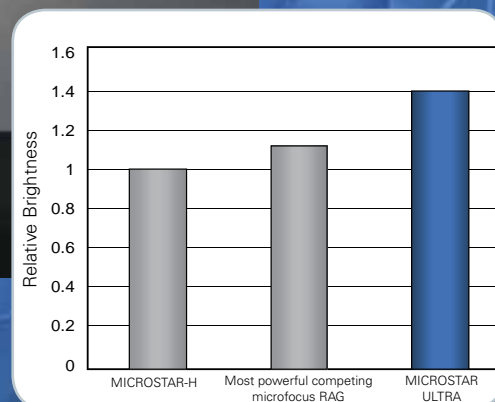
*ACA 2008  
Transactions Symposium  
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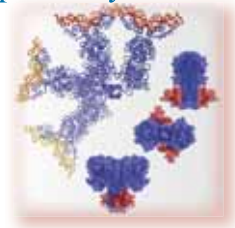
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*President's Column*

This is the final issue of *RefleXions* for this year, and the final President's column that I will write; I will be handing over my quill to Marv Hackert. There have been many issues discussed by Council and raised by the membership over the past year. Although not all questions have been resolved, it has been clear that this is a vital organization, whose members and officers care very strongly about their discipline in all its guises, and about the future of this quintessential interdisciplinary science. Although the present exists because we all stand on the shoulders of those who went before, the future is up to our younger members. I predict a bright future for our science and our organization based on my observations of the revitalization of many of the SIG's due to the energy and enthusiasm of a new generation of scientists. It is tempting to label them the younger generation, however, I may just be underestimating the lengthening of my own teeth. Coupled with this wind of change in the SIG's, there is evidence that many experienced crystallographers are stepping up to the plate to ensure that our tradition of mentoring young scientists continues effectively.

In the winter 2006 issue of *RefleXions*, Bob Bau discussed the risk of crystallography becoming only a black box science, with no one left to teach the foundations of the subject when the "baby boomers" retire. I believe that his concern has been generally recognized, and appropriate steps taken to ensure that "doomsday" does not arrive. Council has decided to put the two ACA summer schools on a more solid foundation by establishing continuing support for four year cycles. The staffing of these schools, and other schools and workshops by volunteers speaks eloquently to the mentoring tradition. These activities are largely outside traditional academic programs but I am pleased to report that at a recent joint meeting of the US National Committees for Crystallography and for Chemistry, the lack of crystallography in the ACS guidelines for undergraduate chemistry education was discussed. I believe that we have now begun a useful dialog between the respective education and training committees. This discussion is very timely as the ACS is currently working on a revision to their guidelines. Watch out you chemists, you may have to move into reciprocal space!

Although the above refers to the intellectual vitality of our discipline, I would be remiss in not commenting on the health of the ACA as an organization. Due to the efforts of our Chief Financial Officer, S.N. Rao, and the current and past Treasurers, Bernie Santarsiero and Doug Ohlendorf, the association is on a sound financial footing. In particular, we have started to build a "rainy-day" fund to ensure continuity of operations should there be an unexpected financial downturn. We have also built a significant endowment for our many award funds, and streamlined the funding of our business office. To ensure continuity of operations, the planning of annual meetings has been extended

further into the future with negotiations for as far out as 2012 currently underway.

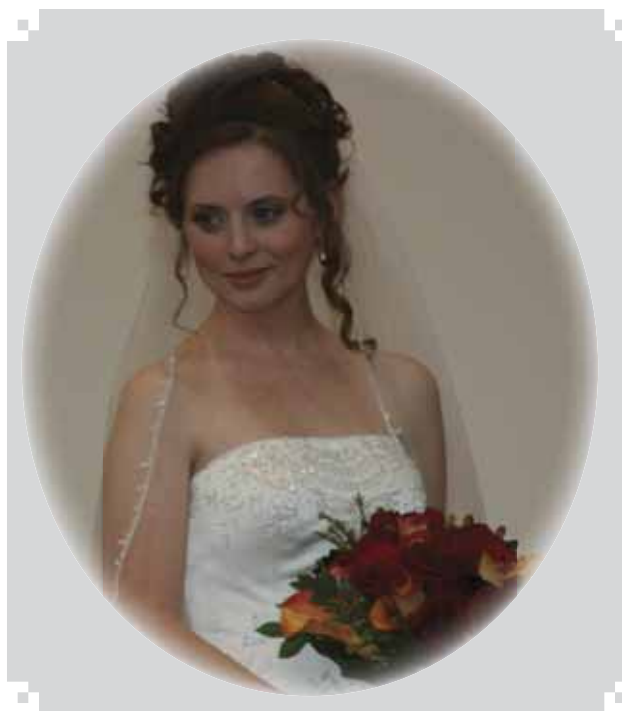
As we go to press, I now have the results of our recent elections. Please join me in congratulating our new Vice-President, Bob Von Dreele, three new members of standing committees, Peter Mueller (Continuing Education), David Harrison (Data and Standards) and Allen Oliver (Communications), and the new Canadian Representative to Council, Jim Britten. For details, see pp. 18 - 20.

In closing, let me say that I hope to see many of you at the Knoxville meeting in the spring. New tools, new ideas, and new results will undoubtedly generate an adrenalin surge, not only in the younger generation, but also in those not as spry as they once were. From this you will understand that there is indeed some vital life force associated with crystals; so come to Knoxville to be revitalized!

*Alan Pinkerton*



*Congratulations Jen*



*Meanwhile - Back in Buffalo ACA's Jennifer (Jen) Curtis became Mrs. Ben Shepard in October. Congratulations and all the best from the ACA family to Jen and Ben.*

## 2008 ACA Meeting Climate Neutral

The scientific evidence is clear: our global climate is warming due to the presence of increasing amounts of greenhouse gases in our atmosphere. Public and political awareness of the consequential dangers have been increasing and it is very fitting that the 2007 Nobel Peace Prize was awarded to the Intergovernmental Panel on Climate Change and one of Tennessee's most famous citizens, Al Gore "for their efforts to build up and disseminate greater knowledge about man-made climate change, and to lay the foundations for the measures that are needed to counteract such change". The challenge to address global climate change is perhaps the greatest of our time. For everything we do we should always consider alternative ways that may lessen our climate and environmental impact.

We therefore hope that members and sponsors of the ACA will join our effort to make the 2008 meeting Climate Neutral. We cannot prevent all greenhouse gas emissions, but we can ensure that the net result of our activities decreases rather than increases the amount of CO<sub>2</sub> in the atmosphere. This goal can be achieved by offsetting the CO<sub>2</sub> released as a consequence of attendees and vendors flying to the meeting and use of the conference center and hotels. We plan to do this by continuing the campaign begun last meeting. We have selected the national Carbonfund organization ([www.Carbonfund.org](http://www.Carbonfund.org)) to make the ACA 2008 annual meeting a CarbonFree event. Carbonfund.org is dedicated to fighting climate change, making it easy and affordable for any person or organization to eliminate their climate impact and hastening the transformation to a clean energy and technology future. They work to achieve this by providing climate change education and cost-effective solutions to carbon reductions that include saving energy and carbon offsets.

The ACA 2008 Climate Neutral Campaign will use the carbon offsets program of Carbonfund.org to help compensate the CO<sub>2</sub> emissions associated with this meeting. Our purchases of Carbonfund.org carbon offsets will support three types of carbon offset projects: renewable energy, energy efficiency, and reforestation. While each is different, they all play an important role in the fight against climate change. All of Carbonfund.org's offset obligations are matched against projects that meet or will meet the Climate, Community and Biodiversity Alliance (CCBA), Environmental Resources Trust (ERT), or United Nations Framework Convention on Climate Change (UNFCCC) Joint Implementation (JI) standards. Detailed information on these programs can be found at the Carbonfund.org website.

Preliminary estimates indicate that to make our ACA 2008 meeting Climate Neutral we will need to offset 475 tons of emissions or approximately 1600 lbs for every attendee (84% of the emissions are travel, the remainder hotel, venue and meals). On average an individual campaign purchase of \$4 worth of carbon offsets per attendee will allow us to reach our goal. Contributions can be made with ACA meeting registration and on a special CarbonFund.org web page '[www.carbonfund.org/site/pages/land/aca\\_2008](http://www.carbonfund.org/site/pages/land/aca_2008)' setup to collect and track the effectiveness

of this campaign. Moreover, donations to this campaign are tax deductible. This campaign is also an effective mechanism to mitigate other sources of emission. For example, electricity used by an average university worker (\$30/year), an average US household's electricity (\$30/year), an average US family's total direct fossil fuel use, excluding air travel, (\$90/year).

We hope that you will join our efforts to make the 2008 ACA Knoxville meeting a Climate Neutral event. It's easy - just go to [www.carbonfund.org/site/pages/land/aca\\_2008](http://www.carbonfund.org/site/pages/land/aca_2008).

*Jason Hodges, Dean Myles, Paul Butler*

*Bob Bau, Bryan Chakoumakos, Leighton Coates, Ed Collins, Joseph Curtis, Graciela Díaz de Delgado, George DeTitta, Cathy Drennan, Judy Flippen-Anderson, Anna Gardberg, Chris Hill, Christina Hoffmann, Jim Kaduk, Tom Koetzle, Joe Luft, Peter Mueller, Allen Orville, Thiyaga Pappannan, Connie Chidester Rajnak, Claudia Rawn, John Rose, Tim Rydel, Bernie Santarsiero, Liang Tong, Jill Trehwella, Carrie Wilmot, Mark Wilson.*

*Note:* We are advocating a specific campaign because we believe that it is the most cost effective option for individuals to offset their CO<sub>2</sub> emissions and because it allows a campaign approach in which ACA members and friends can work collectively to achieve a significant goal. It is important to note, however, that there are many other programs that one might choose to support, including those listed here.

Carbon Offsets: [www.terrapass.com](http://www.terrapass.com), [www.gocarbonzero.org](http://www.gocarbonzero.org), [www.carbonfootprint.com](http://www.carbonfootprint.com), [www.carbonfund.org](http://www.carbonfund.org), [www.nativeenergy.com](http://www.nativeenergy.com), [www.paxnatura.org](http://www.paxnatura.org), [windpower.utah.edu](http://windpower.utah.edu)

Buying Greenpower: [www.eere.energy.gov/greenpower/](http://www.eere.energy.gov/greenpower/)

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14. I certify that all information furnished on this form is true and complete. (signed) Marcia Colquhoun for American Crystallographic Association, Inc.

**To the Editors:**

Lyle H. Jensen writing on the topic of Intelligent Design/Creationism (*RefleXions*, fall 2007), says of Michael Denton's 1985 non-peer-reviewed book "Evolution: A Theory in Crisis" that it "provides a good summary of the evidence challenging Darwinian evolution which had arisen from within various scientific fields prior to 1985 when it was first published." I have read Denton's book and my impression of it is much different.

The blurb on the back cover of my copy reads, "What will be most embarrassing to the neo-Darwinians... will be Denton's revelation that the evidence from his specialty, molecular biology, lends them no support. - *The Spectator*." As it happens, I have a degree in molecular biology, which has been quite useful to me in my practice of protein crystallography. I invite Jensen to open his copy of Denton's book to chapter 12, "A Biochemical Echo of Typology." One would think that a molecular biologist would be able to interpret a sequence comparison, and yet Denton flubs one after another. In the first example (page 278 in my edition) Denton tabulates sequence differences of cytochrome C from various species, and notes that various eukaryotes (horse, pigeon, tuna, silkworm, wheat, yeast) all have an approximately equal number of differences in comparison to bacteria (*R. rubrum* C2). Denton is disturbed by the "dramatic absence of intermediates" (p. 280). This is puzzling until an informed reader realizes that Denton apparently imagined the evolutionary interpretation of life as a ladder, rather than a tree! With a proper understanding of evolution, it is clear that all of the eukaryotes listed share a common ancestor with each other more recently than they do with bacteria. The intermediates are those common ancestors, which are buried deep in the past. Thus the sequence results agree very well with Darwinian predictions, but not with Denton's erroneous interpretation.

Every other sequence comparison listed by Denton, when properly interpreted, likewise fits readily into a Darwinian framework. If Denton had graphed these comparison as branching trees rather than his favored Venn diagrams, it would be readily apparent that phylogenetic trees drawn up on the basis of protein or nucleic acid sequence comparisons agree very well with those drawn from fossil and anatomic comparisons, although based on entirely different methods. This constitutes independent verification.

This interpretation of sequence comparisons as ladders instead of trees is a stunning error which was apparently picked up and repeated by the authors of *Of Pandas and People* (Davis & Kenyon, 1989), the supplementary textbook which was at issue in the Dover, Pennsylvania trial in 2005.

I will restrict myself to this one example which lies inside my area of competence, but I suggest to Jensen that he discuss any other material in Denton's book or other Intelligent Design/Creationism sources, which he finds to be convincing with competent experts in the relevant field of science.

*David J. Schuller*

**To the Editors:**

Lyle H. Jensen's letter (fall 2007, *RefleXions*) is of great interest. However, it is worth pointing out that both the original works of Darwin and the works of Jun-Yuan Chen (the most eminent palaeontologist in China as described by Prof. Jensen) are macroscopic studies, in contrast to the studies we crystallographers, hopefully, arrive at, which are on the molecular scale. Our molecular scale enables casting a very distinct and unique understanding of the concept of "evolution" as applied to all forms of life, much to the credit of Linus Pauling whose pioneering work has been so admirably extended by none other than Lyle H. Jensen himself.

The second letter (from Fanwick and Krause) following after that of Prof. Jensen, brings to mind the ACA Annual Meeting in Seattle, on the campus of the University of Washington. Here is an example where one did relish the resort like experiences in the evenings and where the seriousness and focus of science was enhanced by the campus setting.

*Brahama D. Sharma*

***You Say You Want an Evolution? A Role for Scientists in Science Education***

**Abstract:** The Coalition of Scientific Societies recently conducted a national survey of likely U.S. voters to examine acceptance of evolution, attitudes toward science and scientists, and opportunities for promoting science education. Most respondents accepted that life evolved, many accepted that it evolved through natural processes, and more favored teaching evolution than creationism or intelligent design in science classes. The majority ranked developing medicines and curing diseases as the most important contributions of science to society, and they found promoting understanding of evolutionary science's contribution to medicine to be a convincing reason to teach evolution. Respondents viewed scientists, teachers, and medical professionals favorably, and most were interested in hearing from these groups about science, including evolution. These data suggest that the scientific community has an important role to play in encouraging public support for science education.

*Editors Note: A full paper has been published on the results of the survey<sup>1</sup>. What follows here are some selected extracts from that paper.*

Although evolution is firmly established as one of the most important, integrative, and robust concepts in science, teaching evolutionary science and related subjects (e.g., the origins of the universe, the age of the earth, plate tectonics) has been challenged in school districts across the United States. These challenges—whether introducing religious beliefs as "alternatives" to science, labeling evolution or the big bang as "theory, not fact," or singling out scientific subjects for "critical analysis"—jeopardize science education. Recognizing the harm such actions pose to science education and, ultimately, to the foundation on which scientific advancement is based, 17 scientific societies, representing the

physical, chemical, biological, and social sciences and science teachers communities, established an unprecedented coalition to explore opportunities for collective understanding and action. As part of this effort, they engaged a professional research firm to conduct a national survey of approximately 1,000 likely U.S. voters<sup>1</sup> that examined attitudes toward science and scientists, views on evolutionary science in the context of education, and means through which the scientific community can effectively bolster support for teaching evolution and related subjects.

Recent studies show that Americans' views on evolutionary science have been relatively stable over the past several decades, being almost equally split between those accepting human evolution<sup>2-3</sup>, and those favoring a Biblical creationist account of the origins of life<sup>3</sup>. For example, when people were asked to choose whether humans developed over millions of years either with or without guidance from God, more selected evolution with guidance. In another form of the question, however, respondents were asked if they thought humans evolved or were created in their present form. Those who accepted evolution were then asked if they thought it occurred through natural processes or with guidance. When asked this way, fewer reported that evolution occurred with guidance than through natural selection<sup>3</sup>.

We anticipated that acceptance of evolutionary science would also be influenced by the distinction between human and non-human species. We asked half of the respondents about their views on the evolution of "all living things" and found that 61% accepted that "all living things have evolved over time." Of those, 36% thought all living things "evolved due to natural processes such as natural selection" and 25% thought "a supreme being guided the evolution of living things for the purpose of creating life in the form it exists today." We asked the remaining respondents to consider human evolution and found that 53% accepted that "humans and other living things" evolved. This majority included 32% who accepted that humans and other living things evolved through natural processes and 21% who thought they had evolved with guidance. Compared to other surveys<sup>3</sup>, we found weaker overall support for creationism: 28% and 31% agreed with statements that "all living things" or "humans and other living things," respectively, were created in their present form.

