

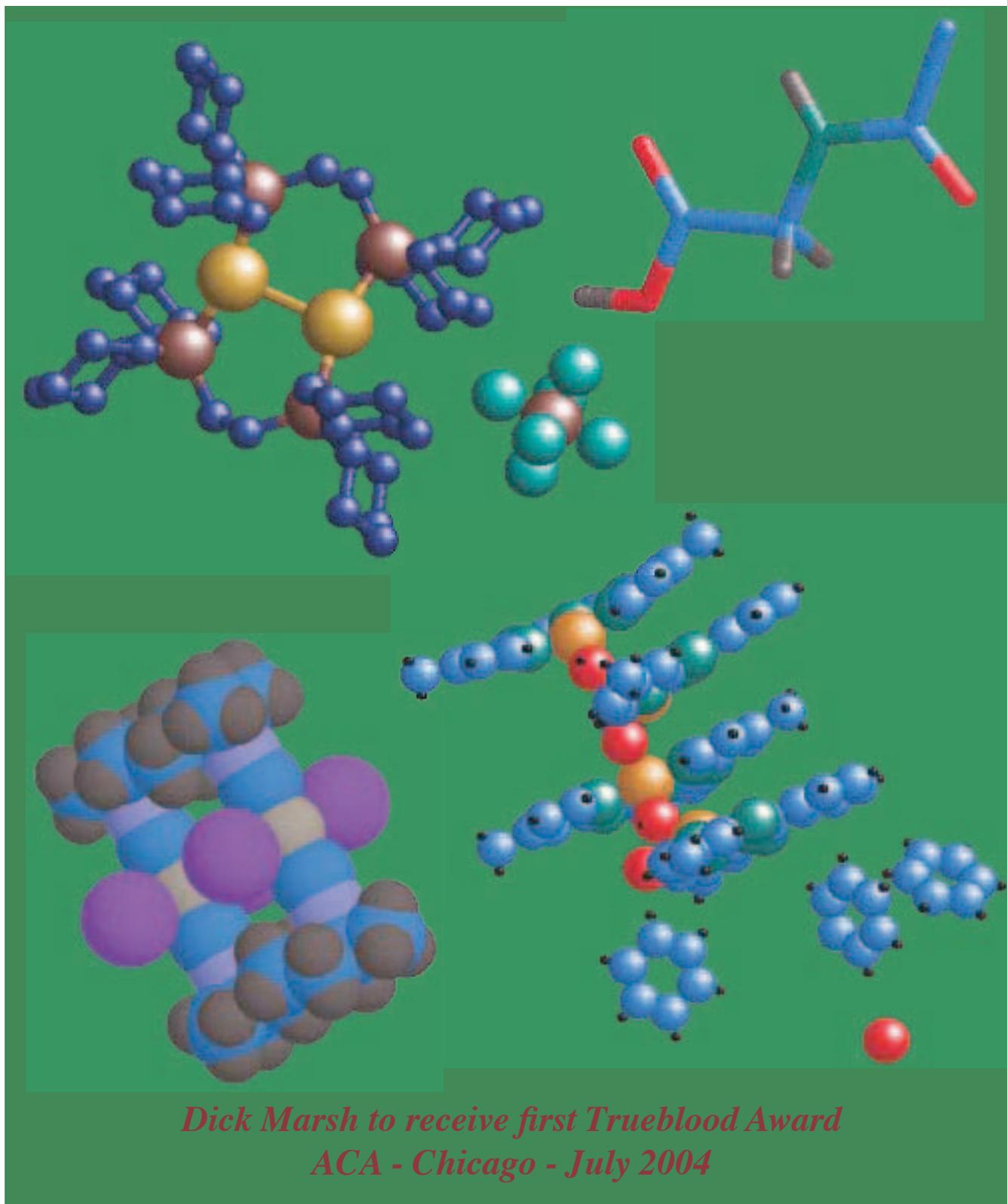


AMERICAN CRYSTALLOGRAPHIC  
ASSOCIATION

# NEWSLETTER

Number 4

Winter 2003



*Dick Marsh to receive first Trueblood Award  
ACA - Chicago - July 2004*

*Inside front cover*

*Diversified*

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**President's Column**

In my first column as ACA President last spring, I remarked on the willingness of ACA members to work on behalf of our science and our organization. I didn't know the half of it! I have been so gratified by the opportunity to see, again and again throughout this past year, the depth of dedication of our mem-

bers and the variety of tasks that they so willingly assume (and often originate!) to make the ACA the vibrant and rewarding association that it is. Despite the risk of omitting individuals or groups deserving our recognition, it is appropriate for me to end these columns as I began them, with words of appreciation for some of the many things done so well by our members for our association.

Our annual meetings continue to grow, not just in numbers of attendees and complexity of arrangements, but also in their central aspect -- the range, quality, and imagination of the science presented. The continually improving scientific vitality at our meetings is due in large part to the increasing roles that the SIGs now play in program planning. Beginning two years ago in Los Angeles, the general structure of the following year's meeting program has been worked out in an intensive session involving the program chairs and representatives from the SIGs. These planning sessions have progressed from a somewhat tentative start in 2001 to an exciting and provocative exchange of ideas at Covington for next year's meeting in Chicago. The enthusiastic and innovative participation of the SIGs is responsible for the success of this mode of meeting planning. A most positive result of this approach is the cooperative organization, by two or more SIGs, of joint sessions that are of interest to a wider variety of our members. Indeed, such cooperative ventures promise to breathe fresh viewpoints, and hence fresh vitality, into the SIG structure itself. Special symposia, especially those built around the interests of major award recipients, continue to be focal points of our meetings, and we are especially appreciative of the extensive efforts of members who organize these symposia. The foresight, the flexibility in the face of shifting program and financial requirements, and the inexhaustible attention to detail of the meeting chairs and their planning committees are critical to continued success of our meetings. Thanks to all those taking part in organizing our annual meetings.

Student participation continues to be an important aspect of the ACA's activities, both at its annual meetings and throughout the

year. I thank the Young Scientists SIG for its increasingly active role, both in encouraging students and other young scientists, and in the more general activities of our association. You will see elsewhere in this *Newsletter* some interesting notes from our student travel awardees about their attendance at the Covington meeting. (This reminds me of the necessity for our prospective meeting attendees from abroad – students and others -- to submit their visa applications as early as possible; six to nine months lead time is recommended.) In the general area of crystallographic education, we are grateful to the many members who worked so hard to put on two very successful ACA Crystallography Summer Schools this year. You can read more about those important efforts elsewhere in this issue.

I have expressed before, and reiterate here, our appreciation to our growing list of corporate members and exhibitors for their continued and varied support of the ACA's activities, both at annual meetings and throughout the year.

We cannot express enough appreciation for the effort that the *Newsletter* Editors voluntarily commit to this important activity. They continue to amaze me with their technical and editorial skills, but even more with the patience and determination they bring to the huge job of collecting the articles, reports, graphics, photos, and calendars that make this a superb newsletter.

Though the ACA (like other organizations and most individuals) is not yet sailing in clear economic waters, our financial position remains cautiously tenable. Many of the most important activities of the ACA are made possible by donations to particular ACA funds (for awards, for student travel, for support of our Latin American initiative). This newsletter contains a long list of donors to ACA funds, and I'm sure you join me in appreciation of the generosity that motivates such contributions.

I give special thanks to Charlie Carter, who is now finishing his term as ACA Past President and three years on the ACA Council, both for his service to ACA and the excellent example he has set for me as an ACA officer. Charlie will continue his service to the ACA as its appointed representative to the American Institute of Physics, while Narasinga Rao, the ACA Financial Officer, has accepted another term on the governing board of the AIP.

Following the recently concluded ACA election, I also welcome the return of two ACA Council members – Doug Ohlendorf, who has been elected to another term as ACA Treasurer, and Louis DelBaere, who has been elected ACA Vice-President. Louis had previously served on the ACA Council as Canadian Representative. Full election results are available elsewhere in this newsletter. Congratulations to the successful candidates, and a special appreciation to all who agreed to stand for election to ACA or SIG offices.

Finally, though I became an ACA student member more than 40 years ago, this past year has given me both a broader and a deeper appreciation of this important, challenging, and supportive organization, but most especially of the people that are the American Crystallographic Association. I thank you for that opportunity.

Ray Davis

## NSF Wants You For Peer Review



Through peer review mechanisms, the NSF Division of Chemistry allocates funds to support basic research and education in the chemical sciences. Doing this

**Arthur Ellis**

effectively requires expert program officers and many volunteers, who serve as

reviewers of proposals. To carry out the peer review process in the most effective way, NSF needs your help

Many more proposals of high quality than can be funded are received from the chemical sciences community. To ensure that the best possible funding recommendations are made, program officers solicit thoughtful reviews from respected members of our community. This process requires substantial service from our community, because the division requests nearly 10,000 reviews a year. Reviewers are called upon to submit timely, constructively critical *ad hoc* reviews that enable principal investigators to enhance the quality of their science. Reviewers are also asked to serve on review panels that may require demanding travel. We thank those of you who have served as reviewers, and we will continue to count on your assistance.

If you have not served as a reviewer and desire to do so, let us know. A qualified reviewer is an established professional who typically possesses a doctorate in chemistry or an allied field. Up-to-date research experience is also required, as it enables the reviewer to provide knowledgeable evaluations of cutting-edge research proposals in his or her particular areas of expertise.

There is no restriction on reviewers based on their employment. Indeed, the breadth of perspectives from scientists in academe, industry, and government laboratories is a great strength of our peer review system. We also welcome participation in the reviewing process by qualified international colleagues. The Division of Chemistry has established a website [www.nst.gov/mps/divisions/che/news/reviewerinfo.htm](http://www.nst.gov/mps/divisions/che/news/reviewerinfo.htm) for prospective reviewers. Please contact us through this website if you would like to review proposals for us.

Once reviews have been obtained, NSF program officers are asked to weigh the responses and to make judicious funding recommendations. Our program officers and support staff are enormously talented and dedicated. About half of the program officers are permanent staff members who provide important institutional perspectives. The other program officers, rotators, will typically spend one to three years with us and help us stay in touch with our community's perspectives.

For the community to have confidence in our decision-making, it is critically important that we continue to attract respected scientists to serve as program officers. NSF offers the kind of stimulating, high-tech environment that would be associated with any outstanding multidisciplinary institution with global reach. Program officers help to launch new areas of research in the chemical sciences and, through mentoring, to contribute to the professional development of principal investigators. Program officers help shape the direction of our chemical research and education enterprise through their service.

Rotators are able to maintain their research programs and pursue funding opportunities during their stay at NSF. NSF provides time, travel, and technology to enable rotators to continue to interact at their home institutions. Rotators who have worked at NSF cite as benefits the opportunities for scientific and professional growth and for establishing new research directions. I urge you to consider providing this important service to your community. See [www.nsf.gov/oirm/hrm/jobs/rotators/start.htm](http://www.nsf.gov/oirm/hrm/jobs/rotators/start.htm) for additional details.

The chemical community plays a critical role in implementing the peer review system. With limited funds, it is more important than ever to make the wisest possible investments in basic research and education. My colleagues and I in the NSF Division of Chemistry hope that you will continue to help us when we call upon you, and we thank you in advance for your assistance.

*Arthur B. Ellis*

*Director, Division of Chemistry, NSF, on detail from the Univ. of Wisconsin, Madison. Views expressed the author's and do not necessarily reflect the views of NSF*

*Reprinted from the March 24, 2003 edition of C&E News with permission from the American Chemical Society.*

## News from Canada



ACA members residing in Canada have an opportunity to make a tax-deductible contribution to be used towards students in Canadian laboratories who attend ACA meetings. In your dues package, there is an insert describing the award. With the cooperation of the Canadian National Committee of the IUCr, funds will be collected under the auspices of the L.D. Calvert Memorial Trust Fund. In order to minimize administrative overhead and the amount of funds needed to get going, we decided to start with a poster award. This could be expanded to travel awards depending on contribution levels. Initially, for the poster award, the judging will 'piggy-back' on the ACA student poster awards (ie the Pauling Prizes). That is, the poster judging committee will have at least one member nominated by the Canadian Division of the ACA, and the highest-ranked poster by that committee by a student from a Canadian laboratory will be awarded the Canadian prize.

In order to fulfill Canadian regulations for such donations, they should not be sent to Buffalo but should be sent to:

### **L.D. Calvert CNC/IUCr Trust Fund**

*c/o Dr. Jean-Pierre Charland, Treasurer CNC/IUCr  
Dept of Nat. Res. Canada, CANMET Energy Tech. Centre  
1, Haanel Drive, Bldg no. 3 Ottawa ON K1A 1M1*

### **CanadaQuirks: Gairdner Awards**

In this item, your correspondent will attempt to clarify Canadian terms, organizations, issues, etc. that might be of interest to the crystallographic community.

The Gairdner Foundation International Awards for Medical Research, often a harbinger of Nobel Prizes, are awarded in Toronto in November of each year, during a two-day symposium featuring major speakers of the highest stature. A number of distinguished structural biologists, including crystallographers, have been honoured in the past, including **Rod MacKinnon** (2001), **Pam Bjorkman** and **Don Wiley** (1994), and **Michael Rossmann** (1987). One of this years awardees was **Wayne Hendrickson**, for contributions to the development of macromolecular crystallography, including the MAD phasing technique, as well as for the structures of several molecules of medical importance. Another feature of the presentation is that some awardees travel across the country, lecturing in a number of major centers. For more information, see [www.gairdner.org](http://www.gairdner.org).

*David Rose*

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## Crystallography Web Watch

A number of people have written in with their favorite web sites. Here are some of them. Thanks to all those who have contributed!

Members of AAAS have free access to a number of web sites of interest. For instance, [[www.sageke.org](http://www.sageke.org)], the Science of AGing Knowledge Environment web site, has a resource link to teaching resources, grant information and web links to related sites. This web site features a wide variety of topics including information on Alzheimer's disease and anti-oxidants.

The web site for the Expert Protein Analysis System proteomics server of the Swiss Institute of Bioinformatics [[us.expasy.org](http://us.expasy.org)] has links to databases and tools for analysis, such as similarity searches, pattern and profile searches and sequence alignment. It also has some links to molecular biology resources.

Now you can calculate most anything you have wondered about! The Calculator On-Line Center, [[www.martindalecenter.com/Calculators3.html](http://www.martindalecenter.com/Calculators3.html)] claims to contain over 17,835 calculators. These calculators encompass more kinds of things than you can imagine – orientation of insects in pheromone plumes as well as the acid-base titrations, wine-making calculations as well as molecular biology protocols.

Two interesting interactive sites are SuMo [[sumo-pbil.ibcp.fr](http://sumo-pbil.ibcp.fr)] from the IBCP in Lyon, France that lets you screen the Protein Data Bank (PDB) finding ligand binding sites matching your structure. Another is PSQ [[pqs.ebi.ac.uk/pqs-quick.html](http://pqs.ebi.ac.uk/pqs-quick.html)] from EMBL/MSDB which looks for likely quaternary states for structures.

[www.structure.llnl.gov/mattprob/](http://www.structure.llnl.gov/mattprob/) is a very handy web-based Matthew's Probability Calculator. It is very convenient and has a nice graphical interface.

[www.ProteinCrystallography.com](http://www.ProteinCrystallography.com) is the new information portal for structural genomics and protein structure technologies. Featuring dedicated company, event, and new product news, it aims to keep researchers and business leaders up to date on what's happening in this important sector. A detailed company index makes finding special products and services easy. For reference, there are links to research centers, relevant journals, books, papers and reviews.

Crystallography resource — A nice resource page for x-ray crystallography can be found at the Department of Earth and Planetary Sciences at the University of New Mexico: [[epswww.unm.edu/xrd/resources.htm](http://epswww.unm.edu/xrd/resources.htm)]. Other useful crystallographic links can be found at [[link.bubl.ac.uk/crystallography/](http://link.bubl.ac.uk/crystallography/)] and at the Biomolecular Structure Center/University of Washington School of Medicine: [www.bmsc.washington.edu](http://www.bmsc.washington.edu)

Peter Mueller mentioned a number of tutorials in his presentation at the ACA meeting two of which are by Kevin Cowtan; *Fourier cat and duck* and *structure factor tutorial* [www.yorvic.york.ac.uk/~cowtan](http://www.yorvic.york.ac.uk/~cowtan). We have previously mentioned the many tutorials by Mike Sawayas [[www.doembi.ucla.edu/~sawaya/tutorials/tutorials.html](http://www.doembi.ucla.edu/~sawaya/tutorials/tutorials.html)] and by Bernhard Rupp [[www.structure.llnl.gov/Xray/101index.html](http://www.structure.llnl.gov/Xray/101index.html)].

The SHELX website [[shelx.uni-ac.gwdg.de/SHELX](http://shelx.uni-ac.gwdg.de/SHELX)] contains a number excellent tutorials including Thomas Schneider's high-resolution protein refinement tutorial, Regine Herbst-Irmer's tutorial about twinning, and Peter's own tutorial about the refinement of disorder with SHELXL.

Have a favorite site you would like to see in a future column (and maybe linked on the ACA web site)? If so, send the web address and a short (1 or 2 sentence) description to **John Sack** ([john.sack@bms.com](mailto:john.sack@bms.com)).

John Sack, Jeanette Bauer, Kay Onan  
and Louis DelBaere

## Concept Clearance of the PSI-2 Production Phase

Plans for the next phase of the NIGMS Protein Structure Initiative (PSI) were announced at the recent NIGMS Council meeting ([www.nigms.nih.gov/news/reports/council-psi-sept03.html](http://www.nigms.nih.gov/news/reports/council-psi-sept03.html)).



This phase will begin in 2005 with the grant announcement expected for early 2004. It is envisioned as an interacting network with large-scale research centers that will operate

as high throughput structural genomics pipelines for protein production and structure determination. The plans approved by the Council also include the establishment of specialized research centers for development of new methods, technology, and approaches for the production and structure determination of especially challenging proteins, such as membrane proteins and proteins from humans and other higher eukaryotic organisms, as well as for projects to address technology barriers to high-throughput operation.

Since 2000, the NIGMS has funded nine pilot structural genomics research centers as part of its plan to reduce the costs and increase the success of the structural determination of proteins. The long-range goal of the PSI is to make the three-dimensional atomic-level structures of most proteins easily obtainable from knowledge of their corresponding DNA sequences. The pilot projects have focused on high throughput methods for structure determination in order to achieve these goals. [www.nigms.nih.gov/psi](http://www.nigms.nih.gov/psi)

## Structural Biology Roadmap RFA

Structural biology is also prominent in the plans of the NIH Roadmap for Medical Research ([nihroadmap.nih.gov/structuralbiology/index.asp](http://nihroadmap.nih.gov/structuralbiology/index.asp)). The roadmap includes an RFA (request for applications) for Centers for Innovation in Membrane Protein Production. Letters of intent are due by February 5, 2004 with applications due by March 11, 2004.

## NSF Custom News Services

In order to receive NSF program announcements, vacancy announcements newsletters or other information as soon as they are published, you can subscribe to the NSF Custom News Services. You pre-select as many key words as you like; every time an NSF document containing one or more of your key words is published, you'll receive email notification with a link to the appropriate web page. For further information, please visit the Custom News Service website: [www.nsf.gov/home/cns/](http://www.nsf.gov/home/cns/)

*Inside*  
*Wyatt - right side*



In recognition of the growing international and interdisciplinary nature of structural biology, three organizations have formed a collaboration to oversee the newly formed worldwide Protein Data Bank (wwPDB; <http://www.wwpdb.org/>). The Research Collaboratory for Structural Bioinformatics (RCSB), the Macromolecular Structure Database (MSD) at the European Bioinformatics Institute (EBI) and the Protein Data Bank Japan (PDBj) at the Institute for Protein Research in Osaka University will serve as custodians of the wwPDB, with the goal of maintaining a single archive of macromolecular structural data that is freely and publicly available to the global community.

The wwPDB represents a milestone in the evolution of the Protein Data Bank (PDB; <http://www.pdb.org/>)<sup>1,2</sup>, which was established in 1971 at Brookhaven National Laboratory as the sole international repository for three-dimensional structure data of biological macromolecules. Since July 1, 1999, the PDB has been managed by three member institutions of the RCSB: Rutgers, The State University of New Jersey; the San Diego Supercomputer Center at the University of California, San Diego; and the Center for Advanced Research in Biotechnology of the National Institute of Standards and Technology.

The wwPDB recognizes the importance of providing equal access to the database—both in terms of depositing and retrieving data—from different regions of the world. Therefore, the wwPDB members will continue to serve as deposition, data processing, and distribution sites. Deposition procedures will not be altered by the formation of the wwPDB; data can still be deposited using ADIT at the RCSB and PDBj or by using AutoDep at the EBI.

To ensure the consistency of PDB data, all entries will be validated and annotated following a common set of criteria. All processed data will be sent to the RCSB, which distributes the data worldwide. All format documentation will be kept publicly available and the distribution sites will mirror the PDB archive using identical contents and subdirectory structure. However, each member of the wwPDB will be able to develop its own web site, with a unique view of the primary data, providing a variety of tools and resources for the global community.

An Advisory Board consisting of appointees from the wwPDB, the International Union of Crystallography and the International Council on Magnetic Resonance in Biological Systems will provide guidance through annual meetings with the wwPDB consortium. This board is responsible for reviewing and determining policy as well as providing a forum for resolving issues related to the wwPDB. Specific details about the Advisory Board can be found in the wwPDB charter, available on the wwPDB web site.

The RCSB is the 'archive keeper' of wwPDB. It has sole write access to the PDB archive and control over directory

structure and contents, as well as responsibility for distributing new PDB identifiers to all deposition sites. The PDB archive is a collection of flat files in the legacy PDB file format<sup>3</sup> and in the mmCIF<sup>4</sup> format that follows the PDB exchange dictionary (<http://deposit.pdb.org/mmCIF/>). This dictionary describes the syntax and semantics of PDB data that are processed and exchanged during the process of data annotation. It was designed to provide consistency in data produced in structure laboratories, processed by the wwPDB members and used in bioinformatics applications. The PDB archive does not include the web sites, browsers, software and database query engines developed by researchers worldwide.

The members of the wwPDB will jointly agree to any modifications or extensions to the PDB exchange dictionary. As data technology progresses, other data formats (such as XML) and delivery methods may be included in the official PDB archive if all the wwPDB members concur on the alteration. Any new formats will follow the naming and description conventions of the PDB exchange dictionary. In addition, the legacy PDB format would not be modified unless there is a compelling reason for a change. Should such a situation occur, all three wwPDB members would have to agree on the changes and give the structural biology community 90 days advance notice.

