

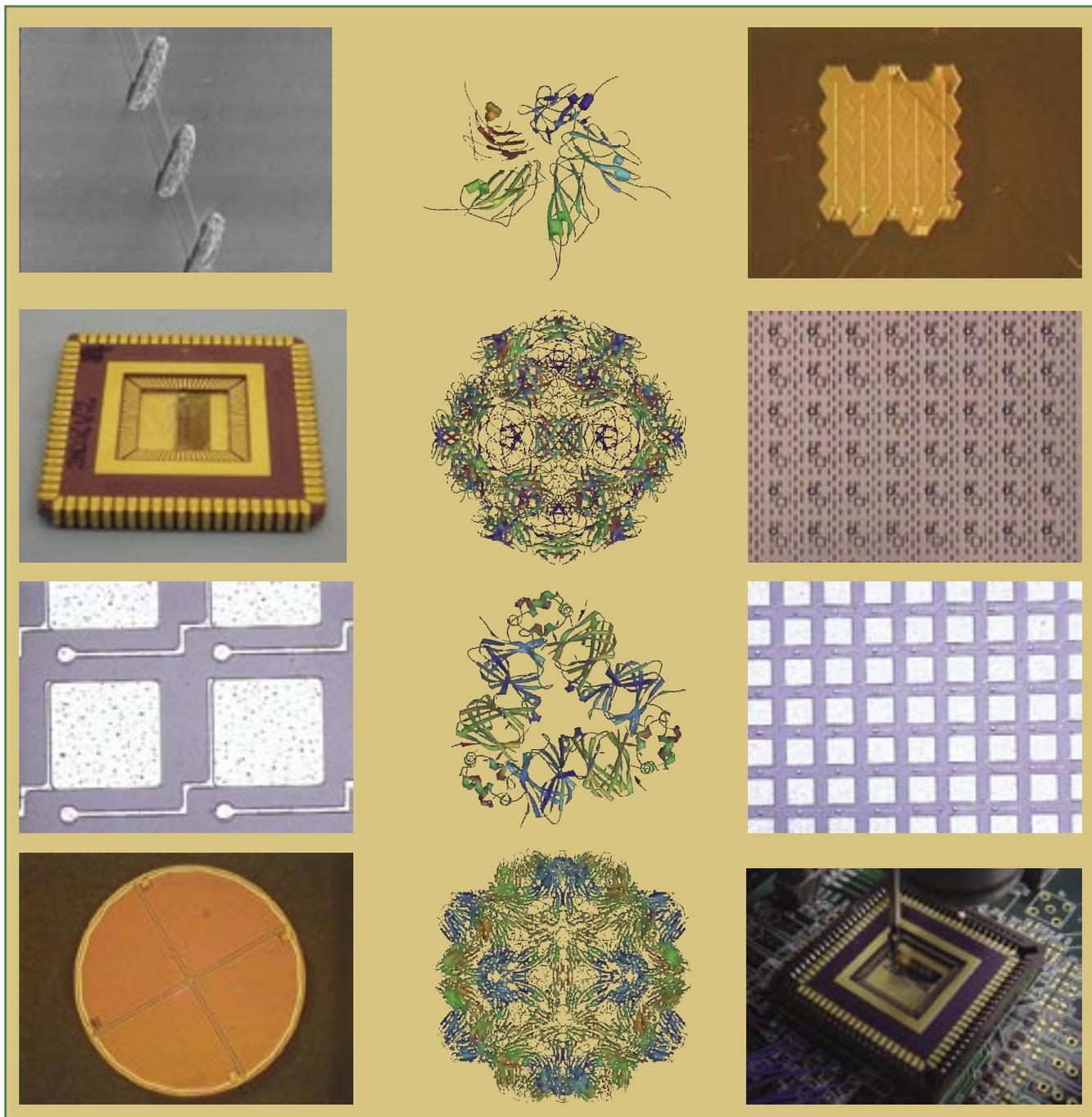


AMERICAN CRYSTALLOGRAPHIC
ASSOCIATION

NEWSLETTER

Number 2

Summer 2004



*ACA 2004
Supper Award
Trueblood Award
Fankuchen Award*

Table of Contents

President's Column 1,40
 Guest Editorial 2
 Open Access to IUCr Journals 4
 2003 Warren Symposium Papers in Zeitschrift..... 4
 News from Canada & Latin America6-8
 Open Data - RapiData 2004 10
 Steacie Award - 2004 Etter Award 11
 Crystallographers Elected to National Academy 11
 ACA Balance Sheet 12
 Pittsburgh Diffraction Society 14
 Web Watch - Contributors to This Issue..... 14
 ACA 2004 Travel Winners - Sponsors - Exhibitors 15
 NIGMS Protein Structure Initiative 16
 NIGMS Protein Crystallization Workshop..... 16-18
 2005 Patterson Award to Alwyn Jones 19
 ICDD News 21
 Notes of a Protein Crystallographer 22-23
 What's on the Cover 26
 Index of Advertisers 26
 ACA Candidates for Offices in 2005..... 28-35
 Wood Science Writing Award to Oliver Sacks..... 37
 Book Reviews 38-40
 Communicating with Congress 43
 Strengthening US Innovation Infrastructure 43-44
 Integrity of the Scientific Advisory System 44-46
 ACA Corporate Members..... 47
 Future Meetings 48

Editors:

Connie Chidester 2115 Glenwood Dr. Kalamazoo, MI 49008	Judith L. Flippen-Anderson 3521 Launcelot Way Annandale, VA 22003
tel. 269-342-1600 fax 716-852-4846 conniechidester@earthlink.net	tel. 703-560-7436 fax 301-738-6255 flippen@rcsb.rutgers.edu

Articles by e-mail or on diskettes are especially welcome. Deadlines for newsletter contributions are: February 1 (Spring), May 1 (Summer), August 1 (Fall) and November 1 (Winter). Matters pertaining to advertisements, membership inquiries, or use of the ACA mailing list should be addressed to:

Marcia J. Colquhoun, Director of Administrative Services
 American Crystallographic Association
 c/o Hauptman-Woodward Medical Research Institute
 73 High Street, Buffalo, NY 14203-1149
 phone: 716-856-9600, ext. 321; FAX: 716-852-4846
 E-mail marcia@hwi.buffalo.edu

ACA HOME PAGE <http://www.hwi.buffalo.edu/ACA/>

ACA Newsletter (ISSN 1958-9945) Number 2, 2004. Published four times per year in the spring, summer, fall and winter for the membership of the American Crystallographic Association, P.O. Box 96, Ellicott Station, Buffalo, NY 14205-0096. Membership in the ACA includes a non-deductible charge of \$1.75 from membership dues to be applied to a subscription to the ACA Newsletter. Periodicals postage paid at Buffalo, New York. POSTMASTER: Send address changes to ACA, c/o 73 High St., Buffalo, NY, 14203.

President's Column

In this issue, I want to focus on two topics. The first is ACA membership and the second is the coming national elections and the impact it may have on ACA members.

As I mentioned in my last column, ACA membership is declining, despite an increase in the number of practicing crystallographers nationally and worldwide. At the Spring ACA Council meeting, an afternoon was devoted to discussing what the ACA can or should offer to retain members in the ever changing world of science. In fact, it is a germane question for the entire readership and a topic on which I hope members will contribute their thoughts at the ACA business meeting on Wednesday, July 21 at 5 PM in Chicago. At present, dues are \$90 per year, for which an ACA member receives monthly issues of *Physics Today*, quarterly *ACA Newsletters*, reduced costs for ACA publications and member registration rates at ACA meetings. In addition, the ACA strongly supports student and young scientist participation in the form of travel grants, poster and early career awards, and the opportunity to orally present preliminary as well as mature crystallographic research. The ACA is also blessed with the membership of many established senior scientists who have long recognized the benefits, not to mention friendships, of a professional society, for themselves as well as their students. It appears that during the intermediate stages of a member's career, the ACA becomes less relevant. This is the period during which the scientific reputation is being built beyond the boundaries of crystallographic research and into a broader realm of science. By necessity, this means more non-crystallographic scientific meetings to attend to publicize the impact of one's crystallographic research on a broader area of science. How then can the ACA maintain its relevance to the crystallographer at the busiest time of his or her career? Does the ACA need to shift its core focus away from crystallographic techniques to applications? Should the ACA publish manuscripts for more sessions? Would sessions on clever, but failed experiments be helpful? Should the ACA offer laboratory or institutional discounts on dues? Would discounted dues entice members to sign up for multiyear memberships? What more can the ACA do to help younger scientist find jobs and learn valuable lessons through professional networking? What more can the ACA do to help all of its members? These questions and other topics will be discussed at the next business meeting. I invite you all to attend and to share your ideas. If you cannot attend, don't hesitate to pass them onto me at jurnak@uci.edu or to any one of the ACA Council members.

The second topic is highly unusual for an ACA president, but particularly for me. I am an apolitical animal at heart, as science has always been so much more fun. However, recently I had the privilege of attending a meeting of the Council of Scientific (continued on page 40)



Guest Editorial: An Electronic Journal for Macromolecular Crystallography



The ubiquity of the internet has produced a number of challenges for scientific publishing. There are few journals worth the name that do not now make possible online access to their entire content, past to present. The journals of the International Union of Crystallography (IUCr) have been leaders in this and conversion to full online access for all IUCr journals was completed in 2000.

The IUCr journals have also been innovative in the area of fully electronic publishing. When the press of new papers and the demand for rapid publication became acute in the small molecule community, the IUCr created a new all-electronic, no-paper journal, *Acta Crystallographica*, Section E, to parallel its popular Section C. By all measures, this strategy has been an unqualified success. In 2002, the total number of papers published in C and E was about twice the number before E was created and, remarkably, both sections were roughly equally popular in the eyes of authors and readers.

The IUCr is now faced with a similar challenge in the macromolecular arena. To meet this challenge, the IUCr is about to launch the first all-electronic journal for macromolecular structures, an *Acta Crystallographica*, Section F. The new journal will streamline publication of protein structure communications generated by structural genomics studies and iterative structure studies such as those used for drug design. It will also provide a forum for rapid publication of crystallization communications.

The advent of structural genomics, a coordinated press for structures of proteins identified in newly sequenced genomes, promises a deluge of new structure papers demanding rapid publication and rapid deposition in the Protein Data Bank. With the encouragement and cooperation of RCSB, a special feature of the new Section F is planned: the facilitated transfer of data required for publication from the database, which will request it at deposition, via the depositors to the journal, where they can be published in tabular form, thereby eliminating duplication of effort on the part of the authors. This new procedure is also expected to facilitate review since the data checking software of the database will signal discrepancies and, if the deposition of required data is incomplete, any data that are missing will be easily identified for follow-up by the editor. (The benefit of providing data required for publication at time of deposition should also mean a higher percentage of more completely documented structures in the database.) All this without sacrificing standards: conclusions must still be supported by experiment, although novelty will take on a somewhat different character as the function of the macromolecule may be unknown.

For two decades now, the pharmaceutical industry has used protein structure to facilitate drug design. Estimates vary, but there must be several thousand unpublished and inaccessible structures in company databases at this point. These are mainly structures

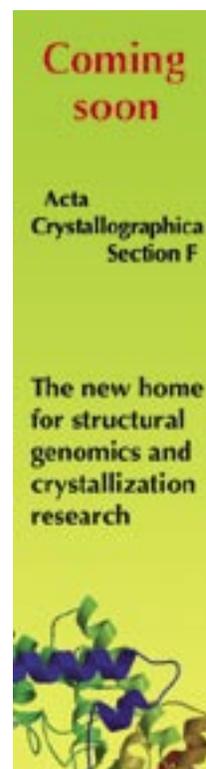
done to characterize as clearly and quickly as possible the mutual adjustments of potential drug molecules and their target proteins to produce binding and function. They come in sets of as few as ten to more than a hundred and contain a wealth of data about protein-ligand interactions. While refinement may sometimes be less than uniformly complete by current standards, the data sets used for these structures are generally the best obtainable by current methods. It is possible that an all-electronic journal with streamlined publication will help to capture more of these structures for the database and make them available to all.

The publication of crystallization communications has been a tradition since the earliest days of protein structure determination. These papers provide detailed documentation of an increasingly important part of the structure determination experiment, a part that is often suppressed or truncated by other journals. And for those who specialize in the crystallization of novel proteins and complexes whatever the result of initial screening trials, the collections of these papers in Section D provide a quick and ready reference to be gleaned for new techniques and new approaches to crystallization. And they continue to serve their original purpose, which is to announce that structural studies have been undertaken and minimize duplication of effort by other groups. The fact that half the typical issue of Section D is now devoted to crystallization communications is testimony enough to their continued popularity. Authors and readers of these papers, however, are now subject to fairly strict limits in terms of space and number of figures and to the luck of the draw in terms of the use of color. It has been proposed that the new all-electronic journal would offer a better home for these papers with fewer constraints on size and color. It would also allow Section D to return to a more structure and technique oriented content, while providing a streamlined and rapid publication path for communications announcing the crystallization of new molecules.

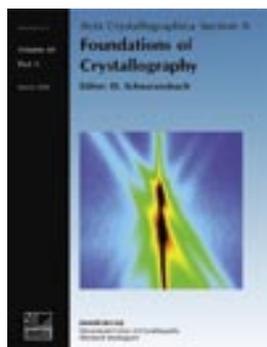
Each communication in Section F will be assigned volume and page numbers and will look online just like it would if it were on paper. If you have any questions about the result, just look in Section E. To prevent artificial fission of the readership, it is envisioned that subscribers to Section D will automatically have access to the all-electronic Section F. And Section D will continue to publish papers on crystallization methodology.

The current trend toward electronic publication continues to gain momentum and expression in the form of new journals and new procedures. The new Section F, together with Section E, will place IUCr journals in the mainstream, perhaps even the forefront, of this trend.

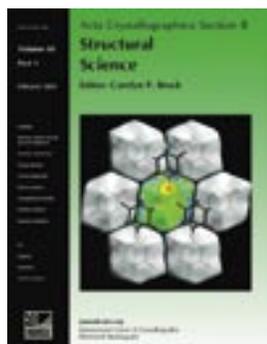
Howard Einspahr



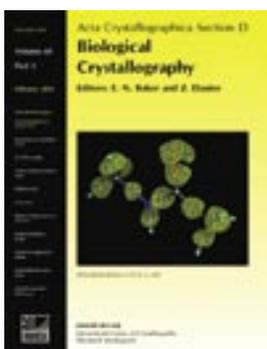
Open-access charges waived for one year for UK staff publishing in IUCr journals



The International Union of Crystallography (IUCr) is delighted to announce that it has been awarded funding from the Joint Information Systems Committee (JISC) to support open-access delivery of its journals, *Acta Crystallographica Sections A–E*, *Journal of Applied Crystallography* and *Journal of Synchrotron Radiation*, via its **Crystallography Journals Online** service. The award will mean the waiving of open-access publication charges for UK higher education staff who publish in these journals for a one-year period from 1 March 2004. This will make UK research more visible worldwide, assisted by the international standing of IUCr journals.