There is considerable uncertainty about what to teach in public school science classes, particularly with regard to including certain religious perspectives: 32% of respondents in our study were unsure about teaching creationism and 41% were uncertain about teaching intelligent design. By comparison, 22% expressed uncertainty about teaching evolution. Consistent with other studies<sup>5</sup>, however, more respondents favored teaching evolution (53%) than creationism (36%) or intelligent design (27%) in public school science classes. These data show that a majority of people favor—and even more may be open to—teaching evolution in science classes.

Why don't more Americans accept evolutionary science? Like other studies<sup>3</sup>, this survey shows a connection between respondents' views on evolution education and their answers to three scientific questions. Although 69% had some college

education, only 23% gave correct responses to all three of the following statements: the continents or land masses on which we live have been moving for millions of years and will continue to move in the future (79% correctly agreed); antibiotics kill viruses as well as bacteria (43% correctly disagreed); the earliest humans lived at the same time as the dinosaurs (53% correctly disagreed). Respondents who answered all three questions correctly were much more likely to respond that humans and other living things evolved (78%) than that they were created in their present form (11%), and more favored teaching evolution (78%) than creationism (27%) or intelligent design (24%). In contrast, respondents who answered fewer than two questions correctly were less likely to accept that life evolved (36%) than to believe it was created in its present form (47%), and they were about as likely to favor teaching evolution (36%) as creationism (38%) and intelligent design (29%).

Americans value the contribution that scientific research makes to eliminating diseases<sup>4</sup>, and they value the relationship between evolutionary science and medicine. We found that 63% of respondents ranked developing medicines and curing diseases as the most important contributions of science to society and 61% thought that understanding the contribution of evolution makes to modern medical science, including to understanding and treating diseases such as avian influenza, was a convincing reason to teach evolution in science classes. This finding, together with Americans' consistently strong support of medical research<sup>4</sup>, suggests that making the connection between evolutionary biology and advancing other areas of medical research (e.g., understanding human gene function or the mechanisms by which antibiotic resistance develops) might be equally compelling. People may also appreciate the contributions that evolutionary science makes to other fields, including agriculture, forensics, and even software engineering, although these were not examined in this study.

Teaching evolutionary science may also enhance science pedagogy, as it "offers educators a superb opportunity to illuminate the nature of science and to differentiate science from other forms of human endeavor and understanding"<sup>6</sup>. The tools and techniques that scientists employ to study evolution—gathering evidence from various sources, making logical inferences, establishing and testing competing hypotheses—are the hallmarks of science and necessary for everyday decision-making. Data from this survey suggest that the public values these learning opportunities: a majority of respondents rated thinking critically, learning to draw conclusions from evidence and learning how science is conducted as very important purposes of public school science education. Communicating the value of learning science, including evolution, for developing analytical skills that are widely applicable beyond the classroom may strengthen public support for all types of science.

The scientific community plays a key role in communicating the importance of science education to the public. Sixty nine percent of respondents had favorable feelings toward scientists and even more viewed medical researchers (72%) and doctors (76%) favorably. While fewer people (59%) rated public school science teachers highly, public school teachers in general were the most widely favored group (79%).

When it comes to scientific issues, the scientific community commands the attention of the public. Among respondents presented with a list of people who might explain science to the public, 88% expressed interest in hearing from a scientist, and almost as many were interested in hearing from a science teacher (85%) or a doctor or nurse (84%). On the topics of evolution, creationism, or intelligent design, most respondents expressed interest in hearing from scientists (77%), science teachers (76%), and clergy (62%). Fewer people were interested in hearing from Supreme Court Justices on evolution (37%), or from school board members and celebrities either on science (34% and 16%, respectively) and evolution (30% and 11%, respectively). These data indicate that Americans respect the expertise of science and education professionals and also look to clergy for guidance on scientific issues of potential relevance to religion. The value of encouraging each of these groups—including scientists who hold religious beliefs—to become involved in promoting quality science education cannot be overstated.

In communicating the value of science, scientists must emphasize the outcomes that matter to people—advancing medicine, improving health, fostering critical thinking—and they must do so clearly and understandably. Technical expositions on scientific topics will not get the attention of the public or policy makers who lack relevant expertise. If researchers can not communicate their findings in ways that are comprehensible, meaningful, and relevant to non-scientists, their message to the public—and their effectiveness as spokespeople for science—is lost<sup>7</sup>. There are ample opportunities for scientists to develop and exercise their communication skills and, whether writing letters to local newspapers, speaking with school boards or community groups, or partnering with educators to design curricula, many scientific and professional societies have trained staff or other resources to help.

There is a clear need for scientists to become involved in promoting science education. Challenges to teaching science undermine students' understanding of the scientific method, how scientific consensus develops, and the distinction between scientific and non-scientific explanations of natural phenomena. If we are to continue to develop the talent necessary to advance scientific and medical research, we must ensure that high standards in science education are maintained and that efforts to introduce non-science into science classes do not succeed. Failure to reach out effectively to a public that is supportive of science and open to information from the scientific community is not just a missed opportunity; it is a disservice to the scientific enterprise.

### References

- [1] The complete article and the list of "Coalition of Scientific Societies" members are available online at [evolution.faseb.org/sciencecoalition](http://evolution.faseb.org/sciencecoalition)
- [2] J.D. Miller, E.C. Scott, S. Okamoto, *Science* (2006) **313**, 765-766.
- [3] "Reading the Polls on Evolution and Creationism" (The Pew Research Center for the People and the Press, Washington, DC, 2005; [peoplepress.org/commentary/display.php3?AnalysisID=118](http://peoplepress.org/commentary/display.php3?AnalysisID=118)).

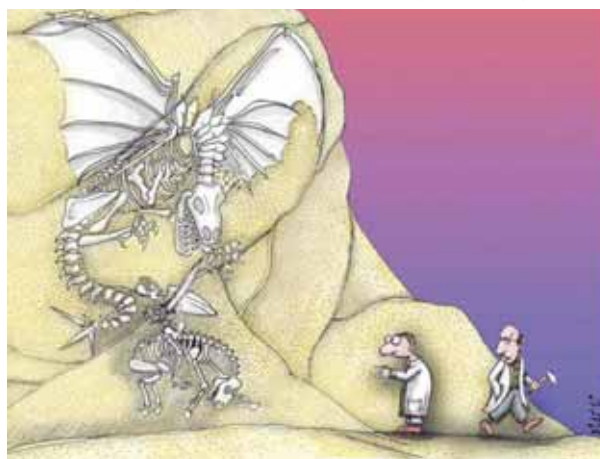
- [4] *America Speaks* (Research!America, Alexandria, VA, 2007; [www.researchamerica.org/publications/AmericaSpeaks/AmericaSpeaksV8.pdf](http://www.researchamerica.org/publications/AmericaSpeaks/AmericaSpeaksV8.pdf)).
- [5] *Evolution, Creationism, Intelligent Design* (The Gallup Poll; [www.gallupoll.com/content/default.aspx?ci=21814](http://www.gallupoll.com/content/default.aspx?ci=21814)).
- [6] National Academy of Sciences, *Teaching About Evolution and the Nature of Science* (National Academies Press, Washington, DC, 1998).
- [7] M.C. Nisbet, C. Mooney, *Science* (2007) **316**, 56.

### Web Resources

- American Association for the Advancement of Science  
[www.aaas.org/news/press\\_room/evolution/](http://www.aaas.org/news/press_room/evolution/)
- American Institute of Biological Sciences  
[www.actionbioscience.org/evolution/index.html](http://www.actionbioscience.org/evolution/index.html)
- American Physiological Society  
[www.the-aps.org/pa/policy/bioissues/evolutionTeach.htm](http://www.the-aps.org/pa/policy/bioissues/evolutionTeach.htm)
- American Society of Human Genetics  
[www.genednet.org/pages/k12\\_evolution.shtml](http://www.genednet.org/pages/k12_evolution.shtml)
- Federation of American Soc for Experimental Biology  
[www.evolution.faseb.org](http://www.evolution.faseb.org)
- Howard Hughes Medical Institute  
[www.hhmi.org/biointeractive/evolution/index.html](http://www.hhmi.org/biointeractive/evolution/index.html)
- National Academies  
[nationalacademies.org/evolution/](http://nationalacademies.org/evolution/)
- National Center for Science Education  
[www.natcensci.ed.org](http://www.natcensci.ed.org)
- PBS Evolution Website  
[www.pbs.org/wgbh/evolution](http://www.pbs.org/wgbh/evolution)
- Understanding Evolution (UC Museum of Paleontology)  
[evolution.berkeley.edu/](http://evolution.berkeley.edu/)

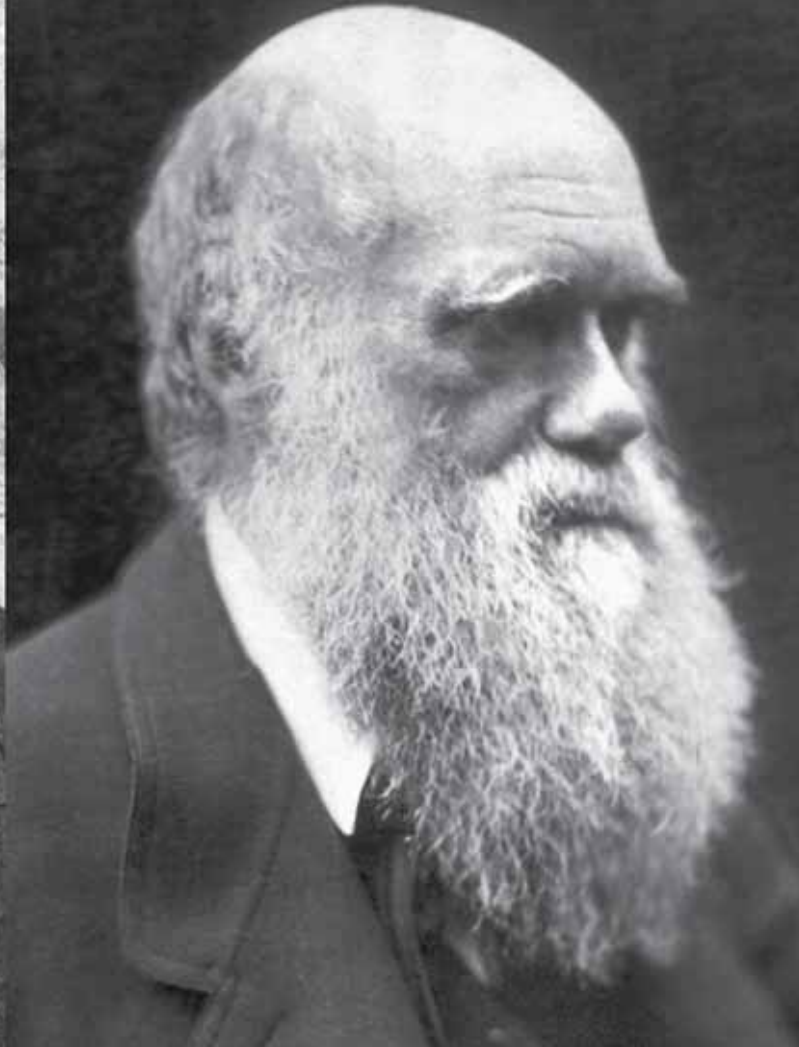
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For more information contact  
Jennifer A. Hobin - [Jhobin@faseb.org](mailto:Jhobin@faseb.org)



Ignore it Henderson, It's Unscientific - by Nick. D. Kim, U. Waikato, New Zealand. See [nearingzero.net/res.html](http://nearingzero.net/res.html)





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### 2009 Art in Crystallography Prize

ACA *Reflexions* Editors are accepting entries to the **2009 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 2009 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 July 1, 2008.

Nominations for both the **Martin Buerger Award** and the **B. E. Warren Award** are due by May 1, 2008.

Nominations for the **Margaret C. Etter Early Career Award** are due by September 1, 2008.

Full details describing the criteria for all ACA awards can be found on the website ([www.AmerCrystalAssn.org](http://www.AmerCrystalAssn.org)) and on page 12-13 of the fall 2005 *Newsletter*. All Nominations should be sent the ACA office ([marcia@hwi.buffalo.edu](mailto:marcia@hwi.buffalo.edu))

### 2008 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)**

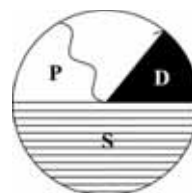
### Nominations for ACA Offices for 2009

In the fall of 2008 we will elect a new Vice-President, Secretary and one person to each of the ACA Standing Committees (Continuing Education, Communications, and Data, Standards and Computing). Suggestions (due by February 1, 2008) should be sent to either of the Nominating Committee Co-Chairs: **Jeanette Krause** ([krauseje@email.uc.edu](mailto:krauseje@email.uc.edu)) and **Louis Delbaere** ([louis.delbaere@usask.ca](mailto:louis.delbaere@usask.ca))

### Summer 2008 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 (5) 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 May 4, 2008 ([www.rigaku.com/protein/postdoc.html](http://www.rigaku.com/protein/postdoc.html)).



The Pittsburgh Diffraction Society announces that it will make travel awards to outstanding graduate students who plan to attend and participate in the Osaka IUCr Congress. Applications for the awards, which are competitive, can be made by reference to the Pittsburgh Diffraction Society website ([www.pittdifsoc.org](http://www.pittdifsoc.org)). Click on the link for the George Jeffrey Award and carefully follow the application instructions. The awards honor the memory of George A. Jeffrey, an influential crystallographer who believed strongly in promoting graduate studies in diffraction sciences and in the importance of international cooperation.

### TRAVEL FELLOWSHIPS for Osaka IUCr Meeting, 23-31 August 2008

The U.S. National Committee for Crystallography, in cooperation with the ACA, will provide partial support for travel to the International Union of Crystallography Meeting in Osaka, Japan. To be eligible, applicants must be graduate students, post-doctoral fellows, or untenured faculty members in any of the crystallographic, diffraction, and imaging Sciences affiliated with the IUCr. Undergraduate students will be considered in exceptional cases. Applicants must be training at a U.S. institution. Recipients are expected to submit a short report in return for their support after the meeting.

An application should include the following:

- (1) Cover page indicating name, address, telephone number, fax, and e-mail address of the applicant and name and address of mentor;
- (2) A current *Curriculum Vita* of the applicant;
- (3) Abstract including title and authors, with applicant as presenter, submitted for presentation at the 2008 IUCr meeting;
- (4) A paragraph by the applicant describing where they are in their career and why they want to attend the Osaka meeting;
- (5) A letter of recommendation from the mentor detailing the group's travel funding and explaining why funds from the USNCCr are needed.

**Deadline: 1 March 2008.**

Send applications to: Cora Lind  
Department of Chemistry, MS 602  
The University of Toledo  
Toledo, OH 43606  
(419) 530-1505  
fax: (419) 530-4033  
[cora.lind@utoledo.edu](mailto:cora.lind@utoledo.edu)

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**Canadian Light Source News (from the CLS E-News, [www.lightsource.ca](http://www.lightsource.ca))** The first and second issues of *InnoVision*, the new Canadian Light Source business newsletter, can be obtained from [www.lightsource.ca/enews/pdf/InnoVision\\_may2007.pdf](http://www.lightsource.ca/enews/pdf/InnoVision_may2007.pdf). Distributed quarterly, each issue showcases business opportunities and successful partnerships with industry, and profiles team members and infrastructure.

The 2005-2006 edition of the CLS Activity Report was released during the summer of 2007. The Activity Report can be downloaded from the CLS website in its entirety or as thematic sections from [www.lightsource.ca/brochures](http://www.lightsource.ca/brochures). The second CLS Corporate Annual Report, covering the 2006-2007 fiscal year, has just been released; it can be downloaded from [www.lightsource.ca/pdf/annual\\_report/cls-annualreport-2006-2007.pdf](http://www.lightsource.ca/pdf/annual_report/cls-annualreport-2006-2007.pdf).

After a very successful term as Executive Director of CLS, Bill Thomlinson will retire in June 2008. The CLS Board of Directors has begun an international search for a new Executive Director. The search committee is chaired by Arthur Carty, Chairman of the Board and National Science Advisor, Industry Canada, and composed of stakeholders including CLS Board members, CLS management and representatives from the international synchrotron community, as well as industry and user community representatives.

The CLS Board of Directors welcomes the following new members: Dr. Lorne Babiuk, Vice-President (Research), University of Alberta; Dr. W.E. (Ted) Hewitt, Vice-President (Research & International Relations), University of Western Ontario; and Mr. Glen Veikle, Acting Deputy Minister, Saskatchewan Industry and Resources. For more information regarding current Board membership please visit: [www.lightsource.ca/aboutus/board.php](http://www.lightsource.ca/aboutus/board.php).

The Fifth International Workshop on Mechanical Engineering Design of Synchrotron Radiation Equipment and Instrumentation (MEDSI) and the Fifteenth Pan-American Synchrotron Radiation Instrumentation (SRI) Conference will be held in Saskatoon June 10-13, 2008. It will be held in conjunction with the CLS Annual User's Meeting June 9-10. [www.lightsource.ca/medsi-sri2008/](http://www.lightsource.ca/medsi-sri2008/).