The creation of the wwPDB formalizes the international character of the PDB and ensures that the archive remains single and uniform. It provides a mechanism to ensure consistent data for software developers and users worldwide. We hope that this will encourage individual creativity in developing tools for presenting structural data, which could benefit the scientific research community in general.

**Acknowledgments:** The RCSB PDB is supported by funds from the National Science Foundation, the Department of Energy, and the National Institutes of Health. The MSD-EBI is supported by funds from the Wellcome Trust, the European Union (TEMBLOR, NMRQUAL, SPINE, AUTOSTRUCT, and IIMS awards), CCP4, the Biotechnology and Biological Sciences Research Council (UK), the Medical Research Council (UK), and the European Molecular Biology Laboratory. PDBj is supported by grant-in-aid from the Institute for Bioinformatics Research and Development, Japan Science and Technology Corporation (BIRD-JST), and the Ministry of Education, Culture, Sports, Science and Technology (MEXT).

*Helen Berman<sup>1</sup>, Kim Henrick<sup>2</sup> & Haruki Nakamura<sup>3</sup>*

<sup>1</sup>RCSB, Piscataway New Jersey, Rockville Maryland, and La Jolla California, USA. <sup>2</sup>MSD-EBI, Hinxton, UK. <sup>3</sup>PDBj, Institute for Protein Research, Osaka University, Osaka, Japan.

**References :** 1. Berman, H.M. *et al. Nucleic Acids Res.* **28**, 235–242 (2000). 2. Bernstein, F.C. *et al. J. Mol. Biol.* **112**, 535–542 (1977). 3. Callaway, J. *et al. Protein Data Bank Contents Guide: Atomic coordinate entry format description.* (Brookhaven National Laboratory, 1996). 4. Bourne, P.E., Berman, H.M., Watenpugh, K., Westbrook, J.D. & Fitzgerald, P.M.D. *Methods Enzymol.* **277**, 571–590 (1997).

*Reprinted with permission from Nature Structure Biology (2003) 10, 980.*

*Inside*

*Bruker 1*

## PDB Poster Prize

This summer, the inaugural PDB Poster Prize was awarded at each of the meetings of the IUCr Regional Associates--the American Crystallographic Association (ACA), the Asian Crystallographic Association (AsCA), and the European Crystallographic Association (ECM). This poster prize was designed to recognize the best student poster presentations involving macromolecular crystallography.



ACA: The first-ever PDB Poster Prize was awarded at the ACA meeting to **Ty Gould** (Univ. of Colorado Health Sciences Center,

Denver- on the left in the photo). The competition was so tight that a runner-up award went to **Paul Hubbard** (Medical College of Wisconsin, Milwaukee). See page 15 in the Fall 2003 ACA Newsletter for more details



ASCA: **Janet Dean** won the prize for her poster "Crystal structure of a complex of FLINC4, an intramolecular LMO4:LDB1 complex" (Janet E. Deane, Megan Maher, J. Mitchell Guss, and Jacqueline M. Matthews, School of Molecular and Microbial Biosciences, University of Sydney).



ECM: The poster "Structural Studies of the Enzymes of Pantothenate Synthesis" won the award for **Carina Lobley** (Carina Lobley<sup>1</sup>, Mairi Kilkenny<sup>1</sup>, Florian Schmitzberger<sup>1</sup>, Michael Webb<sup>2</sup>, Chris Abell<sup>2</sup>, Alison Smith<sup>3,1</sup>, and Tom Blundell<sup>1</sup>; 1. Department of Biochemistry, Cambridge; 2. University Chemical Laboratory, Cambridge; 3. Department of Plant Sciences, Cambridge).

This year, the award consisted of two educational books -- signed copies of *Biochemistry - Vol. 1* by Donald and Judith G. Voet and *Introduction to Macromolecular Crystallography* by Alexander McPherson.

Special thanks to all of the PDB Poster Prize Committee members and organizers -- Vivien Yee, Victor Young, Tom Koetzle, Sylvie Doublet, Marvin L. Hackert, and Jeanette Krause Bauer at ACA; Ted Baker, Peter Colman, Janet Smith, Mark Spackman, Colin Raston, and Yu Wang at AsCA, and G. Davies, C. Kenyon, E.F. Garman, and A. Roodt at ECM.

The PDB Poster Prize contest will resume in 2004 - further details will be announced in the PDB web site news.

Christine Zardecki

## Mini Book Reviews

*Landing Your First Job - A Guide for Physics Students* is an AIP publication written by John Rigden. It is designed exclusively to assist students who are preparing for their first job. This publication will help assess skills and interests and identify ways to look attractive to prospective employers. It contains advice on writing cover letters and resumes, interview preparation, salary negotiation, information on job hunting resources, networking and employment statistics. The regular price is \$19.95. ACA Members can buy it for \$15.96 (20% discount). ACA Members must mention code 187499 to receive the 20% discount.

*Underneath the Bragg Peaks Structural Analysis of Complex Materials* (Pergamon Materials Series, V. 7) by Takeshi Egami, and S. J. L. Billinge, Hardcover: 650 pages, Elsevier Science Ltd; (January 2004), ISBN: 0080426980. Editorial review (from the publishers site): This book focuses on the structural determination of crystalline solids with extensive disorder. Well-established methods exist for characterizing the structure of fully crystalline solids or fully disordered materials such as liquids and glasses, but there is a dearth of techniques for the cases in-between, crystalline solids with internal atomic and nanometer scale disorder. Egami and Billinge discuss how to fill the gap using modern tools of structural characterization. While this subject might sound rather narrow, the fact is that today this problem is encountered in the structural characterization of a surprisingly wide range of complex materials of interest to modern technology and is becoming increasingly important.

*Last Sorcerers: The Path from Alchemy to the Periodic Table* by Richard Morris, Hardcover: 224 pages, Joseph Henry Press; (November 2003), ISBN: 0309089050 Editorial review From *Publishers Weekly*: Though the stories in this volume have been told before in other books, Morris manages to make the history of the periodic table's conception fresh and quirky one more time. He does this by focusing his narrative on early alchemists, who were among the first to investigate the composition of metals and who were widely perceived to be practitioners of mysterious arts. Bernard of Treves, for one, squandered his life and money questing for the secret that would turn ordinary metals into gold. Another alchemist, Paracelsus, was the first to use the word "chemistry," though his egomania and devotion to truth earned him nothing but trouble. Hennig Brandt collected buckets of human urine trying to make gold but ended up producing phosphorus. In Morris's account, even Robert Boyle, "generally considered to be the founder of modern chemistry," was an alchemist. It wasn't until the 18th century, Morris writes, that "alchemy was supposedly superseded by chemistry." Thus the more familiar legends of chemistry, featuring scientists like Davy, Priestly and Lavoisier-appear later in this volume, which recounts the formation of our basic ideas about chemical compounds, elements and molecules. Dimitri Mendeleev, the organizer of the periodic table, gets special treatment. Morris finishes up this delightful tale of science history by sweeping through the 20th century chemists whose discoveries were beyond the wildest imaginings of the ancient Greeks, but who still couldn't make gold from lead. Copyright 2003 Reed Business Information, Inc.

***Napoleon's Buttons: How 17 Molecules Changed History*** by Penny Le Couteur and Jay Burreson, Hardcover: 384 pp, J. P. Tarcher; (April 24, 2003), ISBN: 1585422207, Editorial Review from *Booklist*: Women who use birth control pills probably care more about their effectiveness than about how they actually work, and although ignorance here may be bliss, it also cheats one of a good science story, involving a driven chemist making a serendipitous discovery about cortisone. Le Couteur and Burreson roll out 17 episodes selected for their salience in affecting health as well as history at large. This pair of chemists doesn't overinterpret a particular chemical as a historical influence but makes speculating on, say, piperene, a sporting diversion. Piperine is the molecule that causes taste buds to sting from pepper. Venice had a monopoly on the pepper trade, which rivals wished to break, motivating the voyages of discovery. Although connections frame the authors' tales (the title refers to tin buttons, which contributed to Napoleon's defeat in Russia), each story dwells on its molecular protagonist. The authors diagram the formula and shape of each, from the polymer behind the sheen in silk to the ionic bonds in the taste of salt. Well-conceived, well-done popular science. Gilbert Taylor Copyright (c) American Library Association. All rights reserved.

***The Pathological Protein: Mad Cow, Chronic Wasting and Other Deadly Prion Diseases*** by Philip Yam, Hardcover: 304 pages, Copernicus Books; (June 2003), ISBN: 0387955089, Book Description from *amazon.com*: In 1996, British doctors were horrified to discover that mad cow disease (BSE), an affliction that had been plaguing British cattle for ten years, had jumped the species barrier and was appearing in humans as variant Creutzfeldt-Jakob disease (vCJD). Not unlike the mad cows, victims of vCJD suffer from a degenerative neurological disease that peppers the brain with microscopic holes, causing dementia, loss of motor control, and certain death. What alarms researchers and public health officials worldwide is that the incubation period for vCJD may be as long as 10 or even 15 years, and during this period those infected are symptom-free. And because the disease is so far undetectable except by autopsy, there is no way of knowing with certainty how many people have already been infected. In fact, even travelers who spent time in the U.K. from the early 1980s through the mid-1990s are still considered to be at some risk. What's more, although the U.S. has not detected any mad cows within its borders, there are plenty of "mad deer" running free in several states, and the disease afflicting them is a BSE-type neurological disorder. Called chronic wasting disease (CWD), the illness in these deer has yet to be linked with any human deaths. But given BSE's ability to jump species, there are no guarantees.

In *The Pathological Protein*, Philip Yam describes how, in this atmosphere of uncertainty, scientists have discovered that the agent of disease in vCJD and a host of other devastating neurological disorders is a bizarre, misshapen version of a protein called a prion. Once introduced into the human neurological system, malformed prions recruit the body's own normal prion proteins, giving them the same pathological ability to destroy brain tissue. Unlike the better-known pathogens that afflict humans -- bacteria, viruses, and parasites -- prions have so far proved resistant to drug

therapies and even standard sterilization. No amount of cooking infected meat will prove effective against them.

In a medical detective story with an undercurrent of urgency, Yam describes how the mysterious prion was discovered, how it has been linked to a number of exotic and poorly understood illnesses, and how likely it is that scientists will soon find effective tools for controlling its spread, diagnosing its presence, and treating the devastating disorders it causes.

***Molecular Modeling: Basic Principles and Applications*** by Hans-Dieter Holtje, Gerd Folkers, Wolfgang Sippl, Didier Rognan, Paperback - Second Edition, September 2003, 228 pp John Wiley & Sons, Incorporated, ISBN: 3527305890. Editorial review from the publisher: Written by experienced experts in molecular modeling, this book describes the basics to the extent that is necessary to reliably judge the results from molecular modeling calculations.

Without unnecessary overhead it leads the reader from simple calculations on small molecules to the modeling of proteins and other relevant biomolecules. The beginner is guided through the first modeling experiment, and the routine user of modeling software is provided with invaluable troubleshooting hints. A unique resource for students, researchers and lecturers, now available in an all-new and enlarged edition.

***The National Institute of General Medical Services of the NIH*** publishes several educational booklets that can be downloaded in pdf format at [www.nigms.nih.gov/news/sciend\\_ed/](http://www.nigms.nih.gov/news/sciend_ed/). Print copies may also be at [www.nigms.nih.gov/news/publist.html](http://www.nigms.nih.gov/news/publist.html). Some of the booklets available are: "***The Structures of Life***"



geared toward an advanced high school or early college-level audience, explains how structural biology provides insight into health and disease and is useful in creating new medications. The booklet also features "Student Snapshots" designed to inspire young people to consider careers in biomedical research. "***The Chemistry of Health***"

describes how basic chemistry and biochemistry research can spur a better understanding of human health. The publication highlights the research of a number of chemists and includes questions at the end of each chapter, "***Medicines by Design***"



describes how drugs work in the body, and presents some of the latest research developments in the field. "***Genes and Population***" explains in question-and-answer format why genetics researchers sometimes study identified populations to identify links between genes and diseases. (Also available in Spanish, "***Genes y Poblaciones.***") and "***Genetic Basics***"

includes descriptions of how genes work, "strange but true" exceptions to the traditional rules of genetics, why basic research is important and worthwhile, some of the connections between genes and diseases, and the excitement of genetics research in the 21st century.

*Inside*

*Rigaku/MSD 1*

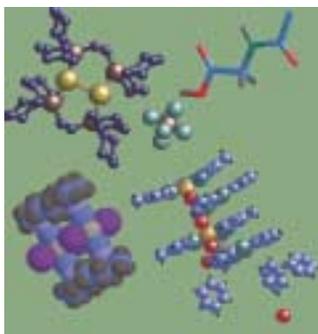
**Rigaku/MSK, Inc. and HKL Research, Inc. Announce Development & Distribution Partnership for HKL-2000 X-ray Diffraction Data Analysis Software**

Rigaku/MSK, Inc has announced a worldwide development and distribution partnership with HKL Research, Inc. to provide optimized and enhanced HKL-2000 software for data processing with Rigaku products. Available with all Rigaku/MSK detectors, the HKL-2000 software package provides crystallographers with several important benefits related to: strategy and simulation, 3-D processing, mosaicity refinement during processing, as well as variable spot size. Due to its 3-D processing strategy, HKL-2000 can handle data from crystals with high mosaicity, which can be of critical concern in macromolecular (protein) crystallography.

**Rigaku/MSK, Inc. and RoboDesign® International, Inc. Announce Distribution Partnership for CrystalMation**

Rigaku/MSK, Inc. announced they have entered into a worldwide marketing partnership with RoboDesign International, Inc. to distribute RoboDesign's CrystalMation line of products for protein crystallography research. CrystalMation is an ever-expanding line of modular products focused on addressing the needs of protein crystal analysis. Each facet of the process: plate handling, image collection, image storage and analysis, crystallization data collection and analysis, is now part of a seamless process. At the core of the system is the RoboMicroscope™ II, an ultra-high resolution imaging system that can quickly and consistently image "hanging," "sitting," or "micro-batch" drops in all plate types.

**What's on the cover**



The cover features molecules solved by Dick Marsh and his collaborators. They were selected from molecules that came up from a search of the Cambridge Data Base (April 2003 release with 3 updates). A search using R.E. Marsh turned up 162 hits. Included the text 're-interpretation' with the search increased the number of hits to 754. Coordinates were retrieved for the molecules selected by editor (based solely on what she thought would make 'pretty pictures'). The illustrations were prepared using RasMol v2.6 (for Macintosh) by Roger Sayle, BioMolecular Structures Group, Glaxo Research & Development, Greenford, Middlesex, UK, June 1994.

The editor would also like to acknowledge Bohdan Schneider who provided a critical mini-tutorial in the use RasMol for small molecules. The molecules featured are:

**upper left:** SONGOR - Bis( $\mu_2$ -1-2-bis(Dicyclohexylphosphine)ethane, P,P')-gold(bis(hexafluorophosphate) W. P. Schaefer, R. E. Marsh, T. M. McCleskey, and H. B. Gray (1991) *Acta Cryst.*, **C47**, 2553,

**upper right:** ACYGLY - Nacetyl glycine J. Donahue and R. E. Marsh (1962) *Acta Cryst* **15**, 941

**Lower left:** COLVOO - Bis( $\mu_2$ -1-8-Di-isocyano-p-methane-C,C')tetraiodo-di-palladium (ii) Chi-Ming Che, F.H. Herbstein, W. P. Schaefer, R. E. Marsh and H. B. Gray (1984) *Inorg. Chem.* **23**, 2572.

**Lower right:** HXCIUM - Tris( $\mu_2$ -Hydroxo) (tris(1-3-bis(2-(4-methylpyridyl)-imino)-isoindolinato)(1-(2-(4-methylpyridyl-6-olato)-isoindolinato)))tetra-copper(ii) benzene solvate monohydrate R. R. Gagne, R. S. Gall, G. C. Lisensky, R. E. Marsh and L. M, Spetz (1979) *Inorg. Chem.*, **18**, 771.

**Dick Marsh - 1st Ken Trueblood Award**

In recognition of his exceptional achievement in computational and chemical crystallography, **Richard E. Marsh** is the selected as the inaugural recipient of the **Kenneth N. Trueblood Award**. The following is a slightly amended version of the nomination that was submitted by two ACA members.

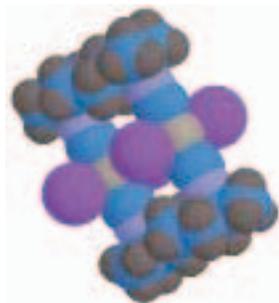


Dick Marsh has been one of the most important contributors to the field of crystallography during his long professional career, dating back to his first publication with J. D. McCullough in 1950. His work has included numerous publications with Linus Pauling, collaborations and publications with Verner Schomaker, David Shoemaker, Dave Duchamp, Wally Cordes, Jenny Glusker, Bill Schaefer and many others. His emphasis on the proper choice of space groups, as well as the need to pay attention to symmetry in the crystallography process, is legendary.

Richard E. Marsh was born in Jackson, Michigan in 1922. He obtained a B.S. in Applied Chemistry at the California Institute of Technology in 1943.

After brief service in the U.S. Navy, he completed a Ph.D. degree at UCLA with J. D. McCullough in 1950. Dick then accepted a position at Caltech as a Research Fellow in 1950 where he has been ever since. He is currently an active Senior Research Associate, Emeritus.

Dick has been a major force in the development of the small molecule x-ray crystallography laboratory at Caltech and a major contributor to crystallographic research there. His work ranged from studies with Linus Pauling on small amino acids, hydrogen bonding and protein structure, to other diverse, challenging problems such as the structures of complex alloys, for example NaPb and NaZn<sub>13</sub>. In the early 1960's he helped to develop and write the crystallographic suite of programs, CRYRM (CRYM), based on a least-squares refinement against F<sup>2</sup> that is still in use at Caltech today. He has been a major contributor to the small molecule structural program for understanding protein structure. He designed and taught the x-ray crystallography course at Caltech for many years where his lecture material and problem sets are still the basis for the crystallography course taught there today.



Dick has been an active member of the American Crystallographic Association for many years, contributing much to the operation and stature of the association. He was elected president of the ACA in 1993. He has been a member of subcommittees of the ACA and of the IUCr, and has lectured at the ACA Summer School. Dick continues to serve and support the

activities of the association. Dick has authored or coauthored over 275 publications, of which 175 have been in *Acta Cryst.* He has reviewed books, coauthored the obituary for Arthur Lindo Patterson, and continues to review manuscripts, critique journal articles, and in general be a friendly and objective voice stressing that all researchers pay careful attention to the features that make the "art" of crystallography a wonderful endeavor.

Dick's reputation for a keen and profound understanding of chemical crystallography coupled with his attention to detail has earned him a special recognition: chemists and crystallographers have honored him with an eponym. Being "marshed" means that errors have been found in publications due to an improper choice of space group and the lack of attention to inherent crystal symmetry, bond distance anomalies or unusual ADP's, or other details. Many of us doing crystallography today pay more careful attention to symmetry and the proper choice of space groups and to the "correctness" of our structures because of the influence of Dick and his insistence that we all do good science.

Dick Marsh, like Ken Trueblood, has been an outstanding teacher, researcher and an exemplary crystallographer to all those who have learned crystallography the easier way by using CCD detectors to measure intensities, PC's and sophisticated software to process and solve structures, and graphics to display complex, three-dimensional structures. It is safe to say there are relatively few crystallographers today who have the ability to see spatial or

symmetry relationships just by looking at a list of fractional cell coordinates, or who could model complex, disordered solvent molecules from Fourier sections or who indeed, could predict heavy atom positions from an oscillation photograph or from a list of unit cell intensities. Dick Marsh is a rare individual among crystallographers, an outstanding teacher and researcher who has greatly influenced so many students and faculty, as did Ken Trueblood during his 50 year career.

Jenny P. Glusker, Chair Award Selection Committee

## Madeline Jacobs - 2004 ACA Public Service Award

The ACA Public Service Award recognizes a non-crystallographer for contributions to science policy, to science funding, or to communication of crystallography to the general public. It is awarded on an irregular basis at the discretion of the ACA Council. Past winners are **Purnell Choppin**, President Emeritus of the Howard Hughes Medical Institute (2000); **Senator George Brown** (CA) in recognition of his efforts to protect the environment and his strong support of government funding for scientific research (1998); **Mike McCormack**: in recognition of his leadership and expertise in science and energy while a member of the U.S. Congress and for his continued efforts in support of science and the scientific community (1989); **William Nelson**: Support of funding fundamental science in particular, crystal growth experiments aboard space shuttles (1988).

At the 2004 ACA Meeting in Chicago the Public Service



Award will be presented to **Madeline Jacobs**, currently the director of the of Chemical and Engineering News magazine group of the American Chemical Society (ACS). The Chemical & Engineering News Magazine Group is a newly formed unit

that consists of *Chemical & Engineering News* (weekly, circulation 161,000), *Today's Chemist at Work* (monthly, circulation 96,000), *Modern Drug Discovery* (monthly, circulation 40,000), and the Production & Imaging Group that provides composition

and imaging support to the three magazines and to all ACS journals. When she became managing editor of *Chemical & Engineering News* she was the magazine's first woman editor-in-chief and she has brought the publication to its highest level of editorial excellence in its 80 year history. She has recently been named by the ACS, the world's largest scientific society, to be their next executive director, effective January 1, 2004.

She received a B.S. in chemistry at George Washington University (Washington, DC), in 1968. She did graduate work in organic chemistry and immunology at the University of Maryland and at NIH and received an honorary Doctor of Science degree from George Washington in 2003. Since 1972 she has also found time to be a freelance writer/editor, consultant, and seminar speaker. She has written and edited for a number of organizations and publications, including the American Association for the Advancement of Science, *Physics Today*, TRW, National Bureau of Standards, Pharmaceutical Manufacturers Association, and *Smithsonian Magazine*. She has presented seminars on the challenges of editing, *Chemical & Engineering News*; diversity topics; challenges for women scientists in the new millennium; attracting the best and the brightest into careers in the sciences; and "The Two Cultures, Zen, and the Art of Motorcycle Maintenance" at universities and colleges, corporations, professional society meetings, and government agencies.

In addition to the honorary doctorate, Jacobs has received dozens of other honors and awards in her career as a writer, editor, innovator, and motivator of young people, including the ACS Award for Encouraging Women in Careers in the Chemical Sciences and the New York Academy of Sciences Women's History Month Award.