JISC is a committee of all UK further and higher education funding bodies, and is responsible for supporting the innovative use of information and communication technology to support learning, teaching and research. In December 2003, publishers were invited to tender for open-access funding of £150,000, the first round in a three-year programme designed to encourage as much open-access delivery of research findings as possible. This initiative coincides with the IUCr's support of open standards as a means to promote its statutory objective of disseminating crystallographic information to the widest possible audience. From the beginning of 2004, authors publishing papers in IUCr journals have been given the opportunity to make their papers open access on **Crystallography Journals Online**, i.e. free of charge to all readers. Open-access papers will appear alongside standard subscriber-only papers for the foreseeable future.

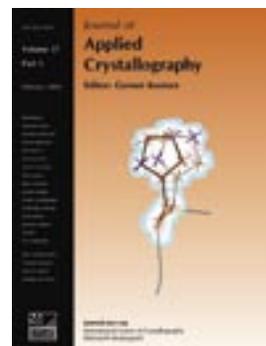


The normal charge for making an article open access is £500. This charge is based on the average cost for the IUCr to produce the first copy of the article, excluding printing and distribution costs, and includes a contribution to the cost of the long-term preservation and access of the publication. Revenue generated from open-access payments will be used to keep subscription costs as low as possible. Open-access articles

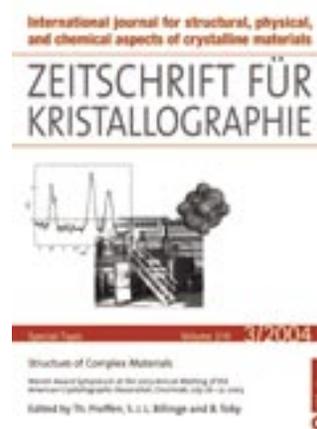
will be clearly marked in contents pages and search results, and because they are freely available, are likely to be cited more frequently.

The IUCr is one of four publishers to have made successful bids for this funding, the other three beneficiaries being the Public Library of Science (PLoS, for *PLoS Biology*), Institute of Physics Publishing (*New Journal of Physics*) and Lancaster University (*Journal of Experimental Botany*).

The IUCr journals, the first of which was established in 1948, appear consistently at the top of the ISI citation rankings for crystallography, and have a deserved reputation for high publication standards. They are published in conjunction with Blackwell Publishing. For information about submitting articles, please visit journals.iucr.org. More information about the IUCr's open-access policy is available at journals.iucr.org/services/openaccess.html.



Warren Award Symposium Contributions Published in *Z. Krist für Kristallographie*



Last year, **Takeshi Egami** received the triannual Warren Award “for his pioneering use of pair distribution functions (PDF) from diffraction data in imperfect crystals leading to new understanding of the physics of complex materials”. In his honor a special symposium was held at the 2003 ACA meeting in Covington, KY to give an overview of the history as well as the current state of structural investigations of complex matter. These contributions are now collected in the special issue of *Zeitschrift für Kristallographie*, “Structure of Complex Materials”, edited by **Thomas Proffen**, **Simon Billinge** and **Brian Toby** (*Z. Krist.*, **219** - www.oldenbourg.de/verlag/zkristallogr/). The cover of the issue features the neutron powder diffractometer NPDF at the Lujan Neutron Scattering Center at Los Alamos National Laboratory. Takeshi Egami was the principle investigator behind a recent upgrade of this instrument, opening the door to new applications of the PDF technique to study intermediate range order in complex materials.

Thomas Proffen

News from Canada, May, 2004



The government of Canada, through NSERC, has announced a new program called CRYSTAL. Not our usual use of the word, it stands for Centres for Research in Youth, Science Teaching and Learning . The goal is to form partnership groups in order to improve the level of teaching of science and engineering in primary

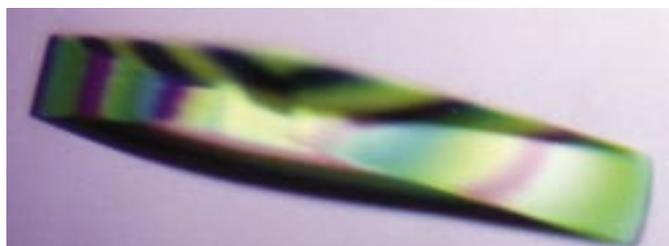
and secondary schools (K-12).

To quote from the website: www.nserc.ca/initiatives/crystal/crystals_e.htm "Each centre will be hosted by one or more of the faculties of education, science and engineering of the lead university(ies). The group must include researchers from education and researchers from science, mathematics and/or engineering, and possibly other areas, as appropriate (such as program evaluation, communications and the arts ...)

Partners from the "user community" must also be actively involved, such as teachers, students and parents from primary and secondary schools, school boards, provincial ministries of education, colleges, non-governmental organizations involved in science promotion, museums, science centres, learned societies, policy makers, curriculum developers and text book publishers. Partners will play a key role in all stages of the research (development of the proposal; planning, direction and conduct of the research; and application of results), through ongoing interaction with the university researchers. Each centre will also be involved in the practical application of research results and the transfer of expertise to the user community, by evaluating, developing and providing outreach activities related to its research theme. Some examples are: professional development for primary and secondary school teachers; innovative tools, materials, textbooks, workbooks and other aids for classrooms; career planning for secondary school students; internships, workshops and exchanges for science, mathematics and engineering university students to develop expertise in education, and for education students to develop expertise in science, mathematics and engineering; and mentorship programs (e.g., university students mentoring secondary school students, secondary school students mentoring young children, accomplished teachers mentoring recent teaching graduates)."

A new type of **CRYSTALlography** that we should be interested in!

David Rose



International Conference on Aperiodic Crystals, Brazil, September 2003

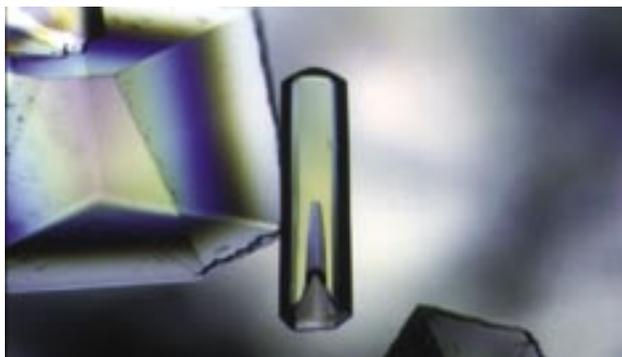


Aperiodic 2003 was held at the Institute of Physics, Universidade Federal de Minas Gerais, Belo Horizonte, Brazil, September 8-13, 2003. The conference was designed to promote research on aperiodic systems, both from experimental and theoretical points of view, and to encourage scientific exchange among groups working in the various fields of aperiodic materials. The conference was well attended with 90 participants representing 22 countries from 5 continents. There were an equal number of contributions from students and senior researchers. Presentations covered the following topics: incommensurate modulated structures, incommensurate composites, quasicrystals, mathematical modelling and symmetry, physical properties, structure determination, polytypes, and applications. The sessions were organized into tutorials (4), oral presentations (20 of which were invited) and posters. Most of the oral presentations were followed by very interesting discussions. Abstracts and proceedings of the congress are available at the congress site (agora.grude.ufmg.br/aperiodic2003). The proceedings will be published by Francis & Taylor as a special issue of *Ferroelectrics*.



A total of 19 scientists were granted partial support for travel and living expenses (2 from Brazil, 1 from Czech Republic, 1 from France, 1 from Germany, 2 from Mexico, 2 from Poland, 1 from Romania, 6 from Russia, 1 from Switzerland and 1 from Vietnam). In addition, 18 young scientists had their registration fee waived and ten students were partially or totally supported thanks to the funds granted by the IUCr.

Nivaldo Speziali and Iris L. Torriani



**International School on Crystal Growth,
Characterization and Applications (ISCGChA)
9-13 December, La Pedrera, Uruguay**

The International School on Crystal Growth was sponsored by the IUCr, UNESCO, and the Scientific Research Commission (CSIC) and Chemistry Department of the Universidad de la República, Uruguay. The attendees were graduate students and researchers from Latin America (Argentina, Brazil, Chile, México, Uruguay and Venezuela) plus some young researchers from France, Italy and Germany.



The total number of participants was 49. 17 grants were awarded to participants from Latin American countries. "A crystallographic approach to the crystalline state" was the title of the opening lecture by **Raúl Marízcurrena** (Universidad de la República, Uruguay). The school included a short course on crystal growth fundamentals titled "Thermodynamics, Kinetics and Defects Characterization" taught by **Peter Rudolph** (Institut

für Kristallzüchtung, Berlin, Germany). The subject of crystal growth morphology was presented by **Robert Sekerka** (Carnegie Mellon, USA), with examples of computed results, ranging from



microstructures in castings to snowflakes. A tutorial on crystal growth modeling was presented by **Jeffrey Derby** (University of Minnesota, USA), showing results of modeling of melt and solution growth systems. Other important subjects included in the plenary lectures were: basic aspects of MOVPE growth (**Mateo Bossi**, Italy), laser heated pedestal growth (**A.C. Hernandez**, Brazil), thick films of heavy metal iodides (Laura Fornaro, Uruguay), local vs. extended structure determination (**A.W. Momburu**, Uruguay) and 2D and 3D characterization of biomolecules and biomaterials (**Abel Moreno**, México). The workshop included



At the poster session: Mabel Giles (Uruguay) and Diógenes Reyes Ardila (Brazil)

a poster session with 39 participants. Prizes were given to four young scientists from Uruguay and Latin America, two one year complimentary ACA memberships were awarded to participants from Uruguay and México, and one-year electronic access to the IUCr journals was granted to the Facultad de Química de la Universidad de la República, Uruguay, as an incentive to the groups that organized this school. Covering other aspects of the meeting, one should mention the hospitality of the local organizing committee, the many young students who took care of all details, and the beauty of the ISCGChA-2003 location: a very small beach town on the coast of Uruguay, just north of Punta del Este.



Does open data better serve the crystallographic community?

The many crystallographic databases, PDB, CSD, ICSD, CRYSTMET, ICDD, AMCSO, NDB (etc) are invaluable tools in crystallography. Essential uses for these tools are too numerous to list. Unfortunately, many researchers do not have access to some of these data collections (open access being ensured for PDB, AMCSO and NDB only), which is detrimental to making good science (reviewers of crystallography papers may not be able to perform a correct evaluation, chemists will try to republish already known structures, etc). Further, the delays between publication and distribution of structures can be quite long, reducing the value of the tools for recent results. Following the ideal PDB, AMCSO and NDB models, the Crystallography Open Database (COD) wishes to establish a public domain web repository and index for published and unpublished structural results (inorganic and organic, excluding proteins and nucleic acids covered by PDB and NDB). The COD advisory board members wish to open a discussion within the community of crystallographers on how this can best be accomplished.

We would like to see crystallographers deposit CIFs with the COD prior to publication, with the understanding that this

disclosure should not be considered “prior publication” when a paper is prepared for journal publication.

We would like to see the IUCr provide copies of CIFs for published papers to the COD, as the IUCr does with the other crystallographic databases. If this would endanger IUCr journal revenues, an alternative would be to only allow the COD to include information on recent structures in the COD indices for some period after publication. During this period, the COD would provide a URL pointer to the CIF on the IUCr site, where access could be restricted to journal subscribers. An outside organization of volunteers would bring new ideas for locating structural information, beyond what the IUCr can afford to develop internally for searching the IUCr’s collection of CIFs. These innovations will be available to the established databases, strengthening their tools as well. For instance, an increasing COD subset is devoted to CIFs of predicted crystal structures (zeolites, etc). If the IUCr takes a direct stance on open access to crystallographic data, we think that this will establish the ethical standards for structure disclosure within the field, and that this can be used to encourage non-IUCr journals to also offer similar access.

COD website: www.crystallography.net

Armel Le Bail on behalf of the COD Advisory Board

RapiData 2004



As predictable as daffodils, crystallographers from around the world gathered at Brookhaven National Laboratory this spring as students in RapiData 2004. This week-long course is offered by BNL’s Biology and National Synchrotron Light Source (NSLS) Departments to introduce students to the best people, newest equipment, and latest techniques in the field of macromolecular x-ray crystallography. Running this year from April 25 - 30, the course began with two days of lectures and tutorials taught by scientists from BNL, industry, academia, and other national labs. Then, the same instructors and others acted as hands-on advisors for a marathon, 60-hour data-collection session on nine NSLS beam lines. Half of the 48 students came with their own specimens to analyze, while the other half learned as observers.

Six students left with solved and potentially publishable structures. The course was organized mostly by **Bob Sweet** and **Denise Robertson** (Biology Dept), but it should be emphasized that its success absolutely depended on enthusiastic help from most of the 20 members of the PXRR (the Biology and NSLS Macromolecular Crystallography Research Resource), NSLS staff members, plus a dozen outside teachers. Major funders of the course were the National Institutes of Health’s National Center for Research Resources and the Office of Biological & Environmental Research within DOE’s Office of Science, with support from the NSLS, equipment vendors, and drug companies. For more information, go to: www.px.nsls.bnl.gov/RapiData2004/.

Bob Sweet

Steaacie Prize to Natalie Strynadaka



Belated congratulations to **Natalie Strynadaka** of University of British Columbia, who was awarded Canada's 2002 Steacie Prize (www.steaacieprize.ca). The award cites her work on beta-lactamase antibiotics. We learned of this award now because she is featured in a full page ad in the 30 April 2004 issue

of *Science* recruiting faculty to UBC.

Natalie is an associate professor of Biochemistry and Molecular Biology at the University and is an associate member of its Biotechnology Laboratory and a member of its Centre for Blood Research. She is also an Investigator of the Canadian Institutes of Health Research, a Burroughs Wellcome New Investigator, and a Howard Hughes Medical Institute International Scholar.

The Steacie Prize is a Canadian award presented to a young scientist or engineer for outstanding scientific work. The winner is selected by a panel appointed by the E.W.R. Steacie Memorial Fund, a private foundation dedicated to the advancement of science and engineering in Canada.

2004 Etter Early Career Award to Leonard MacGillivray



Leonard MacGillivray (Dept. of Chem, U of Iowa) has been selected to receive the 2004 Margaret C. Etter Early Career Award. He will deliver two lectures: "Linear Templates: Tools for Directing Reactivity in the Solid State" will be the opening lecture in the **Etter Symposium** during the Chicago ACA Meeting and "Metal-Organic Polygons, Polyhedra, and Extended Frameworks

Derived from Molecules Constructed in the Solid State" as part of the **Transactions Symposium**.

Editor's note: *Leonard's ladderane structure was featured on the cover of the spring 2004 ACA Newsletter (see page 29 cover story). Since the 2005 ACA meeting in Orlando is a spring meeting, all submission deadlines will be earlier than they are for a summer meeting.*

Nominations for the 2005 Etter Award should be sent to ACA council as soon as possible, but no later than September 1, 2004. Details on the award criteria can be found on the ACA website: www.hwi.buffalo.edu/ACA/. Nominations can be sent by e-mail to marcia@hwi.buffalo.edu.

Crystallographers Elected to the National Academy

The National Academy of Sciences has announced the election of 72 new members and 18 foreign associates from 13 countries in recognition of their distinguished and continuing achievements in original research. Election to the Academy is considered one of the highest honors that can be accorded a U.S. scientist or engineer.