CLS Educational Outreach has two opportunities for collaboration between researchers and students. In the first, teachers from across Canada who attended the CLS Summer Workshop have volunteered their students to help researchers collect samples. In the second, NSERC's PromoScience has funded a CLS initiative to give Canadian students the chance to perform experiments on CLS beamlines. For more information please contact [tracy.walker@lightsource.ca](mailto:tracy.walker@lightsource.ca).

On September 25, in Ottawa, an agreement was signed by the Government of India with the CLS and the Univ. of Saskatchewan to promote cooperation between Indian and Canadian researchers in synchrotron science. The agreement opens the way to explore joint projects including materials research, earth and environmental sciences, and biomedical and life sciences. Other opportunities may see Indian researchers travelling to the CLS as customers to use the facility, as well as learn about the operations

and design of experimental equipment at Canada's synchrotron. For the full press release please go to [www.lightsource.ca/media/media\\_release\\_20070925.php](http://www.lightsource.ca/media/media_release_20070925.php).

A Canadian/German team is developing soft x-ray spectroscopy as a new tool for the investigation of one of the key areas of soil science: the chemistry of nitrogen. Collaborators from the Universities of Saskatchewan (Fran Walley) and Rostock (Peter Leinweber) have combined to produce the necessary first step, a reference fingerprint library to determine the nature of unknown nitrogen in environmental materials (see Leinweber et al. 2007, [journals.iucr.org/s/issues/2007/06/00/issconts.html](http://journals.iucr.org/s/issues/2007/06/00/issconts.html)). This is part of the commitment of the CLS to accommodate "dirty" real-world samples that has also brought researchers from the USA and Australia to Saskatoon.

**Faculty Position in Neutron Scattering Studies of Condensed Matter, McMaster University :** The Department of Physics and Astronomy at McMaster University invites applications for a tenure track faculty position in experimental condensed matter physics using neutron scattering techniques. All applications will be considered, with preference given to an appointment at the Assistant Professor level. The deadline for applications is February 4, 2008. For more information please see: [physwww.physics.mcmaster.ca/?page=neutronsctteringad07.html&type=](http://physwww.physics.mcmaster.ca/?page=neutronsctteringad07.html&type=)

**The Larry Calvert CNC/IUCr Trust Fund Award:** The Canadian National Committee for Crystallography will soon be sending out an advertisement for applications to the Larry Calvert CNC/IUCr Trust Fund Award. There are limited travel funds to contribute to the sending of graduate students to the IUCr meeting in Osaka in 2008, as explained on the website: [www.cins.ca/cncc/calvert.html](http://www.cins.ca/cncc/calvert.html). At the present time the CNC/IUCr can provide two subsidies of \$750 (or one of \$1500). Donations to the travel fund are accepted and will be split 50% to awards and 50% to increase the fund's principal. Donors may request other splits, including having their donations go entirely to a travel award. Income tax receipts will be provided. Contributions must be made to the L.D. Calvert CNC/IUCr Trust Fund and sent to:

L.D. Calvert CNC/IUCr Trust Fund - CNCC  
c/o Dr Marie Fraser, Treasurer  
Department of Biological Sciences  
University of Calgary  
2500 University Drive NW,  
Calgary, Alberta, T2N 1N4 Canada

**Last Column:** On a personal note, this will be my last column in *RefleXions*, since my three-year term as Canadian Representative to the ACA Council is coming to an end. It has been a pleasure to work with the ACA Staff and Council members and to interact with crystallographers from across North America. **Jim Britten** will be serving in this position from 2008-2010.



Lee Groat

*The 16<sup>th</sup> Annual BHT (Buffalo-Hamilton-Toronto) Regional Crystallography Meeting, McMaster University, Hamilton, Ontario, November 9, 2007.*



*BHT Speakers: Front row (l to r) John Rubenstein, Rachel Hanna, Dea Shahinas, Lisa Pell, Alex Vecchio; Back row (l to r) Frank Sicheri, Joaquin Ortega, Sara Andres, Rene Jorgensen, Dmitri Svergun. Photo courtesy of Rob Thorne.*

This year's theme was "Complementary Diffraction Methods for Macromolecular Structure". The morning session consisted of an inspiring and educational review of Small Angle X-ray Scattering from **Dmitri Svergun** (EMBL-Hamburg). Dmitri described the progress in the ability to derive from SAXS such information as *ab initio* structure determination, filling in portions of incomplete structures, validation of 3-D structures from crystallography or NMR, combining multiple "domain" structures into a macromolecular complex, and deciphering stoichiometric information of mixtures or assemblies of structures. Dmitri's lecture was followed by an enthusiastic discussion.

The first part of the afternoon session consisted of brief presentations of research results by trainees. **Alex Vecchio** (Malkowski, Buffalo) presented structural insights into endocannabinoid metabolism by COX-2, followed by **Sara Andres**' (Junop, McMaster) new structure of human XLF, involved in DNA NHEJ. **Rene Jorgensen** (Merrill, Guelph) described the rather convoluted story of how the exotoxin A-eEF2 complex was determined. The calpain-2 complex with calpastatin inhibitor was described by **Rachel Hanna** (Davies, Queen's), and **Dea Shahinas** (Christendat, Toronto) unveiled her structure of aquifex prephenate dehydrogenase. **Lisa Pell** (Howell, Toronto) then discussed the assembly of bacteriophage lambda tail, featuring the structure of the tail terminator protein. Obviously, from the speakers and attendees, participation extends far beyond the nominal founding cities of the symposium. Indeed a very impressive group of trainees has been emerging from the entire southern Ontario, Western New York area.

The final presentations were two spirited talks by **Joaquin Ortega** (McMaster) and **John Rubenstein** (Sick Kids, Toronto) on cryo-electron microscopic reconstruction techniques. Both cryo-EM and SAXS attracted envious attention, especially from trainees, because they don't need crystals! Nevertheless, Qiagen still generously laid on a wine-and-cheese reception (complete with draw and give-aways), which kept attendees from fighting the traffic during rush hour.

The meeting was made possible by generous contributions from Qiagen, VWR, Rigaku, Bruker AXS, Axygen, Hampton Research and (new this year) MiTeGen. Thanks are also due

to this year's Chair, **Frank Sicheri**, whose strict hand kept the timing precise. The Junop/Guarne labs at McMaster provided their usual expert local organization, and **Lynne Howell** and the support group from Sick Kids, Toronto made the whole meeting happen. Finally, **Rob Thorne** (MiTeGen) kindly and spontaneously acted as official photographer. All are welcome to join us for next year's symposium on November 14, 2008, at which the special topic will be Structure-based Drug Design.

*David Rose*

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*XVIII International Conference on the Chemistry of the Organic Solid State (ICCOSS-XVIII), Mérida, Venezuela, July 2007*



The conference was held July 8-13, 2007 in Hotel Belensate, in the beautiful city of Mérida, in the Venezuelan Andes. During the previous week the "First School on Materials Applications of the Organic Solid State" (SMAOSS) was conducted. Participants included graduate students and young scientists from Venezuela, Colombia, Brazil, and Poland. These activities were sponsored by the IUCr, the ICDD, Taylor & Francis, FONACIT-Venezuela, Fundacite-Mérida, Bruker AXS, and Universidad de Los Andes. Awards for the best posters were provided by **Edward Tiekink** (University of Texas, San Antonio) who donated a copy of the book "Frontiers in Crystal Engineering" and by the RSC-*Crystal Engineering Communications*.

The School topics included fundamentals of crystallography, solution and solid state NMR, fundamentals of powder diffraction, data collection and structure solution from powders, use of databases, and solid state reactivity. For ICCOSS XVIII, invited and contributed papers were presented in oral and poster sessions that covered a wide range of topics: reactions in crystals (photochemical, thermal, high energy radiation, etc.), crystallization phenomena (crystal growth, biomineralization, habit control), crystal engineering and supramolecular interactions, metal organic frameworks, polymorphism and phase transitions, functional crystals (magnetic, metallic, semiconductors, photonic, etc.) and pharmaceutical solids, among others. **Roger Bishop** (The University of New South Wales, Australia), **Silvia Bracco** and **Piero Sozzani** (University of Milano-Bicocca, Italy), **Jesús Valdés-Martínez** (Universidad Nacional Autónoma de México, México), **Miguel García-Garibay** (UCLA), **Mark D. Hollingsworth** (Kansas State), **Mingcan Xu** (Cardiff University, UK), **Frank van Meurs** (Bruker AXS BV, the Netherlands), **Alexander Briceño** (IVIC, Venezuela), and **Asiloé Mora** (ULA, Venezuela) delivered invited lectures. **Delia Haynes** (University of KwaZulu-Natal, Republic of South Africa), **Edyta Kolodziejczyk** (Institute of Physical Chemistry of the Polish Academy of Sciences, Poland), and **Weverson Ferreira** (Instituto de Ciências Exatas, Universidade Federal de Minas Gerais, Brazil) also participated in the meeting. The conference

proceedings will be published in a special volume of *Molecular Crystals & Liquid Crystals*.

The XIX ICCOSS will be organized by **Piero Sozzani** in Italy, in July 2009. Watch [www.iccoss.org](http://www.iccoss.org) for information.

*José Miguel Delgado and Graciela Díaz de Delgado*

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*2007 ACA Summer Course on Small Molecule Crystallography., Duquesne University, July 9-18, 2007*

*Summer School participants: Row 1: Andrey Yakovenko, Idaliz Rodriguez, Debasis Banerjee, Will Eckenhoff, Daniel Lima, Daniel Coelho, Michael Moore. Row 2: Bo Li, Cecilia Silva, Elvis Neves, Marta Dabros, Oana Luca, Luisa Chan, Jesse Spencer. Row 3: Dave Duchamp, Nathan Winter, Antonio Scatena, Rocio Santos, Eranda Perera, Lori Fields, Jen Aitken, Jenny Glusker, Jim Kaduk. Row 4: Peter Mueller, Lee Daniels, Bernd Hammann, Ron Benson, Kibong Kim, Bryan Craven, Charles Lake, Curt Haltiwanger*

The 2007 course provided extensive coverage of both single crystal and powder diffraction. 20 students from the United States, South Korea, Mexico and Brazil attended the 10-day course that included 8 days of instruction (lectures in the morning, workshops in the afternoon and computer tutorials at night), a day to tour Pittsburgh and a day for final student presentations. An old ACA Course tradition was resumed when students were treated to a picnic at the Penn Brewery in downtown Pittsburgh. Our highly dedicated teaching staff of 18 individuals from academia, national laboratories and industry made it a priority to provide a strong scientific education in the basic principles of crystallography. This is sorely needed in the modern scientific community because the demand for crystallographic information is increasing rapidly even as the opportunities for a crystallographic education are steadily decreasing.

18 of the 20 students answered a questionnaire providing feedback that has been instrumental in our continued growth and development. The questionnaire was rated on a scale of 1-5, with 5 being excellent and submitters unanimously judged the course as highly successful and stated that they would recommend the course to others. The students gave a very high rating to the category "Did you enjoy the course scientifically" (4.89) and the category "Did you enjoy the course socially" (4.83).

This year, four diffractometers were available to the students. Rigaku-Americas Inc. continued their strong support by bringing a MiniFlex powder diffractometer (Supported by *Lori Fields*) and a SCXmini Benchtop X-ray Crystallography System (Supported by *Ron Benson* and *Lee Daniels*). Duquesne University possesses an x-ray facility which houses a Bruker APEX II diffractometer (Supported by *Bruce Noll* and *Peter Mueller*) and a PANalytical X'Pert Pro powder diffractometer (Supported by *Curt Haltiwanger* and *Jeff Nicolich*). All three

vendors contributed strongly toward the success of the course and clearly support the crystallographic community.

*David Duchamp* and *Jenny Glusker* continued their tradition of giving the essential lectures on the basic foundations of crystallography. Besides being excellent role models, they are outstanding scientists and inspiring lecturers and they contributed much to the success of the course. *Jen Aitken* provided an excellent introduction to powder diffraction and our powder diffractionists, *James Kaduk* and *Brian Toby* continued to provide an excellent education on powder diffraction and showed their usual excitement and tremendous dedication to the field. *Peter Müller*, besides his usual highly dedicated efforts of working one-on-one with the students into the "wee" hours of the morning presented two very interesting lectures on "difficult structures" and "twinning". *Bob Blessing* made an appearance to discuss the latest advances in probability methods and *Sue Byram* and *Lee Daniels* presented a pair of lectures explaining the inner workings of diffraction equipment. *Bryan Craven* presented a very informative talk on atomic displacement parameters and *Bob Stewart* showed his mathematical wizardry while educating students on the principles of least squares analysis. Exposing modern students to basic mathematics is crucial for the survival of science in the United States! *Curt Haltiwanger* gave a strong introduction to single crystal data processing and *John Woolcock* discussed the various crystallographic data bases. The students responded very favorably to the lecture series (4.78). In all, the faculty presented more than 27 lectures covering a wide range of single crystal and powder topics. 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. These materials were rated highly by the students (4.89).

**Curtis Haltiwanger**, **Peter Müller** and **Lee Daniels** presented a series of tutorials on SHELX. **James Kaduk** and **Brian Toby** ran a set of tutorials teaching students how to index powder patterns, and how to use GSAS/EXPGUI and Rietveld analysis. **David Duchamp** presented a tutorial on his powerful CRYSTMOL structure evaluation software and gave all participating students a copy. The experimental sessions were highly successful due to the indispensable services of **Lori Fields**, **Ron Benson**, **Bruce Noll**, **Peter Müller** and **Jeff Nicolich**. These individuals worked one-on-one with students individually into the wee hours of the morning collecting and processing data.

The organizers and students are extremely grateful for the direct financial support provided by the ACA, USNCCr, PDS, Bruker-AXS, Rigaku Americas, PANalytical Inc., IUP and Duquesne University. Their generous donations supported student scholarships and course infrastructure. We would especially like to thank **Joseph Ferrara** and **Thomas McNulty** from Rigaku-Americas. The USNCCr contribution covered travel awards to gifted South American scholars. We are also grateful to **Scott Field** (Cephalon, Inc.) for allowing us to recruit the indispensable services of **Curtis Haltiwanger**.



**Students supported by the USNCCr: Elvis Neves, Cecilia Silva, lecturer Brian Toby, Daniel Lima, Rocio Santos, Daniel Coelho, Idaliz Rodriguez and lecturer Jim Kaduk**

Finally, we would also like to thank **Antonio Scatena** (IUP Chemistry student) for volunteering to provide van service to the students and faculty and making sure that all attendees had an enjoyable, productive time during the course. We are thankful for the tremendous support staff at Duquesne University; **Daniel Bodnar**, **Sandy Russell** and **Jeffrey Palaastro** were contributed significantly to the success of the course. We also thank **Gerald Buriok** (Dean of the College of Natural Sciences and Mathematics at IUP) and **Jeffry Madura** (Chemistry Department Chair at DU) for their support of our activities.

Overall, we feel that the course at Duquesne University was very successful and achieved its goals. Next Summer we are tentatively planning to offer the Small Molecule Course again at IUP with the dates of July 7<sup>th</sup> – 16<sup>th</sup>. Full Details and application forms are available on the ACA website ([www.AmerCrystalAssn.org](http://www.AmerCrystalAssn.org))

*Charles H. Lake, Jennifer Aitken  
and Bryan M. Craven*

### ICCD Distinguished Fellow



At the Plenary Session of the recent Denver X-ray Conference, **Ting C. Huang** was presented the 2007 International Centre for Diffraction Data (ICDD) Distinguished Fellow Award for his extensive contributions to the ICDD for more than thirty years. Since 1999 he has served as Editor-in-Chief of *Powder Diffraction*; since 1988, he has been Editor-in-Chief of *Advances in X-ray Analysis*; and is a Director-at-Large of the ICDD Board of Directors (2004-2008). Ting has served the crystallographic community in many other roles including Consulting Editor of the *Powder Diffraction File* (1994-1996); ICDD Representative to the USNCCr (1994-1996) and the IUCr Commission on Crystallographic Data (1992-1994). He received an ACA Service Award in 1991 and chaired the Applied Crystallography SIG in 1992.

He is currently a Research Staff Member Emeritus, IBM Almaden Research Center, San Jose, CA, USA. Other professional activities include Assoc. Editor-in-Chief of the *Rigaku Journal* (2002 to present) and Co-Chair of the Organizing Committee of the Denver X-ray Conference (2002-2007).

### Ludo Frevel Crystallography Scholarships

To encourage promising graduate students to pursue crystallographically oriented research, the ICDD has established the Ludo Frevel Crystallography Scholarship Fund. Recipients are selected on a competitive basis, each receiving an award of \$2,500. One of the the 2007 recipients is ACA member **Katherine Snoda Ryan**. Kaity is pursuing her PhD at MIT working on RebC and RebP.