### ***1st Charles Supper Award to Nguyen-Huu Xuong***

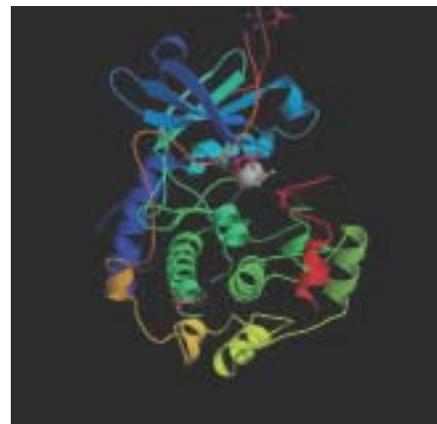


The ACA Council is pleased to announce that the first recipient of the ***Charles Supper Award*** is ***Professor Nguyen-Huu Xuong*** of the University of California, San Diego. Professor Xuong is cited for his pioneering work in "filmless" x-ray detection methods which have revolutionized x-ray diffraction data collection for macromolecular crystallography.

He earned his bachelor's degree in electrical engineering from the École Electricité Industrielle de Marseille in Marseille, France in 1955; three master's degrees, including electronic engineering in 1957, mathematics in 1958 and physics in 1961; and a Ph.D. degree in physics in 1962 from the University of California, Berkeley. He accepted a position as an assistant professor of physics, biology, & chemistry and biochemistry in 1962 at the University of California, San Diego and rose through the ranks over the years. He has been the re-

recipient of a Guggenheim Fellowship (1965), NATO Fellowship (1977), Fogarty Fellowship (1984), and a UCSD Chancellor Associate Award (1992). He has been active in the Vietnamese Alliance Association and has served as chairman of the Boat People SOS Committee.

His research includes his pioneering work in the development of the multiwire area detector for rapidly collecting x-ray diffraction data. For many years, he operated the first national facility at which macromolecular crystallographers could collect data on their protein samples. The collection efficiency and quality of the multiwire data were superior to film methods at the time and thus enabled many crystallographers to speed up their crystallographic analyses. Over the years, he has collaborated extensively with other scientists. His long-standing collaboration with Susan Taylor (*figure is of PDBID 1L3R - Nature Structural Biology (2002), 9, 273*) has resulted in numerous publications on the structure and function of the catalytic (C) and regulatory subunits of cAMP-dependent protein kinase. In addition, Professor Xuong's lab has continued to develop new instrumentation, not only for protein crystallography but also for the new and equally exciting field of cryo-electron microscopy.



*Fran Jurnak*

### ***ACA Elections - 2004***

#### ***Call for Nominations***

The ACA nominating committee is starting the process of selecting candidates for the 2004 elections. The positions to be filled are Vice-President and one member for each of the ACA Standing Committees: Continuing Education, Data, Standards and Computing and Communications/

Suggestions are welcome and can be sent to any member of the nominating committee:

***Victor Young (chair) - young@chem.umn.edu***

***Charlie Carter - carter@med.unc.edu***

***Kathy Kantardjieff - kkantardjieff@fullerton.edu***

## Call for Nominations

**The A.Lindo Patterson Award** was established to recognize and encourage outstanding research in the structure of matter by diffraction methods, including significant contributions to the methodology of structure determination and/or innovative application of diffraction methods and/or elucidation of biological, chemical, geological or physical phenomena using new structural information. Lindo Patterson's 1934 paper in *Phys. Rev.*: "A Fourier Series Method for the Determination of Components of Interatomic Distances in Crystals," signalled a major step forward in understanding diffraction theory; the Fourier series on  $F^2$ , or Patterson function, greatly enabled subsequent structure determination. Other research interests included particle-size line broadening, structures of biological interest, and homometric structures, which are different atomic arrangements having the same Patterson function. His section on Fundamental Mathematics in *International Tables*, Vol. II was another important contribution to the community. After working for the government during the war, and then teaching at Bryn Mawr, he moved in 1949 to the Institute for Cancer Research where he worked until his untimely death in 1966. Lindo Patterson was President of ASXRED in 1949 and played an important role in the formation of the ACA in 1950. The award, established in 1980, is given every three years, and consists of an honorarium plus travel expenses to accept the award and present a lecture at the Annual ACA Meeting. The next Patterson Award will be presented at the 2005 ACA meeting in Orlando. **The selection committee for the 2005 Award consists of James Stewart, chair, Wim Hol, Brian Patrick and Janet Smith.**

Previous winners of the A.L. Patterson Award: 2002 **Douglas Dorset**, 1999 **Gerard Bricogne**, 1997 **Christer E. Nordman**, 1993 **George Sheldrick**, 1990 **Michael M. Wolfson**, 1987 **David and Lieselotte Templeton**, 1984 **Jerome Karle and Herbert Hauptman**, 1981 **Wayne A. Hendrickson**

**The Margaret C. Etter Early Career Award** recognizes outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career. The award was established to honor the memory of Margaret C. Etter (1943-1992), who was a major contributor to the field of organic solid-state chemistry. Her work emphasized the use of hydrogen bonds and co-crystals. In addition to a large body of experimental work she was the major force in devising a set of rules known as graph sets to describe hydrogen bonds in a way that revealed similarities between structures without being tied up in the crystallographic details. Her experience in both industrial and academic settings gave her an unusually broad perspective from which to mentor students and to support and encourage colleagues. She had a love for people, for science, and especially for people who do science, that we honor. Established in 2002 as an annual award, it consists of an honorarium plus travel expenses to accept the award and present a lecture at the ACA meeting.

Scientists involved in crystallographic research in the broadest sense will be eligible for the award. At the time of the closing date for nominations, nominees must be no more than 10 years

beyond the awarding of their Ph.D. degree, not including career breaks, and must have begun their first independent (not post-doctoral) position within the past 6 years. Nominees employed in tenure-track academic positions must not yet have received tenure. Nominations must include as a minimum a nomination letter clearly indicating the accomplishments of the individual since beginning their independent career and assessing their future potential. Additional supporting letters and a c.v. may be provided but are not requirements. Self-nominations are not permitted. Nominees may be employed in regular academic positions, as service crystallographers, in industrial positions or in government laboratory positions.

Since the 2005 ACA meeting will be a spring meeting nominations are being solicited for both 2004 and 2005.

The 1st Etter Early Career Award was presented at the 2003 ACA meeting to **Julia Chan**.

**Margaret C. Etter Student Lecturer Award.** Each ACA Special Interest Group (SIG) may select one student to receive an award and to present a lecture in one of the sessions organized by that SIG. Selections are based upon submitted abstracts and are independent of whether the student presenter originally requested an oral or poster presentation. Award winners are determined by the elected officers of the SIGs. Students who are selected receive a monetary award of \$250, which is independent of any requests for support via the ACA Travel Awards. The nominee must be a student at the time abstracts are submitted.

2003 winners: **Monica Allain, Firas Awwadi, Peter Chupas, David Lodowski, and Jennifer Padilla**

Nominations for all awards should be sent to the ACA Administrative Manager, **Marcia Colquhoun (marcia@hwi.buffalo.edu)**

## 4th European Crystallography Prize



The European Crystallographic Association (ECA) invites nominations for the 4th European Crystallography Prize to recognize a significant achievement in crystallography in the past 5-10 years. Nominees should be affiliated or identified with the European crystallographic community, as broadly defined in the charter of the ECA (see the ECA-news site [www.ecanews.org](http://www.ecanews.org))

The prize, including a monetary award and certificate of recognition, will be awarded at the opening ceremony of the 22nd European Crystallography Meeting (ECM-22) to be held in Budapest, Hungary, 26-31 August 2004.

The previous laureates are 2000 **Ada Yonath**, 2001 **Jochen R. Schneider** and 2003 **Carmelo Giacovazzo**

Nominations should include a statement of the nominee's contribution for which the prize is to be awarded and a short cv. Send by e-mail or regular mail no later than **Feb. 28, 2004** to:

**Anders Liljas**  
**Center for Chemistry and Chemical Engineering**  
**Lund University**  
**Box 124, SE-221 00 Lund, Sweden**  
**Fax: +46-46-222 46 92 / e-mail: anders.liljas@mbfys.lu.se**

**Howard F. McMurdie, 75 years at NBS/NIST!!!**

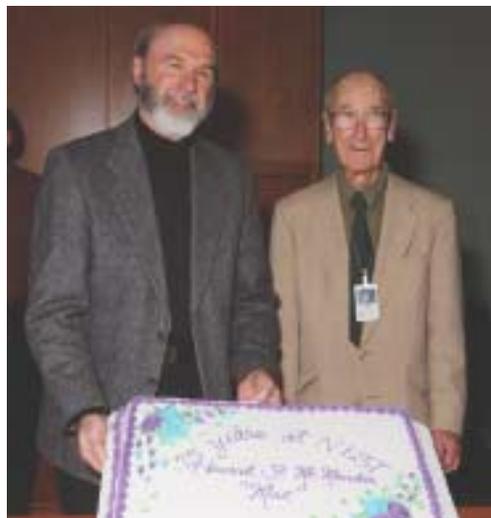
Howard F. McMurdie is a legend at NBS/NIST. Howard, more familiarly known as “Mac” by his colleagues, was born on February 5, 1905 in Detroit, Michigan. Shortly after graduating from Northwestern University, Mac joined the National Bureau of Standards (NBS) on April 2, 1928 as a chemist. His initial activities at NBS were with the Lime and Gypsum Section of the Clay and Mineral Products Division. In mid 1933, after a brief assignment in the Chemistry Division to learn chemical analysis of mineral products, Mac was transferred to Riverside, California. There, he spent two years testing cement for meeting specifications for the Boulder Dam project. After returning to NBS in Washington, Mac was assigned to the Petrographic Laboratory, which was part of the Glass Section. His study of Portland cement was the start of what was to develop into a lifetime interest in “phase diagrams.” In those early days, Mac also pursued the use of x-ray powder diffraction and electron microscopy for phase analysis of solids. These activities paved the way for Mac to become the Chief of the Crystallographic Section.

During his tenure as Chief, Mac oversaw diverse but interesting projects which included: (1) the investigation of crystals (AgI) used for rain making, (2) phase characterization in cement clinker and the hydration products of cement, (3) crystal growth of thallium iodide and bromide (of interest to the Bureau of Ships), and (4) the crystal structure of a variety of single crystals using x-ray diffraction methods. He was instrumental in developing a high-temperature x-ray powder diffraction camera for studying clays and  $MnO_2$  (an early battery material) and in using low-temperature x-ray diffraction for studying free radicals. The group also helped the National Institutes of Health in the examination of a series of roof tiles, which had been exposed to the atomic bomb blast in Nagasaki, in order to determine the temperatures created by the explosion.

Clearly, McMurdie contributed significantly to many areas of research throughout his 75 years at NIST/NBS. He considers three projects as especially important, and was closely related to two of them since his formal “retirement” from NBS in 1966. The first concerns NBS’s connection with the International Centre for Diffraction Data (ICDD), which publishes the Powder Diffraction File (PDF) for identification of crystalline solids. In 1953 he established an ICDD Research Associateship in the Crystallographic Section. For more than 30 years, this Associateship, under his guidance and leadership, prepared a broad set of important, accurate, and widely used powder diffraction patterns. After his retirement, Mac joined the Associateship and served as an editor for the PDF. The second important project was his work on refractory oxides. It was through this work that he established a relationship with the American Ceramic Society (ACerS) and started the publication of the series “Phase Diagrams for Ceramists.” This cooperation is still going strong today and Mac continued to be an editor for the phase diagrams after his retirement. The third important activity, which was initiated in the Crystallographic Section, is the study of materials at high pressure. His vision together with the ingenious work of a group of world-class scientists at NIST/NBS led to the development of

the diamond anvil cell (DAC), the high-pressure single-crystal x-ray diffraction technique utilizing the DAC, and an optical ruby fluorescence method to measure very high pressure in the DAC. This work earned NBS/NIST an international reputation in the field of high-pressure science and technology and also a Department of Commerce Gold Medal Award for the NBS scientists involved in the work.

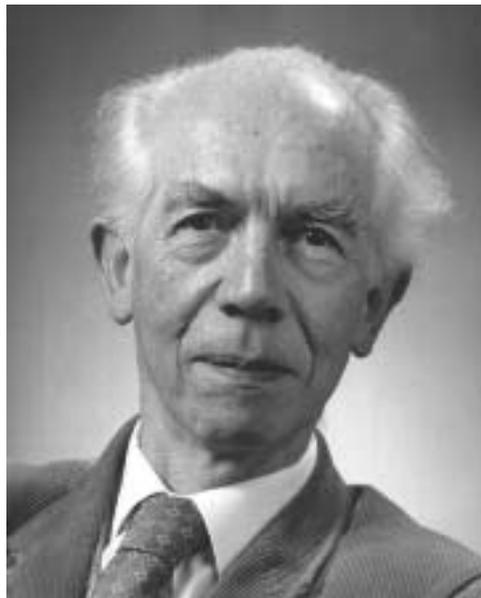
Howard McMurdie has set a superb example for the younger generation of scientists. Not only is he a dedicated, efficient and hard working scientist, he is also a very thoughtful and generous person who is well-liked at NIST. In addition to science, he has many other interests. At home he is a gourmet cook who still cooks weekly for his large extended family (3 children, 6 grandchildren and 5 great grandchildren). He is an accomplished photographer who occasionally serves as a judge at local photography competitions. His boundless energy and sharp mind are sometimes even better than many people half of his age. His ability and desire to keep up with the latest computer and digital camera technology is amazing. He has been heard to remark “I don’t understand why some young people in their 60s and 70s don’t even know how to use a computer.” Over the years, he has made substantial monetary contributions to benefit various organizations such as ICDD, ACerS, and the NIST Association of Asian Pacific Americans. A special biannual “Howard McMurdie” award related to the Powder Diffraction File has been established by ICDD in his honor. He is, indeed, a remarkable individual.



**Howard McMurdie with Director of Materials Science and Engineering Laboratory, Leslie Smith, during the celebration of his 75<sup>th</sup> year at NIST**

During his NIST “retirement” party in April 2003, he was awarded a special certificate of appreciation “for his significant contributions to the Materials Science and Engineering Laboratory of NIST during the past 75 years.” The certificate noted that McMurdie’s “research interests encompassed areas such as measurements of phase equilibria and reference powder x-ray patterns, characterization of solid-state materials, compilation and evaluation of data for Phase Equilibria Diagrams, and for the Powder Diffraction File”.

*Winnie Wong-Ng - Alan Mighell - Gasper Piermarini*

*William Cochran (1922-2003)*

Bill Cochran was born on a remote sheep farm, some 15 miles south of Glasgow. Forebears of the Cochran family had farmed in the area continuously since the middle of the seventeenth century although Bill's father took the family to a new farm, some eight miles west

of Edinburgh in 1928. As Bill himself said "It is surprising, particularly as I have no brothers, that I did not become a farmer." Had he done so it would have been a sad loss to science.

Bill was educated at Boroughmuir High School where his first interest was in languages, but the fortunate gift of a Mecanno set turned his interest first to engineering and later to physics. He entered Edinburgh University in 1939 to read physics, graduating in 1943. He made repeated efforts to become involved in the war effort but he was always directed towards academic activity and from his graduation until 1946 he was an Assistant in the Edinburgh Physics Department, mainly involved in teaching electronics. For the first part of that period he worked under the direction of Professor C G Barkla who had won the Nobel Prize for Physics in 1917 for his work on the characteristic emissions of x-rays. When Professor Barkla died in 1944, Bill moved to the Chemistry Department to do research in x-ray crystallography under the guidance of Arnold Beever. After an exhaustive, but unsuccessful attempt to solve the native sucrose structure, Bill succeeded in solving the isomorphous NaCl and NaBr adducts of sucrose, which enabled him to obtain his PhD.

In 1946 Bill moved to Cambridge as research assistant to Sir Lawrence Bragg. The research group was under the direction of W H Taylor and also contained June Broomhead and C J B Clews. Professor Alexander Todd of the Chemistry Department had suggested to Bragg the problems of solving the structures of pyrimidines, purines, nucleosides and nucleotides as a way of throwing light on the structure of DNA. Cochran and Broomhead found that they could determine the electronic structures of pyrimidines and purines sufficiently accurately to find the positions of hydrogen atoms and Bill found that this was greatly improved by the use of an ( $F_o - F_c$ ) Fourier synthesis that removed the effect of termination errors. Later he built a Geiger-counter diffractometer with which he measured the electron density in salicylic acid to reveal the presence of hydrogen atoms and electron density associated with covalent bonding.

In 1949 Bill met David Sayre, an Oxford-based American postdoctoral worker, and this began his interest in direct methods of solving the phase problem. As early as 1948 papers on inequality relationships by Harker & Kasper, Gillis and others had appeared in *Acta Crystallographica* but such relationships were restricted to very small and simple structures. In 1952, in one issue of *Acta Crystallographica*, there appeared three papers separately written by Sayre, Cochran and Zachariasen that could be said to be the starting point of modern direct methods.

In 1951, after an extended visit to the USA, Bill was promoted to a full Lecturer in Cambridge and so obtained the tenure and stability he needed to anchor his subsequent research career. Travelling home by ship from Stockholm after the second International Congress on Crystallography in 1951, Bill met his future wife, Ingegerd Wall, and they married in Sweden in 1953. Also, at about this time, he collaborated with Henry Lipson in the production of *The Determination of Crystal Structures*, a very influential text for many years.

In the 1950s Bill acted as a consultant to the protein crystallography group in the Cavendish Laboratory and in 1952 he, Francis Crick and Vladimir Vand published a notable paper on the diffraction pattern of atoms on a helix. It was this paper that enabled Crick and Watson to interpret Rosalind Franklin's diffraction photographs of the A-form of DNA.

Bill saw quite early the potential of computers as a crystallographic tool and in 1955, with Sandy Douglas, he applied EDSAC, a primitive early computer, to a direct method for solving centrosymmetric structures. This pointed the way to the subsequent development of computer applications in this field, which had an important impact on structural crystallography.

In the mid-1950's Professor Dingle had created a bit of a stir by expressing doubts about the validity of the 'twin paradox' in relativity and for some time Cochran and Dingle carried out a lively public debate which ended in Cochran's favour. During this period Cochran was becoming somewhat disenchanted with direct methods and had concluded, incorrectly as he later conceded, that they could not solve more than very simple structures. Protein crystallography was clearly the future but, having decided early on that it too was unlikely to succeed, he was reluctant to "climb on the bandwagon" now that it was rolling successfully. By 1958 Cochran was ready to embark on a new field.

In 1957, at the fourth International Congress on Crystallography in Brookhaven, Bill had attended a lecture by Bert Brockhouse on neutron diffraction applied to lattice dynamics. He arranged to spend a year at Chalk River, funded by Atomic Energy of Canada, where Brockhouse, later to win a Nobel Prize, was just using his newly-designed triple-axis spectrometer to measure phonon dispersion curves for sodium iodide. Bill spotted a theoretical paper by Dick and Overhauser on the dielectric constant of alkali halides and he realized that their shell model was just what was needed to explain the lattice dynamics of sodium iodide. Later he extended the theory to germanium and two papers he wrote at this time became classics in the field. Later development, while he was still in North America, led to the idea of the soft-mode concept for the onset of ferroelectricity.

*Inside*

*Gilson*

On returning to Cambridge in 1959 he briefly dallied with the phase problem once more but then turned his full attention to lattice dynamics. He was fortunate in having two gifted research students, Stuart Pawley and Roger Cowley, later to become colleagues at Edinburgh. In the next few years, work was done on the lattice dynamics of molecular crystals, the theory of the lattice dynamics of sodium, and the shell model was extended to GaAs. At this stage Bill was at the forefront of the lattice dynamics field and it was almost inevitable that, at the comparatively early age of 40, he was elected a Fellow of the Royal Society in 1962.

In 1964 he was appointed Professor of Physics at Edinburgh and quickly established a research group on Condensed Matter Physics. Further work was done on phase transitions leading to the onset of ferroelectricity, mainly using the Chalk River facility for neutron spectroscopy. For the next ten years Bill and his group established a leading position in the general field of lattice dynamics. He also developed a new model for the structure of amorphous materials.

In 1975 Cochran succeeded Norman Feather as the Professor of Natural Philosophy and Head of Department in Edinburgh. Although his research activity continued for a while it quickly tailed off as he bore an increasing administrative burden.

Cochran's work was recognised by several awards and appointments to scholarly bodies. He was a Fellow of the Royal Societies both of Edinburgh and London and an Honorary Fellow of Trinity Hall, Cambridge. He was awarded the Hughes Medal of the Royal Society, the Guthrie Medal of the Institute of Physics and the Potts Medal of the Franklin Institute. Amongst his many interests were the writing of poetry and tracing the genealogy of his family. He leaves behind his wife, Ingegerd, and children Margaret, Robert and Jennifer, to whom he was a devoted husband and father.

*Michael Woolfson*

*Reprinted from the Winter edition of the British Crystallographic Association Newsletter*

### **Harold Wyckoff (1927 – 2003)**

*This came in as this issue was on the way to the printer – a full obituary will appear in the Spring Newsletter.* Harold W. Wyckoff died in Connecticut on November 27, of pancreatic cancer. He was the husband of Andrea, father of Richard and Benjamin. He is also survived by three grandchildren. Harold (Hal) was born in Niagra Falls. He obtained his PhD from MIT and was the author of a number of publications of interest to the crystallographic and medical communities dating back more than fifty years. He was a professor emeritus of molecular biophysics and biochemistry at Yale, a fellow of Berkeley College, and a former president (1980) of the American Crystallographic Association and for a number of years was a member of the board of the Orchestra of Mew England.

### **Bertram Neville Brockhouse (1918 – 2003)**

On an ordinary Wednesday morning in October 1994 Bert



Brockhouse got out of bed at his usual time—about 6:45. As he stretched a bit to loosen the overnight aches of his 76-year-old body, he saw the little red light blinking on the answering machine.

Who could have called in the middle of

the night? he wondered, as he pressed the play button. He listened to a voice announcing that it was from Stockholm: “B. N. Brockhouse and C. G. Shull have been selected as recipients of the 1994 Nobel prize for physics.” Brockhouse was stunned. For a moment he thought, Oh that’s interesting, but then he realized, I am B. N. Brockhouse, and he called his wife Dorie, to listen to the tape again with him.

The next year was one of travel, awards, banquets, and lectures. Brockhouse was simply beamed out of quiet retirement. In his annual Christmas letter to friends that year, after describing all the festivities in Stockholm, Brockhouse said, “If anyone cares, we got a new car in the summer, a Chrysler Neon.”

The origins of Brockhouse’s Nobel Prize could be traced back to 1951. Fresh out of the University of Toronto with a PhD in Physics, Brockhouse sat at his desk in a faded blue-shingled wartime hut at Chalk River, Ontario, home of Canada’s Atomic Energy Project funded by the National Research Council.