The Academy is a private organization dedicated to the furtherance of science and its use for the general welfare. It was established in 1863 by a congressional act of incorporation, signed by Abraham Lincoln, which calls on the Academy to act as an official adviser to the federal government, upon request, in any matter of science or technology.

Crystallographers included among the new members are:

Barry H. Honig; investigator, Howard Hughes Medical Institute; and professor, department of biochemistry and molecular biophysics, Columbia University

Stephen L. Mayo; associate investigator, Howard Hughes Medical Institute; and professor of biology and chemistry, California Institute of Technology

Venkatraman Ramakrishnan; group leader, Structural Studies Division, Laboratory of Molecular Biology, Medical Research Council, Cambridge, U.K.

Robert J. Birgeneau; president, University of Toronto, Ontario (Canada) was elected a foreign associate.

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION, INC.
BALANCE SHEET - December 31, 2002 and 2003

	CURRENT FUNDS (2003)		TOTAL	
	Unrestricted	Restricted*	All Funds	
			2003	2002
ASSETS				
Current Assets:				
Cash	32,532		32,532	52,302
Investments	442,328	318,281	760,609	554,327
Inventory	3,600		3,600	3,600
Total Current Assets	478,460	318,281	796,741	610,229
Fixed Assets:				
Computers and Printers	6,500		6,500	6,500
Office Equipment	1,300		1,300	1,300
Accumulated Depreciation	0		0	-0
Total Fixed Assets	7,800		7,800	7,800
TOTAL ASSETS	486,260	318,281	804,541	618,029

Liabilities:

Deferred Dues Income			0	0
Total Liabilities	0		0	0
Fund Balance:				
Unrestricted	486,260		486,260	317,531
Restricted		318,281	318,281	300,498
Total Fund Balance	486,260	318,281	804,541	618,029
TOTAL LIABILITIES				
& FUND BALANCE	486,260	318,281	804,541	618,029

* Current Balances in individual restricted funds - as of December 31, 2003

Buerger Award	31,065
Etter Award	56,120
Fankuchen Award	62,035
Patterson Award	33,563
Pauling Award	27,352
Supper Award	10,039
Trueblood Award	27,574
Warren Award	24,688
Wood Science Writing Award	45,845

A more detailed report on the ACA finances may be obtained by sending a written request to the ACA office in Buffalo, PO Box 96, Ellicott Station, Buffalo, NY 14205-4846.

Pittsburgh Diffraction Society Election Results



From left: Alan Pinkerton (President-Elect), G. David Smith (Past-President), Bryan Craven (Member-at-Large), Allen Oliver (Secretary) and Tom Emge (President). Not shown: Charles Lake (Treasurer)

2004 Pittsburgh Diffraction Conference and Call for Nominations for the Sidhu Award

The Pittsburgh Diffraction Society is pleased to announce that their next annual conference will be held in Pittsburgh, at the Holiday Inn University Center from October 28 through October 30, 2004. The major symposium will celebrate the career of Robert F. Stewart who will be retiring from his position as Professor of Chemistry at the Carnegie-Mellon University this fall. Many of his friends and colleagues from around the world have agreed to participate in this one day – “Bob Day” – affair. Three additional half-day symposia are planned - “New Synchrotron Applications and Optics”, “Recent Developments in Neutron Diffraction” and “Protein Dynamics from Crystallography”. Again, an international list of speakers has accepted invitations to participate in these events. The complete list of speakers and titles will be announced shortly (www.rutchem.rutgers.edu/PDS). There will be a reception and poster session on October 28. The Chung Soo Yoo Award will be made for the best graduate student poster. A banquet and award ceremony will take place on October 29, during which the Sidhu Award will be made. Nominations are herein requested for the Sidhu Award, which is made in honor of Professor Surhain Sidhu, to a scientist within 5 years of the PhD who has made an outstanding contribution to crystallography or diffraction. For further information and to submit nominations, please email apinker@uoft02.utoledo.edu or mail to A. Alan Pinkerton, Department of Chemistry, Mail Stop #602, University of Toledo, Toledo OH 43606

NAS Marian Koshland Science Museum

Take a look inside the new National Academy of Sciences' Marian Koshland Science Museum, which opened to the public Friday, April 23 in Washington, D.C. Explore the museum's website, which offers a sneak peak at the inaugural exhibits on global warming, DNA sequencing, and the nature of discovery. [/www.koshland-science-museum.org](http://www.koshland-science-museum.org)

Crystallography Web Watch

The ACA Communications Committee encourages the entire crystallographic community to participate in the “Crystallography Web Watch”. Please email the web address and a brief description of any sites to Jeanette Krause (jeanette.krause@uc.edu) that could be informative and/or entertaining.

Compilations of sites dealing with all matters in crystallography including educational resources are at:

- a) physics.designerz.com/physics-crystallography-education.php
- b) dir.i-une.com/Science/Physics/Crystallography/
- c) dir.nodeworks.com/Science/Physics/Crystallography/
- d) www.nebulasearch.com/directory/go/Science/Physics/Crystallography/
- e) paloweb.com/Science/Physics/Crystallography/Education/
- f) xray.utmb.edu/Education.html
- g) [www.cristal.org/course/---Internet Course on Powder Diffraction](http://www.cristal.org/course/---Internet%20Course%20on%20Powder%20Diffraction)
- h) cms.lanl.gov/K_12list.html

New Reports available from the National Academy

Electronic Scientific, Technical, and Medical Journal Publishing and Its Implications: Report of a Symposium
www.nap.edu/catalog/10969.html?do_se108
 The Mathematical Sciences' Role in Homeland Security: Proceedings of a Workshop
www.nap.edu/catalog/10940.html?do_se108
 A Patent System for the 21st Century
www.nap.edu/catalog/10976.html?do_se108
 Digital People: From Bionic Humans to Androids
www.nap.edu/catalog/10738.html?do_se109
 University Research Centers of Excellence for Homeland Security: A Summary Report of a Workshop
www.nap.edu/catalog/10984.html?do_se109
 Jeanette Krause

Contributors to this Issue

Cele Abad-Zapatero, Paul Anderson, Bob Beau, Gloria Borghstahl, Patti Colley, Marcia Colquhoun, Zygmunt Derewenda, Howard Einspahr, Tom Emge, James Fettingner, Lee Groat, Annie Heroux, Michael Jennings, Fran Jurnak, Chris Kenney, Jeanette Krause, Armel LeBail, Alex McPherson, John Norvell, William Ojala, Rose Oughtred, Alan Pinkerton, Thomas Proffen, S.N. Rao, David Rose, Bernhard Rupp, Nivaldo Speziali, Alexei Soares Richard Staples, Jim Stewart, Bob Sweet, Iris Torriani and Ed Westbrook

ACA 2004 Travel Awardees

Ekaterina Anokhina
University of Houston, USA

Jason B. Benedict
Univ. of Washington, USA

Kent Brown
University of Minnesota, USA

Kacey Claborn
University of Washington, USA

Teresa De La Mora-Rey
Univ. Of Minnesota, USA

S.A. Fasilova
Uzbekistan

Janaina Ferreira
University of Sao Paulo, Brazil

Suzanne Fisher
University of Florida, USA

Lakshmanan Govindasamy
University of Florida, USA

Franklin Hays
Oregon State University, USA

Ryan Justice
Univeristy of Cincinnati, USA

Olga Kanderall
Ukraine

Tiffany Kinnibrugh
New Mexico Highlands U, USA

Janel W. Laidman
UCLA, USA

Brock Levin
Kansas State University, USA

Anna Makal
Warsaw University, Poland

David Murray
Oregon Health and Sci. U., USA

Ashwini Nadkarni
The University of Georgia, USA

Helena Napolitano
Instituto de Quimica de Sao Carlos,
Brazil

Dmytro Nesterov
National Taras Shevchenko U.,
Ukraine

Cara Nygren
University of Tennessee, USA

Lindsay Odell
Johns Hopkins School of Med., USA

Rositza Petrova
Georgetown University, USA

Jesse L. C. Rowsell
University of Michigan, USA

Debra Salmon
Kansas State University, USA

Nate Schultheiss
Kansas State University, USA

Macy Shen
Cal State Fullerton, USA

Cynthia Sides
University of Arkansas, USA

Michelle Smith
Kansas State University, USA

Jay Stork
U of California Davis, USA

Leopoldo Suescun
Universidad de la Rep`blica,
URUGUAY

Rachael Summerfield
McMaster University, CANADA

Yogesh Surendranath
University of Virginia, USA

Soheila Vaezeslami
Michigan State University, USA

Helen Walden
St Jude Children's Research Hosp.,
USA

Zhanhui Yuan
University of Newcastle, UK.

Peter Zhivkov
Dowling College, USA

Sponsors

3-Dimensional Pharmaceuticals

**Donors of The ACS Petroleum
Research Fund**

Blake Industries

BP Amoco Chemicals

**Bristol-Myers Squibb Bruker
AXS, Inc.**

Genentech

GlaxoSmithKline

Hampton Research Corp.

Hewlett Packard Company

ICDD

IUCr

Merck Research Laboratories

Monsanto Company

Pfizer

Rigaku/MSC, Inc.

Structure

Structural GenomiX, Inc.

Exhibitors

**3D Molecular Designs & MSOE
Cent. for BioMolec. Modeling**

Accelrys

Area Detector Systems

Art Robbins

Beevers

Biophysics Collab. Access Team

Blake Industries

Brandel

Bruker AXS Inc.

CCDC

CCP4

Corning Incorporated

Cryo Industries of America

deCODE Genetics

Delong America Inc.

Diamond Wire Technology

Diversified Scientific

Douglas Instruments

Fluidigm

Formulatrix

Genomic Solutions

Gilson, Inc.

Greiner Bio-One, Inc.

Hewlett Packard

Innovadyne Technologies

IUCR

Malvern Instruments

MAR USA, Inc.

MicroCal LLC

Molecular Dimensions, Inc.

Nextal Biotechnologies

Osmic, Inc.

Oxford Cryosystems

Oxford Diffraction

Precision Detectors

Prooterion Corporation

RCSB Protein Data Bank

Rhombix/Kendro/DCA/Hamilton

Rigaku

RoboDesign International

**Shamrock Stuctures LLC
(SER-CAT)**

Springer Academic Publishers

Tecan

TriTek Corp

Veeco Instruments

VizEveryWhere

Wyatt Technology Corp

Xenocs SA



**Production
Phase of the NIH
Protein Structure
Initiative**

The National Institute of General Medical Sciences (NIGMS) initiated the Protein Structure Initiative (PSI) in 2000. 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. Nine pilot structural genomics research centers were funded as part of the plan to reduce the costs and increase the success of the structural determination of proteins. The pilot projects have focused on high throughput methods for structure determination in order to achieve these goals.

Plans for the next phase of the PSI have been developed over the past year. This production phase will begin in 2005 as an interacting network with three components. Large-scale centers will focus on the production and structural determination of unique proteins, as well as methodology and technology development to reduce costs and increase success rates. The second component comprises specialized research centers focused on the development of new methods, technology, and approaches for the production and structure determination of especially challenging proteins, such as membrane proteins, small protein complexes, and proteins from humans and other higher eukaryotic organisms. These centers will also seek to overcome major barriers to high-throughput operation. The third component of the PSI involves disease-targeted research centers. These centers will be an integral part of the NIH Structural Biology Roadmap. Information on the PSI is at: www.nigms.nih.gov/psi

At the ACA meeting, **John Norvell**, director of the PSI, will describe the development of the production phase of this project. He will summarize the two recently issued Requests for Applications (RFAs) that will support the first two components of the PSI.

NIGMS Protein Structure Initiative 2004 Protein Production and Crystallization Workshop, Bethesda, MD, March 29-31, 2004

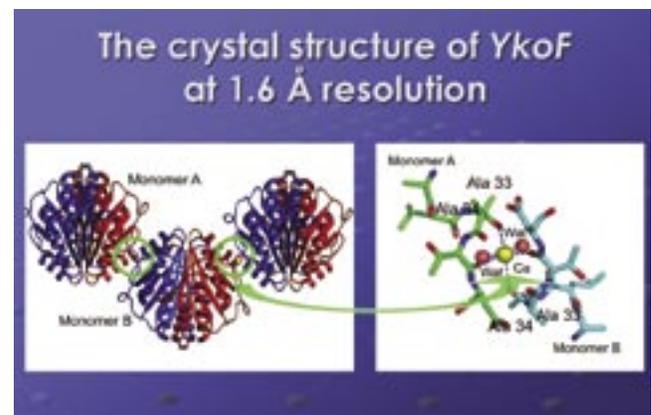
The third annual Workshop included representatives from the nine NIH PSI structural genomics centers, from academic labs and from industry. During the first two years, the structural genomics centers were mainly focused on building the necessary infrastructure for their projects. The different sites have made major progress in incorporating new technologies for protein expression and purification. They now have their pipelines in place and much of the production has been automated. An increasing number of proteins are being produced and more data is emerging. According to several attendees, the presentations this year contained more detailed protocols and data compared to previous years.

With the thousands of proteins being cloned and expressed, no single affinity tag has been found that works for all proteins. However, most of the targets are being expressed as His-tagged

proteins in both prokaryotic and eukaryotic expression systems. Many of the structural genomics sites have developed more flexible cloning and expression strategies. Since only ~30% of eukaryotic proteins can be expressed successfully in *E.coli*, some centers are expressing their targets in yeast, insect cells, eukaryotic cells, or cell-free expression systems. Interestingly, new techniques have made it possible to clone and express proteins of interest in insect cells within 48 hours compared to using baculovirus methods that usually take 2-3 weeks. An improved cell-free wheat germ expression system is being used by the CESG to express eukaryotic proteins. The new cell-free system pipeline involves a fully automated protein synthesizer and so far the procedure looks very promising for high-throughput protein production.



Although many centers have been successful at purifying protein targets, they have encountered problems obtaining proteins that are soluble, properly folded and/or crystallizable. In fact, the average protein to crystal success rate for all of the structural genomics projects is 45.5%, and the average protein to structure success rate for all of the centers is only 6.6%.



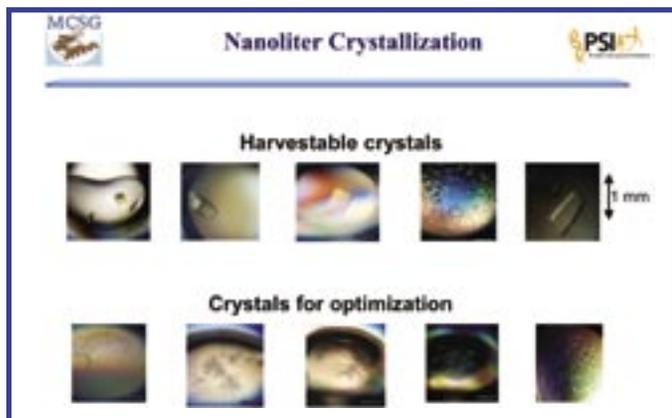
One method that seems to improve the folding and solubility of proteins involves co-expressing them in *E. coli* with a chaperone. Another approach being carried out by the SGPP involves using multiple species to obtain homologues of "difficult" proteins from different protozoa. Although many of the homologues are from 65% to 95% identical, small changes in the sequences of the proteins significantly increase their solubility and crystallization. In cases where full-length proteins are insoluble, some centers are attempting to solubly express selected domains. The SGPP has developed a computational prediction program to help define these domains and have had some success expressing domains

of insoluble proteins. The SECSG, on the other hand, relies on experimental methods such as spontaneous degradation or limited proteolysis of purified proteins to obtain stable domains that are soluble and crystallize well.