Her research centers on using crystallography to investigate enzymes that biosynthesize a class of anti-tumor natural products called indolocarbazoles. Using structural data, she studies the mechanisms by which these enzymes interact with unstable substrate molecules, acting to both prevent spontaneous, unwanted chemistry and to promote the production of desired compounds. This work should help understand how nature builds these molecules, which might lead to new synthetic strategies or to studies in protein engineering.



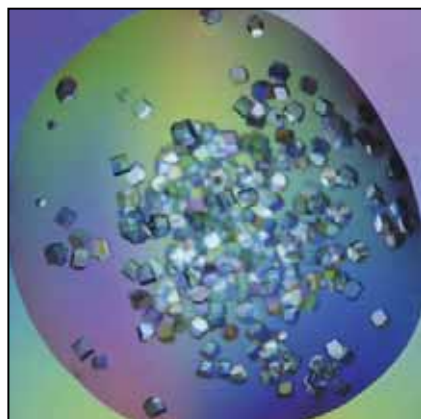
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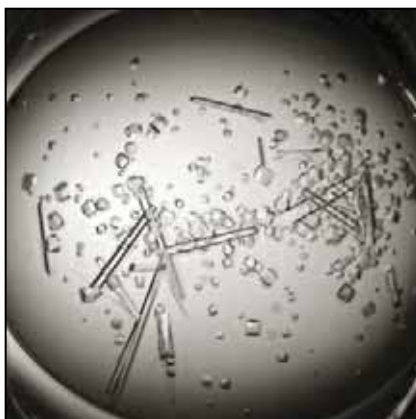


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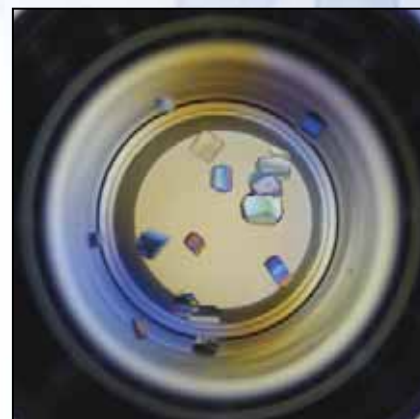
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*Gerald Bunick (1947-2007)*

Gerald John Bunick, Research Professor at the University of Tennessee/Oak Ridge Graduate School of Genome Science and Technology, died on Sept. 19, 2007 at Methodist Medical Center of Oak Ridge after a valiant eleven year battle against multiple cancers. He was born on May 27, 1947, in Boston, Massachusetts, graduated from Newton South High School, and then went to the University of

Massachusetts at Amherst where he obtained a B.S. in chemistry in May 1969. He had summer jobs as a chemist at Monsanto Company and at Polaroid Corporation working on photographic emulsions. His graduate studies in biological chemistry were carried out at the University of Pennsylvania, where he was the first graduate student of Donald Voet. His thesis studies, resulting in a Ph.D. in 1975, involved the crystal structures of antibiotics such as 9- $\beta$ -D-arabinofuranosyladenine and 9-[3-(3-indolyl)-propyl]adenine, models for protein-nucleic acid interactions. His macromolecular thesis studies of structure at the University of Pennsylvania were on the enzyme yeast inorganic pyrophosphatase together with some preliminary studies on the enzyme  $\Delta^5$ -3-ketosteroid isomerase.

In August 1977 Gerry took a position in the Chemistry Division at Oak Ridge National Laboratory, and he was a Staff Member in the Solid State Division from 1982 to 1990. He then became a Senior Staff Member in the Biology Division of the Life Sciences Division where he had several tasks including work on the Advanced Neutron Source Project (1990-1995) and as Program Leader for Structural Biology from October 2001 on. He also had appointments at the University of Tennessee-Oak Ridge Graduate School of Biomedical Sciences, now the University of Tennessee/Oak Ridge Graduate School of Genome Science and Technology where he was a Research Professor. Recently he moved his laboratory there. Gerry was active professionally until his death. He was a member of numerous professional societies and was past president of the small-angle scattering special interest group of the ACA. He leaves a wife, Elaine M. Bunick, an endocrinologist, a son, Christopher G. Bunick and his wife, Lilia and a daughter, Elissa Bunick-Fleming and husband, Scott D. Fleming.

Gerry has been recognized and lauded for his work nationally and internationally. He was meticulous in his laboratory work. His father was a research machinist at MIT and Gerry inherited

an amazing ability to use complicated instruments and to service them when they failed. This was very useful to him in the course of his career, and was a skill he inculcated in those working in his group. He always made certain that every scientific detail was supported to his satisfaction, and his standards were very rigorous. He was a wonderful colleague and friend and will be missed by many.

The majority of Gerry's crystallographic studies can be described in the following three categories: methods for improving the diffraction quality of macromolecular crystals, determination of the structure of the nucleosome core particle and, thirdly, neutron diffraction structural studies of biological macromolecules, particularly enzymes.

As a dedicated experimentalist Gerry investigated methods for producing better macromolecular crystals for diffraction studies. He pioneered the use of macromolecular crystal annealing to reduce any mosaicity acquired by crystals during flash cooling. In this technique a flash-cooled crystal is transferred to a droplet of the original cryoprotectant solution at ambient temperature for about three minutes and then is reflashed to a cryogenic temperature. Details of the method were worked out by Gerry. Joel Harp, Gerry's graduate student, writes: "The annealing discovery came about while working with the nucleosome core particle. The best diffraction was obtained with an MPD level that was marginally useful for cryoprotection so we often had to flash cool 5 to 10 crystals to get one that had an acceptable mosaicity. I was measuring crystal dimensions prior to flash-cooling and diffraction. One crystal had not flash-cooled well but I had forgotten to measure it. I took the crystal off and put it back into cryoprotectant for measurement under the microscope. The crystal after flash-cooling appeared optically clearer than I had remembered it being and wondered if optical improvement could mean diffraction improvement. I flash-cooled the crystal again and took another diffraction image. The difference was astounding! The crystal went from well over 1 degree mosaicity to about 0.4 degree. I don't recall the exact values but the difference leapt off the screen. Gerry immediately saw the importance of the discovery and directed me to divert time from the nucleosome core particle project to a study of the phenomenon that we eventually called macromolecular crystal annealing."

In order to obtain better crystals Gerry also experimented with conditions for growing crystals in space. In microgravity conditions in space it was found that crystals grow more slowly and that the growth is controlled by diffusion alone. Better crystals may be obtained as a result. He has grown macromolecular crystals in space, initially nucleosome crystals in a 1995 NASA space flight. Subsequently several such crystal-growing experiments on NASA and MIR space flights were made; some of the crystals that were obtained were suitable for neutron diffraction experiments.

Gerry focused his interests on chromatin structure and gene regulation, and concentrated his crystallographic studies on the nucleosome core. Nucleosomes package DNA in the nuclei of cells and control how this DNA is used in gene expression. Each nucleosome consists of double-helical DNA (146 base pairs) wrapped around four pairs of histones. These eight histones and DNA constitute the nucleosome core. Such cores are linked

by another histone, H1, so that they appear under the electron microscope as “beads on a string of DNA.” Gerry worked for many years with Joel Harp, Leif Hanson and David Timm on the structure of the nucleosome core particle. It was a huge task as it was necessary to determine how to prepare and crystallize the material and make DNA suitable for binding. He was not the first to publish the entire structure, which was reported in 1997 at 2.8 Å resolution, but Gerry's work provided much additional information when his 2.5 Å structure was published in 2000. New data were provided about the structure of the N-terminal histone tails and useful details were provided on hydration and ion binding. The structure he worked on was composed of twofold symmetric molecules, native chicken histone octamer cores and a DNA palindrome, a crystal resolution feature pioneered by Gerry and his group and essential to an atomic position model of the nucleosome core particle (*Acta Cryst.* (1996) **D52**, 283). As originally theorized palindromic DNA was expected to form a perfectly twofold symmetric nucleosome core particle. In fact, interestingly, the result was found to be asymmetric because of the manner in which the DNA binds to the protein surface and the way nucleosomes pack in the crystal.

Gerry continued his studies of enzyme mechanisms by tackling the determination of hydrogen positions in enzymes that transfer hydrogen ions as part of their mechanism of action. In analyses of D-xylose isomerase he compared the structure at 0.94 Å resolution obtained at 100 K from x-ray diffraction data, with time-of-flight neutron diffraction data measured at room temperature at 1.8 Å resolution at Los Alamos on a deuterated enzyme crystal. The high-resolution x-ray data were for a crystal with bound glycerol, a truncated substrate. This bound near one metal ion but had no atoms that could bind in the isomerization area of the active site. As a result possible side-chain motions were indicated in the disorder found at the isomerization site. From the neutron data Gerry demonstrated that Laue diffraction geometry with time-of-flight neutrons could be used to study larger macromolecules than previously possible. He showed the protonation state of one histidine residue, ready to act on the substrate and open its ring structure. He also showed that the other metal ion binds a water molecule (rather than hydroxyl group even though the pH was 8.0) and that one lysine has only two, rather than three, hydrogen atoms attached to its terminal nitrogen atom. This work showed how productive a comparison of x-ray and neutron diffraction results can be.


Gerry played a central role in aggressively pushing back the experimental limitations of macromolecular neutron crystallography. This technique for providing unique information about hydrogen atom positions in biological macromolecules had been limited by the relatively weak flux of beam lines and by a lack of dedicated beam lines at reactor neutron sources. When the Protein Crystallography Station (PCS) was built at Los Alamos, breaking new ground for structural biology by becoming the first of its kind in the world at a spallation neutron source, Gerry was the first official user, collecting a data set from D-xylose isomerase which, back in 2003, was the largest enzyme ever studied by neutron crystallography. There was great excitement at the beam line as Gerry and his team, including

Amy Katz and Leif Hanson, along with PCS scientists Benno Schoenborn and Paul Langan, huddled around the computer monitors to witness, for the first time ever, the beautiful patterns gradually appearing that are made by the wavelength-resolved diffraction data from a protein. This was one of the pivotal days in the development of neutron protein crystallography. On the basis of this success, a number of other beam lines are currently being designed and built at next generation spallation sources throughout the world. The experimental capabilities for macromolecular neutron crystallography are experiencing a level of investment and a period of growth never seen before. Gerry was at the heart of developing the case for a new neutron beam line at the next generation spallation neutron source (SNS) at Oak Ridge. With the SNS ramping up in power to become the worlds most powerful neutron source and the Macromolecular Neutron Diffraction (MaNDi) beam line in the first stages of design and construction, perhaps the biggest impact of Gerry's influence in this field will only be realized in 4-5 years time when MaNDi and the SNS are operating at full speed.

Jenny P. Glusker and Paul Langan


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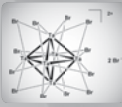
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**Jim Britten**

**Standing Committees**

**Communications**  
**Allen Oliver**

**Continuing Education**  
**Peter Müller**

**Data and Standards**  
**David Harrison**

**SIGS**

**Biological Macromolecules**  
**Chair-elect: John Horton**

**General Interest**  
**Chair-elect: Bruce Noll**

**Industrial**  
**Chair-elect: Herbert Klei**  
**Secretary: Sue Byram**

**Materials Science**  
**Chair-elect: Pamela Whitfield**

**Neutron Scattering**  
**Chair-elect: Thomas Proffen**

**Powder Diffraction**  
**Chair-elect: Ashfia Huq**

**Service Crystallography**  
**Chair-elect: Dale Swensen**

**Small Angle Scattering**  
**Chair-elect: Kenneth Littrell**  
**Secretary: Thomas Weiss**

**Small Molecules**  
**Chair-elect: Jeanette Krause**

**Synchrotron Radiation**  
**Chair-elect: Ernst Bergmann**

**Young Scientist**  
**Chair-elect: Bobby Huether**

**Robert B. Von Dreele, Vice-President**

*Senior Physicist, Argonne National Laboratory; joint appointment with the Intense Pulsed Neutron Source (IPNS) as Instrument Scientist for the Special Environment Powder Diffractometer (SEPD) and the Advanced Photon Source (APS) in the Materials Characterization Group of the X-ray Science Division.*

**Statement:** I was humbled and flattered to be asked to follow in the footsteps of the giants of our community when I was nominated as a candidate for the Vice-President of the ACA. I've been a member of the ACA since joining as a graduate student in the early 70's and it has been the one professional society with the broadest coverage of the

science of crystallography. In that time crystallography has changed dramatically from the time when doing a crystal structure or two could suffice for a publication or even a thesis project to what is now a "technique" on a par with the various spectroscopies commonly available in a chemistry laboratory. This change has been driven by developments in instrumentation and more especially by extreme improvements in computational power and software so that most crystallographic structure determinations can now be performed in a "black box" mode with very little human crystallographic intervention. Even protein structure determination has succumbed to this drive toward automation. While this has been happening for single crystal crystallography, powder diffraction has been transformed out of all recognition from a qualitative/quantitative phase analysis tool done largely in industrial laboratories to a very powerful structural probe usable under extreme conditions on samples that do not normally exist as single crystals. The scope of powder diffraction is rapidly expanding and even proteins are not out of bounds. Moreover, powder diffraction is now used to address bulk properties such as stress/strain and texture in polycrystalline objects which is of great interest to ceramicists, geologists and metallurgists. We have also seen the development of dedicated user facilities in neutron and x-ray scattering constructed at national laboratories that provide brilliant sources and exceptional instrumentation. The explosion of crystallographic information that has resulted from all this is truly staggering; almost 50,000 protein structures are now in the PDB, over 400,000 structures in the CCDC; and over 250,000 entries in the PDF-4+ powder diffraction file offered by ICDD.

Now the bad news: Crystallography is a dying discipline in many universities; many chemistry, physics and geology departments do not have (or want) faculty whose research is driven by a basic grounding in crystallography. The common choice is to relegate crystal structure determinations to departmental staff or else have structures done by mail order. While this does "get the job done" for routine structure determination, the loss is that training in basic crystallography for graduate students and postdocs becomes very spotty at best and completely absent in many locales. I recently saw in the MSA e-mail list many comments from mineralogists about this loss from geology and in some cases describing the complete obliteration of the discipline at their university. Is this a dead end for crystallography?

As I'm sure you know, I develop and maintain a significant crystallographic computer program (GSAS). In fact, I had interrupted my work on this statement to chase down a user reported bug! Much crystallographic software was originally written many years ago by a very small number of folks who had essentially taken this up as a "hobby" and, in one way or another, let the larger community use the fruits of their labors. These codes are commonly in FORTRAN and are becoming more difficult to maintain as that expertise dies. We now want our software to be GUI based and easy to use "black boxes" which requires that all of the accumulated crystallographic "tricks" be somehow coded into them. This requires a new combination of crystallographic and software engineering talents that may be hard to come by.

To meet these challenges, I believe the ACA needs to continue to have an active role in encouraging the development of new ways of providing this needed training and education in crystallography through workshops, summer courses, web-based courses and, of course, the program offered at our Annual Meeting. Perhaps we can learn from the experience of the Rietveld e-mail list where questions (and sometimes contentious comments) are posted by list members about powder diffraction; students in particular almost always receive helpful replies from others. We should have something like this for all of crystallography where e-mail list membership is automatically offered to all ACA members.

In my own particular path through crystallography, I have increasingly become very impressed with the wide variety of tools and techniques that have been developed by the various parts of our community to aid in solving the central problems of crystallography. However, I suspect that much of this knowledge gained in one corner of our science remains unknown and unavailable to the others. The role of the ACA should be to be sure that cross-fertilization occurs between the various subdisciplines within crystallography so that all of us can benefit from this hard-won knowledge. I would encourage future Program Chairs for our Annual Meetings to find ways for our

various disciplines to "mix it up" so we can learn from each other as well as encourage participation (especially by students!) from all corners of crystallography. In my own experience there are incredible scientific riches in the spaces between our various disciplines and the ACA should be there to help us find them.

### *Peter Müller, Continuing Education*



*Director, X-Ray Diffraction Facility, Massachusetts Institute of Technology, Cambridge, MA 02139, pmueller@mit.edu.*

**Statement:** X-Ray Structure Determination is a key method in the life sciences, chemistry, materials sciences and other disciplines and one would expect crystallography to be an important part of the education of every scientist working in those fields. Strangely, however, serious courses in crystallography cannot be found on many curricula. If crystallography is taught at all, it frequently is a marginal part of a physical chemistry class, and only a few hours are available to introduce the method. This is unfortunate, as a majority of scientists relying on crystal structures do not understand the method well enough to evaluate the results of or to draw their own conclusions from crystallographic data. Basic crystallographic education can start as early as in high school and should be taught to undergraduates. In any case, crystallography should be offered as an 18- to 24-unit course to all graduate students of the disciplines mentioned above. Together with the NSF, USNCCr, ACS and the IUCr's Teaching Commission, the ACA should play a prominent role in



fostering crystallographic education at all levels and should help to establish basic teaching standards. I will work in this direction as a member of the Continuing Education Committee.