He gazed out the window at the snow. It was winter, but he felt warm inside the hut. He just sat there thinking, mulling things over in his mind. The other night he had been at the home of Donald Hurst, his boss and head of the Neutron Spectrometer section. They had been reading a 1944 paper about neutrons—subatomic particles with no electric charge that, together with protons, make up the nucleus of an atom. The existence of neutrons had only been verified about 12 years before. Not much was known about them. Brockhouse didn’t quite understand the theories in the paper, but he felt it had a lot of interesting ideas. He was supposed to be working on something else, but he couldn’t stop thinking about the concepts in the paper and how he could do experiments at Chalk River to try out some of the new theories.

He fiddled with some math on his notepad for a while and then went to the coffee room. As he passed the lab that housed the radioactive nuclear pile, a controlled nuclear reaction that emitted one of the most powerful sources of neutrons in the world at the time, he wondered whether he could put it to use. In the coffee room he met Hurst. Brockhouse went up to the blackboard and

said, “Don, there’s something I’d like to show you.” He sketched out some equations on the blackboard. The math described a device they could build that would use a neutron beam as a better type of spectrometer, a kind of flashlight that could probe into the mysteries of crystal structures and other solids such as metals, minerals, gems, and rocks.

In the 1920s Bert Brockhouse’s family moved to Vancouver. After high school, instead of going to university, Brockhouse worked as a radio repairman. Then World War II came along and he used his radio skills as an electronics technician in the Canadian Naval Reserve. When the war ended, Brockhouse went to the University of British Columbia, majoring in Math and Physics. After marrying Dorris Miller, a film cutter at the National Film Board, Brockhouse finished his PhD and the newlyweds moved to Chalk River.

(Extracted, with permission, from [www.science.ca/scientists/scientistprofile.php?pid=4](http://www.science.ca/scientists/scientistprofile.php?pid=4))

In July 1950 Brockhouse joined the staff of the Atomic Energy Project of the National Research Council of Canada, later to become Atomic Energy of Canada Limited (AECL), at the Chalk River Nuclear Laboratories about 130 miles northwest of Ottawa.

In the early months of 1952 Brockhouse put together what he described as a “large aperture double spectrometer”, in reality a triple-axis machine, hoping to be able “to measure the as yet unknown frequency distribution of normal modes” in a crystal. Much effort was put into trying to get the machine to work, including attempts to produce monochromator crystals with higher reflectivity, and improvements to the shielding, but by the end of the year the spectrometer was not producing results.

In 1953 Brockhouse took advantage of an unexpected shutdown of the NRX reactor to spend ten months as the first foreign guest scientist in the Reactor Department at Brookhaven National Laboratory. On his return to Chalk River, Brockhouse again set up his crude triple-axis spectrometer, using a fixed angle monochromator facility with an aluminum crystal monochromator, a makeshift sample table, and the old single-axis instrument acting as the analysing spectrometer. The scattering angle at the sample position was fixed for a give set of measurements but could be changed by turning the sample table and moving the analysing spectrometer on a set of rails. The machine was used successfully, thanks in large part to its improved monochromator, for studies of the phonon frequency distribution of vanadium and of the inelastic scattering by liquid lead and light and heavy water: these measurements were reported at the January 1955 meeting of the American Physical Society in New York City. The energy dependence of the paramagnetic scattering by materials such as the manganese oxides was also studied.

In the early months of 1955, “preliminary measurements (were made) of energy distributions scattered by an aluminum single crystal in several different orientations”. This work, in collaboration with A.T. Stewart, led to the first successful determination of a phonon dispersion curve. It provided the first convincing demonstration of the power of the triple-axis method, at a time when groups at Saclay and at Brookhaven were concentrating

their attention on a complementary time-of-flight technique.

Brockhouse next turned his attention to the possibility that neutrons might be used to investigate the “thermal disturbances of the magnetized arrays of...coupled magnetic moments (which) can be described by means of quantized wave excitations called spin waves”. The ferrimagnetic material magnetite was chosen, for the very good reason that large single crystals were available. The measurements of scattered neutron energy were carried out for 12 different orientations of the crystal, using 1.52 Angstroms incident neutrons and a scattering angle of 18 degrees, and it was concluded that the observed excitations were not phonons, but indeed “in the spin system itself”. This was the first experimental determination of a magnon dispersion curve.

A new type of high resolution time-of-flight instrument was devised by Brockhouse at about this time, following a conversation with D.G. Hurst. This was the rotating crystal spectrometer, first mentioned in an AECL Physics Division progress report in late 1957. The first version of this machine was installed at the NRX reactor, and an improved version, fitted with a cooled quartz filter and initially located at the NRX reactor, was later set up at the N5 hole of the new reactor NRU (National Research Universal). R.N. Sinclair, who had worked with Brockhouse as a postdoctorate fellow, built a similar machine at Harwell on his return from Chalk River.

The rotating crystal spectrometer was initially used for a detailed study of the quasi-elastic component of the scattering by water. The results were consistent with earlier Chalk River results, and strongly suggested that the supposed fine structure in the data of D.J. Hughes and his collaborators was spurious. The spectrometer was also used for an extensive series of experiments, by D.G. Henshaw, on liquid helium: the first inelastic work on helium at Chalk River had been undertaken using the filter-chopper spectrometer. Other early work using the rotating crystal spectrometer included phonon measurements on lead and sodium iodide.

The famous C5 triple-axis spectrometer, immortalized in Kittel’s “Introduction to Solid State Physics”, was installed at the NRU reactor in 1958. This machine remained in use for more than twenty years and was an important training ground for many present day triple-axis spectrometrists. The first material to be studied using the C5 machine was a single crystal of silicon; lead was also studied, supplementing the earlier work on the rotating crystal spectrometer.

With the capability to vary the incident neutron energy of the C5 spectrometer, a new method for the study of high energy excitations became possible. This was the beryllium filter detector method, which was first tried at Chalk River in early 1960. At about this time the N5 rotating crystal spectrometer was modified so that both the incident energy and the angle of scattering could be continuously varied.

In 1962 Brockhouse moved to McMaster University where he was a professor of Physics until his retirement in 1984.. At McMaster he took an active part in teaching, and was able to communicate his enthusiasm for physics to undergraduate and graduate students alike. He received many honors over the

years, including the Tory Medal (Royal Society of Canada), the Buckley Prize (American Physical Soc.), the Duddell Medal and Prize of the (British) Inst. of Physics and Physical Society “for excellence in experimental physics”, and the Centennial Medal of Canada. He was a Foreign member of the Royal Swedish Academy of Sciences.

We owe a tremendous debt of gratitude to Bert Brockhouse. He inspired many people to accept the challenges of neutron inelastic scattering, and to work long and hard to improve methods, materials and equipment in order to be able to do experiments properly and convincingly. Throughout his career he demonstrated an honesty, thoroughness and scientific passion which are an example to us all. The “absent-minded professor” stories are plentiful, and amusing, but the stories of his insistence on good experimental technique, and of his concern that time and money be efficiently used, are perhaps more to the point. His intuition, dedication to research, and kindness and concern for his fellow workers, were frequently mentioned by those who had the pleasure to work with him.

(Extracted, with permission, from [www.physics.mcmaster.ca/people/fs3\\_people\\_Brockhouse\\_BN.html](http://www.physics.mcmaster.ca/people/fs3_people_Brockhouse_BN.html))

**Felix Bertaut (1913 - 2003)**

*As we were going to press the following was received from Theo Hahn:* It is with great sorrow that I have to inform you of the recent death of our old friend and co-author Felix Bertaut of Grenoble, France. Felix was our “Senior” among the International Tables Vol. A editors: he died at the age of 90 years.

”We all will remember Felix as a very friendly and inspiring active scientist, both in theory and experiment, and this is clearly evident in his contributions to Vol. A which deals with the symbols of space groups for various settings and coordinate systems, as well as with the subgroup relations among space groups. In particular, I recall his lively discussions during all our editorial meetings, esp. the final “Aachen meetings” in 1978 and 1979.

Felix was a very good friend since we met first 50 years ago in the USA, when he spent some time at Penn State in Ray Pepinsky’s lab and I used their analogue computer X-RAC, and this friendship has continued through the years.

With deep sorrow about this loss I send you all my cordial greetings and best wishes for the coming Christmas Season and the year 2004

Yours Theo Hahn

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	Average No. Copies each issue during proceeding 12 months	Single issue nearest to filing date
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7. I certify that the statements made by me above are correct and complete. (Signed) Marcia Colquhoun for American Crystallographic Association, Inc.

### Protein Production and Crystallization Workshops

The Protein Structure Initiative (PSI) aims to provide one or more representative structures from each of the several thousand protein-domain families found in living organisms. PSI is in its third year, and the nine PSI pilot research centers have identified a number of important bottlenecks that need to be addressed in efforts to meet the goals of the program. For example, it is accepted that a major challenge to high-throughput determination of protein structure is the production of protein samples and crystals that are suitable for structural analysis.

To facilitate an effective exchange of developments and advancements, the National Institute of General Medical Sciences (NIGMS) has organized annual workshops on gene cloning and protein expression and purification. The first such meeting took place in March 2002 at the National Institutes of Health (NIH), in Bethesda, Maryland ([www.nigms.nih.gov/news/reports/protein\\_production.html](http://www.nigms.nih.gov/news/reports/protein_production.html)). In a second workshop the scope of the meeting was expanded to include crystallization. The Protein Production and Crystallization Workshop was held at NIH, in Bethesda, in April 2003.

The 2003 NIGMS Protein Purification and Crystallization Workshop was organized with the main goal of providing an effective platform for scientists to share and exchange ideas and data, to discuss progress and problems, and to address the most challenging bottlenecks. Another purpose of the workshop was to encourage contacts and collaborations among the participating groups. The meeting brought together representatives from all nine P50 center grants and two P01 program project grants and several recipients of NIH R01 and SBIR grants in the area of structural genomics methodology and technology development. Other attendees included representatives from similar international efforts in Canada, Europe, and Japan; NIGMS and other components of NIH; and other Federal agencies. A total of 110 participants met at this workshop. Nine invited speakers presented research results in areas relevant to the meeting topic, and representatives of the research centers and program projects described the bottlenecks in the research process and presented the study results. In addition, experts from the international community were invited to provide initial discussion points in all critical areas pertinent to the main topics of the workshop. Discussions focused on progress in high-throughput methods for cloning, production, purification, and crystallization of proteins for x-ray crystallography and NMR studies.

Workshop topics included the following:

- \* Cloning technologies
- \* Statistics on DNA sequence quality and error rates for polymerase chain reaction
- \* Vectors and host strains
- \* Complementary DNA (cDNA) clones or reagents
- \* Technologies for eukaryotic expression
- \* Approaches to solubilizing or refolding proteins or both
- \* Issues related to metalloproteins and post-translational modification

- \* High-density fermentation and scale-up of fermentation
- \* Protein production and purification and parallel approaches to purification
- \* Homogeneity and quality control of protein samples
- \* Expression of membrane proteins
- \* Reconstitution of proteins into membrane environments
- \* Crystallization of membrane proteins
- \* High-throughput crystallization
- \* Crystallization optimization
- \* Sample storage, reagent archiving, and record keeping
- \* Robotic platforms for these procedures
- \* Failures, problems, and bottlenecks

The proceedings of the workshop will be published in the *Journal of Functional and Structural Genomics* (in early 2004). The organizing committee for the meeting has compiled information about research methods, technology, instrumentation, and contacts and has posted this resource on the PSI Web page (see [www.nigms.nih.gov/psi/meetings.html](http://www.nigms.nih.gov/psi/meetings.html)).

A video archive of the 2003 workshop is available on the NIH Videocast Web site ([videocast.nih.gov](http://videocast.nih.gov)) for each of the workshop's three days. (Note: The videocasts require free RealPlayer software and 220Kbps LAN or 56Kbps dial-up bandwidth.)

The 2004 workshop will take place at NIH from March 29-31, 2004. Details will be available at [www.nigms.nih.gov/psi/meetings/](http://www.nigms.nih.gov/psi/meetings/)

### Contributors to this issue

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*Inside*

*Osmic*

### ACA 2003 Election Results

**Vice-President** Louis Delbaere  
**Treasurer** Doug Ohlendorf

#### Standing Committees

##### Continuing Education

Cathy Drennan

##### Data, Standards, and Computing

Ward Smith

##### Communications

Simon Billinge

#### Canadian Division

**Chair** Jim Britten  
**Secretary** Pawel Grochulski

#### Special Interest Groups

##### Biological Macromolecules

**Chair-elect:** Steve Ginell

##### General Interest

**Chair-elect:** Jeanette Bauer  
**Member-at-Large:** Peter Mueller

##### Neutron Scattering

**Chair-elect:** Jason Hodges

##### Powder Diffraction

**Chair:** Abe Clearfield  
**Chair-elect:** Alex Yokochi  
**Secretary:** Peter Zavali

##### Service Crystallography

**Chair-elect:** John Bollinger

##### Small Angle Scattering

**Chair-elect:** Gregory Beaucage  
**Secretary:** Susan Krueger

##### Small Molecules

**Chair-elect:** Allen Oliver  
**Secretary:** Jeanette Bauer

##### Synchrotron Radiation

**Chair-elect:** Henry Bellamy

##### Young Scientist

**Chair-elect:** Chad Haynes

**By-law change** Passed

### Louis Delbaere - New ACA Vice-President



Louis Delbaere is of Belgian ancestry and is very proud of his roots. Thus, he likes to be known by the Belgian pronunciation of his name (Loo-ee Del-bar, NOT Loo-iss Del-bear). This can be committed to memory by associating Louis' name with the best place to find him at a conference—in the bar. Delbaere in the bar.

Louis is a native of Winnipeg, Manitoba. He received his Bachelor's degree in Chemistry (1965) and Doctorate in Chemical Crystallography (1970) from the University of Manitoba. Although he had learned his crystallography studying organometallic compounds, he went to Oxford in 1970 to do post-doctoral work with Dorothy Hodgkin in macromolecular crystallography. After 2 years with Dorothy, Louis began post-doctoral appointments with Ray Lemieux and then Mike James at the University of Alberta. After four years he became a research associate with Mike James. He became a Sessional Lecturer at the University of Alberta in the Department of Biochemistry in 1977. In 1979, he moved to the Biochemistry Department at the University of Saskatchewan in Saskatoon, Canada, as an Associate Professor, the position being funded by a Medical Research Council (MRC) of Canada fellowship. He was promoted to Professor in 1984 and became Department Head in 1998. He has spent two separate sabbatical years as a Visiting Professor at the Biozentrum of the University of Basel in Switzerland working with Hans Jansonius on the mechanism of catalysis by vitamin B6 enzymes. In 2001 he was awarded a Tier 1 Canada Research Chair in Structural Biochemistry which is renewable in 2008. He finished his term as Department Head and is presently on leave, working in Oxford with Louise Johnson and he will be spending four months after Christmas in Auckland with Ted Baker.

Louis' interests in structural biology are broad, ranging from drug binding of calmodulin to saccharide receptor sites in lectins and including the HPr system and phosphoenolpyruvate carboxykinase. Louis keeps an active lab running, but finds time for many professional contributions. He has served as an editor of the *Canadian Journal of Chemistry* (1992-94). He has spent 4 years as an MRC Regional Director (1994-96, 1997-99). He was chairman of the MRC Biochemistry and Molecular Biology Grant Committee (1993-96). He found time to be Program Chair of the 1998 ACA Meeting in Washington, DC and served as the Canadian Representative on the ACA for three years.

It is an old saying that "If you have an important job that needs doing, give it to a busy person." Louis is that busy person who always finds time to do another job. The list of activities in the previous paragraph is but a sampling of Louis' many activities. He doesn't limit himself to just professional jobs. He and his wife

Carol energized the Christopher Leadership and Public Speaking Course in Saskatoon and have kept it going while hundreds of graduates have benefited. Louis worked tirelessly (with many others) to bring the Canadian Light Source to the University of Saskatchewan (it will be in operation in 2004).

I have worked with Louis for over 23 years, since he came to Saskatoon. In that time, I have always found him willing to take on jobs that had to be done and he never lets the side down. He is generous with his time and I have benefited greatly from that generosity. If any characteristic stands out, it is that you work with Louis, never for him. I am certain that the ACA will benefit from Louis' gift for giving others energy and direction.

*Wilson Quail*

### **Doug Ohlendorf - Re-elected ACA Treasurer**

Doug Ohlendorf is a faculty member in the Department of Biochemistry, Molecular Biology and Biophysics at the University of Minnesota in the Twin Cities. He was program co-chairperson for the year 2000 ACA meeting in St Paul and is currently finishing up his first term as treasurer of the ACA during which he also represented the ACA on the USNCCr. Doug has always been an active ACA member and is currently on the editorial board of the *Journal of Applied Crystallography*.



Raised in southern Illinois, he won a scholarship to Caltech and spent his freshman year in Pasadena. Doug left there after his 1st year having missed the mid-western climate. For the remaining years as an undergraduate he studied in the Physics Department at Washington University in St. Louis, Mo. In four years, Doug graduated *summa cum laude* with both a B.S. and an M.S. His master's thesis in crystallography dealt with the use of computations to simulate molecules and living processes. He then joined the graduate program in biochemistry at Washington University. A true physicist, at that point he had but a single course in biology. His Ph.d. thesis involved image reconstruction of a crystalline lipoprotein.

Doug did post-doctoral studies at the Molecular Biology Institute -University of Oregon. In addition to his work in protein crystallography, Doug used model-building techniques to propose one of the earliest models for protein:dna interactions. He then became a Senior Research Scientist at the Genex Corporation in Maryland. One of the earliest biotech companies, the group was one of the first in protein engineering. While there he pioneered the development of software for one of the early area detectors. He later moved to take a principal investigators position at DuPont in Delaware. At DuPont he solved the crystal structure of protocatechuate dehydrogenase 3,4-dioxygenase and hence began his interest in metallo-enzymes. Wanting to

return to academics, he joined the faculty at the University of Minnesota in 1991 and is currently a full professor. Carrying on his structural studies of metalloproteins, he has also developed a research effort aimed at understanding the structure/function relationships of super antigens and other virulence factors in gram positive pathogens.

In addition to his faculty position, he is a fellow of the Minnesota Supercomputer Institute. He is an active member of a number of professional societies and has served as a reviewer for several granting agencies.

Doug Ohlendorf is a talented musician who plays the bassoon, sax, piano and organ. He is married to a scientist (Cathy Earhart). He is an avid skier- a product of those good old Keystone meetings. In Minnesota besides his science and crystallography, he has taken to being an active party member in a certain (un-specified) political party.

*Len Banasak*

### **U.S. Physics Team**

The American Assoc. of Physics Teachers and the AIP sponsor a competition each year for high school students to represent the US at the International Physics Olympiad Competition.

The 2003 team visited Taipei, Taiwan in August for the international competition. Our five-member team won nine different honors. Although the country scores are not formally tallied in the competition, the cumulative score of the five U.S. students was the highest in the world for the first time in the competition's history.

**ACA Executive Officer Bill Duax** received the following note from **Natalie Quets** of the AIP thanking the ACA for its donation to the U.S. team.

Thank you for providing encouragement for our program. We have some exciting news to report - the US was the top ranking country for the first time ([www.aapt.org/olympiad2003/](http://www.aapt.org/olympiad2003/)). Without the American Crystallographic Association's support of the Team, we would not be able to succeed so well.

We thank you very much for your support of the U.S. Physics Team this year. The Team won five medals and four special prizes. Fifty-four other nations participated. [//www.insidescience.org/reports/2003/071.html](http://www.insidescience.org/reports/2003/071.html)

Pavel Batrachenko (Rochester, MN) was the absolute winner (1st prize) and also received the best score in the 'experiment' competition. Daniel Gulotta, (Aurora, IL), had the best score in the 'theory' competition and Emily Russell (Wallingford, CT) was the best female participant. All five students placed in the top 10%. Batrachenko (1st), Gulotta (ranked 13th), and Chintan Hossain (Wilmington, DE) (19th) received gold medals. Russell (ranked 22nd) and Immanuel Buder (Alexandria, VA) (ranked 23rd) received silver medals.

### Cool Structure Session - ACA 2003

This year's cool structure half-day session started with a presentation about structure and magnetic properties of new transition metal cluster compounds as single crystal magnet (SMM) by **John Bacsa**. He pointed out that the orientations of the Jahn-Teller distortion of the Mn (III) centers in the two  $Mn_{12}$  clusters have a significant impact on their magnetic property. Then we heard a lecture by **Marilyn Olmstead** on structures and nomenclature of diamondoids with the formula  $C_{26}H_{32}$  separated from petroleum. These miniature diamonds have potential application as electronic devices. **Xiang (Sean) Ouyang** on behalf of Deyuan Kong gave a talk on the structure and property study of a family of newly synthesized macrocyclic ligands with hexaaza and octaaza donors and their metal complexes. *In Vitro* studies indicate that the dinuclear copper complex of 30-membered octaazamacrocyclic ligand BTBD shows antitumor activities towards pBR 322 DNA in the presence of hydrogen peroxide. **Graciela Díaz de Delgado** described structure studies in their lab using metal carboxylates. Under room temperature condition and hydrothermal reaction, they obtained the same crystalline product with Ca carboxylates. They got different products when Ba



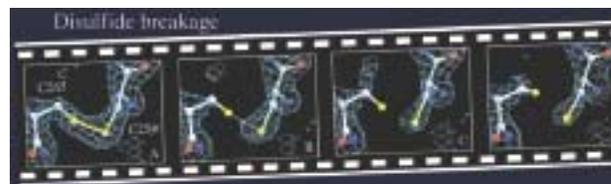
carboxylates were used. Margret C. Etter Student Lecturer Award winner **Firas Awwadi** gave us insights into halogen – halogen interactions in crystal engineering through a series of structure studies. Many new materials were synthesized based on the halogen-halogen interactions theory, including the longest known planar bibridged oligomer,  $Cu_{10}X_{22}$ . **Charles J. Simmons** gave us a lecture on historical and new research in the modeling study of Cobalt-Dioxygen complexes that mimic the active site of natural oxyhemoproteins. Dioxygen-Co bonding angles and the frequency of the dioxygen molecules were used to probe the nature of the dioxygen bonds in different model compounds. We thank all presenters for providing cool structures and insights of their specialized fields.

*Xiang (Sean) Ouyang*

### Macromolecular Crystal Growth and Perfection

The past few years have seen a revolution, fueled by the application of new physical techniques, in our understanding of how protein crystals nucleate and grow, of why they stop growing, and of the important sources and kinds of crystalline disorder that limit diffraction resolution. With advances in expression and purification on the one hand and X-ray data collection and analysis tools on the other, these issues now present more of a bottleneck than ever, and so recent insights should be quickly adopted into general practice. This year's extremely well-attended session focused on closely related problems of crystal degradation after growth caused by crystal soaks, by cryoprotection and freezing, and by radiation damage that often limit the quality of the structural information that can be obtained.