The bottleneck for many sites is the crystallization step. Unfortunately, a significant fraction of target proteins are being “left behind” because they do not produce diffraction-quality crystals. The SECSG is attempting to rescue some of their targets by re-purifying them or by trying different techniques such as reductive methylation of lysines. They managed to salvage 10% of their failed proteins using these methods. At other sites, rational mutagenesis is being performed on high value targets to modify the protein surfaces and thereby enhance crystallization. The SGPP is exploring the use of recombinant antibody and target protein complexes to facilitate crystallization. They are producing high-affinity single chain recombinant antibodies using phage display instead of relying on Fab fragments derived from regular monoclonal antibodies. The phage antibody technology apparently yields useful antibodies in about a week, which is much less time-consuming than conventional methods for isolating monoclonal antibodies.

A few centers have successfully expressed functional membrane proteins in *E. coli* and in eukaryotic systems. The JCSG has been able to express 20% of the membrane proteins from *T. maritima* using *E. coli*. However, they have been unable to do so in a high-throughput manner due to the many detergents that need to be screened to solubilize the membrane proteins. They will eventually be using NMR spectroscopy to determine the structure of small membrane proteins of 16 KDa or less.

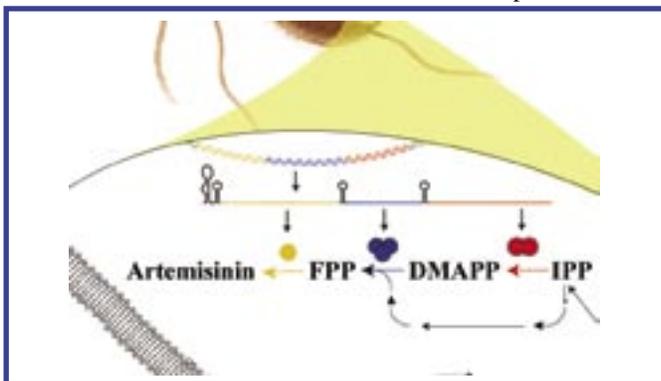
Some data mining is being performed on the data that is already available from the structural genomics projects. Attempts are being made to correlate protein properties and crystallization conditions with crystallization success. However, access to the data from all of the different sites is very limited and large-scale data mining is therefore very difficult to carry out. The integration of different pipelines with laboratory information management systems (LIMS) and databases is a serious issue



that still needs to be addressed. Although many centers have their own database system in place, some are still in the process of building their own database. Many centers with databases also continue to store some of their data and protocol details in spreadsheets or laboratory books.

It was generally recognized that centralizing all of this protein expression, purification and crystallization data in the PEPCdb

database will not only permit the sharing of data between different sites, but will also be invaluable for data mining purposes. It was also emphasized that successful and unsuccessful attempts at cloning, expression, purification and crystallization should be captured in the PEPCdb database. Obtaining standardized protocols from each center will be helpful, however it will be critical to obtain details about any modifications to the protocols that were made in order to deal with “difficult” proteins.

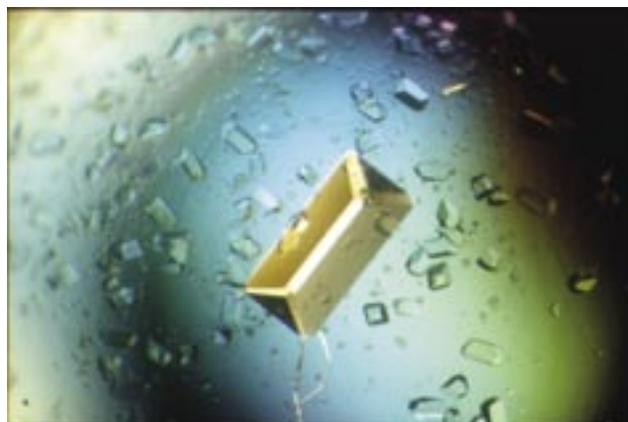


Aside from the increased number of structures being produced, much of the value coming out of the structural genomics projects lies in the increased knowledge and technology being produced. New techniques, computational methods and robotics have been developed that have completely revolutionized structural biology. Indeed, the centers seem to be heading towards robotic visual imaging systems for evaluating the thousands of crystals being produced by multiple high-throughput conditions, thereby automating one of the few remaining steps in the pipeline that remains very labor intensive.

For more information see: www.nigms.nih.gov/psi/meetings/ppcw2004.html.

The figures were selected from presentations given at the workshop. The YkoF figures are from "Protein Crystallization Using the Surface Entropy Reduction Approach" by Jacob Bielnicki (University of Virginia). The nanoliter crystallization image is from "Crystallization Strategies in the Midwest Center for Structural Genomics" by Irina Dementieva (Argonne National Laboratory). The Artemisinin image is from "Genetic Tools for Metabolic Enzyme Production in *Escherichia coli*" by Jay Keasling (University of California, Berkeley).

Rose Oughtred



2005 ACA Patterson Award to Alwyn Jones

The 2005 Patterson Award in Crystallography goes to **Alwyn Jones**, Professor of Structural Biology, Department of Molecular Biology, Uppsala University, Sweden. The A. Lindo Patterson Award is made 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.



This award derives from the work of A. Lindo Patterson. His 1934 paper in *Phys. Rev.*: “Fourier Series Method for the Determination of Components of Interatomic Distances in Crystals”, signaled a major step forward in understanding diffraction theory; the Fourier series on $|F|^2$, the Patterson function, greatly enabled subsequent structure determination. Previous winners have included: 2002 **Douglas Dorset**, Correlations, Convolutions and the Validity of Electron Crystallography; 1999 **Gerard Bricogne**, Intensities, Phases and Structures: The Role of Mathematics in Crystallography; 1997 **Christer E. Nordman**, Travels in Patterson Space; 1993 **George Sheldrick**, Direct Attempts to Solve Protein Structures; 1990 **Michael M. Woolfson**, Direct Methods and Macromolecular Structures; 1987 **David and Lieselotte Templeton**, Theory, Measurement, and Use of Anomalous Scattering; 1984 **Jerome Karle and Herbert Hauptman**, Direct Methods of Crystal Structure Determination; and 1981 **Wayne A. Hendrickson**, Use of Anomalous Dispersion Effects in Phasing Protein Diffraction Data.

The contributions of Alwyn Jones in the field of macromolecular crystallography have revolutionized the methodology of protein structure determination. He was a pioneer in the application of computer graphics to the construction of atomic models from an electron density map. While other graphics software has been developed, Alwyn’s programs, in addition to being among the first, have set the standard for ease of use and, most importantly, continued support and development. His first popularly distributed program, *FRODO*, permitted the placement and modification of atomic positions directly within the computer, rather than in the “Richards box” or on perspex sheets. This made the whole process faster and much more accurate.

The impact of *FRODO* was followed by a series of further developments in the automation of various aspects of the fitting

procedure, first backbone tracing and then side chain identification. This evolved into the program package ‘*O*’, now used by many crystallographic laboratories worldwide, and served as a model for other programs. The package provides for many aspects of automated fitting, local model refinement and validation of both the fit and stereochemical quality of the model. This last aspect has led Alwyn and his team in Uppsala to release a series of programs and routines in structure validation, which have, in many cases, eliminated serious errors from protein models.

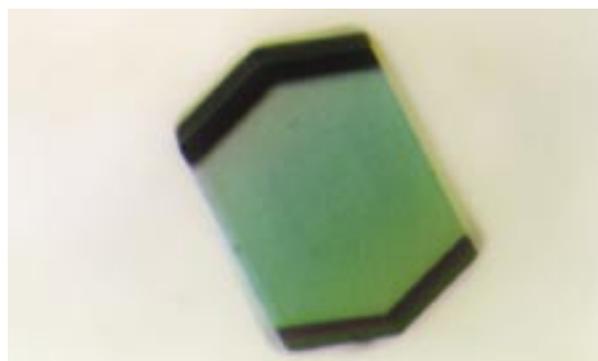
The implications of these procedures are enormous, not just for crystallographers but for any investigators using atomic models of proteins generated by crystallography or other techniques. It is impossible to imagine macromolecular crystallography without computer graphics techniques, and it would certainly be impossible to even conceive of the current wave of “high throughput” approaches without the automation of model building and verification that came out of these advances.

Alwyn Jones was born in Glamorgan, Wales, and completed his primary and secondary education there. Among his list of GCE subjects are French, Latin, English Language and English Literature, which may have been a foundation for his deep interest in Tolkien. Jones completed both his undergraduate degree in Physics and graduate degree in Biophysics at King College, London, receiving his PhD in 1973. He spent 1977-1978 as a Systems Analyst and Research Assistant with Robert Huber in Munich, before moving to the Department of Molecular Biology, Uppsala University in 1979. He is now Professor of Structural Biology at Uppsala. He is married to Sherry Mowbray, also a well-known structural biologist, and they have two children.

Among other honors, he is a Fellow of the Royal Society, EMBO Fellow, member of the Swedish Royal Society, and recipient of the Aminoff Prize awarded by the Swedish Royal Academy of Sciences in 2003. He has served on several international journal editorial boards, including *Acta Cryst A* and *D*, and *Structure*.

Alwyn is author on over 135 peer-reviewed publications. He was involved in some of the earliest macromolecular crystallographic work on trypsin/BPTI and antibody fragments. His earliest methodological work related to the refinement of crystal orientation parameters. The landmark paper in *J. Appl. Cryst* in 1978 on a graphics model building and refinement system for macromolecules set the stage for his major contributions in graphical building and quality analysis of macromolecular structures.

Patterson Award Committee 2004: *Wim Hol, Brian Patrick, Janet Smith, and James Stewart, chair.*



ICDD Spring Meeting

During the week of 22-26 March 2004, ICDD members gathered at the Newtown Square Headquarters office for the Annual Spring Meeting.

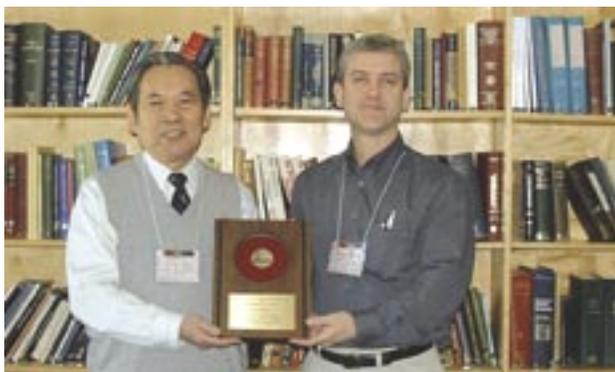
This year's Plenary Session focused on Advanced Instrumentation. Speakers at the plenary session included: **Bob He** (USA): Two-dimensional X-ray Diffractometer: Convention, Components and Configuration, **Martijn Fransen** (The Netherlands): Advanced Optics and Detection Systems, What Do They Offer the Research Community?, **Hideo Toraya** (Japan): A High-Performance Silicon Photodiode Detector for Fast X-Ray Counting, and **Pierre Villars** (Switzerland): New Structural Prototyping System used by the LINUS PAULING FILE and proposed for the Powder Diffraction File (PDF)



Bob He (BrukerAXS), Martijn Fransen (PANalytical), Hideo Toraya (Rigaku Corporation), and Pierre Villars (Materials Phases Data System)

The poster session was the most successful Spring Meetings' poster session to date. Approximately 30 posters were on display, allowing attendees yet another venue to communicate their studies and exchange information with fellow scientists.

Several awards were also announced at the meeting. **Shao Fan Lin** of the Nankai University, People's Republic of China was recognized for his 17 years as a participant in the ICDD Grant-in-Aid Program as he was named the 2004 Distinguished Grantee Recipient. He has published approximately 700 patterns in the PDF.



Shao Fan Lin, 2004 Distinguished Grantee and Dr. Tom Blanton, Chairman of the ICDD Grant-in-Aid Committee

Following more than 30 years of service to the ICDD, **Robert Snyder**, Georgia Institute of Technology, was named as the 2004 Distinguished Fellow. Bob has served the organization in various capacities: as a member and leader on various committees, subcommittees, task groups, and most recently as Chairman of the Board of Directors. Over the years, he has often been referred to as the "ICDD ambassador to the world" and his relentless energy and vision have served as catalysts in bringing a new dimension to the PDF.



Robert Snyder, 2004 Distinguished Fellow

ICDD Board of Directors - 2004 - 2006

- Chairman - **James Kaduk**
- Vice Chairman - **Paolo Scardi**
- Treasurer - **Julian Messick**
- Corporate Secretary - **Terry Maguire**
- Executive Director - **Timothy Fawcett**
- Chairman, Technical Committee - **Raymond Goehner**
- Directors-at-Large, Board of Directors - **Evgeny Antipov, Tom Blanton, Herbert Goebel, Ting Huang, and Daniel Louër**
- Past Chairman - **Camden R. Hubbard**



Front row: Antipov, Blanton, Maguire, Scardi, Kaduk, Goehner, Louër, Back row: Goebel, Fawcett, Hubbard (Not shown - Huang)

Notes of a Protein Crystallographer - Our Unsung Heroes

For the new generations of protein crystallographers, beamlines dedicated to protein crystallography are taken for granted, the more the better. Few of the younger generation of crystallographers are familiar with the history of the technological developments that were necessary to have routine access to experimental stations permitting rapid and reliable data collection of excellent diffraction data from protein crystals. Moreover, the names and efforts of the people involved in this pioneering work are probably unknown to them. A recent essay (Cele Abad-Zapatero, *Structure* (2004), **12**: 523-527) gives the background and historical perspective to those scientific achievements with a personal point of reference. A brief excerpt from the essay (*Reprinted with permission from Elsevier*) is printed below. Students and newcomers to the field are encouraged to read the entire article. The article is dedicated to the people who designed, built and currently work at synchrotron beamlines

In her delightful book *Longitude*(1), Dava Sobel details the troubles and tribulations that John Harrison (1693-1776) had to endure to claim the award money for having solved the most important technological problem of the 18th century- measuring longitude. And yet, the humble name and superb technological achievement of John Harrison is generally not recognized.

In history books, narration glorifies kings, presidents, generals, oligarchs, lawmakers and others but never the humble instrument makers, craftsmen who made possible dramatic societal advances with their quiet, unpretentious work. I fear that in the history of science we have the tendency to do the same. Are we going to tell the story of crystallography and structural biology the same way? Are we only going to recognize the principal investigators that solved the structure(s) of the largest supra-molecular assemblies? What about the people who built the instruments that made all those discoveries possible? What about the people who built the unique synchrotron beamlines that we take for granted? There are legions of such unsung heroes and, in this brief essay, I would like to focus on one who epitomizes these talented scientists, and extend my appreciation and modest homage to all.