A different aspect of crystallographic education is the training of scientists who want to determine crystal structures not only occasionally and under the guidance of a trained crystallographer, but fully on their own. The training of a professional crystallographer reminds me of that of a Jedi Knight: the practical knowledge only goes from the master's mouth to the apprentice's ear and it can be difficult for the outsider or autodidact to become adept without a local guru's help. At the same time, modern software has become so good and fool proof that many routine structures can be determined without any skill other than the ability to repeatedly hit the carriage return key while simultaneously ignoring occasional error messages. To overcome this black box phenomenon is a key challenge for the ACA and crystallographic education must continue well beyond the regular classes mentioned above. The annual ACA Summer Courses as well as workshops held at the annual ACA meetings are important for the development of the crystallographic community, but I would like to see the ACA put an even higher emphasis on education. Several attempts to establish an Education Special Interest Group have failed in the past years. As the current Chair of the General Interest Group I will try to amend the bylaws of this group to include an educational mandate. As a member of the Continuing Education Committee I will use my experience in organizing and teaching to work towards offering, promoting and sponsoring a broader range of workshops and courses and to make education one of the top priorities of the ACA.

**David Harrison, Data and Standards**



*Department of Chemistry and Biology, Rosalind Franklin University of Medicine and Science, Chicago, IL*

**Statement:** As the field of macromolecular x-ray crystallography becomes more like that of small molecule x-ray crystallography, it becomes more and more important that crystallographic data be able to stand on its own without the need to rely on accompanying publications. Data standards make it possible for automated bioinformatics programs to work on public databases without intervention by researchers and programmers. The two issues that I will focus on are data quality and data standardization. In college, I spent my summers doing database programming in FORTRAN for a financial management company. From this experience I gained a solid understanding of the nuts-and-bolts of database programming, which has given me insights into how data standards may ease database design. I also spent a short time as a small molecule crystallographer and I am aware how data standards have been used to allow systematic characterization of bond lengths, bond angles, and non-bonded interactions. Since I have also spent several years as a producer of macromolecular crystallographic data. I am aware of how important it is that the standards not unduly interfere with the process of model refinement and data deposition. Further, in light of recent events, it seems to me that standards must be adopted for

the submission of experimental phases as well as the routine deposition of derivative and MAD datasets in addition to the deposition of native data. It should be possible for researchers to objectively view crystallographic data without model bias in the case of controversial publications. I look forward to the opportunity to work with this committee.

**Allen Oliver, Communications**



*Research Crystallographer, Department of Chemistry and Biochemistry, University of California Santa Cruz, Santa Cruz, CA 95064*

**Statement:** I am honored to have been elected to the ACA Communications Committee. Communicating concepts, information and results are vital to any society; both within the society and to the public at large. Today's crystallographic research covers a diverse range of topics and we need to be able to present our ideas to those within and outside of our field of specialization. I will endeavor to work with the committee to promote more interdisciplinary discussions to strengthen our understanding of the fields within our chosen profession. Furthermore, I will endeavor to raise public awareness of the ACA and what we provide to the greater community

**Jim Britten, Canadian Representative to Council**



*Assistant Professor, Department of Chemistry and Brockhouse Institute for Materials Research, Manager, MAX Diffraction Facility, McMaster University, Hamilton, ON, Canada L8S 4M1*

**Statement:** It is an honour to have been elected the Canadian Representative to ACA Council. Crystallography development, promotion, and education in Canada are experiencing advances and barriers similar to those seen in the US. The production of high quality data for protein, chemical, material, and scattering analyses is increasing steadily. A set of beamlines for scattering and diffraction experiments at the CLS has been funded. The demand for crystallographic analyses is growing faster than the capacity to train and fund independent crystallographers. As the Canadian Representative to Council, I will bring Canadian ideas and perspectives to the table, and encourage Canadian ACA members to become more involved in the ACA and in the continuing success of our meetings. We are excited about hosting the 2009 meeting, and will make every effort to ensure its success.



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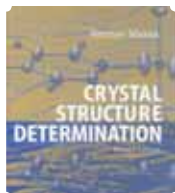
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## The 10 "Must Read" Book List for X-ray Crystallographers

As I was sitting in my office at Texas A & M University, pondering where I was going to go for lunch, a student approached and we began a conversation on x-ray crystallography. The student asked a very interesting question. He said, "Given my limited lifespan (only 70 or so more years), I can only afford to read ten books on any given subject. What ten books on x-ray crystallography would you recommend?" Unfortunately the answer that I gave the student was unsatisfactory, due to the fact I was overwhelmed by hunger, but I vowed to find a better answer.

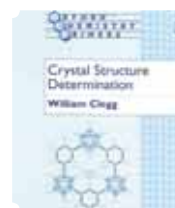
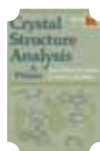
With this in mind, I posted the same question to my colleagues on a user group newsgroup. The response that I saw was fantastic and here is the list that we produced. Keep in mind that this is an informal survey of very wise old masters with many years of research and teaching under their ever-expanding belts and consequently there may be a few good books that we have not included. I call this the "must read book list" and I recommend that students and experts alike should consider this list when choosing their top ten books to read on the subject of x-ray crystallography.

The books are listed in no particular order. The remarks are from actual readers and do not necessarily reflect my opinion, but who am I to disagree with the old masters.



[1]. *Crystal Structure Determination* by: Werner Massa (March 31, 2004) ISBN-10: 3540206442 "My favorite introduction to Crystallography." "It's the one book I would force into a student hands!"

[2]. *Crystal Structure Analysis* by: Jenny Glusker and Kenneth Trueblood (August 1992 ISBN-10: 0195035313 "A good starter for the common scientist."



[3]. *Crystal Structure Analysis: Principles and Practice* (IUCr Monographs on Crystallography) by Peter Main, William Clegg, Alexander J. Blake, Robert O. Gould. (January 28, 2002) ISBN-10: 019850618X "One of my favorite and informative book(s). "Crystallographers should read this book first."

[4]. *The Determination of Crystals Structures* by: H. Lipson & W. Cochran (June 1966) ISBN-10: 080140276X "It is still an amazing book!" "Today's crystallographers could garner a new perspective and appreciation of the subject."



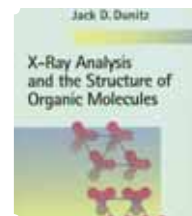
[5]. *Fundamentals of Powder Diffraction and Structural Characterization of Materials* by: Vitalij Pecharsky and Peter Zavalij (March 3, 2005) ISBN-10: 0387241477 "Only book that I know of that explains indexing and indexing programs. "A must own book for the powder and single-crystal diffractionist!" "A gotta-have book for people interested in the bigger picture."

[6]. *Structure Determination by X-ray Crystallography* by: Mark Ladd and Rex Palmer (September 30, 2003) ISBN-10: 0306474549 "I have given Ladd and Palmer to non-crystallographers who needed to gain a basic understanding of the process."



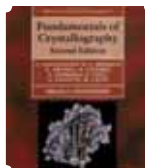
[7]. *X-ray Structure Determination* by: George Stout and Lyle Jensen (April 24, 1989) ISBN-10: 0471607118 "A good, practical book for the student after they are into the subject." "My first book and the most recent book I have re-read on crystallography!"

[8]. *X-ray Analysis and the Structure of Organic Molecules* by: Jack Dunitz (December 16, 1996) ISBN-10: 3906390144 "A great book (even for an inorganic chemist) and it is filled with Jack's usual wit!" "The section on weighting schemes in least squares is a must read"



[9]. *Protein Crystallography* by T.L. Blundell and L. Johnson (January 28, 1976) ISBN-10: 0121083500 "It is required reading for the scientist in the area of protein crystallography."

[10]. *Fundamentals of Crystallography* edited by C. Giacovazzo (July 15, 2002) ISBN-10: 019850958 "A MUST HAVE for a lab! "For more advanced students Giacovazzo is a must."



### Short books quite useful for beginners

*Introduction to Crystallography* by Donald E. Sands (January 7, 1994) ISBN-10: 0486678393 "A good addition to a practical methods course."



*Crystallography Made Crystal Clear* by: Gale Rhodes (February 16, 2006) ISBN-10: 0125870736 "For the novice/macromolecular user."



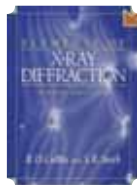
*Crystal Structure Determination* by: William Clegg (June 18, 1998) ISBN-10: 0198559011 "First time crystallographers should read this book."



**For General X-ray Powder Diffraction**



*Introduction to X-Ray Powder Diffractometry* by Ron Jenkins and Robert L. Snyder (June 28, 1996) ISBN-10: 0471513393 "A bit dated but still a good read."



*Elements of X-Ray Diffraction* by B.D. Cullity and S.R. Stock (February 5, 2001) ISBN-10: 0201610914 "This book is very inclusive on the subject of X-ray Diffraction."

**And finally a good book for SHELXL users**



*Crystal Structure Refinement: A Crystallographer's Guide to SHELXL* by Peter Müller, Regine Herbst-Irmer, Anthony Spek, Thomas Schneider, Michael Sawaya (August 14, 2006) ISBN-10: 0198570767 "Regine's section on twinning is marvelous!"

This list is certainly not all inclusive and is specific for x-ray diffraction and in particular to small molecule crystallography. This list should not be considered the only list the reader could consult. Every scientist is unique and will require their own personal library tailored to their needs. This list is a starting point that can be used to build or expand that library and to give the investigator the information they need to do their science.

*Joseph Reibenspies*

**Book Review: Live-Net by David M. Blow. (2005). Edward Gaskell, publishers, Lazarus Press, ISBN 1-898546-75-4, 126pp**

**A Parable of Electronic Hobbits and Humans:** Imagine your reaction if one morning, your almost finished manuscript on the biological implications of the structure you just solved had been significantly altered in your sleep. What would your reaction be? What would be the personal, political and social implications of this act of 'computer piracy'? How would you solve it? These are some of the issues that D. M. Blow explores in his brief novella 'Live-Net' [for the full review see reference <sup>1</sup>].

Indeed, this is the same David Mervyn Blow (1931-2004) who is one of our professional heroes and who, by the power of his intellect, was a key contributor to (MIR) <sup>2</sup> and Molecular Replacement (MR) <sup>3</sup> both of which played a fundamental role in the development of macromolecular crystallography. His group solved soon thereafter the atomic structure of one of the first enzymes, chymotrypsin, unveiling the 'catalytic triad' (Ser-Asp-His), which has been found to be widespread in nature. Many well deserved honors were bestowed upon him in the years that followed.

But *Live-Net* unveils another, more accessible, David. Blow. The novella reveals a reflective person who has allowed his imagination to fly from what we know and do with computers today towards what might happen in the near future. The story develops a brief but well-connected plot where all the critical elements

of society are present. Younger generations are represented by two of the main male characters, cousins Nick Stone and Rob Price, both students in Cambridge. Their respective girlfriends, Tina and Diana, are also significant protagonists of the story. Tina speaks with the voice of biology in an environment biased towards computational and technical viewpoints and explanations. Diana is a well-connected, savvy and shrewd assistant to Alec Fowler, the director of Microsoft in Cambridge. The academic establishment in computer intelligence and security is Rob's PhD adviser, Jim Logan. The high brass of government security is represented by General Hocking.

*Live-Net* is an imaginative, well interwoven story of computer fiction and biological thoughts with an underlying layer of philosophical reflection on what is 'living' and 'non-living'. It is the product of a brilliant and fertile imagination written at a time when most humans have settled down into other more terrestrial pursuits. I truly recommend this brief novel to any reader interested in computer science-fiction and especially to the younger generations. The situation presented in the opening sentence might well happen in the near future.

References

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Cele Abad-Zapatero - caz@uic.edu

**Crystallography 101: Tutorials, applets, and movies for the structural biologists**



Crystallography 101, the popular tutorial website by Bernhard Rupp ([www.rupweb.org](http://www.rupweb.org)), began in 1993 when the web was an untapped educational resource, Google didn't exist, and Mosaic was all the rage.

The website has been enhanced with new material over the years, and Crystallography 101 is widely used in various workshops including those sponsored by the National Science Foundation and in lectures at the EMBL PEPC courses. The tutorial includes units on crystallization and crystal mounting, diffraction basics, phasing, model building, and structure validation. There are also informative interactive modules on symmetry, space groups, structure factors, Fourier and Patterson transforms and calculation of electron density maps. A special section harbors useful little applets for numerous quick calculations including the Matthews probabilities calculator (*Prot. Sci.* **12**:1865, 2003). A number of crystallization and ligand soaking movies make interesting discussion material. Crystallography 101 has been visited by more than 515,000 students and scientists worldwide. If you are looking for material to accompany a course or for a handy reference on space groups, the Patterson function, anomalous absorption edges, or even FORTRAN cgi scripts, visit Crystallography 101.

The web site will be completely updated to accompany Bernhard Rupp's new textbook (publication late 2008).

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## US National Committee for Crystallography



*USNCCr meeting in Salt Lake City: Standing (l-r): Ron Stenkamp, Scott Misture, Kathie Bailey-Mathae, Doug Ohlendorf, Bill Duax, Paul Voyles, Cheryl Klein-Stevens, Bernie Santarsiero, Alan Pinkerton, Brian Toby, Bob von Dreele, Jennifer Swift, Joe Ng, Seated (l-r): Cora Lind, Julia Chan, Jim Kaduk, Kathy Kantardjieff, Chris Cahill, Vic Young. Background photo courtesy of Kathy Kantardjieff.*

The US National Committee for Crystallography (USNCCr-[www7.nationalacademies.org/USNC-IUCr](http://www7.nationalacademies.org/USNC-IUCr)) is the body which represents the United States (on behalf of the National Academy of Sciences) to the International Union of Crystallography (IUCr) ([www.iucr.org](http://www.iucr.org)). It tries to represent the breadth of crystallographic science in the U.S. There are no individual members of IUCr, only countries. Because the ACA is a Regional Associate of the IUCr and because ACA and the USNCCr work closely with each other, there is sometimes confusion between the two.



Over the next year, many of the activities of USNCCr will be devoted to preparing for the 21<sup>st</sup> Congress and General Assembly (GA) of the IUCr in Osaka. The USNCCr intends to propose six changes to the IUCr Statutes and By-Laws ([www.iucr.org/iucr-top/iucr/statutes.html](http://www.iucr.org/iucr-top/iucr/statutes.html)). The intent of these proposed changes is ensure maximum diversity in the membership of the Executive Committee and to emphasize the role of the General Assembly as the forum at which crystallographers direct the work of the Union.

The proposed changes, with our rationale, are:

[1]. Statute §6.1g, add: *one representative from each of the Regional Associates.*

The Regional Associates (RA) are defined in Statute §1.2i. Representatives of the Regional Associates may attend the General Assembly (By-Laws 1.4), but have no voting power. The three current Regional Associates – the American, Asian, and European Crystallographic Associations – are becoming

more important to crystallographers and to the Union. We believe that this growing importance should be recognized by permanent representation on the Executive Committee. The benefits of broader representation on the Executive Committee should exceed the relatively minor increased costs. It has been noted that this change will introduce to the Executive Committee members who have not been elected by the General Assembly. We view this as a good thing, as these representatives will have been chosen by an even larger electorate than the General Assembly.

[2]. Statute §6.4, insert a paragraph describing how these members will be chosen: *The representative of each Regional Associate will be that person elected by his or her respective association membership. They are not eligible for immediate re-election to the same office.*

Our intent is that each of the Regional Associates will determine their own selection process. Because the other members of the executive Committee serve from GA to GA, it may be best for each RA to create a new office, rather than have the President serve as the Executive Committee representative.

[3]. Statute §6.2, add a third paragraph: *The representatives of the Regional Associates are not considered when determining whether there are two or more officers from any one country.*

The intent of the “not more than two” restriction is clear, and enhances diversity. We see no reason to change it because additional diversity has been incorporated into the membership of the Executive Committee.

[4]. By-Law §1.4, amend to remove the following phrase *but they shall not take part in the discussions, unless specifically invited or permitted to do so by the Chair, and they shall have no voting power.*

This change is to emphasize that it is the right of any crystallographer to speak at the General Assembly, and not a privilege granted by the Chair (though it is up to the Chair to manage the discussion).

[5]. By-Law §8.5, amend the second paragraph to have: *At least two nominees shall be presented to the General Assembly for consideration as candidates for election to one of these offices* replace *If there is only one candidate for one of these offices, his or her nomination shall be presented to the General Assembly and the candidate shall be considered as elected.*

[6]. By-Law §8.6, amend to delete the following. *If there are not more candidates than vacancies, the nominations shall be presented to the General Assembly and the candidates shall be considered as elected.*

The deletion in §8.6 articulates the election process in light of the changes proposed in §8.5. The point of these changes is to emphasize that the Executive Committee is responsible to the GA. The duties of the GA are not merely to endorse the recommendations of the Executive Committee (such as a slate of candidates), else there is little reason to have a GA. We believe that there is no shortage of qualified crystallographer candidates, and are very gratified that the Executive Committee has nominated multiple candidates for the election in Osaka. We see no reason that this should not be the case in future General Assemblies, and would like to enshrine that notion in the By-Laws.