**Martin Weik** described specific kinds of radiation damage seen in electron density maps obtained at  $T=100$  K. Disulfide bonds are broken and elongated, and Cys and acidic residues like Glu and Asp show large B factor increases. These effects vary with the residue's location. Martin also discussed the behavior of solvent when crystals are slowly warmed from below water's glass transition. In crystals with large solvent channels the unit cell volume and ice ring intensity jump abruptly near  $T=155$  K whereas crystals with small solvent channels show no such jump, demonstrating that solvent behavior is strongly modified by its proximity to the protein surface.



**Disulfide bond breakage in acetylcholinesterase (AChE) with increasing radiation dose**

**Raimond Ravelli** discussed an alternative phasing method based on the specificity of radiation damage. Rather than relying on structure factor changes due to addition of heavy atoms or



to wavelength changes near absorption edges of Se and S, one can simply compare low and moderate radiation dose data sets to locate preferentially damaged residues. This radiation-induced phasing (RIP) solves structures of native crystals at arbitrary energy, but will require greater understanding of radiation damage to become a generally applicable method. **The**

**figure illustrates an on-line microspectrophotometer at ESRF for characterizing radical formation during x-ray illumination**

**Sergei Kriminski** described a theoretical analysis of heat transfer from protein crystals during flash cooling. In all but the largest crystals, heat transfer from the crystal is limited by the rate of external convection and internal crystal temperature gradients and associated thermal stresses are small. Factors affecting cooling times can be ordered from most to least important as crystal solvent content and composition, crystal size and shape, amount of residual surrounding liquid, choice of cooling agent, and flow speed. Since the portion of the crystal outside the illuminated volume acts like a heat sink, heating by intense x-ray beams can be minimized by using plate-like crystals with dimensions much larger than the beam diameter.

**Doug Juers** showed evidence that changes in solvent content are behind the success of "flash" annealing, in which the cold



stream is briefly interrupted, allowing the crystal to warm to near room temperature. Multiple annealing cycles cause a steady increase in cell volume and an increase and then a decrease in diffraction quality. Using humidity control, the optimum diffraction was found to correspond to an optimum solvent content. This provides evidence that the optimal cryoprotectant concentration for cryo-cooling allows the bulk solvent contraction to best compensate

for the protein and lattice contraction *The figure illustrates a humidity-controlled sample chamber for characterizing effects of water absorption and transport during flash annealing*

The next two presentations focused on the elastic properties of protein crystals, which determine their response to stresses caused by impurity incorporation, soaks and flash cooling and thus determine crystal mosaicity. *Alexander Chernov* analyzed why static or low frequency dynamic measurements result in much smaller elastic moduli than high-frequency measurements. Since intra-crystalline water and protein molecules have different moduli, inhomogeneous stresses induce water redistribution with an estimated relaxation time of  $10^{-7}$ - $10^{-8}$ s, much longer than thermal vibration periods  $\sim 10^{-10}$  s. High frequency measurements thus primarily probe intramolecular rather than intermolecular properties. *Sergio Speziale*, an Italian graduate student at Princeton, was deemed a sufficient threat to national security to deny him a re-entry visa, and so the session chair gave his talk describing the use of Brillouin scattering to determine the complete elastic constant tensor of tetragonal lysozyme. This non-contact light scattering technique can be performed on crystals in their native environment, and provides information about inter- and intramolecular elasticity that should be useful in modeling protein dynamics.

The last two talks in the session addressed problems in crystal growth. Chernov presented results on behalf of *Alexander Malkin* showing that HPLC purification improves the resolution of canavalin crystals to 2.22 Å from 2.55 Å. This improvement correlated with dramatic changes in step morphology on the growing crystal face as analyzed by AFM – from strongly jagged and, on average, isotropic steps to strictly polygonized steps. This polygonization is explained assuming a lack of kinks on polygonized short step segments between two impurity stoppers. Finally, *Jeff Habel* described crystallization experiments on Pfu-35386. Twinning was found to result because of excessive growth rates following nucleation. By streak seeding into metastable solutions and slowing evaporation during growth, maximum growth rates were reduced and untwinned crystals were obtained

*Robert E. Thorne*

### ACA 2003 - Travel Awardees Share their Stories



I would like to give you my impressions about the ACA 2003 Meeting, suggesting new ideas to strengthen the Latin America Initiative.

This meeting is a rare opportunity for us from Latin America to become up-to-date with new developments and technologies in crystallography and, particularly, structural biology, my research field. This year, I had the chance not only to

present part of my work as an oral presentation but also to attend interesting talks. In addition, the meeting is an auspicious occasion to meet researchers in your area, those people who you know from papers but have never met. Sometimes, a few words can help you to clarify points of your own work. All of this would not be possible without the financial support from ACA, IUCR and generous donors and I acknowledge them for receiving a travel grant.

I think that the Latin America Initiative is a great idea and it should be continued. However, in my opinion it should be seen as part of an overall strategy to join the crystallographic communities in the continent. In this regard, I feel that there is a place for more collaborations to be established between US and Latin America labs. At the same time, I think that it would be worthwhile to make an effort to eliminate possible misconceptions about our science, giving US lab scientists an opportunity to know us and our capacity to work. The ACA Meeting and the Initiative may be important in this sense as well.

From my point of view, one reason for the Latin America Initiative to be successful in the long term would be if US labs could benefit from it. What I am suggesting here would be an effort in this direction.

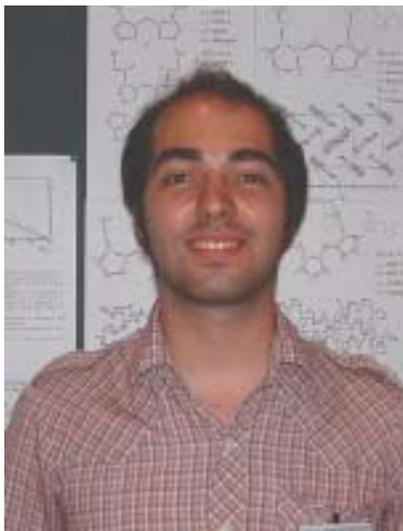
Thank you very much for the opportunity to attend the ACA 2003 Meeting.

*Ricardo Aparicio*

I arrived to the meeting on Friday 25 of July, because next day I was going to attend the workshop about twinning of crystals. The first day I walked along the streets of Covington. The next day at the workshop they demonstrated how we can treat x-ray data from twinning crystals, using a new program Crystals.

Each day I attended many presentations. The lectures from Konstantin Udachin about the clathrate hydrates, and Christer Aakeroy about supramolecular synthesis were very interesting. Also, I enjoyed the presentation from Herbert Hauptman about

the phase problem in neutron crystallography. Most of the presentations were devoted to protein structures. I attended them,



but they were difficult to follow. I have only dealt with crystallography of small organic molecules. This year I am taking a Biochemistry class at my university, in hope of finding this field of crystallography clearer for me.

I enjoyed the demonstrations given by the firms. I had a very interesting and useful talk with presenters from Accelrys and they explained some features of their program which

had not been clear before. At the meeting I met many Russian coworkers with whom I had worked in the Moscow x-ray laboratory of the Nesmeyanov Institute of Organoelement Compounds. Now they are working in different places in the USA. It was very nice to see them again.

From this meeting I obtained new information about crystallography, and met some interesting people. I hope to attend the ACA meeting next year.

#### *Boris Averkiev*

Attending the ACA meeting was very obliging in terms of helping me learn how to solve twinned structures, knowing the hot topics in crystallography, expanding my horizons, improving my skills in giving talks as well as listening to other speakers, and giving me the opportunity to know new people. I attended many seminars and one workshop. The most helpful event was the crystal and twinning workshop. I learned how to use the programs CRYSTAL and ROTAX. ROTAX program is very obliging

in solving twinned structures. So, I expect it will be very helpful, since I frequently encounter twinned crystals, usually I cannot solve the structure due to twinning, and spend a lot of time looking for a single crystal. In most cases I give up. I wish I would attend more workshops on solving twinned structures.

I attended many seminars. Two were very exciting. The one about determination of the adiabatic potential energy surfaces of copper(II) Jahn-Teller complexes using temperature dependent

copper-ligand bond lengths. The authors were able to calculate these surfaces using the vibronic coupling model. The second most exciting seminar was the one about using multi beam synchrotron radiation to get better data set by increasing the redundancy in the dataset, and hence obtaining an accurate structure.

I gave a talk titled "The role of the aryl C-Br...X<sup>-</sup> synthon in the crystal structure of copper(II) halide salts". These types of interactions have received much interest, due to their importance in holding the structural units inside the crystal. We have investigated the crystal structure of tetrahalocuprates(II) with monobromopyridinium counterions (n-BrPyH)<sub>2</sub>CuX<sub>4</sub>. (x=Cl or Br, n=2,3 and 4). The C-Br...X<sup>-</sup> synthon is invariably characterized by essentially linear C-Br...X<sup>-</sup> angles with Br...X<sup>-</sup> contacts 0.3-0.4 Å less than the sum of van der Waals radii. Accordingly, our results indicated that these contacts play an important role in determining the crystal of all the studied model structures.

Finally, I would like to thank the American Crystallographic Association for giving me the opportunity to attend such a great event by giving me a travel grant. In the future, I wish ACA would give me the opportunity to attend more workshops about solving twinned and difficult crystal structures.

#### *Firas Awwadi*

I would like to express my gratitude to the ACA for providing financial support to attend the 2003 meeting in Cincinnati.



This support was critical and I would not have been able to attend without it, especially as my mentor has just retired and no longer has funds available for travel to meetings.

The atmosphere at ACA was wonderful for presentation of scientific results, and I was pleased with the interest in my poster presentation.

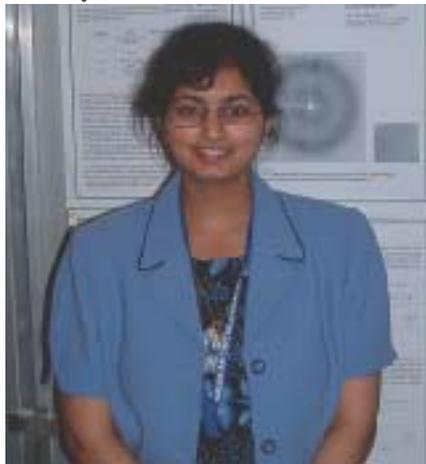
The poster session provided me an opportunity to meet many new people and share with them my dissertation research. I was pleasantly surprised to be recognized with a Pauling poster award for my work.

The sessions at the meeting were incredible, and many days were difficult to schedule due to concurrent sessions on very interesting topics. I am always in awe of membrane protein structures, and this session was a nice way to start the week. The breadth of information on neutron scattering with macromolecules was impressive, as well as the other complementary methods presented throughout the week. It was also refreshing to learn about the status of the high-throughput methods and progress, as well as the large number of new and interesting structures. I

think the most revealing session I attended was on crystal growth and perfection, and in particular the presentation by Raimond Ravelli on solving crystal structures by using radiation damage for phase information. Amongst the scientific information, there was time for social interaction and it was nice to visit with friends and meet new people. I am indebted to ACA for their support, and I look forward to many future ACA meetings!

*Christina Bourne*

Firstly, I would like to thank the ACA for providing me the



travel award which gave me the opportunity to attend my first ACA meeting in Covington, Kentucky. I was able to interact with a large number of scientists from different areas which helped me broaden my perspective. I found the whole experience to be quite enjoyable and exciting.

I found the sessions "Protein Structure, Function, and Dynamics", "Neutron Diffraction", and "Time-resolved Diffraction" extremely interesting. Some of the talks in other sessions were also of interest to me even though they were not related to my area of research. I must say that in many of the presentations I did not understand many parts; however the purpose of the meeting is to bring together people from different areas and to be able to become aware of the happenings in the scientific community. Along with the talks, the poster sessions were highly impressive. It gave me the chance to discuss many topics and address questions with the presenters in great detail. I had the opportunity to present my research and during the session I got some valuable suggestions from scientists as well as graduate students. I hope to incorporate all the new ideas into my research soon.

I sincerely appreciate the efforts put in by the ACA in organizing the "Topics for the Young Scientist" session. The speakers offered important tips on job-searching and gave me a good comparison of industry vs. academics. The panel of speakers in the grant-writing session helped me get an inside-view of how grants are reviewed and processed. It was nice to hear stories from the other side. I also enjoyed all the evening mixers. I would like to thank the organizers for the tremendous amount of hard work they put in. Overall, it has been a stimulating and motivating experience and I look forward to many more of such meetings.

*Sasa Kiran Chilukuri*



This was my first year attending an ACA meeting, and I greatly appreciate the travel award that made my attendance possible. As a young graduate student, I do not have a lot of crystallographic experience yet. This meeting offered numerous valuable learning experiences. I was able to see the vari-

ous applications and techniques of crystallography as well as learn more about protein crystallography which will aid in my own research.

The quantity and variety of posters presented was incredible. It was enlightening to see all the other research going on in the field of crystallography. I also presented a poster involving my complications in determining phases for my protein structure. My abstract was titled "DeNovo X-ray Structure Determination of the Bacterial Quorum-sensing Phosphorelay Protein Lux U". I received a variety of beneficial comments and helpful advice. Thanks to those who contributed.

I found the seminars very stimulating and resourceful. It was exciting to hear seminars from pioneers in the field and from authors of books that I currently reference. I particularly enjoyed the morning session for "Biomacromolecular Crystal Growth and Perfection". These talks offered some useful tips with cryoprotectants, freezing, and radiation damage. Douglas Juers's seminar on cryo-annealing was very intriguing, and I have even attempted some of the cryo-annealing techniques he presented since returning from the meeting. Furthermore, I have been utilizing other techniques that were presented throughout the seminars at the meeting. For example, I have not only used seeding tips from Terese Berfors' "Succeeding with Seeding" seminar, but I have also used the "Sammy the crystallization horse" tail hair from samples she provided to streak seed my protein crystals.

As far as the social activities, I really enjoyed the opening reception held at the Newport Aquarium. It was a nice opportunity to see the aquarium and kick off the ACA meeting. The Rigaku/MSC dinner at Jillians was extremely entertaining, and it gave us the opportunity to meet and hang out with other scientists who joined our bowling team. All the activities provided a comfortable atmosphere to converse and network with fellow crystallographers while having a good time. Furthermore, the awards banquet was a great ending to the meeting with unforgettable memories of how protein dynamics can be choreographed.

Another notable opportunity included all the various vendor exhibits. This showed all the recent technology that is currently

being marketed and used today. I was amazed at how advanced some of these robots and automated systems were. It gave me the opportunity to see these new instruments up close, while also chatting with vendors who supply equipment I frequently use. I was delighted to see that there is now a company who can create physical models of your protein out of carbohydrates. All of these vendor booths allow for us to see the latest wave of technology that is being utilized.

Every aspect of this meeting was very educational and entertaining. I enjoyed the host city Covington, KY as well. From all that I have learned and enjoyed throughout my experiences at this year's ACA meeting, I am grateful I was able to attend and will look forward to next year's meeting in Chicago.

*Jill Dombrauckas*

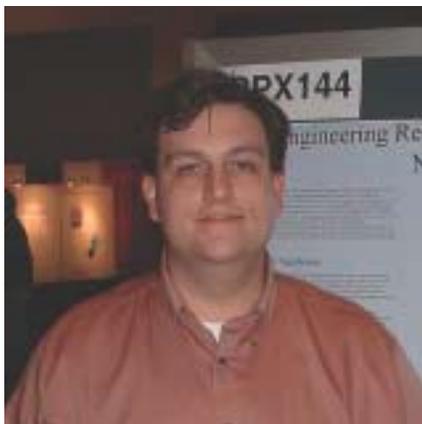


The 2003 ACA meeting in Kentucky was a very nice experience. Although it was not my first conference, I found it to be the most interesting one. I would like to take the opportunity to thank the ACA for providing the financial support that allowed not only me to participate but also an important

number of young scientists from South America. This kind of help is, in fact, vital for the growth and the development of the crystallographic groups of our countries.

The ACA 2003 was an outstanding congregation of academic and industrial researchers. I particularly enjoyed attending the time resolving crystallography session and the presentations concerning new developments in x-ray data management application software. I also found the poster sessions superb. To my surprise, many people came to see my poster. Some of them provided, indeed, very valuable comments that will help me a lot in my research.

*Javier Elena*



The 2003 ACA conference marked the end of my first year working in the field of crystallography. The conference allowed me to see many of the possibilities for research in the field. The weeklong conference not only provided an ample amount of time for me

to see many different areas of research, I was also able to meet many new people. The oral presentations were very interesting and informative. The poster session was a great time to share my work and future ideas with a plethora of knowledgeable people. Seeing other people excited about my work was amazing and made me even more motivated to return home and work even harder! This was the first scientific conference I have attended and it was a great learning experience. I want to thank the ACA for the opportunity to attend this conference, and I look forward to the next conference.

*Daniel Ferraro*



I would like to sincerely thank the ACA for the travel grant that allowed me to attend the annual meeting at Covington, KY. I am grateful for the opportunity to present my work at the poster sessions and I would like to thank everyone who showed an interest in my work and for

the valuable comments and suggestions. The selection of talks covered a broad range of subjects and I had a hard time deciding which ones to go to since many were of interest to me. I found the sessions concerning crystal growth and difficult structures especially helpful. The "Topics for Young Scientists" session was also very useful, giving me insights on my career as a scientist. Last but not least, I also enjoyed the social events and I was most impressed with the Newport Aquarium, the venue for the opening ceremony. Thank you again for your generosity and for a great meeting!

*Desiree Fong*



The latest innovations and discoveries presented at the 2003 annual ACA Meeting have provided me with a new level of motivation and enthusiasm for my research project. It was also a great opportunity for me to meet many established crystallographers and striving students in the field of macromolecular crystallography.

*Inside*

*MAR 1*

*Inside*

*MAR 2*

Among a wide range of topics presented at the meeting, I was particularly impressed by the ability of electron crystallography to effectively solve the megadalton-sized molecular assemblies. I would like to thank the ACA for their generous support in assisting me to attend the meeting.

***Noboru Ishiyama***



Obtaining a travel award for the 2003 ACA meeting in Covington, Kentucky gave me chance to attend my first big conference. It also gave me the opportunity to present my first scientific talk during the time-resolved x-ray crystallography session. This talk presented the research that I am currently conducting

in Andrew Mesecar's lab. I did not realize how big this conference was until the program came in the mail, and I had trouble deciding between which seminars I would attend. At first this made me a little intimidated, because I am a second year graduate student who would be speaking at a meeting with some of the most prestigious scientists in the field. However, I found everyone who attended to be very supportive and encouraging. I was also able to attend many useful seminars in different avenues of crystallography. Although I thoroughly enjoyed all of the lectures I attended, I felt that the series directed towards young scientists to be most beneficial. I was also amazed at the participation of the poster sessions in the evening. A few of the posters that stood out were P129 "*The Impact of the Beam Stop on Data Collection Strategies at Synchrotron Beam Lines*" R.W. Alkire, Robert Schuessler, Frank J. Rotella, John Goczny, Gerold Rosenbaum and PPX146 "*Protein Crystals Grown in vivo*". Nathan Coussens, Barbara Stay, Kenneth Murphy, Games Gray, Jason Telford, Ramaswamy Subramanian.

In addition to all the knowledge that I was able to obtain, I also had a wonderful time at all activities planned after the sessions. My favorites were the opening ceremony at the Newport Aquarium and the Rigaku-MSD dinner at Jillian's.

In the future I will look forward to the annual ACA meeting. It's a great conference that makes it possible to see how the field of crystallography evolves from year to year. I enjoyed getting to know other scientists and graduate students that share similar interests and who will be great contacts for future studies and collaborations. I would like to say thank-you to the International Union of Crystallography and the other generous donors that made it possible for me to participate in this event.

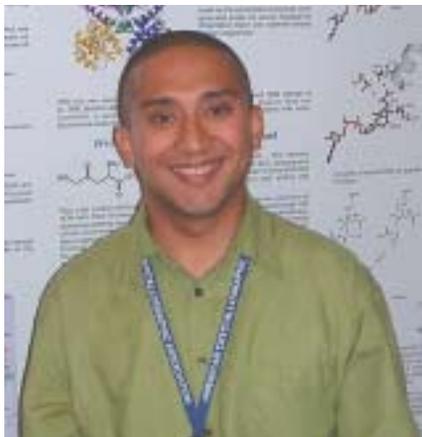
***Sonia Larsen***



First, I need to thank the generosity of the travel grant committee. The travel grant enabled me to attend the ACA meeting and still be able to pay rent and eat the next month. Probably the single best session I saw (other than the General Interest III session, which I chaired) was the Biomacromolecular Crystal Growth and Perfection session. The introduction and post talk summations made this session flow. I only wish there had been a few more talks scheduled. At that session Doug Juers had the best answer to the "What if hypothetical experiment question". The answer was "That's a good idea. You should do that and tell me your results." Jeff Habel's keen mind and sharp eyes were too much for a difficult protein but they were no match for Microsoft, as his computer decided to hibernate near the end of his talk. Additionally, I was surprised at how far the neutron scattering group has evolved over the last two years. At the L.A. meeting, there were some initial neutron results and a discussion of new sources. At this meeting, there were several sessions devoted to neutron scattering. I have not gotten a crystal large enough to try this technique. Tim Mueser demonstrated a novel cost effective approach to doubling the productivity of graduate students. The meeting was also a good time to see people that I generally only get to talk with by email or have worked with at the synchrotron. On the lighter side, I mistakenly missed the charter home from the opening reception at the aquarium along with a couple other people so we went to a few more places before cabbage it home. The next day we all seemed to be suffering from West Nile or some other illness. I think Brandon Collins set a new margin of victory record in winning the Rigaku/MSD fun run. The late night extreme training regimen that he and Steve Tomanichek used paid off. Unfortunately, I missed breakfast with some of the locals at the Waffle House near the end of the meeting. Finally, the Reds actually won the night a group of us went over to see the game.

***Jeffrey Lovelace***

ACA 2003 in Covington KY was my first opportunity to attend an international crystallography conference and what an experience it was. As an aspiring crystallographer I found it refreshing to interact with the movers and shakers in our field. I also very much enjoyed meeting fellow graduate students and learning about what other people are doing and getting the inside scoop on how to grow the perfect crystal. OK, so maybe I didn't come back with the secret recipe but I definitely learned of a few more things to try and hey, even if they don't work at least I'm still



in good company. As a rural kid myself, it was nice to get away from the hustle and bustle of the big city and enjoy Covington and Newport.. especially Newport, the Aquarium was really neat. Well, as anyone who knows me will tell you, I sure do like to talk and one of the coolest things of the

whole conference was being able to share my work with others; from the poster session to a mini-presentation on the plane back to home ACA 2003 provided ample opportunities for me to share and learn from the great crystallographic community. Thanks ACA!