After DESY in the early 70s (*Deutsches Elektronen Synchrotron*, 7.5 GeV), the storage ring DORIS (operating at 3-4 GeV) was about 1000-times brighter at 1.54 Å than a rotating anode source (2). Conceptually and experimentally, the achievement of the pioneers in the field was to bring such an intense but transient radiation from the emitted cone tangential to the trajectory of the moving electrons to an experimental sample a fraction of a millimeter in size, several tens of meters away. The radiation had to be extracted from the ring, monochromatized, focused, directed to the experimental 'bunker', shone on the minute sample and the resulting diffraction pattern had to be recorded, read and stored. Due to the high level of background radiation, all the manipulations had to be done by remote control.

What was the driving force behind these titanic efforts? The driving force was to understand structurally how muscle tissue worked. The goal was to be able to perform small-angle x-ray diffraction experiments with insect flight muscle and specially to be able to follow the changes in the diffraction pattern during

the cyclic oscillations of muscle contraction. These were the interests of two pioneers of muscle research Hugh Huxley and Ken Holmes, who moved to Heidelberg in 1968.

Gerd Rosenbaum was born in Breslau, Germany, on August 22, 1942. He initiated his undergraduate studies in physics at the Freie Universität in Berlin but transferred to the Ludwig Maximilian Universität in Munich to continue his undergraduate degree, where he obtained first the *Vordiplom* (equivalent to B.S., 1965) and later the *Diplom* (equivalent to M.S., 1968). Gerd's primary interest was never to build instruments for their own sake, but in the challenge of solving complex problems (first in physics, then in biology). After finishing his M.S., Gerd decided to leave physics and pursue a Ph.D. in biophysics, which he considered to be full of opportunities. He and Ken Holmes initiated a scientific collaboration in 1969 for the first use of synchrotron radiation for diffraction at low angles with biological samples.



Gerd Rosenbaum, John Barrington Leigh, and engineer Rolf Coors (right to left) celebrating the Richfest (German custom at the completion of the basic structure of a new building) of the EMBL bunker at DESY (ca. 1975).

Gerd, supported by Jean Witz designed, fabricated and put into action the necessary instrumentation to carry out the pioneering experiments on synchrotron radiation as a source for further x-ray diffraction. These test studies were performed at the F41 bunker at DESY. As part of these tests, the first ever x-ray diffraction pattern with synchrotron radiation was recorded. The preliminary results published in 1971 in *Nature* showed that, indeed, the measured radiation intensity emanating from DESY was consistent with previous calculations and amounted to about 300 times the one produced by the most powerful fine-focus x-ray tubes of the time(3).

The rest is history. The review published by John Barrington Leigh and Gerd Rosenbaum(2) in 1976 presented the progress that had been achieved by then in the different sources available at the time, which included the German storage ring DORIS, SPEAR (at Stanford) and DCI in the U.K. It is important to realize that even at that time the most significant advances had been made in low angle x-ray diffraction. There was a small section dedicated to 'other applications' where the initial results on Small-Angle Scattering obtained by the biological group at the SPEAR ring at Stanford were discussed. Within the same section, it was reported that a group at the chemistry department at Stanford had succeeded in taking single crystal precession photographs of different biological macromolecules (6 times faster than a rotating anode!), using a camera at an unfocused beam in one

of the SPEAR beam lines(4). More modest improvements were observed at about the same time by a German group using the radiation from DESY(5). Furthermore, the same group at Stanford had also investigated the anomalous scattering in crystals of rubredoxin. Precession photographs taken with wavelengths just below (1.78 Å) and just above (1.74 Å) the iron K-edge (1.7435 Å or 7.1111 KeV), had shown changes in the average intensities of the Friedel pairs ranging from 4-2% (6). The authors of the review finished the section on protein crystallography with the open-ended sentence 'How far one can apply this method in solving the phase problem in crystallography using synchrotron radiation is not yet clear'. The answer began to emerge a few years later (references 6-8), and now synchrotron experiments tuned to optimize anomalous scattering dominate in *de novo* protein structure determination.

Aren't these beamlines comparable to unique sculptural, architectural or artistic masterpieces? Aren't our current synchrotron beamlines technological icons of our time comparable to the timekeepers that earned Mr. Harrison the prize of the Board of Longitude? And in a different vein, aren't these beamlines the reflection of a creative mind comparable to the best artistic minds of all times? Indeed, each component part has a specific design and purpose within the operation of the whole, but isn't the conceptual design, fabrication and execution comparable to the conception, development and harmonization of the score for an entire symphony? Currently, our work depends on the skills, creativity and dedication of anonymous instrument makers. The number of structures published, refined or deposited at the Protein Data Bank does not measure directly their ingenuity and achievements. Rather, their accomplishments are part of our latest storage rings, the optical components of our newest beamlines, and the elements of our most sophisticated experimental hutches. Our most recent and more spectacular structures may be part of the news and bring honor and fame to many members of the crystallographic community and to crystallography as a field of research. However, we should never forget our unsung heroes who built the storage rings and experimental stations and who made those amazing achievements possible.

Notes

(1) Longitude. "The True Story of a Lone Genius who solved the Greatest Scientific Problem of His Time. Dava Sobel" Walker and Company: New York, 1995.

(2) Barrington Leigh, J. & Rosenbaum, G. (1976). "Synchrotron X-Ray Sources: A New Tool in Biological Structural and Kinetic Analysis" *Ann. Rev. of Biophys. Bioeng.* 5: 239-270.

(3) Rosenbaum, G., Holmes, K. C. and Witz, J. (1971) "Synchrotron Radiation as a Source for X-ray Diffraction" *Nature* 230: 434-437.

(4) Phillips, J. C., Wlodawer, A., Yevitz, M.M. and Hodgson, K.O. (1976) "Applications of synchrotron radiation to protein crystallography: preliminary results" *PNAS* 73: 128-32.

(5) Harmsen, A., Leberman, R. and Schulz, G. E. (1976). "Comparison of protein crystal diffraction patterns and absolute intensities from synchrotron and conventional x-ray sources" *J. Mol. Biol.* 104:311-314.

(6) Phillips, J. C., Wlodawer, A., Goodfellow, J.M., Wa-

tenpaugh, K.D., Sieker, L.C., Jensen, L. H. and Hodgson, K. O. (1977). "Applications of Synchrotron Radiation to Protein Crystallography. II. Anomalous Scattering, Absolute Intensity and Polarization" *Acta Cryst.* A33:445-455.

(7) Hendrickson, W. A. (1985). "Analysis of Protein Structure from Diffraction Measurements at Multiple Wavelengths" *Trans. Amer. Cryst. Assn.* 21: 11-21.

(8) Kahn, R., Fourme, R., Bosshard, R., Chiadmi, M., Risler, J.L., Dideberg, O. and Wery J. P. (1985). "Crystal Structure Study of Opsanus tau Parvalbumin by Multiwavelength Anomalous Diffraction" *FEBS Lett.* 179: 133-137.

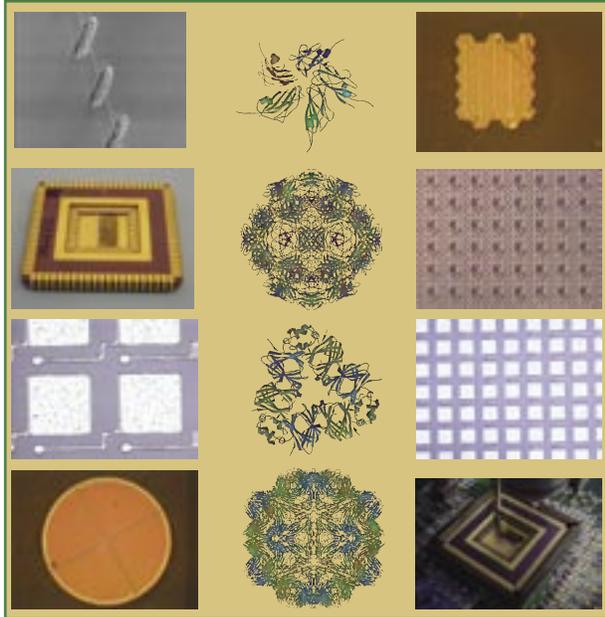
Acknowledgements.

I have felt honored to be Gerd's friend for sometime now. I wish to thank him for the time he devoted to flesh out this article with the factual information about his life accomplishments. The insightful comments and suggestions of W. A. Hendrickson on the manuscript are greatly appreciated.

Cele Abad-Zapatero

Editor's Note: This article is especially timely in light of Nguyen-Huu Xuong being awarded the first-ever Charles Supper Award at ACA Chicago.

What's on the Cover



After **Dr. Xuong (Supper Award winner)** developed the multiwire proportional counter technology for crystallographic applications, he became interested in silicon pixel-array detector (SPAD) technology. He spent most of the 1990's working in this area.

The Molecular Biology Consortium 3DX project - funded by a grant from the NIH-National Center for Research Resources, as was Dr. Xuong's work, is inspired by his early work on SPADs, and is based upon much of what he accomplished. Like Dr. Xuong, we are collaborating with the Electronic Engineering Division of Lawrence Berkeley National Laboratory (LBL) for our application-specific integrated circuit (ASIC) readout electronics. The images on the left and right columns were provided by Ed Westbrook and Christ Keney and should be viewed as an extension of Dr. Xuong's work..

Top row left: A set of three indium bumps. Each pixel of the silicon sensor must be electrically coupled to its readout electronic CMOS (complimentary metal-oxide-semiconductor) chip, which is a separate silicon chip behind the sensor chip. Coupling is made by placing little bumps of indium, a soft, compressible metal, on both the sensor and readout chips, and pressing them together until the bumps merge.

Top row right: A 3D sensor made with hexagonal pixels. This is an alternative geometry for pixels that might provide slightly lower capacitance among the electrodes, yielding better signal-to-noise than square pixels.

Second row left: A sandwich 'flip chip' 3DX sensor, bump-bonded to its readout CMOS chip, wire bonded in a chip carrier. The carrier electronically connects the CMOS chip to its printed circuit board.

Second row right: A close up of part of the 3DX CMOS chip, with under-bump metal deposited on the bump bond pads. After the CMOS integrated circuit is fabricated, the bonding pad must be coated with metal so the indium will bind to it.

Third row left and Third row right: These are sensor elec-

trode squares, attached to bonding pads. The full size array is a 64 x 64 matrix. The sensor pixel raster is 150 microns, but the CMOS pixel raster is 144 microns. This allows the edge of the CMOS chip to be about 0.2mm within the edge of the sensor, so the sensor chips can butt together without causing electrical contact between neighboring ASICs. Therefore there are metal conductors of different lengths connecting each bond pad to its electrode.

Bottom row left: This is a quadrant sensor, which we are developing as a beam position monitor.

Bottom row right: This shows a 3DX CMOS chip being probed at LBL, on a probe station with a micromanipulator. The CMOS is held in its chip carrier, which is plugged into the printed circuit board.

The MBC work is supported by NIH grant 1 R01 RR16230.

The *images in the center* are illustrations of protein structures solved in **Alex McPherson's** (Fankuchen Award winner) laboratory. The images were retrieved from the RCSB Protein Data Bank. *Alex also kindly provided the photos of crystals scattered throughout the Newsletter.*

Top row: Ban, N., McPherson, A.: "The structure of satellite panicum mosaic virus at 1.9 A resolution" *Nat Struct Biol* 2 pp. 882 (1995) (PDBID 1STM)

Second row: Larson, S. B., Day, J., Greenwood, A., McPherson, A.: "Refined structure of satellite tobacco mosaic virus at 1.8 A resolution" *J Mol Biol* 277 pp. 37 (1998) (PDBID 1A34)

Third row: Ko, T. P., Ng, J. D., McPherson, A.: "The three-dimensional structure of canavalin from jack bean (*Canavalia ensiformis*)" *Plant Physiol* 101 pp. 729 (1993) (PDBID 2CAV)

Bottom row: Canady, M. A., Larson, S. B., Day, J., McPherson, A.: "Crystal structure of turnip yellow mosaic virus" *Nat Struct Biol* 3 pp. 771 (1996) (PDBID 1AUJ)

Index of Advertisers

ATPS, Inc	44
Boehringer	35,46
Bruker AXS	43
Bruker/Nonius	Inside front, 20
DCA	13
deCODE Genetics	Outside back
Diversified Scientific	36
Genomic Solutions, Inc.	33
Gilson, Inc.	7
Hampton Research	41
MAR USA, Inc.	24,25
Molecular Dimensions	11,23,42
Oxford Cryosystems	39
Oxford Diffraction	17
Rigaku/MSK, Inc.	9, Inside back
Rigaku/Osmic, Inc	27
RoboDesign	30
Wyatt Technology Corporation	3
Xenocs	5

Candidates for ACA offices in 2005

The Nominating Committee has selected the following candidates for the 2004 elections for ACA offices in 2005

Vice-President: Robert Bau and Zygmunt Derewenda

Canadian Representative to Council: Lee Groat and Michael Jennings

Committees:

Communications: Annie Héroux and Jim Fettinger

Data, Standards & Computing: Bernhard Rupp and Richard Staples

Continuing Education: Gloria Borgstahl and William Ojala

2004 Nominating Committee:

Victor Young (Chair), Charlie Carter and Kathy Kantardjieff

To nominate write-in candidates for any of these offices, write to the ACA Secretary: Lisa J. Keefe, IMCA-CAT, Sector 17, Bldg. #435A, Advanced Photon Source, Argonne National Laboratory, 9700 South Cass Ave., Argonne, IL 60439. (Fax: (630) 252 0521) Letters must be received by September 15, 2004 and must be signed by 5 supporting ACA members and include a signed statement by the candidate describing his or her qualifications. Nominations for the Canadian representative to council must be made by members living in Canada. Statements from all candidates will be included with the ballots which will be sent to all members in October 2004.

metal hydride complexes and the analysis of unusual modes of metal-hydrogen bonding, and this is probably the type of research for which we are best known. Lately we have been exploring the potential of making the neutron diffraction technique more accessible to protein crystallographers, by demonstrating that the new, sensitive neutron detectors that have been developed by various groups around the world (most notably those at JAERI in Japan, the ILL in France and Los Alamos in New Mexico) are capable of locating the hydrogen atoms of a protein at atomic resolution in certain favorable cases.

Statement: First of all, let me say that it is certainly an honor to have been invited to be a candidate for the vice-presidency of the ACA. I have always looked forward to the annual ACA meetings throughout my career, both from the point of view of providing stimulating scientific ideas, as well as their benefits in making contacts and meeting friends and colleagues. Originally coming from a background in organometallic chemistry, I've been involved in crystallographic investigations since the late 1960's, first as a graduate student with Herb Kaesz (UCLA) who stimulated my interest in metal hydride clusters, and Mel Churchill (then at Harvard), who taught me the "basics of the trade". Later as a postdoctoral fellow with Bill Lipscomb (Harvard), I became introduced to macromolecular crystallography as a member of the ATCase team (aspartate transcarbamylase), an interest that has become rekindled in recent years through some work on the neutron diffraction study of small proteins such as rubredoxin.