The USNCCr believes that (although these changes sound picky and bureaucratic) they help ensure that the IUCr becomes more representative and diverse. I would appreciate comments on and support of these proposed changes.

The various National Committees for Crystallography proposed nominees to the IUCr Executive Committee. Based on these nominations, the slate proposed for the elections in Osaka is:

President

C. Gilmore (UK)  
S. Larsen (France)

General Secretary and Treasurer

S. Lidin (Sweden)

Vice-President

P. Colman (Australia)

Three six-year vacancies for Ordinary Members

E. Boldyreva (Russia)  
C. W. Carter (USA)  
V. Cody (USA)  
L. T. J. Delbaere (Canada)  
K. El Sayed (Egypt)  
C. Lecomte (France)  
J. M. Perez-Mato (Spain)  
Xiao-Dong Su (PR China)  
Yu Wang (Taipei)

For the likely one or two three-year vacancies for Ordinary Members: Same list as for the six-year vacancies

In addition to “our own” candidates, we supported the nominations of Chris Gilmore and Peter Colman. The members of the IUCr Executive Committee will be elected by the General Assembly in Osaka.

The USNCCr has also made nominations for members of the various IUCr Commissions that will be selected in Osaka. I was amazed and gratified by the willingness of crystallographers to serve in what are sometimes thankless jobs. Thank you to all those willing to be nominated! If there is anybody out there who wants to be nominated to the XAFS or the Mathematical and Theoretical Crystallography Commissions, contact **Jim Kaduk** at [innovene.com](mailto:innovene.com).

The USNCCr is in the process of selecting the US Delegates to the General Assembly in Osaka. As a category 5 member of the IUCr the US delegation consists of 5 voting members. When named, the delegates, alternates, and I will accept gratefully any input you wish to make on the issues which come before the General Assembly.

The USNCCr is a self-electing committee. New members (for a term of 2008-2010) are: **Julia Chan** (Louisiana State University, re-elected), **Miriam Rossi** (Vassar College, re-elected), **Bernhard Rupp** (University of California-LLNL), and **Steven Sheriff** (Bristol-Myers Squibb). We thank outgoing USNCCr members **Ron Stenkamp** and **Peter Kuhn** for their contributions to lively discussions.

In addition to the “bureaucratic stuff”, the USNCCr tries to do something useful. A major recent thrust (under the leadership of Vice Chair **Katherine Kantardjieff**) has been the preparation of the report *Molecular Structure by Crystallography: Crystallography Education Policies for the Physical and Life Sciences. Sustaining the Science of Molecular Structure in the 21<sup>st</sup> Century*. This document contains curriculum recommendations for both practitioners of crystallography and users of structural information in both the life and physical sciences. The next focus is on implementing these recommendations. Because nothing happens in the chemistry curriculum without the encouragement of the ACS Committee on Professional Training, we were very disappointed with their new draft of *Undergraduate Professional Education in Chemistry: Guidelines and Evaluation Procedures*, which contain no mention of crystallography whatever! We are attempting to work with the ACS CPT to get crystallography back into the chemistry curriculum. The USNCCr Education Subcommittee is beginning to work on assessment tools to assist implementation of the curriculum recommendations, as well as pamphlets on crystallography. We hope that schools supported by the USNCCr will implement the recommendations.

The USNCCr is running a student travel support program for the Osaka IUCr meeting. See page 8 for details. The Committee also supported students from Latin America to attend the ACA 2007 Small Molecule Crystallography Course (see pages 13-14).

In an attempt to identify synergies among National Committees, the USNCCr met jointly with the USNC/IUPAC in Washington on 2-3 November 2007. Both National Committees, as well as both Unions and the National Academies, are interested in strengthening engagement with Latin America.



*The IUCr Executive Committee met in Salt Lake City immediately after the ACA meeting. During the ACA Meeting the USNCCr hosted the members of the IUCr EC for an evening of refreshment and conversation. Standing: Marv Hackert, Bernie Santasiero, Malcom Cooper, Sven Liden, Claude Lecompte, Gautam Desiraju, Chris Gilmore, Gernot Kostorz, Doug Ohlendorf, Jim Kaduk, Bob von Dreele, Victor Young, Alan Pinkerton, Davide Verterbo, Bill Duax, Gernot Heger, Peter Colman. Seated: Kathy Kantardjieff, Iris Torriani, Yuji Ohashi, Cora Lind, Jane Robinson, Mike Dacombe.*

**Eduardo Feller** (NSF Office of International Activities) summarized the NSF programs which facilitate interactions with Latin American scientists.

The two National Committees compared their programs for young scientists. The IUPAC program is geared to encouraging “young” (< 45 years) scientists to participate in the governance of IUPAC, while the IUCr program supports scientific attendance at the Congress. There will, however, be an American Institute of Physics student reporter at the Osaka Congress.

The IUPAC Education Committee was interested in our curriculum recommendations document, and provided suggestions on working with the ACS to get the recommendations implemented. Both Committees are interested in extending their education work to the K-12 arena. If we can get junior high school students (and their teachers) interested in crystallography and chemistry, they can become hooked for life! A particular challenge in implementing science recommendations in the K-12 curricula is that they are managed by the states and not nationally.

We heard a presentation on a report from a New Materials Synthesis and Crystal Growth study committee of the NAS Board on Physics and Astronomy. There was no mention of organic crystal growth or crystal engineering in this inorganic materials-focused report. The USNCCr will attempt to correct that situation! We also heard a report from **Dorothy Zolandz**, Chair of the NAS Board on Chemicals Sciences and Technology, on *The Future of U.S. Chemistry: Benchmarks and Challenges*. The presentation sparked a spirited discussion on just how bright was the future of chemistry in the U.S. There was a summary of current U.S. visa policies from **Kofi Kpikpitse** of the NAS International Visitors Office. The main message was (especially for Cuban scientists) “apply very far in advance.” **Mike Lubell** of the APS Public

Affairs Office gave an enlightening presentation on “Budgets and Politics in Funding Science and Research Facilities”, telling how the system really works.

The joint meeting led to lots of good ideas. Now we need to let them percolate, and see if something real comes from them. Since crystallography is such a fundamental science, we can expect to see additional joint meetings with other U.S. National Committees.

*Jim Kaduk, Chair, USNCCr*

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## ACA 2007 - Workshop WK.01: SHELX



The 2007 SHELX workshop, organized by George Sheldrick and Peter Müller ([web.mit.edu/pmueller/www/ACA2007/WK01/index.html](http://web.mit.edu/pmueller/www/ACA2007/WK01/index.html)) was held on Saturday July 21<sup>st</sup> directly prior to this year's annual ACA meeting in Salt Lake City. With over 100 enrollees it was very well attended. Hoping to provide the opportunity for an exchange of ideas between the two groups, this whole-day event was the first SHELX workshop to focus on both macromolecular and small-molecule topics. Eight experts presented on a multitude of SHELX related aspects.

The first half of the workshop focused on refinement issues with talks about the history and structure of the SHELX package as well as the concept of constraints and restraints (*George Sheldrick*, University of Göttingen), disorder refinement (*Peter Müller*, MIT), twin refinement (*Regine Herbst-Irmer*, University of Göttingen), protein refinement at atomic resolution (*Thomas Schneider*, EMBL Hamburg), SHELXPRO (*George Sheldrick*), preparation of CIF files (*Ilia Guzei*, University of

Wisconsin) and structure validation with PLATON (*Ton Spek*, Utrecht University).

The general theme of the afternoon session was experimental phasing with SHELX. *George Sheldrick* described his programs SHELXD (structure solution with advanced Direct Methods) and SHELXE (density modification and primitive autotracing). *Thomas Schneider* demonstrated his and *Thomas Pape's* HKL2MAP program that works as an automatic front-end to SHELXD and SHELXE, and *Judit Debreczeni* (Astra Zeneca) gave an introduction to the method of SAD and MAD phasing. At the end of the workshop, *Paul Emsley* (University of York) demonstrated COOT, a program written by *Kevin Cowtan* and *Paul Emsley*. COOT stands for Crystallographic Object-Oriented Toolkit and, according to Paul, also refers to the hairstyle of its two authors. It is a very powerful graphics program that displays electron density maps and models. It allows a multitude of model manipulations and has many features that resemble

those of FRODO, O and XtalView's XFIT, however unlike those programs, COOT directly reads and writes SHELX format files.

Most of the feedback received by the organizers was enthusiastically positive, however a few participants felt the workshop could have been more hands-on and practical. While this would have been difficult with the large number of participants in Salt Lake City a smaller, very practical SHELX workshop that will be



Workshop speakers - Back row *Ilia Guzei, Ton Spek, George Sheldrick, Judit Debreczeni, Thomas Schneider*. Front row: *Regine Herbst-Irmer, Peter Müller, Paul Emsley*.



taught by *George Sheldrick*, *Chuck Campana* and *Peter Müller* will be held early next year at MIT in Cambridge, MA. This workshop will focus on refinement and possibly data reduction and will be coupled to the 2008 Bruker/MIT Symposium. For more information, contact *Peter Müller* ([pmueller@mit.edu](mailto:pmueller@mit.edu)), visit the workshop web site ([web.mit.edu/x-ray/bmit08.html](http://web.mit.edu/x-ray/bmit08.html)) and see the announcement on page 48 in this volume of *ACA RefleXions*.

### ***ACA 2007 - Workshop WK.02: Validation of Macromolecular Structures: Updating Standards for Publication of NMR Structures in an IUCr Journal***

***Participants:*** *Howard Einspahr* (*Acta Cryst. F*), *Mitchell Guss*, (*Acta Cryst. F*, Sydney), *Manfred Weiss* (*Acta Cryst. F*, EMBL Hamburg), *Luciano Mueller* (Bristol-Myers Squibb), *Rob Kaptein* (Utrecht), *Eldon Ulrich* (BMRB, Wisconsin), *James Aramini* (Rutgers), *John Westbrook* (RCSB, Rutgers), *Clemens Anklin* (Bruker BioSpin), and *Peter Strickland* (IUCr Journals)

The suggestion of having a workshop on standards for publication of NMR structures in IUCr journals was first discussed among the editors of *Acta D & F* at the IUCr Journal Commission Meeting in Montecatini (Italy) in August 2005. With the publication of the first NMR structure in *Acta Crystallographica Section F*<sup>1</sup>, the need for a workshop became imperative. The objective of the workshop was to arrive at a list of data supplemental to the earlier IUPAC standards<sup>2</sup> that are to be required or recommended for publication in any manuscript that describes a three-dimensional macromolecular structure determined by NMR submitted to *Acta Cryst.*

*Howard Einspahr*, *Manfred Weiss* and *Mitchell Guss* organized the workshop with the help and advice of *John Markley* (Wisconsin) and *Gaetano Montelione* (Rutgers). The participants heard and discussed a series of presentations in the morning and then met as a committee of the whole in the afternoon to draft summary recommendations. These recommendations are now nearing completion and, after review, will appear in an editorial in *Acta Cryst. F*.



***Workshop participants: Clemens Anklin, Peter Strickland, Eldon Ulrich, James Aramini, Luciano Mueller, Howard Einspahr, Mitchell Guss, Manfred Weiss, Rob Kaptein, John Westbrook***

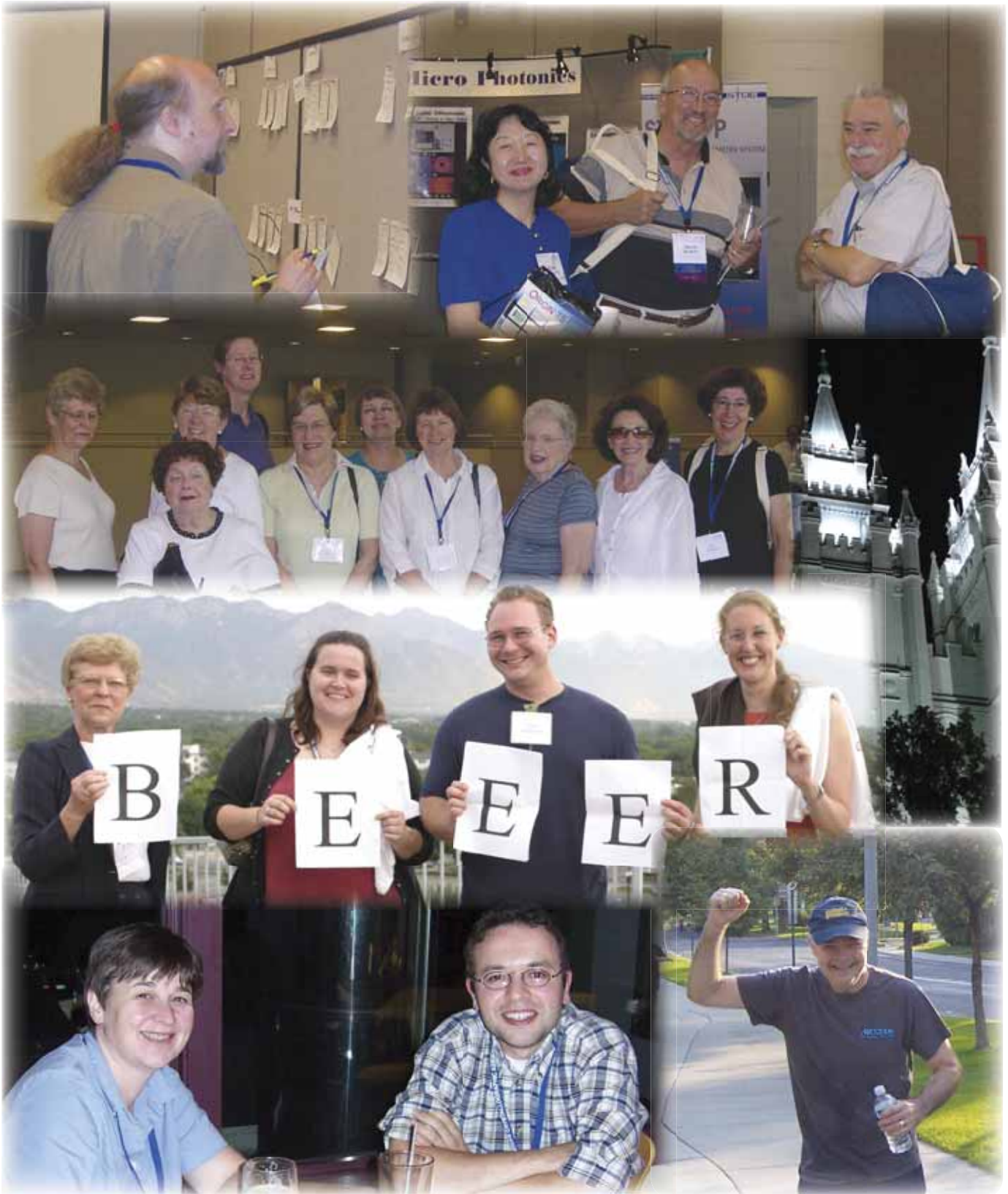
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### ***Howard Einspahr***



***2007 ACA Award Winners and Friends: Back row - Marv Hackert, Bernie Santasiero, Jack Dunitz, Alan Pinkerton, Angelo Gavazotti, Frank Herbstein, Lee Groat, Bob Bau. Front row: Cora Lind, Claudia Cortese, Barbara Dunitz, Amy Michel Herbstein, Lisa Keefe.***



*From the top: Paul Butler working on the program for Knoxville; Winnie Wong-Ng, Marv Hackert and Abe Clearfield at a poster session; The Better Halves: Carol Delbaere, Ruth Clearfield, Florence Quail, Bretna Hackert, Annas Rae, Nancy Fratini, Pamela Salyer-Ibberson, Carol Johnson, Sharon Davis, Sally Springer; the Temple at night; Carol DelBaere, Amy Gindhart, Chris Jurgenson, and Judith Schmiedel at the YSSIG mixer; Carrie Wilmot and Hasan Demirci at the Mentor Mentee dinner; and Charlie Carter surviving the fun run. Beer photo courtesy of Cora Lind.*

*Following are some of the impressions and experiences of the students who received travel grants this summer*



I was among the few that received a travel grant award to attend the ACA Meeting in Salt Lake City. I was also one of the recipients of the prestigious Pauling prize. This was the first and biggest conference of its kind I have ever attended in the history of my educational career. I am very happy to say with joy and satisfaction *A Big Thank You* to all those who spent sleepless nights working to put up such an interesting and successful conference. I had the opportunity to meet with George Sheldrick in particular and a lot of professors in general with whom I was able to share words concerning excellence in education. I had the opportunity to discuss my poster presentation in the presence of some professors who took great interest in what I was talking about. I actually met with a professor from the University of Florida-Gainesville (Aboud Khalil) who after listening to my presentation and finding out I got a Pauling poster prize, promised me a position in his chemistry department and called me "a future graduate student of that University."

I wish to thank the ACA organizing committee of the Salt Lake ACA 2007 conference and to tell them "Bravo" –The Sky is Your Limit.