*Ahmad Mirza*



Attending the 2003 ACA Annual Meeting has been a superb opportunity to interact with both other young scientists and those pioneers who have developed many of the crystallographic techniques widely used today. I am also glad that I was able to listen a lot of interesting talks and

to see many fantastic posters, as well as seeing the latest developments in the vendors exhibition. I would like to express my sincere appreciation to the organizers for financial support which helped me defray the costs. Furthermore the grant received from ACA allowed me to attend the 2003 Summer Courses.

I had the opportunity to present my own work about protein molecular weight determination and to discuss its theoretical aspects with experienced scientists. All these aspects broadened the scope of my doctoral research. I had also the chance to meet many nice and inspiring people, some of whom I knew only from books, papers or crystallographic programs. It was a great and stimulating experience.

*Hamilton B. Napolitano*

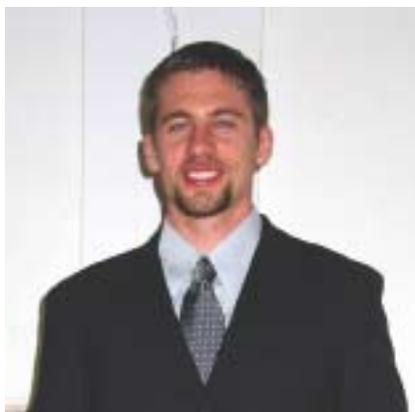
Attending the ACA meeting helped me meet crystallographers from all over the world. This was my first ACA meeting, and I had a great time! I met many talented people and learned about exciting projects. I appreciated all the opportunities to engage fellow scientists in conversations at the Young Scientists Mixer,



the MSC dinner and the poster sessions. These discussions gave me new ideas to try back at the University of Missouri-Columbia, where I am a graduate student. I was fortunate to not only receive a travel grant, but also to have the opportunity to present my work in the "Protein, Structure,

Function and Dynamics" section, chaired by Martha Teeter. My talk went well, and I received encouraging feedback from both professors and other graduate students. I appreciated all the feedback from these scientists, as this was my first oral presentation at a national meeting. All of the sessions were extremely informative, and I enjoyed all the graduate student presentations. I especially liked the "Difficult Structures" and "Structural and Functional Genomics" sections. In "Difficult Structures", Song Tan's presentation was of particular interest, because I have recently started working with a protein that expresses as inclusion bodies. The "Genomics" section covered a variety of systems and introduced me to new computational tools and analyses. Both sections made me excited about my own research and my future as a structural biologist. I look forward to sharing what I learned with my peers in Lesa Beamer's laboratory and to bringing new insight to my work. In closing, I enjoyed being immersed in crystallography topics for an entire week! My experience would not have been possible without the travel grant, which covered all of my expenses. I am very grateful for the funding I received, and I would like to thank the organizers for an excellent meeting. I hope to see you all again next year!

*Catherine Regni*



I would like to extend my gratitude to the ACA for providing me with a travel award that allowed me to attend the meeting this summer in Northern Kentucky. It gave me the opportunity to present my research for the first time to an international audience. Although my

talk was at the end of the conference, it was still reasonably well attended and I received some valuable questions and comments about my work. I learned quite a bit of crystallography from the other presentations at the conference, too. The time-resolved

diffraction sessions made me realize that crystallography can be used effectively to visualize dynamic processes as well as static snapshots, and I especially enjoyed Keith Moffat and Philip Anfinrud's presentations. The difficult structures session was also useful to me as a student to see problems that other people have encountered during macromolecular structure solutions and how they were resolved. The conference seems to be very valuable to those who are learning the technique of crystallography and I'll be back next year!

*Eric Schreiter*



I want to thank the American Crystallographic Association for the travel grant that enabled me to present my research at the meeting in Covington. My favorite sections that I attended were the new structures and difficult structures sections. It is always interesting and useful to see how other researchers have solved difficult crystallographic problems. I

also would like to thank the organizers of the New Structures section for inviting me to present my graduate research. As my first opportunity to present my research at a professional meeting, I would say that I thoroughly enjoyed the experience. I would also like to thank the ACA for giving me a Margaret C. Etter award for young lecturers. Attending the conference allowed me to make many contacts which will be invaluable in my search for a postdoctoral position. I look forward to seeing everyone next year at the ACA 2004 meeting and thank the organizers again.

*David Lodowski*

*In past issues of the Newsletter we have been featuring articles detailing the changes in procedures for obtaining visas to visit the US. In particular we have stressed the need to apply early. Unfortunately, one of our awardees did not get his visa in time for the meeting and sent the following note to the ACA President.*

Unfortunately, I am not going to be able to travel to the US to attend the 2003 ACA meeting. I really appreciated that I was selected by the ACA to receive a travel grant as a student from South America to present a contribution at the meeting. It was really a great pleasure to have received such support.

At this moment, the US Embassy in Caracas just made me the assignment for the interview they carry out with all the applicants to give the US visa entry to USA. Unfortunately, the interview will take place in about two weeks (after the meeting!). For



this reason, I have no other choice than to stay here without being able to attend the ACA meeting. I must say that the process of getting visa to travel to the US has become a very difficult one.

I would like to suggest that my place be taken by another student of our group who also is a co-

author in the work and is in a position to attend the meeting and present the same poster. She is Ana Vivas. In this way, the work titled "Characterization of Sediments from the Ocean Floor of the Venezuelan Atlantic Front Using X-ray Powder Diffraction Techniques". will be presented as programmed for her.

As a young scientist, I hope to be able to go to the USA sometime in the near future. It will certainly be nice to attend future scientific meeting and visit different crystallographic laboratories.

Giving again my thanks to you and the organizers,

*Cesya Cedeno*

*Editors note: Ana Vivas did make it to the meeting and presented the poster. If you need a visa to come to Chicago - Apply Early.*



#### Important dates to remember:

<i>Abstract submission</i>	<i>March 1, 2004</i>
<i>Travel Grant Applications</i>	<i>March 1, 2004</i>
<i>Advance Registration</i>	<i>June 1, 2004</i>
<i>Hotel Reservations</i>	<i>June 15, 2004</i>



**PROGRAM CHAIRS**  
**Christer Aakeröy**  
**and Marilyn Yoder**



**2004 LOCAL CHAIRS**  
**Karl Volz and**  
**Bernie Santasiero**



*Inside*

*Bruker 2*

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

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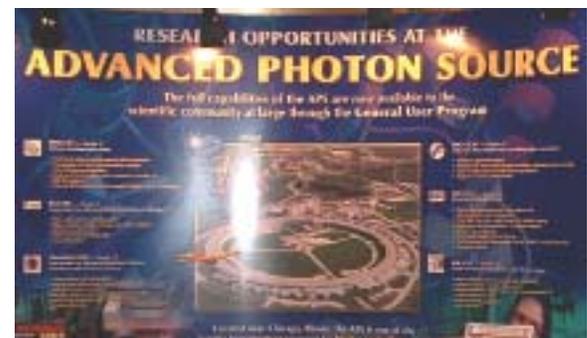
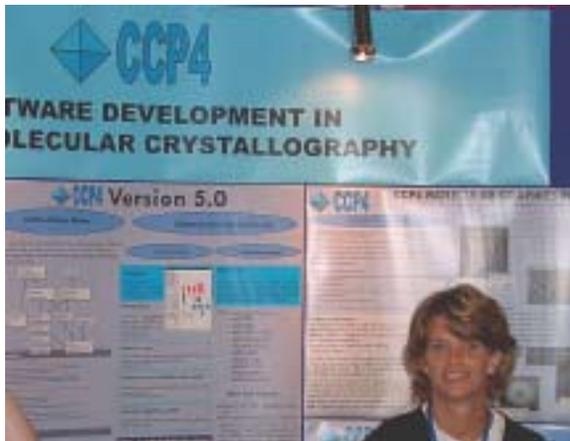
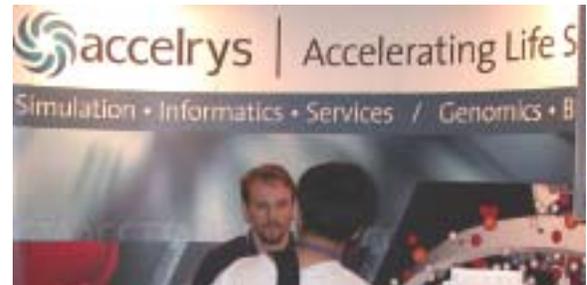
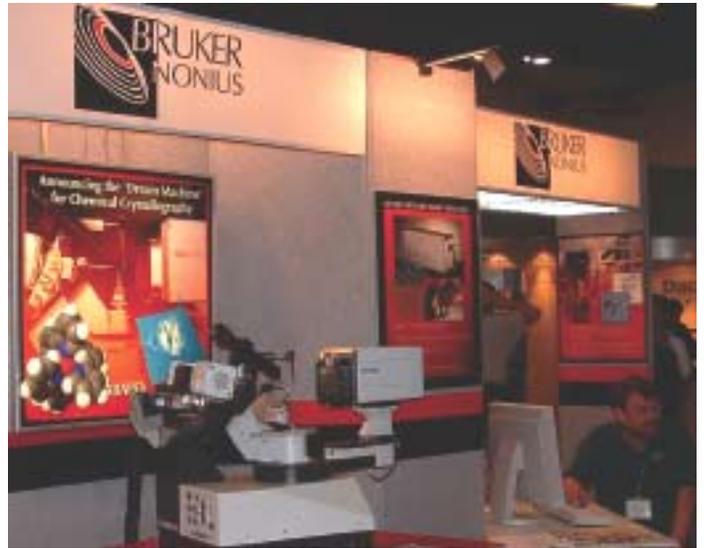
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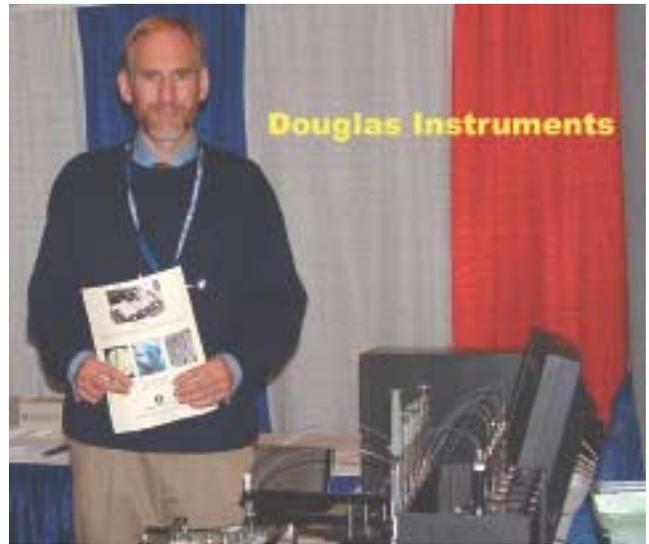
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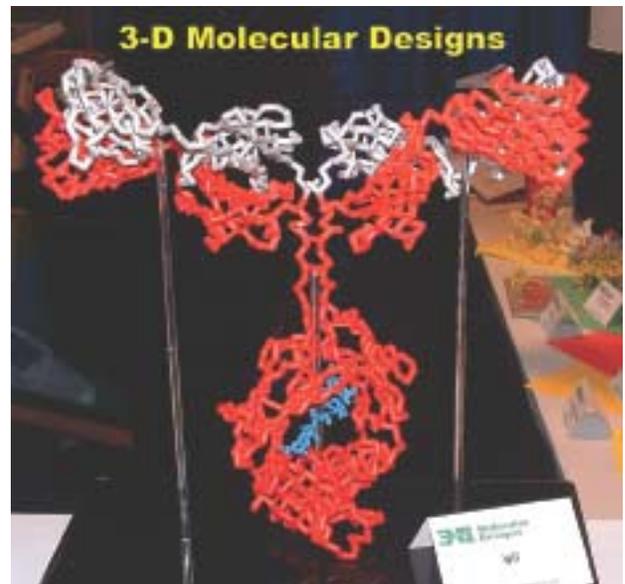
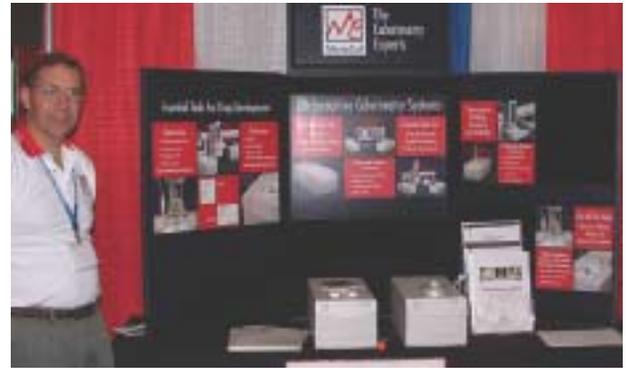
**ACA - 2003 Commercial Exhibits**

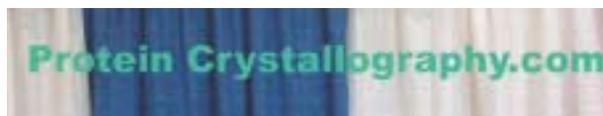
Under the sure hand of Bob Finnegan of the AIP the commercial exhibit at the ACA meeting in Covington set a new record with over 40 companies displaying their products and services. Almost half were new exhibitors, showing products and services that support structural genomics. It's amazing how fast things move from the seeming confusion seen here to the orderly informative exhibits represented on the following pages. Be sure to join us in Chicago where the show will just as exciting if not more so.

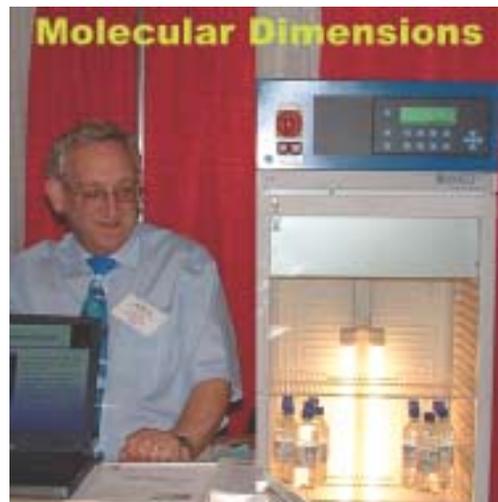
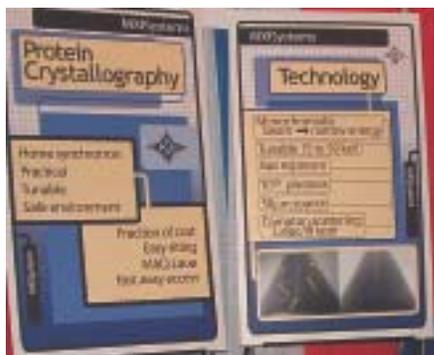














*USNCCr meeting - Covington, July 2003. Back row: Ken Downing, Ray Davis, Jim Kaduk, Ron Stenkamp, John Parise and Howard Einsphar. Middle row: Alex Chernov, Kathy Kantardjieff, Jian-Min Zuo, Tamae Wong, Kathryn Ely, Joel Brock and Cheryl Klein. Front row: Marilyn Olmstead, Charlie Carter, Peter Kuhn, Jon Clardy, Fran Jurnak, Bob Sweet, Bill Duax and Winnie Wong-Ng.*

**Results of recent USNCCr elections**

Members (2004-2006)

- Frank Fronczek** - Louisiana State
- Kathryn Kantardjieff** - California State Fullerton
- Matt Redinbo** - U. of North Carolina, Chapel Hill
- Brian Toby** – NIST

Member (2004)

- Ned Seeman** - New York University

Secretary/Treasurer

**Joel Brock** - Cornell (to serve 2004-2006) The USNCCr is currently seeking nominations for elections in the fall of 2004. Suggestions may be sent to any member of the Nominating Committee

- Ken Downing** ( [kdowning@lbl.gov](mailto:kdowning@lbl.gov) )
- John Parise** ( [john.parise@sunysb.edu](mailto:john.parise@sunysb.edu) )
- Ron Stenkamp** ( [stenkamp@u.washington.edu](mailto:stenkamp@u.washington.edu) )
- Cheryl Klein Stevens** ( [cklein@xula.edu](mailto:cklein@xula.edu) )

The USNCCr will be awarding travel grants for attendance at the IUCr Congress in Florence in 2005. Details will be printed in upcoming issues of the newsletter and posted to their new website [www7.nationalacademies.org/USNC-IUCr/](http://www7.nationalacademies.org/USNC-IUCr/).

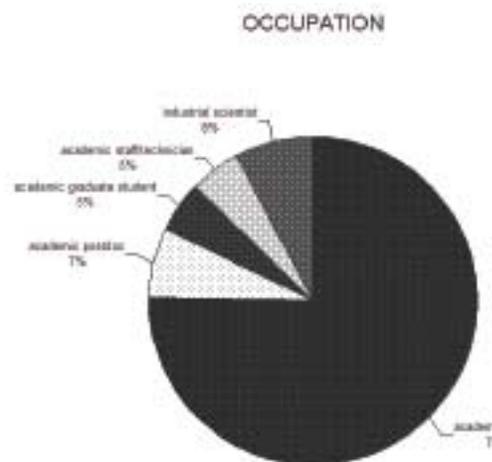
**Crystallography in a College/University Curricula**

The Education Committee of the USNCCr conducted a web-based survey between, April 25 and May 16, 2003. They asked the crystallographic community, through several popular list-serves, their opinions and views about the role and coverage that crystallography should have in an undergraduate or graduate curriculum in various scientific disciplines. There were 141 respondents.

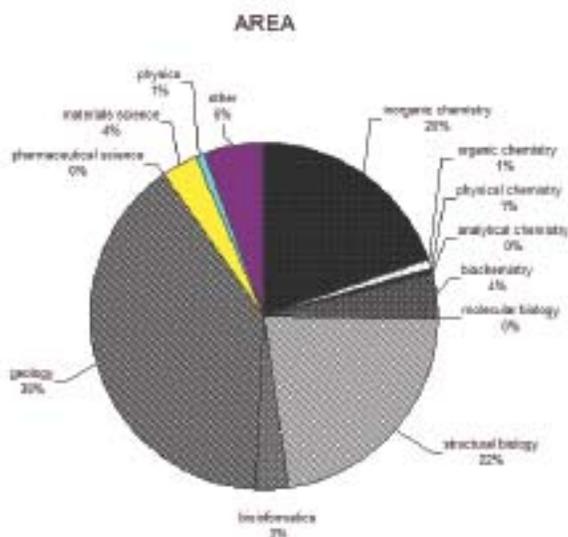
There were a range of comments in the survey, showing that the crystallographic community is somewhat polarized in its views. Crystallography is fundamental to most of what we know about the structure of matter at atomic resolution (including biochemistry), yet it is appalling how little it is covered. Some regard crystallography as no more important than electrophoresis or chromatography, while others feel we have created a generation of button pushers who can't do anything on their own.

*Inside*

*Rigaku/MSD 2*



Although those surveyed felt that they were adequately prepared to do their work, they feel less satisfied with the preparation of those whom they supervise, and across the board, everyone was generally dissatisfied with the coverage of crystallography in the curriculum, at the undergraduate *and* graduate level. There is a clear disconnect between preparation and curriculum.



**Some trends have emerged as “issues” from the results of the survey:**

1. Clients/users of databases thirst for education in critical evaluation/validation/assessment of structures, so that structures are not simply regarded as “gospel truth”, and people can critically read the literature.

2. Placing crystallography in the curriculum with adequate depth of coverage is not a trivial matter. The undergraduate curriculum is already impacted with subject matter and there is little room, not to mention time. Graduate programs are trying to speed the process from entry to PhD.

3. Unless the ACS specifically requires coverage of crystallography, the practice of teaching it will likely *not* be adopted.

4. Those called upon to actually teach the subject are not themselves crystallographers. Universities increasingly do not hire “crystallographers”.

5. Not everyone has instruments, and less people are aware that they can remotely access facilities.

6. There is an apparent paucity of good texts/teaching materials.

7. Increasingly, people rely on workshops and short courses to receive their education/training in crystallography.

**Recommendations of the USNCCr Education Committee:**

1. The USNCCr should seriously pursue submitting recommendations for inclusion of crystallography in the undergraduate curriculum as a requirement for ACS certification (to the same degree as NMR). The content should emphasize the fundamental importance of crystallography to the sciences, interpretation and assessment of structures.

2. Given the increasing practice of attending or sending students and post docs to professional development/training workshops and short courses, the USNCCr should work with the ACA to develop a set of course content guidelines for certification of crystallography workshops and short courses.

3. The USNCCr and ACA must then consider whether graduate education and training should be “certified” through workshops and short courses rather than in addition to completion of formal university courses.

4. Given the universal opinion that hands-on training and “apprenticeship” are essential to crystallographic education, particularly for those planning to practice crystallography rather than casual users, the USNCCr should work with the ACA and the ACS to increase awareness of availability of instruments by remote access, both at the undergraduate and graduate level. Institutions with remotely accessible facilities (particularly undergraduate institutions) need to coordinate efforts better.

5. The USNCCr has been asked to consider sponsoring/creating an online course in crystallography, or at least a repository of endorsed tutorials.

**Additional information:**

*The Journal of Chemical Crystallography* recently published a two-volume special issue 33(5,6) 2003 showcasing work at Predominantly Undergraduate Institutions (PUIs). The forward, written by the guest editor, Greg Grant, eloquently describes the current state of affairs and the near future.

The Center for Workshops in the Chemical Sciences, directed by Jerry Smith at Georgia State University, constitutes a consortium of 12 institutions/PIs (+ 2 discretionary) that host professional development workshops each year for faculty at predominantly undergraduate institutions. The W.M. Keck Center for Molecular Structure at Cal State Fullerton was selected in 2003 to host one of the discretionary workshops, “Crystallography for Chemists (and others!)”. This workshop, attended by 30 faculty, was very well-received, and it has now been added to the consortium, pending NSF renewal. In an open discussion at this workshop, faculty expressed support for the recommendations made in this report.

*Kathy Kantardjieff*

*Inside*

*Oxford cryo*

### 8th Annual Structural Biology Symposium of the Sealy Center for Structural Biology (May 2003)

The symposium, held in the UT Medical Branch in Houston, drew the largest attendance in its history, with more than 325 registered participants and 112 posters. The major topics were measurements of single molecules and methods for following the folding of proteins and RNA. Applications of these methods to drug design were also illustrated.