I believe that I can bring into this office an appreciation for various diverse fields of crystallography. Over the years, our group has been active in both x-ray and neutron diffraction, and we have collaborated extensively with investigators from both the small-molecule and macromolecular communities. Our work has been carried out, not only in our own labs, but also in half a dozen neutron facilities and several synchrotron sources around the world, and this has led to an appreciation of how crystallographic research is done under a wide variety of different experimental conditions. Indeed, many of my former students have acquired positions not only in academic institutions and industrial laboratories, but also in major govern-

Bob Bau, Vice-President



Professor of Chemistry, University of Southern California, Los Angeles, CA 90089

Education: B.Sc., University of Hong Kong (1964); Ph.D. in Chemistry, University of California at Los Angeles (1968); Postdoctoral Fellow, Harvard University (1968-69)

Professional Activities: DOE: Chairperson, IDT (Instrument Development Team) for the construction of a new Single Crystal Diffractometer at the SNS

(Spallation Neutron Source), Oak Ridge, Tennessee. DOE: Member, IDT for a new Macromolecular Neutron Diffractometer ("MaNDi") being proposed for the Spallation Neutron Source. ACA: Member, Neutron Scattering SIG. *Past activities:* NSF: Member, Chemistry Division REU Panel. NIH: Panel Member for Program Project site visit. ACS: Alternate Counselor, Southern California Section. ACS: Alternate Counselor, Inorganic Chemistry Division. Editorial Advisory Board, *Inorganica Chimica Acta*. Editorial Advisory Board, *Chemtracts*. Editor "Transition Metal Hydrides", *ACS Advances in Chemistry Series*, No. 167. External Examiner, Chemistry Department, Chinese University of Hong Kong. *Honors and Awards:* Fellow of the Alfred P. Sloan Foundation. NIH Research Career Development Awardee. Alexander von Humboldt Senior U.S. Scientist Awardee.

Research Interests: X-ray and neutron diffraction studies of transition metal hydride complexes. X-ray and neutron studies of small proteins. Determination of the absolute configuration of isotopically-substituted molecules via single-crystal neutron diffraction. Historically, most of our group's efforts have been directed towards the neutron diffraction analysis of

ment-run national labs, and this again has added an extra dimension to my awareness of different aspects of crystallographic research.

I am currently the Chairperson of the IDT (Instrument Development Team) for the construction of an SCD (Single Crystal Diffractometer for small molecules) at the new high-intensity Spallation Neutron Source currently under construction at Oak Ridge, Tennessee. I am also a member of the IDT for a second instrument (tentatively called "MaNDi") currently in the proposal stage that would be built for neutron protein crystallography. The aim, in both cases, is to utilize the greatly increased neutron flux of the SNS to enable the analysis of crystals an order of magnitude smaller than those currently required for neutron diffraction. If these promises materialize, it would make the neutron diffraction technique much more accessible to the crystallographic community, and would open up this field in a way similar to the manner in which synchrotron radiation has totally revolutionized x-ray data collection. I think these activities provide me with a perspective that would be useful as vice-president and president of the ACA.

The ACA itself is a well-run, efficient organization with a highly professional staff. If I am elected, I intend to use my experience to support synergy among the association's many activities and also with the IUCr. In particular, I would like to make some contributions towards the ACA's continuing education activities. Having taught a graduate level course in x-ray crystallography for the better part of my 35-year career at USC, I feel that I may have something to offer in this area. I have had the pleasure and satisfaction of seeing many fine former students become successful in this field, and it's a rewarding feeling to realize that one had something to do with these scientists' development. I think that as a society the ACA has an obligation to continue to make sure that crystallographic education is actively maintained at a high level, not only at universities across the country but also at other scientific institutions that participate in this worthy activity. Indeed, I believe that my connections developed over the course of a long collaborative career with scientists from national and international government organizations may also be use-

ful in this regard. Many of these research institutions (such as the Argonne and Los Alamos National Labs, the Brookhaven and Stanford Synchrotron Sources, to name a few, and international facilities such as the ESRF and ILL in France and ISIS in England) offer a wide variety of tutorials and summer training programs, and I believe that the scientists who run these highly successful educational programs could provide ideas that would further enhance the already excellent set of workshops and summer courses offered by the ACA.

Zygmunt S. Derewenda, Vice-President



Professor of Molecular Physiology and Biological Physics, University of Virginia School of Medicine, Charlottesville, Virginia

Education: M.S. Biophysics, University of Lodz, Poland (1977); Ph.D. Chemistry, University of Lodz, Poland (1982). Doctoral/Postdoctoral, University of York, UK, Guy G. Dodson (1980-85).

Professional Activities: Canadian Society for Biochemistry and Molecular Biology, Councilor (1993-1996); Canadian Federation of Biological Sciences Annual Meeting, Session Organizer and Chair (1993 & 1994); Midatlantic Crystallography Annual Meeting, Organizing Committee Member (1997 & 2001); ACA Annual Meeting, Session Co-Chair (2002); NIH Special Study Section (2001-2003); APS Sector Review Panels Member (2003);

DOD Neurofibromatosis Program Review Panel (2004); numerous institutional committees at the University of Alberta (1991-1995) and University of Virginia (1996-present); *ad hoc* reviewer for Medical Research Council of Canada, Natural Sciences and Engineering Research Council of Canada, NSF, US Department of Agriculture, Heart and Stroke Foundations of Canada, American Chemical Society, Wellcome Trust UK and BBRC UK. Member of the ACA, ACS, ASBMB and NYAS.

Research Interests: For nearly thirty years I have been driven by intense curiosity about structure-function relationships in biological macromolecules. My first, voracious read of James Watson's 'The Double Helix' at the age of 16, convinced me that crystallography was the most beautiful of all sciences (incidentally, I still firmly believe that to be true). Years later, I was fortunate to be in a position to make contributions to the studies of the haemoglobin function, and the development of insulin variants for diabetes treatment; I worked in a collaborative effort with Novo-Nordisk (Denmark) on the development of enzymes, such as lipases and amylases, for industrial applications; and now, inspired by the recent advances in cell biology, I work on GTPase (RhoA) – mediated signaling; neuronal migration; and molecular basis of neurofibromatosis. Throughout my career I have contributed to methodological advances, such as the use of synchrotron radiation, developments in refinement strategies and in molecular replacement. More recently, I became interested in new approaches to protein crystallization. My aim has always been to do good science, advancing the field as well as our knowledge of the world around us.

Statement: I took my first X-ray diffraction images on a Weissenberg camera in 1976, and attended my first IUCr Meeting in 1978 (Warsaw), thus embarking on an odyssey in crystallography, which would take me through several countries on two continents, and lead me to my present home in Charlottesville, Virginia. I never suspected when I joined ACA in 1991, having just moved to Canada from the U.K., that I might ever be nominated for the Vice-Presidency of the Association. Needless to say, I feel deeply honored by the invitation to stand, but I see it first of

all as a call to duty from an Association to whom I owe many wonderful moments and a plethora of professional opportunities.

Crystallography emerged in the nineteenth century as an independent offshoot of mineralogy, and through the studies of von Laue, and later the Braggs, Pauling, Bernal, Crowfoot, Crick, Watson, Perutz and others, brought about successive revolutions in physics, chemistry, biology, and now medicine. The ACA is charged—along with the other national associations and the International Union—with preserving this heritage and legacy, retaining its traditionally high standard of services to its members, and promoting education in the field. Above all, the ACA is responsible for preserving a unique identity of our profession (and vocation) and for striving to maintain the high standards established by our members in research, teaching and service to the community.

If called upon, I will strive to represent the interests of the entire community. My professional careers spans four different countries and two continents, and I believe that this has given me experience that could be useful in that regard. For a number of years I worked in Chemistry Departments, and since my move to North America I have been affiliated with Medical Schools. As early as 1981, I was among the crystallographers using synchrotron radiation, and throughout the years I have retained a keen interest in experimental methodology. Through my collaborative efforts with industry, I was involved in translational research leading to industrial applications. Thus, I am familiar with many of the diverse facets of crystallography.

The ACA has a wide ranging spectrum of activities and responsibilities. I believe that it is important to maintain the high quality of the scientific program of our annual meetings, while at the same time nurturing the wonderful atmosphere of friendships and collegiality. The Society should make a conscious effort to ensure that—as the crystallographic methodology becomes incorporated into the experimental palette of structural biology, cell biology and drug discovery—the quality of crystallographic endeavors is not exiled, along with data collection tables, into the supplementary material of scientific journals. I also feel that teaching and training presents us with very serious challenges, as high-throughput pipelines

and automated software suites change the way we work. The Society should make itself visible and identifiable early on in young crystallographers' careers. Finally, as asserted by previous ACA leaders, we should continue to work closely with our colleagues in other countries in the Americas and with IUCr.

Lee Groat, Canadian Representative to Council



Professor, Department of Earth and Ocean Sciences, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada

Education: B.Sc., Queen's University (1982); Ph.D., University of Manitoba (1988); NATO PDF, Cambridge University (1989)

Professional Activities: Member of ACA, Canadian Institute for Synchrotron Research (CISR); Editor, *American Mineralogist*

Research interests: Small-molecule crystallography; crystal chemistry of minerals; synchrotron x-ray diffraction; twinned structures; structure solution from powder data.

Statement: This is an exciting time for crystallography in Canada, thanks to construction of the Canadian Light Source (CLS) and improved funding for instrumentation through the Canada Foundation for Innovation (CFI). We need to improve communication in order to make best use of the equipment, and to showcase our research at the national and international levels so that the scientific community is made aware of the impact of the new facilities. If elected as your representative I will do my best to make this happen.

Michael Jennings, Canadian Representative to Council



X-Ray Service Crystallographer, University of Western Ontario, London, Ontario, N6A-5B7

Education: B.Sc., Chem/Math, Simon Fraser University, 1984; Ph.D., Chemistry, University of Western Ontario, 1989; NATO Post-Doctoral Scholarship, Toulouse, France 1990-1991 Crystallographic Mentors: N. Payne (1986-88); Lj. and K. Muir (1988); G. Ferguson (1989)

Professional Activities: ACA member since 1989.

Research Interests: Small Molecule Crystallography, Twinning

Statement: I have been the Service Crystallographer at UWO since July 1998 and have not missed an ACA meeting over the past 6 years. I have certainly got a lot of mileage out of the numerous workshops I have attended. The time and energy expended by the various crystallographers who have shared their expertise with me is greatly appreciated. I feel it is time I put something back into the crystallographic community and representing Canada at the ACA council meetings seems like a good start. As yet, I don't have much of an agenda as a potential Canadian Representative for the ACA. Perhaps I'll have more far reaching goals once I have some experience in the position. I certainly plan to become acquainted with as many Canadian Crystallographers as possible. This should make it easier to address any Canadian issues that might crop up.

**James C. Fettinger, Communi-
cations Committee**



Director, X-ray Crystallographic laboratory, University of Maryland, College Park, Maryland 20742

Education: B.S. Chemical Engineering, State University of New York at Buffalo (1982), Ph.D. Inorganic, Chemistry, University at Buffalo, State University of New York (1987), Post-doctoral fellowship, (James A. Ibers, 1987-1988), Northwestern University, Research Associate (1988-1992) CIBA-Geigy, Basel Switzerland.

Professional activities: Member of ACA (1990-present); Member of ACS (1984-present); Service Crystallography Secretary 2003-present; Radiation Safety Committee member, University of Maryland (1999-present).

Research Interests: Service Crystallography, disordered and twinned structures, large small molecules.

Statement: It is an honor to be nominated as a candidate for the communications committee. With the evolution of crystallographic computing speeds and software the examination of disordered and twinned structures are now becoming more routine. This renaissance concerns the various flavors of data analysis, reduction and optimization that the 'experts' in our field are currently implementing and it would therefore be prudent for such knowledge to be communicated to all so, if elected, it would be a pleasure to serve on the communications committee and participate in this process.

**Annie Héroux,
Communications Committee**



Associates Biophysicist, local contact beamline X26C, Biology Department, bldg 463, Brookhaven National Laboratory, Upton, NY 11973-5000

Education: B.Sc. Chemistry (1990), M.Sc. Chemistry- small molecule crystallography- (1992), Ph.D. Chemistry- fiber diffraction- (1996) Université de Montréal, Canada. Post-doctoral work in protein crystallography from 1997-1999 with David Borhani at Southern Research Institute, Birmingham, AL.

Professional Activities: 2003 NSLS Users' Planning Committee: publicity chair, 2003-2005; Allocation panel for General User time at the NSLS.

Research Interests: For the past year, I have been involved in the *Mail-in* program with Howard Robinson at BNL Structural Biology. The interest for this *RapidAccess* form of data collections for macromolecular crystallography users is growing at an exponential rate. The users benefit from our intimate knowledge of the beamlines and optimization of the time available. This results in a very fast turn around for getting results and insights on what needs to be done to complete the experiments. This creates a very dynamic and stimulating environment for the users and us.

Statement: I look forward to being an active participant in the ACA communications committee. I interact on a daily basis with several different research groups, either directly with users coming to collect data or via emails with remote users. This allows me to get a pulse for what the community is looking for. I would feel privileged to channel this information via the publications and public events related to the ACA.

**Bernhard Rupp, Data, Standards
and Computing Committee**



Macromolecular Crystallography and Structural Genomics, University of California – LLNL, POB 808, Livermore, CA 94551

Education: M.S. and Ph.D. Habilitation (*venia docendi*) in Molecular Structural Biology, University of Vienna, Austria (1988) in Structural and Physical Chemistry; Research and Teaching Associate, Austrian Science Foundation; Lady Davis Postdoctoral Fellow, Racah Institute of Physics, Jerusalem, Israel; Research Scientist at the Nuclear Research Center (KFA) Jülich, Germany, and Neutron Scattering Laboratory (LNS) of the ETH Zürich, Switzerland; University of California - Lawrence Livermore National Laboratory, Postdoctoral Fellow, Synchrotron Group; UC-LLNL, Head of X-ray crystallography group, Biology and Biotechnology Research Program, UC-LLNL; Participating Research Team Leader, Advanced Light Source, LBNL; Macromolecular Crystallography and Structural Genomics Group, UC-LLNL.

Professional Activities: Member of the SSRL Users Organization Executive Committee (1998-2000). Special Session Chair, American Crystallographic Association Annual Meeting 2001, Los Angeles; Member of the NIH PSI TB Structural Genomics Consortium.

Research Interests: My research has been the relation between structure, function, and physical properties of matter ranging from high temperature superconductors to protein drug target structures. Crystallography has always been my prime means of research, using

techniques covering powder diffraction, small molecule crystallography, magnetic neutron scattering, time resolved synchrotron diffraction studies, and, during the past 11 years, macromolecular crystallography, with a focus on development of high throughput crystallization and crystallography in structural genomics of drug targets structures.

Statement: Each of the fields in crystallography has unique needs for computing, presentation of results, and deposition and maintenance of data. My familiarity with a wide range of computational techniques ranging from Rietveld powder refinements to automated validation in high throughput macromolecular crystallography allows me to appreciate the needs and concerns of multiple and diverse interest groups in the ACA community. I also maintain crystallography tutorials on my public web site www-structure.llnl.gov/.

Richard Staples, Data, Standards and Computing Committee



Lecturer and Manager of X-Ray Crystallography, Department of Chemistry and Chemical Biology, Harvard University, 12 Oxford Street, Cambridge, MA 02138

Education: BA (1985) Central Michigan University, Ph.D.(1990), University of Toledo, Postdoc Texas A&M University.