*Ernest Asani*

I'd like to thank the ACA for the travel grant. This meeting was my very first conference to attend and it was a great experience for me. First of all, it was fascinating to listen to all the talks during the "Large and Difficult Structures" session, especially on topics covering the "central dogma of molecular



biology." Understanding structures, such as RNA Pol II and the ribosome is really important; however it is very challenging because of their massive size. I was really impressed with how crystallographers are now able to solve larger and larger protein complexes at high resolution. Additionally, the talks for "Strategies for Crystallization Challenged Macromolecules" were very informative and gave me some insight on how I can go about improving crystallization. The "Crystallography in Industry" session was especially useful for me because I am a graduate student and want to learn of possible career opportunities in crystallography. It was very interesting to learn about a popular method for drug design like "fragment screening". At the same time, I was very fortunate to be able to present a poster and to have a chance to discuss my research with fellow scientists. Thus, I'd like to thank ACA for this great experience again, and I hope to have more opportunities to attend ACA meetings in the future.

*Shiho Tanaka*



The ACA's generous travel awards enable many students like myself to present research at meetings they would otherwise not be able to attend. Not only are the meetings intellectually stimulating, it is also very exciting to see what new

developments have arisen in the field of crystallography. Beyond this, the travel awards also allow students the opportunity for networking and a chance to get feedback on the research they have done. 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. This would not have been possible without a travel award. The travel award also allowed me to give an oral presentation of my research, resulting in an "Outstanding Oral Presentation" award. The chance to give an oral presentation was an invaluable experience, and the meeting was a resounding success. I hope the ACA is able to continue enabling students to travel to meetings around the country.

*Brett Hanson*



I would like to start off by thanking the ACA and its sponsors for providing me with funding to attend the Salt Lake City ACA conference. This was my second experience at an ACA conference and I again found the lectures and posters to be quite fascinating. The climate might not have been as nice as the ACA conference in Hawaii; however the people made it a very rewarding week. I would also like to thank the Materials Science SIG for giving me an Etter Student Lecture Award as well as the ICDD for their extra funding. I was honored to have the opportunity to present my research to such a great crystallographic audience as well as be able to attend activities such as the YSSIG Mixer which was a great place to interact with fellow researchers. Thank you again for this great opportunity.

*Amy Gindhart*



I would like to thank the ACA for providing travel funds allowing me to attend the meeting in Salt Lake City. With such funds I was able to witness some of the great veterans of crystallography give some fascinating talks, as well as some of the younger but equally impressive scientists provide insight into their research. It was also a huge asset being able to talk to people regarding advancement of my own research as well as potential future plans. Thanks again!

*Benjamin Scott*



This ACA meeting was especially productive for me for a number of reasons. In addition to receiving an ACA travel award, I also was chosen for a Pauling Poster Prize. I felt that the ACA had a strong focus on student research, as opposed to simply handing out awards to established scientists. This is a very welcome boost to the early career of young scientists and makes the ACA meeting more attractive for students to attend.

The highlights of the meeting were the mixers which were held nearly every night. MarUSA hosted a dinner at the local science center, and Qiagen sponsored the Young Scientist SIG dinner at the Salt Lake City Public Library. This proved to be a great opportunity to mingle in an informal setting with professors and students alike.

The scientific content of the meeting was exceptional in that many of the presentations addressed some of the pressing issues relating to modern structural studies. The ones that stood out the most for me included the recent advances in using longer wavelength X-rays for sulfur and phosphorous phasing, new developments in micro-diffractometry and the structural basis behind disease and immunity. It was encouraging to see how many new areas of research there are in protein crystallography and that so many are participating in advancing the field.

*Christopher Jurgenson*

I would like to thank the ACA for selecting me to receive a travel award, as well as the organizers of the Etter Early Career Award Symposium for allowing me to give a talk on my research. I thought that the meeting was very well organized, and I was fortunate to meet a lot of great scientists. I especially enjoyed talks that focused on large protein complexes, and I was also very impressed with the



quality of the posters presented at all of the poster sessions. As a graduate student, this meeting was an excellent opportunity to network with other students, post-docs, and principal investigators to learn about the broad spectrum of research that uses structural biology. I am very grateful to the ACA for the travel award which allowed me to take advantage of such a great opportunity.

*Jamie Wallen*

I would like to sincerely thank ACA for funding my travel to the ACA meeting in Salt Lake City and for giving me an opportunity to present my work. As



I would like to thank the ACA for the grant to attend this year's meeting in Salt Lake City. This was my first meeting and I enjoyed the atmosphere of the meeting, as well as Salt Lake City itself. The committee did a fantastic job putting together a meeting with a lot of interesting topics from a variety of areas of research. I particularly enjoyed the sections on "New Structures" and "Structural Mechanisms of Infectious Diseases".

I would also like to thank the organizing committee for allowing me to present a poster. As a graduate student, this afforded me the opportunity to discuss my research with the scientific community. It gave me the opportunity to talk to other graduate students, post-docs, and scientists about their research. I was impressed by the number of great talks and posters. Again, I would like to thank the ACA for making this tremendous experience possible and I look forward to future ACA meetings.

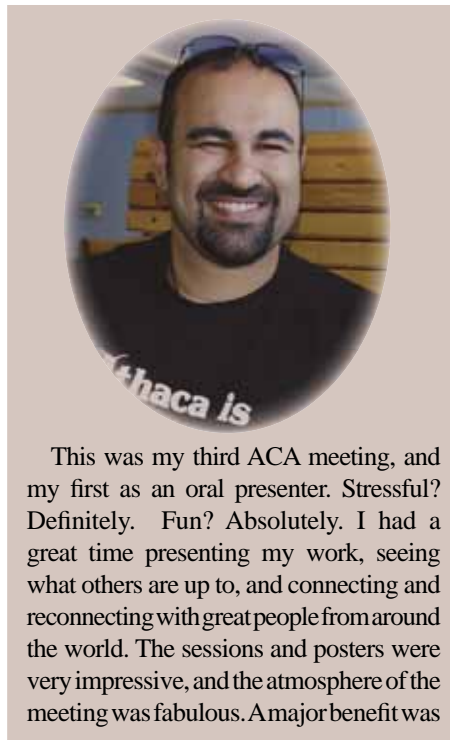
*Timothy Colussi*



this was my first ACA meeting, it was a pleasure to meet people from different parts of the world in person, most of whom I had only known from the literature and bulletin boards of x-ray crystallography. I thank the organizers for putting together an impressive array of sessions on diverse topics. The workshop on *SHELX* and the sessions on "Strategies for Crystallization Challenged Macromolecules", "Large and Difficult Structures", and "Impact of Crystallography in Industry" were particularly interesting and inspiring for me. It was unfortunate that I had to miss some of the talks as they were in concurrent sessions. The young scientist mixer provided an excellent atmosphere to make new connections with other

scientists in a relaxed atmosphere. Overall, the meeting was very informative and enjoyable and I am looking forward to attending the ACA meeting next year.

*Nalam Nadhavi*



the exposure to other trainees to discuss the challenges of a career in science. I must admit, the Salt Lake City area was largely unknown to me before this meeting, but I'll definitely be returning again to take advantage of the great skiing and hiking in the area. Many thanks to the ACA for their generosity.

*Nick Shah*



done in these fields including topics that are less directly related to my research area.

It was very good to talk to several scientists that have experience in areas where I don't, for me to get suggestions for my research. It was also encouraging to see that other people were interested in my research work too.

*Silvina Pagola*



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helped me learn some new approaches, sessions on new structures and impact on industry familiarized me with exciting new opportunities in crystallography. Poster sessions provided an opportunity to meet and interact with numerous people having various backgrounds and interests. It was especially satisfying to see several attendees take a keen interest in my poster and provide valuable feedback. I am thankful to ACA for providing me a travel



grant that made all this possible.

*Satish Singh*

As a PhD student at the lab of Menachem Kaftory (Technion, Israel), my research interests are photochemical reactions carried out in crystalline inclusion compounds. I was invited to give an Etter Lecture in Salt Lake City and am grateful for this opportunity. During the meeting I met many old friends and also made new friends; some showed great interest in my work. The lectures were great. I would like to mention two talks that I enjoyed very much: Larry Falvello on “the Correct Use of Incorrect Space Groups and Unit Cells” and Bruce Foxman on “Solid-state Transformations of Metal Carboxylates”. After my PhD I’m planning to do a post-doc in macromolecular crystallography. At the ACA meeting I was able to hear many lectures on topics that were new to me and will help me “get into the field”. I have been in the USA only twice before this trip (New York and San-Francisco), so it was very exciting to visit again. I found Salt Lake City very interesting, especially the Mormon Temple where I learned many new and interesting things.

*Tali Lavy*



I would like to thank the ACA for funding me to attend the 2007 conference in Salt Lake City. It was a great opportunity to attend

my first crystallography conference. I am also grateful for the chance to talk about my research in the “General Interest” seminar.

I enjoyed the session on “Strategies for Crystallization Challenged Macromolecules” that showed me new techniques and insights for improving protein crystallization. “Informatics in Structural Biology” introduced me to new computational tools for identifying domains and modeling assemblies and functional states.

The “Impact of Crystallography in Industry” lectures taught me about the research and development being done in the industrial sector. It was insightful to learn about the use of crystallography in drug design and in software development for structure determination. I was particularly interested in the lectures during “Fun Lectures for Young Scientists” where the talks gave great introductions to the process of applying for post-doctorate positions, depositing structures to the PDB, and even some history of crystallography.

*Yingsu Tsai*



I would like to thank the ACA for the travel grant that helped me attend this year’s meeting in Salt Lake City. As a newcomer to the discipline of crystallography, it was fascinating to see the variety of projects presented; they provided me with greater insight into the capabilities of x-ray crystallography

as well as an introduction to powder and neutron diffraction, with side trips into drug design, disease mechanisms, and even materials science. I particularly enjoyed the session on radiation damage. Somewhat surprisingly it was both informative and entertaining! It truly was a privilege and a pleasure to witness all of these interesting talks and posters.

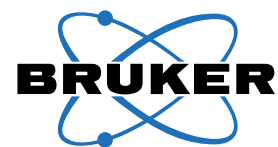
I am also grateful to have been given the opportunity to share my undergraduate project and to have received the AIP award for my presentation. I would like to thank everybody I met – the enthusiasm that people have for their work is infectious, and I hope to see many of you in Knoxville next year.

*Leslie Williams*



The ACA meeting this year was a wonderful learning opportunity and I thoroughly enjoyed the presentations and the socializing at the meeting. The ACA travel award was a great help. Thank you. My favorite session was “Large and Difficult Structures”. The sizes of the structures solved and the challenges associated with their initial phasing are issues which are simply astonishing to imagine. The fun lectures for young scientist series was also very informative and enjoyable. The showcases offered by the many vendors with their latest gadgets were eye-opening, and it made me realize that the technical considerations and challenges associated with these tools will be constantly changing. Lastly, the ACA meeting provided me with the opportunity to see the natural beauties of Utah’s desert landscape and to travel on their scenic routes. I look forward to return to the future meetings that ACA will hold in other places.

*Jimson Wong*



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think forward

Crystallography



The ACA conference was a great opportunity for me to display my research to the scientific community. Through the conference I was able to meet researchers from around the country who were interested in my work and even found a possible collaborator. In addition, the conference was a great experience and I was able to explore some of Salt Lake City's culture and landmarks, as well as meet and interact with other students my age.

*Anubhav Jain*



Flying to Salt Lake City for my first ACA meeting, I was afraid that I would be strangely out of place. Giving a talk about my work using small-angle x-ray scattering in collaboration with an NMR spectroscopist, I felt like the "anti-crystallographer." But this fear was quickly dissipated by the collegial atmosphere of the meeting and by the impressive breadth of the topics covered. Several interesting sessions reported on recent developments and applications of small-angle x-ray and neutron scattering. The small-angle scattering field is developing dynamically due to improvements in instrumentation and algorithms for data analysis and modeling. It was exciting to hear about these developments from the leading researchers in the field. But naturally small-angle scattering was only one of many aspects of the meeting, and I much enjoyed a range of talks about macromolecular structures, computational methods, and bioinformatics. After a memorable awards symposium, I took the plane back to California, now convinced that the ACA meeting has much in store even for the non-crystallographer and I would like to thank the meeting organizers for their invitation and the ACA for supporting me with a travel award.

*Jan Lipfert*

from various parts of the USA. As a young researcher I had the opportunity to present my work and I would like to thank everyone who demonstrated interest in it and for the important comments and suggestions. I came back to Brazil full of new ideas. The meeting allowed me to expand my knowledge of small molecule crystallography and also to enhance my limited knowledge of protein crystallography. Overall, I really enjoyed this meeting. I thank the organizers for their hard work and I hope to meet you again in the near future.

*Janaina Gomes Ferreira*



The Salt Lake City conference, my second ACA meeting, was an enjoyable experience that gave me a lot of inspiration and new ideas I could try with my own work. It was an excellent opportunity to meet fellow crystallographers, many of whom were fellow Canadians. The talks I attended were interesting and diverse. I especially enjoyed the "Young Scientist Sessions", the "Etter Award Symposium" and all the crystallization and phasing technique talks. Some of my favorite highlights of the meeting and of Salt Lake City were: The fireworks and tamales at the YSSIG mixer, Polygamy Porter, the Rigaku Fun Run, the "Sleep by Numbers bed" at the Radisson, Robert Bau's karaoke performance and the 3-D IMAX at the MarUSA event. Finally, I would like to sincerely thank the ACA for the travel grant and for organizing such a great meeting. I'm looking forward to the next one!

*Lyann Sim*

I would like express my thanks to the ACA for their generous support. This was my first ACA meeting and my first time in



I am very grateful for the generous travel grant which allowed me to present my work at this year's ACA Conference. This was my second ACA conference, but it was the first time I was able to present my research there. The feedback and supportive comments from well known scientists and fellow students proved to be invaluable. The many social gatherings, such as the YSIG mixer and mentor mentee dinner, were great opportunities to meet new and interesting people from around the world. Traveling to Utah was also a great experience. It had some great views, especially when seen from the roof of the library. Thank you ACA.

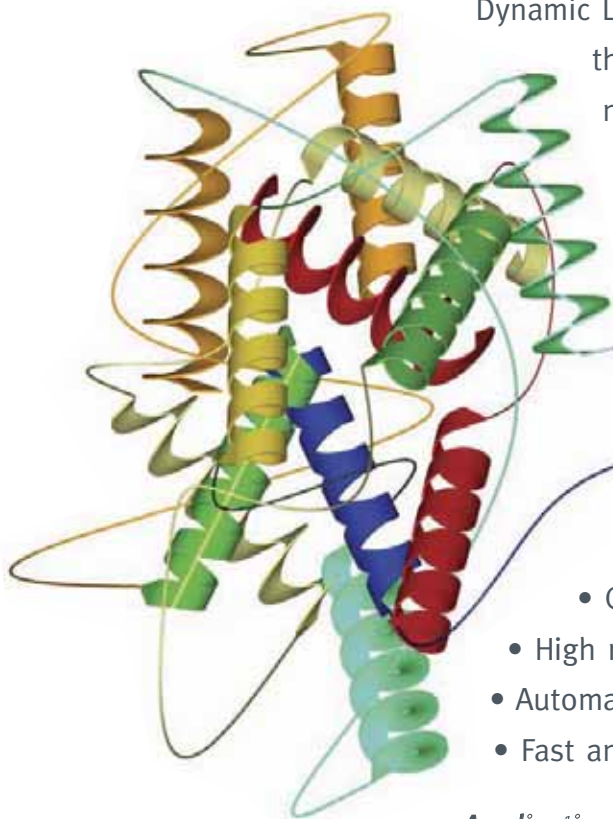
*Bill Bauer*



I would like to thank the ACA for the travel grant that allowed me to attend this important event in Salt Lake City. It was an enriching experience for me. There was a great variety of topics, a high level of research on display, and the possibility to interact with a wide variety of researchers



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Salt Lake City. The workshops were great; I learned a lot. The entire meeting was incredible. I was very happy to meet fellow crystallographers from a variety of backgrounds, and enjoyed talking and discussing science with them. I also had a chance to present my research and got lots of valuable feedback. Salt Lake City is a wonderful place. I enjoyed the beautiful western scenery which is very different from what I see in New England. Many thanks again to the meeting and organizers! I am looking forward to attending the next ACA meeting.

*Hua Li*



I would like to take this opportunity to thank the ACA for the travel award to the 2007 Meeting. I was a little nervous when I arrived but the welcoming atmosphere put me at ease and made asking questions and participating a pleasure. I was especially excited about the technical lectures, as it is rare to have the chance to attend so many interesting talks about cutting-edge technology given by specialists in the field. These lectures allowed me to return to the laboratory with knowledge about recent advances in data collection, different methods used for experimental phasing and novel ideas for the use of nucleants in protein crystallography. My greatest source of motivation, however, was

meeting students from all around the world and seeing their projects and passion for science. The poster session allowed me to make my own contribution to the meeting and share my knowledge of the intricacies of solving a challenging phase problem and obtaining a new crystal form with others. The annual ACA meeting allowed me to grow as a scientist and I would encourage any student to attend it, as they can only benefit. Thank you once again for this wonderful opportunity.