**Grab a single nucleic acid strand by its tail:** Several techniques that can be used to study individual proteins and nucleic acid molecules were presented. **Carlos Bustamante** (UC, Berkeley) opened the symposium with a demonstration of methods developed in his group to follow the packaging of DNA by phi29 phage. While one can find empty capsids, those with their tail assembly attached always contain DNA, indicating the necessity for order in the packaging process to obtain viable phage. In the phage particle, the DNA is compacted 6000x compared to its volume in solution. In order to determine the forces that are put on the DNA during the packaging, they used an optical trap and laser tweezers. The phage packaging system, consisting of a packaging motor (gp10), an ATPase (gp16), and a hexameric packaging small RNA (175 b), moves the ds-DNA into the capsid in measurable spurts, a segment at a time. He estimates that this motor can exert a force up to 55 pN, which makes it extremely strong compared to other biological motors. For example, myosin motors only exert forces of 3-5 pN. He estimates, according to his pressure measurements, that the pressure within the phage head is 10x that of a bottle of champagne.

One of the more interesting questions posed by these findings is why the phage chooses to exert such force to compact the DNA, when it could simply make a 2x larger head to package the DNA in a less condensed form. His answer is that the phage does not need to be efficient, as it uses the ATP of the host cell in the assembly process. Muscle fibers should be much more efficient, by this logic.

Several speakers presented other methods to study individual molecules. **Taekjip Ha** (Univ. of Illinois) presented three examples of how fluorescence energy transfer (FRET) studies, can elucidate the mechanism of folding of polynucleotides. By labeling the ends of each arm of the DNA with different markers, one can measure the energy transfer between the labels to determine the molecular configuration during branch migration. The technique allows them to visualize intermediates, for example, during resolution of a Holliday junction that would not be apparent using ensemble averaging. To study helicase, they have the DNA bound to streptavidin, which in turn is bound to PEG affixed to a glass surface. The helicase, T7 g4, is hexameric and the donut shape appears to move down the individual strands of the dsDNA to separate the duplex. They could also use FRET to follow the folding of single ribozymes.

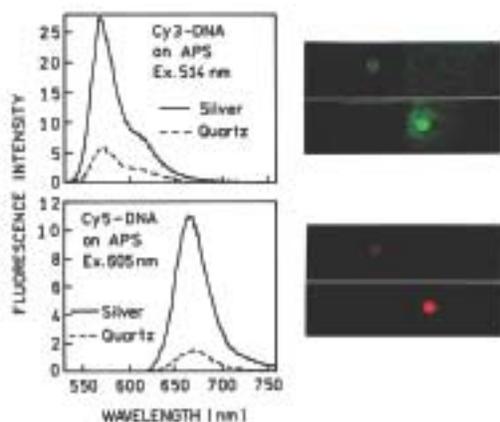
**Timothy Lohman (Washington U, ST. Louis)** showed how single turnover, DNA-unwinding studies could be used to study the mechanism of action of E. coli SF-1 DNA helicases Rep and UvrD. Mutations in the corresponding mammalian enzymes

have been characterized in many diseases, including Werner's and Blooms syndromes and *Xeroderma pigmentosum*. Helicases use the energy of ATP hydrolysis to open up the strands of DNA during replication and transcription. The mechanism for the *Bacillus stearothermophilus* helicase, PcrA, has been characterized as "monomeric inchworm", which means that the protein binds as a monomer and moves progressively down the DNA. However, both the SF-1 helicases, Rep and UvrD, are obligate dimers. While the UvrD protein self assembles into dimers and tetramers in the absence of DNA, the Rep protein assembles into a dimer after addition of DNA. His group showed that as the helicases were forced to a monomeric state by adding more DNA to the system, they ceased to have unwinding activity. Rep and UvrD monomers can translocate along ss-DNA, but cannot unwind duplex DNA. These results were confirmed by FRET measurements of DNA single molecule unwinding, done in collaboration with **Taekjip Ha**. Further, by varying the length of DNA in the assay, they could determine that the kinetic step size was 4-5 bp.

**Michael Brenowitz** (Albert Einstein College of Medicine, Bronx NY) described an approach to follow the folding of RNA molecules into their biologically active conformations with single nucleotide resolution. His model system is the 380-nucleotide *Tetrahymena thermophila* ribozyme, whose compaction can be induced by monovalent or divalent cations. The principal approach used is quantitative hydroxyl radical footprinting in which the solvent exposure of the polynucleotide backbone is determined by its relative reactivity to the hydroxyl radicals. For time-dependent experiments, an x-ray beam generated at the NSLS at BNL is used to generate high concentrations of hydroxyl radicals within milliseconds. RNA samples are mixed with the ions that induce folding and compaction in a special rapid mixing device. The distribution of folded and unfolded RNA molecules are 'sampled' by irradiation with the x-ray beam as a function of time after mixing. Thus, the time-evolution of the inside and outside of the RNA molecule can be quantitated and models describing this process critically tested. The synchrotron x-ray beam is an NIH-supported facility. Those wishing to use this unique resource for relevant research problems can contact Michael directly.

Many of the methods presented rely on detecting fluorescence. **Joseph Lakowicz** (Univ. of Maryland Sch. of Med.) showed that such measurements can be enhanced by using planar metal surfaces to enhance the radiative decay rate of fluorescent molecules and to better direct the radiation toward the detector. As the lifetime of the fluorescence decreases, the intensity of the emitted radiation increases. He showed several examples by which "radiative decay engineering" (RDE), can greatly increase the quantum yield of weakly fluorescent species. For example, the quantum yield of the weak fluorophore, rose bengal, increases in the presence of silver ellipsoids from 0.02 to nearly 0.48, while there is little enhancement of the strongly fluorescent dye rhodamine. The implications for RDE in biotechnology and biophysics are in many cases breathtaking, as increases in sensitivity even allow detection of the fluorescence from naked DNA. He suggested that RDE could be used to develop sequenc-

ing with unlabeled DNA, by using the slightly different emission maxima of each base pair. Yet another area of application is in improving the sensitivity of surface plasmon measurements by improving directional emission. Here, replacing the gold film with a (mirroring) silver one allowed the investigator to obtain an overall yield of emitted light that amounts to 60- 93% of the exciting beam.



*Lackowicz showed how using metal films could enhance fluorescence detection. The emission spectra of Cy3-DNA (left top) and of Cy5-DNA (left bottom) on APS-treated slides, is enhanced by silver island film. The silver film allows the signal to be seen clearly (right).*

**Physical Methods to follow protein folding:** Several elegant studies of protein folding and unfolding were presented. **Andres F. Oberhauser (UTMB)** showed how to use the tools of Atomic force microscopy (AFM) to measure the energy of protein unfolding. His method, which gives a completely different energy function than conventional solution unfolding measurements, is a mimic of the mechanical forces that proteins in the cytoskeleton or extracellular matrix are exposed to in nature. For example, titin, an elastomeric protein found in muscle cells, extends in response to a mechanical force. Many of the proteins that function in response to mechanical forces have a modular structure. These can be IgG like beta-sheet domains (fibronectin (FN), titin) or long alpha-helical domains such as in the spectrin fold. One can determine the force needed to extend single FN molecules. Domains in FN unfold according to their unfolding hierarchy where the weak domains unfold first. By mixing weaker domains of FN and stronger domains from titin, he showed that one could relate the unfolding dynamic curve to the protein architectural elements. The method offers a way to better characterize folding intermediates and misfolded states, and eventually to design proteins with enhanced tensile strength.

Hydrogen exchange methods can provide an atomic level view of the molecular search process of protein folding. **Walter Englander** (Univ. of Pennsylvania) a pioneer of hydrogen exchange (HX) methods, illustrated how HX-NMR could be used to follow the folding of cytochrome c and other proteins. Hydrogen exchange methods can provide a high-resolution view of the folding process at many identifiable amino acid positions

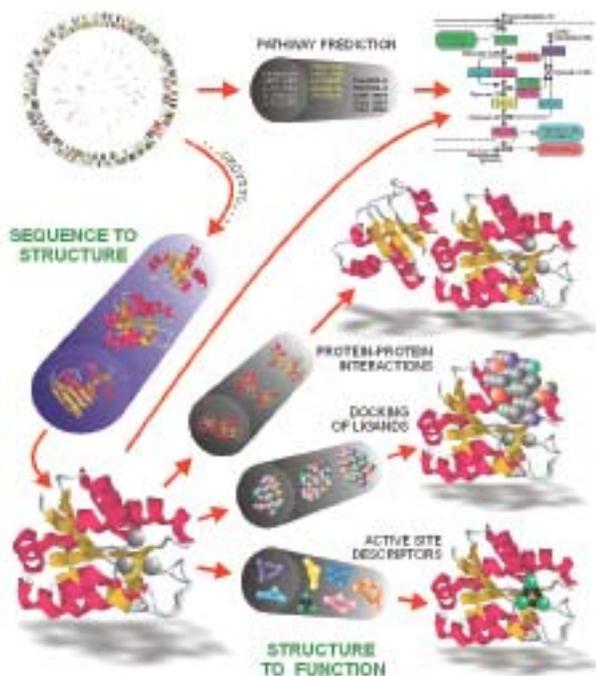
in a protein. In a method called ‘HX pulse labeling’, a transiently populated folding intermediate can be labeled by H-D exchange in a structure-sensitive way during the sub-second folding process. The labeling profile can then be read out later by 2D NMR of the native protein after folding is completed. The results show which amino acids were present in the intermediate. Another method, ‘native state HX’, can be used to follow the continuous unfolding and refolding of proteins even under native conditions. This behavior cannot be detected by other methodologies. By analysis of the labeled hydrogen positions, one can determine the structure of the folding intermediates and their pathway order of folding. In cytochrome c, there are several distinct folding units, which Walter refers to as “foldons”. These are identical to the intrinsically cooperative secondary structural units of the native protein, or groupings thereof. The sequence of pathway events is determined by the way these foldons are organized in the native protein.

Other methods can also be used to follow hydrogen exchange. For example, **Natalie Ahn** (U. Colorado, Boulder), uses mass spectroscopy (HX-MS) to monitor mobility in protein kinases. In one model system, she followed changes in the HX rate in local regions of the protein kinase, ERK2, upon activation by phosphorylation. Briefly, the protein is incubated at neutral pH in D<sub>2</sub>O for various times to allow exchange of protons for deuterons. The reactions are quenched by rapidly lowering the pH and temperature, and the labeled protein digested to peptides, which are separated and analyzed by ESI-LC/MS. By locating the peptides on the x-ray structure, she could follow changes in flexibility of the protein upon activation. The mobility of individual side chains upon enzyme activation was also followed by EPR, after coupling a nitroxide spin label to engineered cysteine residues. Comparison with a related kinase, p38 MAPK, showed similar patterns. However, the changes in HX seen upon phosphorylation/activation are quite different. Thus the patterns of conformational mobility in related enzymes differ. This is a very promising result, as it means that directing design to the mobile residues could lead to specific inhibitors of kinases. For example, regions outside the active site of MAP kinase-1 that show increased flexibility upon enzyme activation coincide with residues that interact with a specific noncompetitive inhibitor.

**Solvent conditions and energy states:** On the computational side, **Ken Dill** (UC, San Francisco) presented a simplified 2-D model of water that can account for some of its anomalous physical chemical properties, with respect to volume and density changes with temperature, and interactions with ions. In the 2D-model, individual molecules of water are viewed as Lennard-Jones disks with three radial arms for the hydrogen bonding potential, emanating from the center, like the Mercedes-Benz logo. Waters are strongly ordered by small (kosmotropic) ions, while large (chaotropic) ions order waters in the same way nonpolar solutes do. The bonds between the water molecules and small ions are stronger than those between ions with larger radii. This means that with smaller ions, the interaction is dominated by electrostatics. For large ions, the distance from the charge to water’s dipole is larger, so the electrostatic effect is less pronounced. The structuring of the solvent is changed due to the effect of

water molecules binding to each other in a “shell” around the large ion. Thus, the larger the ion the more disordering will be its effect on water structure. The model’s ability to account for experimental data (i.e., the effect of various salts on viscosity) indicates it may eventually help to explain the wide differences in the effects of cosolutes on protein stability.

**Peter G. Wolynes** (UC, San Diego) discussed preparing “knowledge based” energy functions that would better mimic how “nature’s” energy landscape determines protein folding. He made the point that the currently used energy functions cannot accurately predict the true structure of a protein as that with the lowest energy state. Thus, they must be missing terms that determine folding in the real world. He also pointed out that real proteins have been selected for solubility, while those that start from a random polymer of amino acids will probably not be. Thus, while a natural protein will have a major energy minimum, an atypical one will have many smaller minima. According to this logic, protein models with a well-defined energy well would be most likely to represent a true biological structure. Thus his group has developed a function that can be used to test whether the folding of a model of a novel protein is consistent with known, native state structures. He illustrated how this function can be used for *ab initio* modeling of proteins (i.e., for those where no clear template is available). The method can also be applied to designing novel proteins and in predicting interprotein interactions.



*The Skolnick group’s approach to obtaining both structure and function from genomic sequence data.*

**Protein modeling and design:** The *Critical Assessment of Techniques for Protein Structure Prediction* (CASP) are biannual competitions where groups submit models for target sequences of proteins whose structure has been determined experimentally but not yet made public. One of the top competitors in CASP5, held last summer, **Jeff Skolnick** (SUNY Buffalo), described

how programs developed in his group can automatically identify protein folds, active sites, and even protein quaternary structure from sequence data. Initially, the TOUCHSTONE program predicts the tertiary structure of the protein, using the PROSPECTOR threading algorithm. If a template is identified, they use their GENECOMP comparative modeling approach to determine structure. The resulting structure is then compared to a library of 3D descriptors of active sites (fuzzy functional forms, FFF) of known proteins to screen for regions that match in geometry and residue type. If they find an FFF match, they can attribute function to the protein. Overall, the CASP5 results were quite promising, even for proteins where the template was less clear. They then let the Threader loose on bacterial and yeast genomic data. The program was able to predict structures for 80% of the ORFs from bacterial genomes and 72% of those for yeast, compared to only 50% that would be possible with PsiBLAST and other conventional approaches.

The last presentation was by **Richard Brennan** (Oregon Health and Science University, Portland) on structural mechanisms of multidrug binding and induction by the transcriptional regulator, QacR from *Staphylococcus aureus*. The Qac family of multidrug transporters are integral membrane proteins that actively efflux mono and bivalent cationic lipids, quaternary amino compounds (hence Qac), disinfectants, antibiotics, and antiseptics, thus limiting the ability of these agents to kill bacterial cells. QacR is a 23 kD plasmid encoded protein, that regulates the synthesis of the QacA/QacB multidrug transporter genes. The mechanism by which QacR binds to DNA has been studied using crystal structures of the complex. The two subunits of the QacR dimer bind to consecutive major grooves and cause them to widen. QacR binds as a dimer of dimers. Binding of the first dimer to the DNA widens the major groove at one position, apparently enabling the cooperative binding of the second dimer to the DNA.

Having established the structure of the complex, they were able to account for how the protein recognizes such a vast array of structurally different substrates. Only one site per dimer is able to bind drugs, as the 2<sup>nd</sup> site is occluded by structural changes. The multidrug pocket is quite wide, about 1100Å<sup>2</sup>, and contains many aromatic and charged residues that allow it to bind positively charged molecules with different shapes. QacR can even bind two molecules at once. On binding of a drug, QacR undergoes a coil to helix transition, expelling two tyrosine residues from the pocket in the process. This structural transition is probably the signal for initiation of transcription from the QacA locus, which initiates the mechanism by which the drugs can then be exported from the bacterium. The structural information can contribute to the design of antibacterials that can elude the QacR signaling mechanism.

**Poster Awards:** This was a record year for posters; more prizes (\$300 each) were awarded in all categories. Winners were **Leila Reynald** (Johns Hopkins), **Payel Das** (Rice), **Matthew T. Auton**, **Wifredo A. Fernandez** and **James B. Hamburger** (UTMB), **Ganesh S. Anand** (HHMI, San Diego.), **Roberto Galletto**, **Jianquan Li** and **Joerg Roesgen** (UTMB).

Catherine Schein

*Inside*

*genomic*

## ACA Summer Course in Small Molecule Crystallography

The Course was held August 3 through August 13, 2003 on the campus of Indiana University of Pennsylvania (IUP), Indiana, PA. The attendees numbered 33 and there were 10 teaching faculty, including a representatives from Bruker-AXS and Rigaku. A questionnaire indicated that the great majority of the students judged the course to be highly successful. All teaching faculty are enthusiastic in urging that the course should be given again in 2004 and all look forward to returning in 2004.



The attendees included 18 women and 15 men (1 undergraduate, 22 graduate students, 3 postdoctoral fellows, 4 academic faculty and 3 from government or corporate labs). Twenty-three were US residents, 2 were from Canada, 4 from South America, 3 from Europe and one from India. Initially, the organizers decided to limit attendance to the first 30 applicants because of concerns about overcrowding the available space and facilities. Eventually, all 37 applicants were admitted, with the notion that many would be unable to accept. In fact 33 actually attended (see photograph). There were some complaints about overcrowding, but these were mainly over the shortage of computers. A computer was available for each of the ten work-groups but no allowance had been made for the daily surge of e-mail traffic for personal correspondence.

Of the ten teaching faculty (see photograph), five were present throughout the course and the remainder were present for six of the eight days in which instruction was given. *Steve Geib* was at IUP for three days and for the remainder was at the University of Pittsburgh collecting data on the Bruker-Axs APEX diffractometer which was electronically linked to the x-ray Lab at IUP. On Sunday August 10, all attendees went to Pittsburgh to visit Steve's lab.

The lecture notes for the 2003 course were almost completely revised from the previous 2000 version. Each morning, three formal lectures were given to all attendees. On some days, lectures on special topics were also given during the afternoon or evening sessions, e.g., on radiation safety and on searching crystal databases (Cambridge, powder diffraction and inorganic). An excellent supplemental lecture on macromolecular crystallography was prepared by *Lynne Howell* and presented by *David Smith*.

Tutorial sessions were presented during the afternoons and evenings. *Curt Haliwanger* (Bruker-Axs) and *Tom McNulty* (Rigaku) were invaluable contributors throughout the Course by presenting tutorials and giving individual help. Tom spoke on powder diffraction emphasizing the diffractometer hardware and software and Curt spoke on the use of the SHELXTL software package. *Pat Woodward* presented a tutorial on the use of the GSAS/EXPGUI and CRYSFIRE software packages. All faculty participated in smaller group or individual instruction, e.g., on symmetry, crystal mounting, probability methods and data collection.

About half the attendees brought single crystal or powder samples for data collection and analysis. The two single crystal diffractometers (CAD4 and APEX) were operational throughout the course. During the first morning coffee break at IUP, attendees surrounded the terminal linked to Steve Geib's lab at the University of Pittsburgh and were rewarded by a graphical data display, followed closely by the first structure determination. It was remarkable. A total of ten data sets were collected. Six structure determinations were completed and presented by attendees on the final morning, although by then, more than half the attendees had left for the airport.

Unfortunately, the two powder diffractometers (Bruker D8 and Rigaku Miniflex) were both plagued with down-time. Both the Rigaku and Bruker representatives made heroic efforts (including many phone-calls) to get their machines up and running. However, only two powder diffraction data sets were collected. These difficulties were offset by data sets that Pat Woodward had brought with him. These provided the opportunity for attendees to analyze powder data, e.g. to carry out Rietveld analyses.

While the experimental side of the powder diffraction initiative was largely frustrated, the idea of including a significant powder component in the course for the first time was clearly welcome. It was only a group of about six attendees who said they were not interested in powder diffraction. Pat Woodward and Tom McNulty are to be commended for their efforts to satisfy the needs of the large majority.

Questionnaires were completed and handed in by 26 of the attendees, most being unsigned. Attendees were asked to respond to each question with a score from 5 (excellent) to 1 (poor). The reverse side of the page invited detailed comments and in many cases these were copious, thoughtful and useful.

All but one person said they would recommend the course to others. Average scores for whether they enjoyed the course were 4.4 (scientifically) and 4.5 (socially). Regarding the duration of the course (Aug 3 to 13), 21 said it was about right. The course location (IUP) received a score 4.4. The course administration scored 4.2 for advance publicity and information and also 4.2 for responsiveness to their needs. Housing scored 4.1 for room assignments (all scholarship students and a few non-scholarship students were assigned to double occupancy apartments), 3.4 for quality (complaints centered on poor pillows) and 4.0 for cafeteria food.

Regarding the instructional program, the highest score (4.7) went for the value of the lecture notes and the lowest (3.1) went for

the adequacy of the computing facilities (12 PC's were available, all preloaded with software). Asked whether the instruction met their needs, the result was 4.1 for the lectures, and 3.7 both for the tutorials and experimental sessions. The lowest score under experimental was 3.4 for the time available for data collection.



*Summer course faculty - Back row: John Woolcock, Dave Smith, Bob Blessing and Bryan Craven. Front row: Charles Lake, Curt Haltiwanger and Brian Wargo. Faculty not in the photo: Patrick Woodward, Tom McNulty and Lynne Howell*

The afternoon tutorial and experimental sessions were not as well received as the formal lectures, as was clear from the written comments of the attendees. The organizers and faculty did their best but they were too few for the job. Many good suggestions came from attendees as to how these sessions could be improved. It is expected that most of the problems in 2003 will be eased by having additional faculty.

The organizers are grateful for direct financial support (\$7500) from the ACA, the IUCr, the Pittsburgh Diffraction Society, Rigaku and IUP. This enabled us to award full scholarships to almost half the attendees. The fee for non-scholars was \$494 which covered lodging, meals and tuition. A carry-over of \$1022 is available for 2004.

We also acknowledge the critically important support not recorded on our balance sheet. This included the presence of the representatives from Bruker-Axs and Rigaku who were indispensable as faculty. IUP Departments provided air-conditioned classrooms (Chemistry), a teaching lab (Geosciences) and computing facilities (Physics). IUP also provided two vans used for airport shuttling and for the excursions to Pittsburgh and to the picnic at the Craven alpaca farm. Brian Wargo was widely appreciated for driving attendees to go shopping, dining out and for dealing with a medical emergency.

The faculty are already discussing improvements and how to build on the successes achieved in 2003. It is planned to offer the Course again following the ACA Meeting in July, 2004.