Research Interests: Structural aspects of inorganic compounds, coordination complexes and potential catalysts. The development of techniques to grow crystals of organic complexes.

Professional Activities: Service SIG chair (2003), organized sessions at recent ACA meetings. Member of ACA, ACS and Protein Society.

Statement: I will try hard to work with instrument providers to improve software implementation so that options are not lost in the automation process that is currently on going. It seems to me that the instrument providers are so intent to simplify the data collection and processing software that there is the possibility of less user control over parameters that in some experiments may be necessary and pertinent. This lack of control is somewhat removed by free software available but this software does not often interact with the manufacturers software to provide seamless information transfer to cif files. This is a second area of concern, as the more and more automated software is developed even some small values need to be adjusted to create a legal cif file in the final result.

Gloria Borgstahl, Continuing Education Committee



Eppley Institute for Cancer Research, 987696 Nebraska Medical Center, 10732A Lied Transplant Center, Omaha, NE 68198-7696

Education: University of Iowa, B.S.E. Biomedical Engineering (1985), University of Iowa, Ph.D. Biochemistry (1992). Thesis advisor: Dr. Arthur Arnone., Postdoctoral Advisors: Elizabeth Getzoff, John Tainer and Tom Terwilliger.

Professional Activities: Member ACA since 1988. Chair of the ACA General Interest Group (GIG) 2001-2.

Research Interests: Cancer, Biochemistry, DNA metabolism, Protein crystallography, Aperiodic modulated crystals,

Super-fine phi slicing, Parallel synchrotron radiation, Crystal mosaicity, and x-ray topography

Statement: I am very pleased and honored to have been nominated to the Continuing Education Committee. I have always thought of the ACA as my home. I have felt indebted to the Association, ever since graduate school, when the contacts and friends I made in those early days in my career really helped me to understand crystallography and to finish my thesis work. That solid education through the Association really paid off in my postdoc years. Now I make a habit of attending the ACA meeting every year and I encourage my students to become members.

To serve on the Continuing Education Committee is a natural choice for me. My personal plan is to stop learning when I die and even then I will learn something. My approach to every day is to learn and I am a continual student. I try to teach my own students and lab members to seek knowledge, to understand and to be understood. Our work week includes many opportunities to learn from each other and to teach each other. One of the greatest rewards in research and mentoring is when your students are successful. As all teachers know, it is only after you have taught crystallography that you learn it through and through.

To the Continuing Education Committee I can offer the rich experiences I have enjoyed in teaching crystallography. I believe that to have a successful crystallography laboratory you have to teach the subject. While an Assistant Professor at the University of Toledo, I developed several courses in crystallography, including: a one semester general overview using Glusker's text with an extensive lab component, a summer session on crystal growth using McPherson's text, and then semester long special topics courses on data issues, phasing, density modification, modeling, refinement and validation using current crystallographic literature. These lectures were attended by students as well as other faculty. Now at the Eppley Institute I am teaching crystallography to an informal "study group" of cancer biologists, that includes graduate students and faculty, who wish to apply our methods to conquering this disease that negatively affects us all. Blow's "Crystallography for Biologists"

is the text. While the chair of the General Interest Group, I organized many sessions for two ACA meetings in a row. I set aside one session at each meeting for educational lectures.

As a member of the Continuing Educating Committee I will continue this natural quest for knowledge and help to pass on the knowledge to future generations of crystallographers. I would enjoy the opportunity to contribute my experience to the committee's assigned tasks and the mission of the ACA.

Bill Ojala, Continuing Education Committee



Chemistry instructor and laboratory teaching/development staff, University of St. Thomas, St. Paul, MN

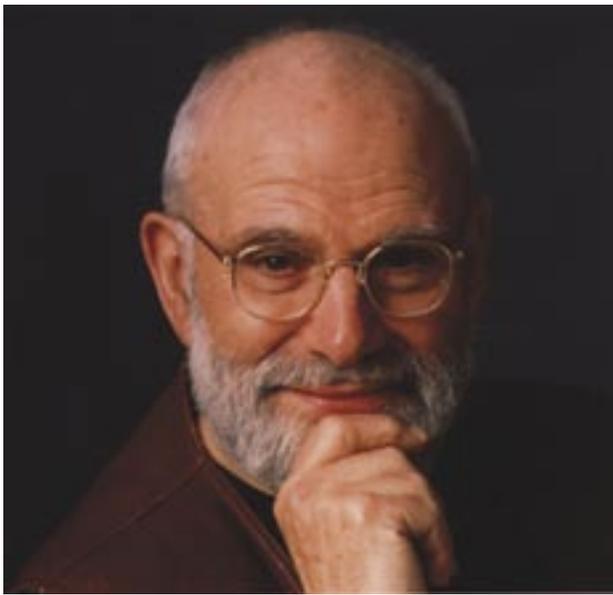
Education: B.S. College of Great Falls, Great Falls, MT (1977), Ph.D. University of Minnesota, Minneapolis, MN (1986)

Professional activities: ACA member since 1993; member, American Chemical Society, American Association for the Advancement of Science, Minnesota Academy of Science, and Council on Undergraduate Research; coordinator of the United States National Chemistry Olympiad for the Minnesota Local Section of the ACS.

Research Interests: Solid-state structures of monosaccharide derivatives; phase transitions in small-molecule organic solids

Statement: Few other scientific fields have undergone so dramatic a transformation in such a brief time as crystallography, progressing from films to CCDs within the span of a typical research career. Keeping pace with this spectacular rate of change makes the field both challenging and enjoyable to those of us who have the opportunity to participate in it. Staying current with these changes can be especially challenging to those of us who work in primarily undergraduate institutions. I am fortunate in that the four-year liberal arts university at which I work is located near a major research center for crystallography (the University of Minnesota) that has faculty and staff who are generous in helping me and my undergraduate research students stay connected with crystallography. I suspect that few other researchers in small colleges and universities similar to mine are so fortunate. In seeking a position on the Continuing Education Committee, I hope I can be of particular help to faculty and staff from small colleges who wish, like I do, to keep up with the rapid progress being made in our science.

ACA Elizabeth A. Wood Award for Science Writing to Oliver Sacks



Oliver Sacks was born in London, England and earned his MD at Queen's College, Oxford. In the early 1960s, he moved to the US and completed an internship in San Francisco and a residency in neurology at UCLA. Since 1965, he has lived in New York, where he is clinical professor of neurology at the Albert Einstein College of Medicine, adjunct professor of neurology at the NYU School of Medicine and consultant neurologist to the Little Sisters of the Poor.

In 1966 he began working as a consulting neurologist for Beth Abraham Hospital, a chronic care facility in the Bronx where he encountered an extraordinary group of patients, many of whom had spent decades in strange, frozen states, like human statues, unable to initiate movement. They became the subjects of his second book, *Awakenings* (1973), which later inspired a play by Harold Pinter ("A Kind of Alaska") and the movie, "Awakenings," with Robert De Niro and Robin Williams.

He is perhaps best known for his 1985 collection of case histories from the far borderlands of neurological experience, *The Man Who Mistook His Wife for a Hat*, in which he describes patients struggling to live with conditions ranging from Tourette's syndrome to autism, parkinsonism, musical hallucination, phantom limb syndrome, schizophrenia, retardation and Alzheimer's disease. (This book later inspired a dramatic work by Peter Brook, "L'Homme Qui. . .")

As a physician and a writer, Oliver Sacks is concerned above all with the ways in which individuals survive and adapt to different neurological diseases and conditions, and what this experience can tell us about the human brain and mind. His books exploring these themes have been bestsellers around the world and are used widely in university courses on neuroscience, writing, ethics, philosophy and sociology. They have served as the inspiration for artists working in forms as varied as poetry, essay, documentary, drama, painting, dance, cinema and fiction.

In 1989, Dr. Sacks received a Guggenheim Fellowship for his work on what he calls the "neuroanthropology" of Tourette's

syndrome, a condition marked by involuntary tics and utterances, and how its symptoms can be perceived differently in different cultures.

He is a regular contributor to *The New Yorker* and *The New York Review of Books*, as well as various medical journals, and is an honorary fellow of the American Academy of Arts and Letters, the American Academy of Arts and Sciences, the New York Academy of Sciences, and Queen's College. *The New York Times* has referred to him as "the poet laureate of medicine," and in 2002 he was awarded the Lewis Thomas Prize by Rockefeller University, which recognizes the scientist as poet.

His books include the following:

Migraine (1970, revised ed. 1992) Paperback, Vintage Books--ISBN 0-375-70406-x An investigation of the many manifestations of migraine, including the visual hallucinations and distortions of space, time and body image which migraineurs can experience.

A Leg to Stand On (1984) Paperback, Touchstone Books, ISBN 0-684-85395-7 Here the doctor becomes a patient, as he chronicles the mountaineering accident which left him with the uncanny feeling of being "legless," and raises profound questions of the physical basis of identity.

Awakenings (1973, rev. ed. 1990) Paperback, Vintage Books, ISBN 0-375-70405-1 The classic account of survivors of the encephalitic lethargica and their return to the world after decades of "sleep." This book was the inspiration for the 1990 film starring Robert De Niro and Robin Williams as Dr. Sacks.

The Man who Mistook his Wife for a Hat (1985) Paperback, Touchstone Books, ISBN 0-684-85394-9 The bestselling collection of clinical tales from the far borderlands of neurological and human experience.

Seeing Voices (1989) Paperback, Vintage Books, ISBN 0-375-70407-8 A journey into the world of deaf culture, and the neurological and social underpinnings of the remarkable visual language of the congenitally deaf.

An Anthropologist on Mars (1995) Paperback, Vintage Books, ISBN 0-679-75697-3 Seven paradoxical tales of patients adapting to neurological conditions including autism, Asperger's syndrome, amnesia, epileptic reminiscence, Tourette's syndrome, acquired colorblindness, and the restoration of vision after congenital blindness.

The Island of the Colorblind (1997) Paperback, Vintage Books, ISBN 0-375-70073-0 An exploration of a society where total congenital colorblindness is the norm, this book is also a meditation on islands and the strange neurologic malady on Guam which resembles parkinsonism and Alzheimer's, and may provide the key to these diseases.

Uncle Tungsten: Memories of a Chemical Boyhood (2001) Paper, Vintage Books, ISBN 0-375-70404-3 Hardcover, Alfred A. Knopf, ISBN 0-375-40448-1 A memoir of growing up in World-War-II England as part of an extraordinary scientific family.

Oaxaca Journal (2002) Hardcover, National Geographic Directions, ISBN 0-7922-6521-1 A trip to see ferns in Mexico turns into a meditation on Mesoamerican civilization, chocolate, agriculture, mescal, amateur naturalists and more.

Eurekas and Euphorias - The Oxford Book of Scientific Anecdotes by **Walter Gratzer** (2002), Oxford University Press, ISBN 0-19-280403-0.

This is a pleasant book to relax with in the evening, on an airplane, or at the beach. It consists of almost 200 short pieces on various famous figures in science. Each piece is from a half page to several pages in length. Some pieces are humorous, others informative, revealing, and sometimes even disturbing. All are interesting.

For the most part, the people mentioned in the stories will be well known to all readers. Archimedes is a player in one of the pieces. Francis Bacon, Newton, and Darwin also are featured. For the most part, however, most of the scientists are of more recent vintage. The fields of chemistry, biology, physics, astronomy, and mathematics are well represented.

Often you will learn about other people who are not as well known as the principal players but who played a role in a discovery. The book certainly corroborates the role of serendipity and accident in the scientific discovery process. For example, a woman named Cesarina Marina, who mopped the floors in Fermi's Italian lab, and abundant Italian marble both played an important role in the discovery of slow neutrons.

The book paints a number of historic figures in a somewhat tyrannical light, usually from the perspective of junior co-workers or through biting verses from anonymous sources.

Many of the stories relate to the interplay of politics, governments, and scientists. The book contains many stories about scientists fleeing Europe in the 1930s. Were you aware that Niels Bohr purposefully dissolved Max von Laue's gold Nobel prize medal in aqua regia in order to hide it? And, did you know that he purposefully left the jar containing the dissolved medal in plain sight in his Copenhagen lab when he fled to Sweden? What is perhaps most interesting is that the container survived the war intact, just as Bohr expected, and that the Nobel Foundation was pleased to recast the medal after the war for von Laue.

There are more stories about governments and scientists than just stories of Europe in the 1930s. The French revolutionary government, the UK government, and the US government also play occasional, not particularly flattering roles.

Another interesting aspect of these stories is that many of them describe interactions and lasting rifts between well-known scientists such as Einstein and Schrödinger.

The pieces typically include a reference to a longer published article or book. I'm intending to locate some that were of most interest to me. I wish I had the time to read more of them. I'm sure everyone who reads more than a tenth of this book will make his or her own list. Happy reading.

Paul Anderson



Oxygen: the Molecule that Made the World by **Nick Lane** (2003), Oxford Prsss, ISBN: 0198508034.

Three hundred million years ago, dragonflies grew as big as seagulls, with wingspans nearly a yard across. Researchers claim they could have flown only if the air had contained more oxygen than today--probably as much as 35 percent. But oxygen is a toxic gas. Fruit flies raised at twice the normal level of oxygen live half as long as their siblings. If atmospheric oxygen reached 35 percent in the Carboniferous, why did oxygen promote exuberant growth, instead of rapid aging and death? This is just one of the puzzles Nick Lane answers in *Oxygen*. Lane takes the reader on an enthralling journey, as gripping as a thriller, as he unravels the unexpected ways in which oxygen spurred the evolution of life and death. The book explains far more than the size of ancient insects: it shows how oxygen underpins the origin of biological complexity, the birth of photosynthesis, the sudden evolution of animals, the need for two sexes, the accelerated aging of cloned animals like Dolly the sheep, and the surprisingly long lives of bats and birds. Drawing on this grand evolutionary canvas, *Oxygen* offers fresh perspectives on our own lives and deaths, explaining modern killer diseases, why we age, and what we can do about it. Advancing revelatory new ideas, following chains of evidence, the book ranges through many disciplines, from environmental sciences to molecular medicine. The result is a captivating vision of contemporary science and a humane synthesis of our place in nature. (Book description at Amazon.com).

Nature's Robots: A History of Proteins by Charles Tanford and Jacqueline Reynolds (2004) Oxford University Press, ISBN: 019860694X.