*Magdalena Korczynska*



I am very grateful for obtaining a travel grant to attend the 2007 ACA meeting. It was so exciting to meet so many crystallographers, especially those that have written books or programs that I have used! They are a source of inspiration for me and make me want to continue my studies. It was my first time in the United States and I enjoyed Salt Lake City very much. Hopefully, I will visit other cities in the future since I am considering doing a postdoc in the US. It felt very good to be able to communicate in English, even though I do not speak it very well. I thank the jury of the poster prizes for their patience with me. I certainly hope to be able to attend the next meeting in Knoxville.

*Julia Bruno-Colmenárez*

***This summer Rigaku Corp also awarded travel grants to young scientists doing crystallographic research. Three of their recipients shared their experiences with us.***

My first ACA meeting at Salt Lake City was truly a rewarding experience and I would like to thank Rigaku Corporation for the generous travel award. Overall, the meeting was well planned and the sessions well organized. It was evident from the high quality of the first talk, which was part of the



*SHELX* workshop, that the entire meeting would be very productive. True to the nature of a workshop, all the speakers balanced the theoretical aspects of crystallography with the practical aspects of day-to-day use of the programs in their talks. Being taught about the nuances of the program by the authors themselves, including George Sheldrick, was indeed an experience!

The various sessions of the meeting were organized such that each attendee had the flexibility to attend talks at different, concurrently running sessions. This made it easier for me, as a macromolecular crystallographer, to attend a few particularly interesting small-molecule talks. In particular the sessions that discussed methodology – "Advances in Data Collection", "Strategies for Crystallization Challenged Macromolecules", and "Radiation Damage" – were helpful in thinking about commonly encountered problems in structure solution in novel and unconventional ways. I was also able to discuss aspects of my research with the speakers during the breaks. Being able to do so with experienced crystallographers was the most rewarding aspect of the meeting. In general, the informal nature of the sessions facilitated open discussions during the Q&A sessions.

I would also like to thank B. C. Wang and Manfred Weiss for inviting me to present my sulfur phasing work at the "Phasing with Longer Wavelengths" session. As my first talk at an international meeting, it was an unnerving and yet an exciting experience. The nervousness was in part due to my being a relatively inexperienced speaker sharing the session with experienced scientists. I am very grateful to Zbigniew Dauter for taking the time to discuss my research before the session. This really went a long way towards giving me the confidence for my talk. The questions I was asked about my talk and

the post-session discussions reinforced the single point that is crucial for being a successful scientist – stay curious.

Once again, I would like to thank the ACA for organizing such a wonderful conference and Rigaku Corporation for providing me with financial support to attend.

*Ganapathy Sarma*

receptor was able to recognize a glycolipid in the context of CD1d, whereas there is currently a wealth of information about how a T cell receptor can recognize a peptide in the context of an MHC. This work was recently published in 'Nature'. I would like to thank Rigaku for offsetting some of the cost of the conference.

*Natalie Borg*



I attended the 'XIX International Symposium on Glycoconjugates' in Cairns in July and gave a presentation titled "NKT cell receptor recognition of CD1d presenting glycolipid."

I presented the three-dimensional structure of two immune system molecules in complex with one another. That is, how a T cell receptor in our body (NKT cell receptor) recognizes a glycolipid when it is presented to our immune system via the CD1d molecule. Until this point, we had no molecular snapshot of how a T cell

I was honored to receive Rigaku's travel award for the 2007 ACA meeting. The conference provided a great set of talks for macromolecular crystallographers focusing on membrane proteins, like myself. There were excellent reports on new structures and other fascinating advances in macromolecular crystallography such as a variety of alternate methods. I found the new techniques used to determine the shape and size of the protein detergent complex especially interesting. This topic is one of the most important questions to those working on membrane protein crystallography. The program this year was very beneficial overall and I was excited to leave with information that can be applied to my own research.

I enjoyed catching up with friends and establishing some new professional relationships at the meeting. I also got to experience Pioneer Day, a unique holiday celebrated on the streets of SLC. Experiencing the culture of Utah and enjoying the ACA meeting was memorable to me and I could have not been there without the help of Rigaku's travel award. Thank you to Jim Pflugrath and Rigaku for making this possible.

*Peter Horanyi*

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www.oxford-diffraction.com



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



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



**Select Biosciences Ltd.**  
www.selectbiosciences.com



**Taylor & Francis**  
www.taylorandfrancis.com



**Thermo Fisher Scientific**  
www.thermo.com



**TriTek Corp.**  
www.tritek.com



**Viscotek Corporation**  
www.viscotek.com



**Wyatt Technology**  
www.wyatt.com



**Xenocs SA**  
www.xenocs.com



**Workshops**

**WK.01 Magnetic Structure Analysis by Neutron Diffraction Techniques**

**WK.02 Neutron Macromolecular Crystallography from Expression to Refinement**

**WK.03 Wise Use of Dose: Structure Solvability vs Structure Integrity**

**WK.04 Structural Biology Without Crystals: Small Angle Scattering Methods**

*May 31- June 5, 2007*

*Knoxville Convention Center  
Knoxville, Tennessee*

**Deadlines:**

*Travel Grant Application: December 31, 2007*

*Advance Registration: April 4, 2008*

*Hotel Reservations: April 15, 2007*

*Full Call for Papers online at  
[www.AmerCrystalAssn.org](http://www.AmerCrystalAssn.org)*



*Local Chair*

*Jason Hodges*

*ORNL - Oak Ridge, TN*

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*Program Chairs*

*Paul Butler*

*NIST, Gaithersburg, MD*

*Dean Miles*

*ORNL-Oak Ridge, TN*

*ACA08@ornl.gov*



**Award Symposia**

**Patterson Award in honor of Bi-Cheng Wang**

**Margaret C. Etter Early Career Award in honor of Radu Custelcean**

**Transactions Symposium**

**Complementary Methods**

**Organizers: Carrie Wilmot and Susan Kruger - Sponsored by the BioMac, General Interest, Neutron Scattering, Powder Diffraction, SAS, and Synchrotron SIGs**

*Speakers: James Stivers, Kylie Walters, Oliver Einsle, James Holton, Jill Trehwella, Doug Tobias, Dominique Bourgeois, Leighton Coates, David Worcester, Shuji Akiyama, Joseph Wedekind, Carole Bewley*



**Microsymposia - Organized by SIGS****Biological Macromolecules****New Structures****Structural Enzymology****Systematic Molecular Anatomy, Structural Phylogeny, and Evolution****Computational Crystallography - Nuts and Bolts***Speakers: George Sheldrick, Jane Richardson***How Structures are Used by Others****Engage Your Brain***Speakers: Z. Dauter, A. Wlodawer, C. Carter, C. Deivanayagam, G. Bricogne, K. Rajashankar***Practical Approaches to Improving the Formation and Diffraction-Quality of Protein Crystals****Difficult Structures****Industrial****Challenges in Industrial Crystallography***Speakers: Robert Dinnebier***Neutron****Structure and Dynamics of Hydrogen Bonded Systems****Small Angle Scattering****Understanding the Nano-scale Using Small Angle Scattering****Macromolecular Dynamics***Speakers: D. Bossev, B. Leheny, H. Nanda, K. Wood, M. Rheinstadter***Fiber Diffraction****Fiber Diffraction and Friends (Neutron/X-ray+EM, SAS, etc)****Small Molecules****Cool Structures****Joint Symposia****General Interest I and II****Incommensurate and Modulated Structures****Solid State Transformations and Reactions***Speakers: Larry Falvello, Ilia Guzei, Alexander Briceno***Structural Biology in Neurological Disorders***Speakers: Greg Petsko, Ray Stevens, Eric Gouaux, Gergely Toth***Diffraction Studies of Correlated Electron Systems***Speakers: Andy Christianson, Igor Zaliznyak, Jaime Fernandez***Modern Teaching Tools for the 21st Century***Speakers: Brian Toby, Bernhard Rupp, Reinhard Neder, Katherine Kantardjieff***Molecular Magnets***Speakers: Joel Miller, Roger Willett***Professional Directions****Catalysis Studies using SAXS and High Energy Scattering with PDF***Speakers: T. Egami, K. Chapman, A. Benedetti, B. Weckhuysen, C. Revenant, S. Lee, D. Tiede***Emerging Opportunities for X-ray and Neutron Scattering: New Sources and Techniques****Supramolecular Chemistry: Organic Crystals from Assembly to Function***Speakers: J. Delhomelle, L. Estroff, B. Kahr, M. Peterson, N. Rodriguez, M. Ward, L. Yu***Powder Challenges: Structures Under Nonambient Conditions****Materials for Energy Applications****Microcrystals****Diffuse Scattering Studies of Local Structure in the Solid State**



**Special Event - Tour of the Spallation Neutron Source**

On Sunday evening, June 1st, there will be an Oak Ridge National Laboratory sponsored tour of the Spallation Neutron Source including hors d'oeuvres and refreshments. Pre-registration is required.

The Spallation Neutron Source (SNS) is the first of a new generation of spallation neutron user facilities, exemplifying a significant increase in both neutron production power and instrument technology. Currently ramping up to full power, the SNS is already producing the world's most intense pulsed neutron beams for materials, physics, chemistry and biological research. The SNS is currently building and commissioning a diverse suite of eighteen instruments for diffraction, small-angle scattering, spectroscopy and reflectometry. These complement the scattering instruments at the recently upgraded High Flux Isotope Reactor (HFIR) neutron source. For more information on both the SNS and HFIR neutron user facilities, please visit <http://neutrons.ornl.gov>.

Registration for the tour is open to ACA 2008 attendees and exhibitors only; there is no charge for this event. Charter buses will bring attendees to the SNS and back. An ACA 2008 conference badge will be needed to board the buses. All participants in this special tour will need to bring photo identification in order to have access to ORNL. Unfortunately due to entry restrictions and the amount of time required for approval of visitors from certain countries, we are not able to accept registration from any foreign national who was born in, or is a citizen of, or employed/sponsored by a company in Cuba, Iran, North Korea, Sudan or Syria.



**Registration fees**

Fee	Advance (before April 4)	Late (after April 4)
<b>Regular Member</b>	\$395	\$595
<b>Retired Member</b>	\$161	\$239
<b>Post doc Member</b>	\$200	\$298
<b>Student Member</b>	\$161	\$235
<b>Nonmember*</b>	\$590	\$883
<b>Post doc Nonmember*</b>	\$298	\$444
<b>Student Nonmember*</b>	\$239	\$356
<b>Guest**</b>	\$ 50	\$ 50

<b>WK.01</b>	\$120 (for all)
<b>WK.02</b>	\$100 (60 students)
<b>WK.03</b>	\$110 (60 students)
<b>WK.04</b>	\$110 (70 students)

<b>Mentor/Mentee Dinner</b>	
<b>Mentor</b>	\$30
<b>Mentee</b>	\$20
<b>Award Banquet</b>	\$55 (\$25 students)

\* The nonmember registration fee includes a complimentary membership to the Association for 2008. Those registering as nonmember post docs or nonmember students must include documentation of this status with 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

[www.AmerCrystalAssn.org](http://www.AmerCrystalAssn.org)

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

**Exhibit Show 2008**

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, May 31 in conjunction with the Opening Reception. The 2008 Show will run through Tuesday evening June 3. The exhibit show will be closed on Wednesday June 4th 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 1NO1, 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 \$400 for one booth. Booth rental is \$1,400 for all others.

Register online at [www.AmerCrystalAssn.org](http://www.AmerCrystalAssn.org)

**MARCH 2008****28-29 II International Workshop on**

**Layered Materials: structure and properties**, Univ. of Piemonte Orientale of Vercelli, (Italy). The workshop

will mainly focus on spectroscopic, diffraction and computational methods to describe the structure of layered materials and on physical tools to monitor their properties in order to enlighten the structure-property relationships. [www.layeredmaterials.mfn.unipmn.it](http://www.layeredmaterials.mfn.unipmn.it)

**MAY 2008**

31-June 5 **ACA Annual Meeting ACA 2008**, Knoxville, TN. Local Chair, Jason Hodges. Program Chairs, Paul Butler and Dean Miles.

**JUNE 2008**

30-13 **15th Pan-American Synchrotron Radiation Instrumentation Conference**, Saskatoon, Alberta, CA. [www.lightsource.ca/medsi-sri2008](http://www.lightsource.ca/medsi-sri2008)

**SEPTEMBER 2008**

20-24 **ICSG 2008 International Conference on Structural Genomics**, Oxford, UK, [www.spine2.eu/ISGO](http://www.spine2.eu/ISGO) sponsored by ISGO, the International Structural Genomics Org. [www.isgo.org](http://www.isgo.org)

**AUGUST 2008**

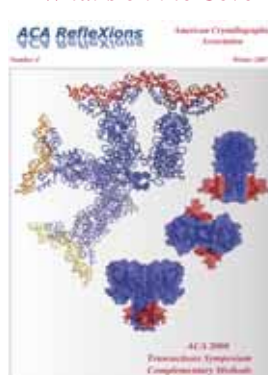
21-28 **IUCr2008: 21st Congress of the International Union of Crystallography**, Osaka, Japan. [congre.co.jp/iucr2008](http://congre.co.jp/iucr2008).

**JUNE 2009**

4-14 **High Pressure Crystallography: From Novel Experimental Approaches to Applications to Cutting Edge**: Erice, Italy. [www.crystalericce.org/2009.htm](http://www.crystalericce.org/2009.htm).

**JULY 2009**

25-30 **ACA Annual Meeting - Toronto, Ontario - Canada Program Chair: Jim Britten (McMaster U., [britten@mcmaster.ca](mailto:britten@mcmaster.ca))**.

**What's on the Cover**

Small-angle scattering and neutron contrast variation from protein complexes in solution complements crystallographic data reveals (upper left) information on the flexibility of a dimeric protein/DNA complex, shown in the crystal form (dark blue) and in the increasingly extended forms observed in solution shown with lighter hues indicating decreasing populations for the most extended forms. Images at lower right show, in three rotated views, the disposition of subunits in a complex of a histidine kinase (blue) complexed with its inhibitor (red) for which the individual component structures are known from crystallography and NMR. Figures courtesy of Jill Trehwella.

**Symposium on Bioinorganic Structural Chemistry and Refinement Workshop**

For over a decade, the Chemistry Department at the Massachusetts Institute of Technology has held an annual symposium dedicated to the cutting edge of chemical crystallography. From the beginning, the meeting was generously sponsored by Bruker-AXS, hence the name "Bruker/MIT Symposium". Originally, this meeting was directed towards chemists and crystallographers from the greater Boston area, but in the last years, the symposium has grown considerably and has drawn participants and speakers from all over the world. The past three symposia were coupled with refinement workshops, contributing to the popularity of the meeting. The 2008 workshop will focus on programs of the SHELX family.

The motto of the 2008 Bruker/MIT Symposium is going to be **X-Ray Crystallography in Bioinorganic Chemistry** and the lineup of speakers for both the workshop and the symposium is going to be great. Among the confirmed speakers are Steven J. Lippard (MIT), one of the pioneers of bioinorganic chemistry, Steven E. Ealick (Cornell) and George M. Sheldrick (University of Göttingen), sole author of the SHELX program suite.

More information about the symposium, as well as an online registration form can be found on the following URL: <http://web.mit.edu/x-ray/bmit08.html>

**Contributors to this issue**

Cele Abad-Zapatero, Jennifer Aitken, Ernest Asani, Bill Bauer, Natalie Borg, Jim Britten, Julia Bruno-Colmenarez, Paul Butler, Timothy Colussi, Bryan Craven, Jose Miguel Delgado, Graciela Diaz de Delgado, Howard Einspahr, Amy Gindhart, Jenny Glusker, Janaina Gomes Ferreira, Lee Groat, Brett Hanson, David Harrison, Jennifer Hobin, Jason Hodges, Peter Horanyi, Anubhav Jain, Christopher Jurgenson, Jim Kaduk, Katherine Kantardjieff, Magdalena Korczynska, Charles Lake, Paul Langan, Tali Lavy, Hau Li, Cora Lind, Jan Lipfert, Dean Miles, Peter Mueller, Nalam Nadhavi, Allen Oliver, Silvina Pagola, Alan Pinkerton, Joe Reibenspies, David Rose, Bernhard Rupp, Ganapathy Sarma, David Schuller, Benjamin Scott, Nick Shah, Brahma Sharma, Jennifer Shepard, Lyann Sim, Satish Singh, Shiho Tanaka, Jill Trehwella, Yingssu Tsai, Bob von Dreele, Jamie Wallen, Leslie Williams, Jimson Wong. Fireworks in Salt Lake City on page 19 by Cora Lind. Spring blossoms in Knoxville on page 20 from [www.nps.gov/grsm/photosmultimedia/index.htm](http://www.nps.gov/grsm/photosmultimedia/index.htm). Photo of SNS provided by ORNL

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