*Bryan Craven and Charles Lake.*

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*Inside*

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**61st Pittsburgh Diffraction Conference October 29  
– November 1, 2003, Rutgers University**

The first session of this year's Conference, "**The Powder-Single Crystal Diffraction Interface**", was chaired by **Qi Bao** (Bristol-Myers Squibb). This intriguing title and the talks during the day emphasized that the boundary between single crystal diffraction and powder diffraction is becoming blurred. Accurate structures that were once only obtainable in the realm of single crystal diffraction are now becoming routinely available using powder diffraction. The first talk of the day by **Peter Stephens** (SUNY Stony Brook) emphasized this point. He highlighted that high quality powder data is obtainable using the new beamlines available for powder work and indeed this higher quality data has often been found to be a necessity for correct structure solution. This was followed by a talk by **Cikui Liang** (Accelrys Inc.) who described the new powerful algorithms incorporated into software available from Accelrys and how these could make formally very difficult problems routine. **Douglas Dorset** (Exxon-Mobil) explained the utility of electron diffraction in removing some of the indexing ambiguities that are common in the field of x-ray powder diffraction of zeolites and that electron diffraction can be also used more quantitatively if more careful data is collected. An interesting talk by **Maxim Lobanov** (LANL) described his work on the characterization of hydrogen clathrates using neutron powder diffraction. The modeling of disordered guest molecules at high temperature using a rotator model was fascinating, as was his introduction to hydrogen fuel cells. **Gu Xu** (McMaster University) introduced some novel methods for obtaining atomic images for nano- and bio- non-crystalline structures including single beam x-ray holography and phasing using Bragg peak profile asymmetry. The use of these new methods in the solution of the structure of multiwall carbon nanotubes was presented. **James Kaduk** (BP Chemicals) presented his work on ammonium salts of carboxylic acids. The usefulness of quantum mechanical calculations in determining hydrogen positions in powder structures was discussed. **Abe Clearfield** (Texas A&M) gave a review of his work with powder diffraction over the course of 25 years. The changes in the field over the period from initial crude attempts to today's use of synchrotron radiation and sophisticated software was enlightening. The final talk of the day by **Rob Grothe** (UCLA) revealed how methods development can come from attempts to solve a very specific problem. His work on determining the structure of amyloid fibers led to an analytical method for extracting intensity data from powder data using an area detector. To do this an explicit model of the sample texture was required and could be extracted using the angular profile of the diffraction rings. It was generally agreed by the audience that his newly developed methodology would be very powerful in many other cases.

Overall the session showed that the interface between crystal and powder diffraction is indeed becoming blurred and the overlap between the two fields will continue to grow as progress in powder diffraction continues.

Friday's session "**Macromolecular Complexes of Biological Interest**" was organized by **Helen Berman** (Rutgers University)

and sponsored by the Protein Data Bank. It opened on a festive note, with **Erica Ollmann Saphire** receiving the 2003 Sidhu Award presented by Tom Koetzle. Erica carried out her post-doctoral work in the laboratory of Ian Wilson and has recently accepted a position of assistant professor at Scripps in the Department of Immunology.



She gave an outstanding presentation on her work with Ian Wilson on the "Crystal Structures of a Broadly Neutralizing Antibody: Implications for HIV-1 Vaccine Design and Immune Effector Function". Her dynamic descriptions of the structure determination of the intact antibody B12 as well as the complex of the Fab of this antibody with a phage-display generated

peptide, B2.1, established a theme carried throughout the day of using "the dance" as Helen Berman described it, to illustrate structural features and re-arrangements. Erica discovered that the power of Ab B12 may lie in its extra long H3 antigen-binding loop and its extended presentation away from the surface of the antibody. In addition, the docking of this antibody's active site with the crystal structure of truncated GP120 using the Scripps program Autodock revealed that B12 is unique among the other phage-display generated antibodies in its ability to bind the oligomeric state of GP120. These conclusions were confirmed by mutational studies. Erica observed that the crystal packing of the intact B12 antibody formed a hexamer through the Fc domains and presented the hypothesis that this is a biologically relevant state by modeling the binding of this hexamer to the hexameric form of C1q. This led to the proposal of a model for complement activity and for the possible binding of the C5 protein with both the C1q and the Fab portion of IgGs.



Following the coffee break, **David Sayre** (SUNY Stony Brook) presented his work on "Diffraction Imaging of the General Particle". He demonstrated that feasibility of performing X-ray diffraction of single particles of small size (<10microns) which may include oligomeric complexes, organelles or even small whole cells.

He laid out the historic progression of the development of this technique that started with his first publication on the possible application to non-crystalline materials in 1980. Since then the methodology has developed substantially and David has shown a synthetic two-dimensional example where the x-ray diffrac-

tion experiment regenerated an object containing letters to high accuracy. The technique takes advantage of the fact that the diffraction is not limited to Bragg spots but rather is continuous, a phenomenon that offers phase solution. He called on the community of crystallographers to partake in this new frontier and to join the 6 laboratories currently investing time and research in making it happen. A measurement of the diffraction of a freeze-dried dwarf yeast cell of about 3 microns was at 12 nm resolution with  $10^9$  over-sampled Fourier terms. The current obstacle to the success of this methodology is the radiation damage to the specimen and the inability to average the information over a number of similar, yet not identical, samples. The solution to this problem might be, according to Dr. Sayre, in the use of very strong radiation and the collection of data over femto-second time scales in which the specimen did not have a chance to be effected by the radiation. For a follow-up review to this intriguing and thought-provoking presentation, see *Structural Chemistry* 13, 81-96 (2002).



**Back row:** Art Olsen, David Sayre, Ada Yonath, Eddy Arnold, Wah Chiu, Erica Sapphire and Cathy Lawson. **Front:** Helen Berman

**Ada Yonath** (Weizmann Institute) gave a wonderful talk about the outstanding structure of the largest non-symmetric macromolecular structure determined – the ribosome. In this talk Ada focused on a few of the amazing features of this complex system and in particular the binding of tRNAs, the translocation of these tRNAs through the three sites of mechanistic importance and the entrance and exits of the mRNA and nascent protein. Ada made her molecules dance in front of us to demonstrate the motion of the ribosome during tRNA incorporation and translocation. The movies are available for a minimal fee at [zoreq@bezeqint.net](mailto:zoreq@bezeqint.net). The ribosome is likened to a duck with a head that changes conformation upon tRNA binding, a neck along which the mRNA rolls like a necklace and two arms (stalks) that pull and push the mRNA through the neck. Various antibiotics affect the process at different stages, some freeze the platform movement thereby stopping translocation while others compete for the tRNA binding or place themselves in the PTC cavity or where the peptide bond is formed. A beautiful presentation of the symmetry of the P region as it relates to the A region demonstrated how the first tRNA must rotate through a two-fold rotation axis to make room for the second tRNA that will then position the amino acids in perfect orientation for peptide-bond formation. Her talk was awe-inspiring, and a tribute to her perseverance.

The first speaker after lunch was **Wah Chiu** (Baylor College of Medicine). His talk, “Electron Microscopy of Macromolecular Assembly at Sub-nanometer Resolution,” revolved around the acrosomal bundle. He referred to the dance in his presentation as that of a courting dance of the horseshoe crab sperm in which a major conformational change in actin filaments afford the incorporation into the egg. He made the case for the ability of electron microscopy to theoretically obtain information beyond 2.5 Å since the wavelength of the instrument is in the sub-angstrom length and the specimen can be frozen as a hydrate while the phase information is directly obtainable. As in David Sayre’s talk, radiation damage is the limiting factor and the solution is to use low dose images in many-fold duplication. Sub-nanometer range was described as that between 10<sup>-7</sup> Å. Data collected on the acrosomal bundle of filaments in the unit cell of 145, 145, 765 Å consisted of 50,000 observations, 16,000 unique from 153 different bundles and a total of 1000 segments. This filament contains actin, scruin and calmodulin. The image reconstruction and the use of the known structure of actin gave rise to the arrangement of actin molecules in the filament with the scruin molecules acting in a binding role. It was seen that actin becomes distorted by the presence of scruin and that causes adaptation and affects the symmetry. The calmodulin molecules were not found. Other projects that Dr. Chiu presented included the bacteriophage P22 with icosahedral T=7 symmetry. Two different states of this virus, the intact and the pro-capsid, demonstrated the conformational re-arrangement of the components through an opening and a twist of the domains. The 5.5 Å structure determination of cytoplasmic polyhedrosis virus (CPV), an insect virus comprised of 5 proteins, required analysis of thousands of particles, while the cryo-EM of GroEL is the gold standard. He clearly presented this breakthrough technology of cryo-electron microscopy as a tool in the forefront of non-crystalline structure determination.

The following presentation by **Arthur Olson** (Scripps) was a multi-media extravaganza. He took the theme of dancing to real-time videography in his talk “Back to the Future – a Tangible Approach to Protein Interactions”. In the first half, Art described the docking programs that have been developed at Scripps, such as Autodock and Surfdock that give reasonable atomic details with no presumption of location and no flexibility. These are rapid techniques in that they use a set of pre-calculated values to describe the environment the ligand will observe as it approaches the stationary target. It uses a stochastic search. As an example, in addition to that presented in the first talk, the interaction between tissue factor (TF) and factor VII in the coagulation process was investigated. “Back to the Future” referred to the pre-computer graphics practices of using physical models as research and communication tools even as far back as 1803 for crystal habits. Harvy, Kekule and Linus Pauling were examples of users of just this type of tool. Interestingly, the Kekule and Hoffman models created with croquette balls had the same color-coding that we use today in computer graphics. Art has embarked on the creation of real physical models with a powder printing technique. These models offer more than computer graphics, especially when used in collaborations, in

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that they engage many senses, encourage social interactions and use natural intuitive behaviors. The beauty of this approach was apparent when Art showed that one can combine the power of the physical model with that of computer graphical information by adding an annotation from the computer database onto the video image of the physical object through the use of ARToolkit markers that label the physical object for the computer's use. This integration of techniques, such as the insertion of drugs into the pocket of the physical model as observed on the video screen, stimulated the audience, as did his thought-provoking lecture on the future of computation and reality.

**Cathy Lawson** (Rutgers University) spoke about the multi-protein, multi-step structure determination of the catabolite gene activator protein (CAP) complexed to other protein and DNA partners in the "Structural Basis of Transcription Activation". CAP recognizes the sequence TGTGA. It is a 45 kDa protein with an N-terminal dimerization domain and a C-terminal DNA binding domain with a helix-turn-helix motif. It was the first transcription activator solved in 1981 by the Steitz laboratory. CAP bends the DNA and it has a kink in it as well. Intriguingly, the crystallographic structure demonstrated that the region of the kink at the second T of the consensus sequence does not directly contact the protein. It is an indirect recognition with very high affinity. A structure of CAP bound to a TGCGA sequence retains the kink while gaining a direct interaction with the protein at Glu 181. Interestingly, mutation of this Glu181 to Asp eliminated the kink. This leads to the conclusion that the DNA structure depends on the DNA-protein interactions. A ternary complex of CAP-DNA and the C-terminal domain (CTD) of the alpha subunit of RNA polymerase was also solved to 3.1 Å. In it there is an apparent water molecule in the minor groove of the DNA as it interacts with  $\alpha$ -CTD. The interactions between CAP and  $\alpha$ -CTD are in agreement with the mutational analysis of these proteins. Kathy presented these complexes so that we could view them from all directions in a "dancing" display in line with the day's theme. Her interesting presentation culminated with the anticipation of a future structure that includes region 4 of the  $\sigma$  subunit of RNA polymerase to form the complex CAP- $\alpha$ CTD- $\sigma$ R4- DNA.

**Eddy Arnold** (Rutgers University) finished off this wonderful session with an exciting talk focused on the "Use of Crystallography to Design Drugs Targeting the AIDS Virus Reverse Transcriptase Enzyme". The fascinating molecular machine that converts the viral genetic material (RNA) into DNA for further replication and integration into the host cell is a moving target. This is a result of the high mutation rate of the enzyme that affords a change every cycle of multiplication. Non-nucleoside reverse transcriptase inhibitors (NNRTIs) have been developed that bind near the polymerization active site but not in place of incoming nucleotides. The binding pocket for these inhibitors is formed by conformational changes to a hydrophobic region of the protein in the presence of the inhibitor. In a structure-based drug design project in collaboration with Paul Janssen of Belgium a new series of NNRTIs was discovered. An important factor in designing potent anti-HIV drugs is their ability to maintain activity even against the escape mutations. Of this new series one drug in particular, TMC125, shows nanomolar activity against

all mutant strains of HIV-reverse transcriptase. Interestingly, the most effective drugs produce poor quality diffracting crystals and Eddy advanced the hypothesis that flexibility may be the key to both the poor quality of diffraction as well as to the ability of the drugs to evade the drug-resistance mutations. The drugs need to be able to wiggle out of constrained conformations formed by the mutations and need to be able to jiggle in the pocket to form strong binding. The wiggle and jiggle dance may be key in this structure-based design of drugs.

At the banquet on Friday night current PDS president, Dave



Smith, presented the Chung Soo You student poster award to Jayita Guhaniyogi for her poster entitled "Structural Analysis of the Chemotaxis Regulator, CheY, with the C-Terminal Peptide of its Phosphatase, CheZ."

On Saturday, **Dr. Kandalam "Chary" Ramanujachary** chaired the final session on "Teaching Diffraction to Undergraduates/Graduates." After opening remarks by Chary, the 1<sup>st</sup> talk of the day was presented by **Joseph Potenza** (Rutgers) who spoke of "Thirty-five Years of Introduction to X-ray Crystallography." Joe gave a very engaging and entertaining talk about where crystallography was 35 years ago, how it has evolved over these decades, where the science is now, and then posed the question: "Where do we think crystallography will be in the next 10-20 years?" He talked about changing from a rigorous 1-year course to a shortened, slightly less mathematical one, but still holding to the principle that students can master this material if they wish.

**Glenn Yap** (University of Delaware) gave a talk describing "Evolving a Conceptual Approach for Introductory Crystallography" which described his teaching of an introductory course for the past 7 years. His main thrust was that students should have a "top to bottom" organization of conceptual units. Here, the students learn each unit and then the postulates used are deconstructed in a regressive fashion to move down the pyramid and get the most physical, theoretical and basic concepts later on. I believe that he only has 10 weeks in which to give the course.

**Feng Chen** (Rider University) presented "Introducing X-ray Powder Diffraction to Undergraduate Students." She spoke of introducing powder diffraction to students at all levels of instruction, in the general chemistry course for science majors, basic instrumentation and data analysis in analytical chemistry lab and advanced inorganic chemistry lab, and also in supervised study and independent research.

**Brian Bahnson** (University of Delaware) spoke on "From Crystals to Protein Function: Seeing the Forest Through the Trees." Brian told us about teaching students in structural biology who are of diverse backgrounds. He integrates protein crystallography with protein production, protein analysis, and crystallization of protein and structure solution; students compare structures using macromolecular NMR.

**Charles Lake** (Indiana University of Pennsylvania) gave a talk in which he described how he has been instrumental in getting XRD related experiments into various courses: phase changes in physical chemistry; standard addition techniques used to determine % composition of calcite in antacids in analytical chemistry. He is getting people in physics, in geochemistry, and in material science to get involved with powder diffraction.

**Robert Pipal** (Alfred University) presented his work with students without access to instrumentation. He has a very small number of students, and teaches the basics of x-ray crystallography. He has a number of data sets that he solves with the students (to show the process), and then gives each student their own data to solve and refine and finally write up as if it were to be sent on to a journal. Finally, he and his students synthesized a new compound, had data collected, and solved and refined the structure.

**David Grossie** (Wright University in Dayton), described his 10-week course in crystallography. Some of the questions he tried to answer were: How deep into diffraction do you go? Do you need Bragg's law? Talk about powder diffraction, or just single-crystal? Is diffractometer necessary? What kind? Hands on or not? Teach students to handle and mount crystals? Software necessary? What do students take away?

*Andrew Brunskill and Roger Lalancette*



On April 24, IUCr President, Bill Duax, was standing on a boulder on the edge of a beach in British Virgin Gorda, when a wave washed over the boulder and threw him 6 ft to the surface of another boulder, breaking his leg. Six ambulances, one ferry boat, two airplanes (including a saber jet), 4 different sets of traction apparatus, 150 medical personnel, and 36 hours later he was in Buffalo where an orthopedic surgeon put his leg back together with a 12 inch titanium plate and 13 screws. Two months later he began walking with the aid of a cane. Then in November, the titanium plate broke (that's probably one for *Ripleys*) and Bill found himself back in surgery. He now has a shorter piece of titanium and fewer screws holding his left together. He's currently using one crutch and should be back to the cane early in 2004. We hope that by ACA 2004 he will have discarded the cane.

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 Gary L Gilliland  
 Elihu Goldish  
 Joseph Xiaomin Ho  
 Hakon Hope  
 Carol P Huber  
 Jeanette A Krause-Bauer  
 Marilyn Morgan Olmstead  
 George M Sheldrick  
 Clara B Shoemaker  
 William C Stallings  
 Cynthia Vianne Stauffacher  
 Robert M Sweet  
 Dale E Tronrud  
 Thomas Webb  
 Mark Whitener

***Warren***

Michael J Bedzyk

Blake Industries, Inc.  
 Abraham Clearfield  
 Henderson Cole  
 Philip Coppens  
 John M Cowley  
 David E Cox  
 William L Duax  
 Takeshi Egami  
 Gary L Gilliland  
 Heinz Jagodzinski  
 Bennett C Larson  
 Allen C Larson  
 Gabrielle G Long  
 Richard J Nelmes  
 Clara B Shoemaker  
 Lester A Siegel  
 Cynthia Vianne Stauffacher  
 Hugo Steinfink  
 Robert M Sweet  
 Michael K Wilkinson  
 Elizabeth A Wood  
 R A Young

***Wood Writing***

S C Abrahams  
 Helen M Berman  
 Robinson D Burbank  
 Connie Chidester  
 Abraham Clearfield  
 Ann S Cooper  
 Gary L Gilliland  
 Jane F Griffin  
 Ethan A Merritt  
 Timothy J Rydel  
 Clara B Shoemaker  
 William C Stallings  
 Robert M Sweet  
 Norman M Walter  
 Elizabeth A Wood

***Undesignated***

Joseph C Calabrese  
 Jon Clardy  
 Abraham Clearfield  
 Edward J Collins  
 Richard D Gilardi  
 Gary L Gilliland  
 Allen N Goland  
 Douglas M Ho  
 Menahem Kaftory  
 G T Kokotailo  
 Saul Krasner  
 Thomas Laube  
 Christian Lehmann  
 James W Pflugrath  
 Marc Lee Pusey  
 David R Rose  
 Michael G Rossmann  
 Nadrian C Seeman  
 Stephen R Sprang  
 Boris Strokopytov  
 Thomas C Terwilliger

### **High Resolution Drug Design Meeting, Bischberg-Strasbourg May 13 - 16 2004**

For more information check the fall issue of the Newsletter or the meeting website at <http://www-igbmc.u-strasbg.fr/HRDDM.html>

### **The XVI International Summer School on the Physics and Chemistry of Condensed Matter entitled Structural Aspects of Solids, Bialowieza, Poland from 1st to 10th July 2004**

Organized by the Institute of Experimental Physics University of Bialystok under the auspices of the Committee of Crystallography, Polish Academy of Sciences.

General information and a registration form can be downloaded from our website:

[/alpha.uwb.edu.pl/schoolXVI/](http://alpha.uwb.edu.pl/schoolXVI/) The School is dedicated to structural properties of solids. Special attention will be paid to:

- \* *charge and spin density distributions in modern materials, biomaterials in particular*
- \* *structure of proteins and pharmacological compounds*
- \* *solid-state reactions*
- \* *structures of solids with highly correlated electrons*
- \* *solids under high pressure*
- \* *structures in excited states*
- \* *chirality in solids*
- \* *software problems in structure determination*
- \* *modelling solids*

### **13th Annual CCP13/Fibre Diffraction & Non Crystalline Diffraction Meeting, 2-4 June 2004**

Institut Laue Langevin/ESRF, Grenoble, France

Contact: Trevor Forsyth ([tforsyth@ill.fr](mailto:tforsyth@ill.fr)) [www.ccp13.ac.uk](http://www.ccp13.ac.uk)

### **Gordon Research Conference on Diffraction Methods in Structural Biology, July 11-16, 2004 at Bates College, Lewiston, Maine**

The 2004 Gordon Research Conference on Diffraction Methods in Structural Biology will be a highly interactive meeting focusing on advances in methodology for macromolecular x-ray crystallography and other diffraction applications, with highlights of particularly significant structural results. All participants will be expected to contribute extensively to discussion, to present either a talk or a poster, and to attend the entire conference.

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

Confirmed topics, session leaders and speakers include:

- \* *Pushing the limits of synchrotron techniques*  
E. Garman/K. Moffat/A. Podjarny/ G. Schertler/ A. Soares
- \* *Long-wavelengths for phasing*  
A. Leslie / M. Weis / Z. Dauter / B.-C. Wang
- \* *Ab initio methods*

V. Lunin / P. Gros / S. Ursumtsev

#### \* *Software development*

R. Grosse-Kunstleve / Z. Otwinowski

#### \* *Data and structure analysis*

G. Kleywegt / T. Yeates / T. Schneider / J. Richardson

#### \* *Substructure determination*

C. Weeks / C. Giacovazzo / G. Sheldrick

#### \* *Phasing and density modification*

E. Dodson / R. Read / G. Bricogne

#### \* *Model building and refinement*

V. Lamzin / A. Perrakis / T. Ioerger / G. Murshudov

#### \* *Medium resolution from different directions*

Paul Adams / S. Ludtke / A. Brunger / K. Bakolitsa

#### \* *Molecular complexes and membrane proteins*

A. Jones / M. Rossmann / J. Tesmer / S. Iwata

#### \* *Dynamics and disorder*

J. Sussman / J. Kuriyan / G. Phillips

### **ACA 2004 - Chicago - July 17-22, 2004**

See page 34 for important information

[www.uic.edu/orgs/aca2004/](http://www.uic.edu/orgs/aca2004/)

### **53rd Annual Denver X-ray Conference, Steamboat Springs, Colorado, August 2-6, 2004**

This year's Plenary Session "Red Hot X-rays" will explore different uses of X-ray analysis in the study of Volcanology.

[www.dxcicdd.com](http://www.dxcicdd.com) - [dxc@icdd.com](mailto:dxc@icdd.com)

### **ICDD's 2004 X-ray Clinics**

Live Instrumentation, Industry-Expert Faculty and Hands-on Training

#### **Practical X-ray Fluorescence Spectrometry**

April 26-30, 2004

#### **Fundamentals of X-ray Powder Diffraction**

June 7-11, 2004

#### **Advanced Methods in X-ray Powder Diffraction**

June 14-18, 2004

[www.icdd.com/education](http://www.icdd.com/education)

[clinics@icdd.com](mailto:clinics@icdd.com)

### **4th International Conference on Inorganic Materials Antwerp, Belgium \* 19-21 September 2004**

Chairs, Kenneth R Poeppelmeier, Northwestern University, Mas Subramanian, DuPont, and Gustaaf Van Tendeloo, University of Antwerp

[www.im-conference.com](http://www.im-conference.com)

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