Proteins are amazing molecules. They spark the chemical reactions that form the basis for life, transmit signals in the body, identify and kill foreign invaders, form the engines that make us move, record visual images. For every task in a living organism, there is a protein designed to carry it out. *Nature's Robots* is an authoritative history of protein science, from the earliest research in the nineteenth century to the most recent findings today. Tanford and Reynolds, who themselves made major contributions to the golden age of protein science, have written a remarkably vivid account of this history. The authors begin with the research of Berzelius and Mulder into 'albumins,' the early name for proteins, and the range all the way up to the findings of James Watson and Francis Crick. It is a fascinating story, involving heroes from the past, working mostly alone or in small groups, usually with little support from formal research grants. They capture the growing excitement among scientists as the mysteries of protein structure and function--the core of all the mysteries of life--are revealed little by little. And they include vivid portraits of scientists at work--two researchers, stranded by fog in a Moscow airport, strike up a conversation that leads to a major discovery; a chemist working in a small lab, with little funding, on a problem no one else would tackle, proves that enzymes are proteins--and wins the Nobel Prize. Written in clear and accessible prose, *Nature's Robots* will appeal to anyone interested in the peaks and valleys of scientific research. (Book description at Amazon.com)

Debunked: ESP, Telekinesis, and Other Pseudoscience by **Georges Charpak, Henri Broch, Bart K. Holland** (Translator) (2004) Johns Hopkins University Press, ISBN: 0801878675

Can you walk over red-hot charcoal without burning your feet? Appear to stop the beating of your heart? Bend spoons using the power of your mind? In *Debunked!* Nobel Prize winner Georges Charpak and physics prof. Henri Broch team up to show you the tricks of the trade and sleight of hand that keep astrologers, TV psychics, and spoon benders in business. Using only the simplest science, they explore the effectiveness of horoscopes the blander the better and why, with a television audience in the millions, any strange, unlikely prediction is almost certain to come true. If such insider information does not impress your colleagues, why not pierce your tongue with a skewer or demonstrate your eerie powers by using telepathy and the telephone to get a distant friend to intuit the number and suit of a card picked at random. Charpak and Broch show you how. Not merely an expose of magic tricks, this book demonstrates how pseudoscientists use science, statistics, and psychology to bamboozle an audience sometimes for fun, sometimes for profit. During the most scientifically advanced period in human history, belief in the paranormal and the supernatural is alarmingly common. Entertaining and enlightening, *Debunked!* is the antidote, vigorously asserting the virtues of doubt, skepticism, curiosity, and scientific knowledge. This lucid translation makes the arguments clear, understandable, and a pleasure to read. The authors have a serious agenda a critique of belief in the paranormal and the supernatural, and the irrational behavior of those who are taken in by such beliefs but address it with a light and good-humored touch. The book provides entertaining and amusing reading while bringing about an understanding of how the simple application of probability theory and science explains ‘amazing’ coincidences and abilities. (John M. Charap at Amazon.com)

The Nature of Design: Ecology, Culture, and Human Intention by **David W. Orr** (2002) Oxford Press, ISBN:019514855X.

The environmental movement has often been accused of being overly negative—trying to stop “progress.” *The Nature of Design*, on the other hand, is about starting things, specifically an ecological design revolution that changes how we provide food, shelter, energy, materials, and livelihood, and how we deal with waste. Ecological design is an emerging field that aims to recalibrate what humans do in the world according to how the world works as a biophysical system. Design in this sense is a large concept having to do as much with politics and ethics as with buildings and technology. The book begins by describing the scope of design, comparing it to the Enlightenment of the 18th century. Subsequent chapters describe barriers to a design revolution inherent in our misuse of language, the clockspeed of technological society, and shortsighted politics. Orr goes on to describe the critical role educational institutions might play in fostering design intelligence and what he calls “a higher order of heroism.” Appropriately, the book ends on themes of charity, wilderness, and the rights of children. Astute yet broadly appealing, *The Nature of Design* combines theory, practicality, and a call to action. (Book description from Amazon.com)

The Double Bond: Primo Levi, A Biography by **Carole Angier**(2003) Farrar, Strauss & Giroux, ISBN 0374528985.

Perhaps the most important writer to emerge from the death camps, Primo Levi spent sixty-five of his sixty-seven years in Turin, Italy, where he worked as a chemist by day and wrote at night in a study that had been his childhood bedroom. Thanks to his memoirs, which include *Survival in Auschwitz*, *The Reawakening*, and the classic *The Periodic Table*, he became widely known and loved as a supremely moral man, one who had transmuted the agonies of persecution into understanding and clarity. The whole world was shocked when he died in 1987, apparently having thrown himself into the stairwell of the house in which he had been born.

Carole Angier has spent nearly ten years writing this meticulously researched, vivid, and moving biography, which illuminates the design of Levi’s interior life: how he lived as a man divided, not only between chemistry and writing but between hope and despair, and how the duty to testify released him to communicate, which was his deepest need (From the publisher at Amazon.com).

President's Column continued from page 1

Society Presidents in Washington, D.C. The organization is headed by Martin Apple, who has his pulse on the local-national political scene. Not only were we treated to outstanding speakers on a wide variety of topics, but we spent a morning on Capitol Hill, talking science budgets and science education with Senator Kit Bond, Representative Roscoe Bartlett and staffers from Senator Bill Frist’s office. One professional lobbyist, who prepared us for the visit, emphasized that this is the year to have an impact. *Why? Because it is election year and your local representatives listen far more carefully to voters in their district than at any other time.* Your issues, be they scientific or other, need to be stated briefly and your request must be specific. From the viewpoint of the ACA, it is important to let your congressional representatives know that the NIH, NSF and science education budgets need to be protected in these difficult fiscal times. Moreover, Congress and the President once promised to double NSF’s budget over the next five years, only to renege on that promise. Remind your congressional representatives of that promise. (*Editor's Note: For more on communicating with Congress see page 43.*)

I am pleased to offer congratulations to Alwyn Jones who will receive the A. L. Patterson award at the ACA meeting in Orlando in 2005. Before that, I hope to see all of you in Chicago. It should be a great meeting, made better by the presence of our numerous award winners: Madeleine Jacobs, ACA Public Service Award; Leonard MacGillivray, Margaret C. Etter Early Career Award; Richard Marsh, Kenneth N. Trueblood Award; Alexander McPherson, Fankuchen Memorial Award; Oliver Sacks, the Elizabeth A. Wood Science Writing Award; and Nguyen-Huu Xoung, the Charles E. Supper Instrumentation Award.

Fran Jurnak

Communicating With Congress: Now is the Time

“Politics is not a spectator sport. Yet far too many scientists and engineers sit on the sidelines while major decisions are being made on science policy and funding.” - Rep. Vernon Ehlers (R-Michigan)

“Too often scientists avoid politics in the same way that many Members of Congress avoid science. This is a formula for failure.” - Rep. Rush Holt (D-New Jersey)

Major decisions are being made concerning the level of federal funding for programs that are of interest to the scientific community. An important factor in determining the amount of money a department, agency, or program will receive is the amount of correspondence and other communications that Members of Congress get from their constituents. Now is the time to act.

The AIP has a science policy website designed to assist you in communicating with Congress. Among this site's features are:

Guidance on corresponding to, and visiting with, Members of Congress. Information on key chairs and their committees and links to locators for your representative and senators, including e-mail addresses, is available. E-mail is recommended because of time-consuming screening procedures for U.S. mail.

Information on the Administration's FY2005 budget request for the Defense Department, Energy Department, NASA, National Institute of Biomedical Imaging and Bioengineering, National

Institute of Standards and Technology, National Science Foundation, U.S. Geological Survey, and science education programs can be found at www.aip.org/gov/budginfo.html.

Information on the latest congressional budget action on the Administration's budget requests for the above departments, agencies and budgets is at www.aip.org/gov/budginfo.html.

An archive of 2004 issues (and earlier) of FYI, as well as a search engine for FYI can be accessed at www.aip.org/enews/fyi/.

Sixteen AIP exhibits highlight the important links between federal funding for basic and applied research and development and their economic benefits to society. Hard copy versions of these Physics Success Stories are available without charge. See www.aip.org/success/.

Policy statements issued by different science coalitions to which AIP and some of its Member Societies belong recommend funding levels for the science and technology programs of the Department of Defense, the Office of Science of the Department of Energy, National Science Foundation, and the Education Department's Math and Science Partnership Program. See www.aip.org/gov/polstates.html

Links to public policy sites for six of AIP's Member Societies are at <http://www.aip.org/gov/pubpol.htm>

Richard M. Jones

The American Institute of Physics

Recommendations for Strengthening the U.S. Innovation Infrastructure

“Unfortunately, the U.S.’s ability to adapt, compete and innovate alongside emerging workforces in countries such as China and India is threatened by a systematically weak education system, a dearth of R&D funding, visa policy that discourages the brightest foreign minds and a business climate heavy with regulatory and tax burdens.” This is the conclusion of a new report by the Electronic Industries Alliance (EIA), an alliance of approximately 2,500 electronic and high-tech companies and associations. “The best hope for the U.S. to maintain its edge against rising global competition is by fostering and expanding our most prized intellectual asset: innovation,” the report says. “If we want to ensure that successive waves of innovation begin in the U.S., and that U.S. workers are first to benefit from ‘the next big things,’ we have to have the necessary innovation infrastructure in place.” The EIA report includes the following recommendations::

INTERNATIONAL BUSINESS AND TRADE ENVIRONMENT: Use the WTO legal system more aggressively; encourage trading partners to more aggressively enforce intellectual property protections; support policies for voluntary, open standards, including international standards on product design; and bring cases of improper trade practices to the attention of high-ranking government officials.

VISA AND IMMIGRATION POLICY: Provide adequate funding and resources to streamline the visa processes and maintain appropriate statistics; strengthen enforcement of existing regulations; and tighten restrictions on the L-1 category for foreign workers with “specialized knowledge.”

WORKFORCE ASSISTANCE AND TRAINING: Implement a “human capital investment tax credit” to encourage worker training by industry; revise the Trade Adjustment Assistance program to provide workforce assistance for all displaced workers regardless of business sector; subsidize high-tech workers who choose to work in K-12 science and math education; and establish industry-community college partnerships to train workers for technology careers.

K-12 MATH AND SCIENCE EDUCATION: Require industry involvement in the Education Department’s Math and Science Partnerships and industry input to relevant school district policies; encourage students to pursue teaching careers in math and science through tax credit, loan forgiveness, and professional development programs; support school choice policies; and revise the “No Child Left Behind” Act to ensure testing requirements do not lead to a “race to the bottom.”

RESEARCH AND DEVELOPMENT: Strengthen and make permanent the R&D tax credit; increase funding and speed the award process for the Small Business Innovation Research (SBIR) program; enhance industries’ ability to collaborate with and commercialize federally funded research; improve technology transfer practices; and support longer-term funding of a more balanced federal portfolio of basic research. programs.

Audrey T. Leath

The American Institute of Physics

Ensuring the Integrity of the Scientific Advisory System

Based on allegations that administrations officials have, for political and ideological reasons, manipulated scientific advisory committees, reports, and information, several Members of Congress asked the General Accounting Office (GAO) to review the federal government’s policies for staffing scientific advisory committees. At a May briefing, Reps. Eddie Bernice Johnson (D-TX), Ranking Minority Member of the House Science Subcommittee on Basic Research, and Science Committee member Brian Baird (D-WA) released the GAO’s report, which makes a series of recommendations to better ensure the independence and balance of scientific advisory committees and the transparency of the committee appointment process. It is of note that, in April, White House Office of Science and Technology Policy Director John Marburger issued a rebuttal of many of the allegations referred to above.

“The American public deserves to see its government receive the best advice available,” Johnson declared at the briefing. “Every area of life is touched upon by the work of these advisory panels - the environment, our food supply, public health and safety, education, research programs in a wide array of fields - so this is more than just an academic debate,” she said. The U.S.’s national security, economic future and health, Baird said, depend on “integrity” within the scientific advisory system, and “political respect” for that system. Rep. Rush Holt (D-NJ) added that “there must not be confusion” between the gathering and analysis of scientific information and the political work of balancing different interests.

During President Bush’s tenure, a number of scientists have charged that Administration officials took actions to alter the membership of scientific advisory bodies, censor or suppress scientific information, and selectively consider data, to an extent not seen in previous administrations, to concur with ideological, political, or religious views. These allegations have led to several reports by critics of the Administration that attempt to document such abuses. One such report was issued by Rep. Henry Waxman (D-CA), Ranking Minority Member of the House Government Reform Committee (see www.house.gov/reform/min/politicsandscience/report.htm). Another was prepared by the Union of Concerned Scientists (UCS), and accompanied by a February 18 statement signed by over 60 leading scientists, including 20 Nobel laureates and 19 National Medal of Science winners. The UCS report alleges a “pattern of suppression and distortion of scientific findings,” an “effort to manipulate the government’s scientific advisory system,” and censorship of government scientists. The accompanying statement acknowledges that “other administrations have, on occasion, engaged in such practices,” but it alleges that those practices were not as systematic “nor on so wide a front” as those of the current Administration. The UCS report and related statement can be viewed at www.ucsusa.org/global_environment/rsi/index.cfm.

In April Marburger issued a rebuttal of the UCS’s charges. His response, available at www.ostp.gov/html/ucs.html, states in part that many of the “suppressed” items of information were removed from public access for revision and were, or will be,

subsequently re-posted with updated scientific information, and that changes in committee membership and the elimination of certain advisory panels were part of the regular advisory committee process and not intentional manipulation. (It is worth noting that, according to GAO, the law allows for individuals to be selected for a scientific advisory committee to represent certain interest groups or stakeholders, in addition to members selected for their expertise in relevant areas, and requires that such bodies be “fairly balanced” across points of view.)

The GAO report does not address any of the allegations nor their validity, but instead reviews the federal processes and procedures for appointing advisory committee members, and makes suggestions to improve those processes for consistency, transparency, and to better ensure independent and balanced committee membership. Robin Nazzaro, GAO Director for Natural Resources and Environment, stated that, “independent of the facts and issues, the perception alone [that committees are not independent and balanced] is problematic,” and may “jeopardize the value of the committees’ work and call into question the integrity of the advisory system itself.”

GAO recommends that the Office of Government Ethics give federal agencies additional guidance to clarify the difference between those members designated as “special government employees,” who are invited to serve on advisory committees for their expertise and are subject to conflict of interest regulations, and those designated as “representatives,” who are invited to serve as the voice of an interest group or community of stakeholders, and are expected to have “a particular and known bias.” The report further recommends that the General Services Administration provide guidance on what types of information should be collected in a systematic, consistent way on potential advisory panel members in order to ensure that, as required by the Federal Advisory Committee Act, committees are - and are perceived to be - “fairly balanced in terms of points of view presented and the functions to be performed by the advisory committee.” (However, the report does not address how wide a range of views should be represented in order for a panel to be considered balanced.) Additionally, the report identifies several “promising practices” for enhancing independence, balance, and transparency: seeking committee nominations from the public; using a clearly defined process to review information on nominees’ viewpoints and possible conflicts of interest; and developing a structured prescreening interview to ensure appropriate questioning of nominees.

Addendum: The UCS has subsequently issued a response to Marburger, which can be found on the UCS web site at www.ucsusa.org/global_environment/rsi/page.cfm?pageID=1393.

The GAO report, “Federal Advisory Committees: Additional Guidance Could Help Agencies Better Ensure Independence and Balance,” can be found at www.gao.gov/new.items/d04328.pdf.

Audrey T. Leath
The American Institute of Physics

ACA Corporate Members

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

Art Robbins Instruments
www.artrobbinsinstruments.com

ATPS Inc.
www.atpsinc.com

*Bibliothek Technische Hochschule
Hannover, Germany*

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

Bruker AXS Systems
www.bruker-axs.com

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

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

Corning, Inc.
www.corning.com/lifesciences

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

Crystal Logic Inc.
www.xtallogic.com

Crystal Systems, Inc.
www.crystalsystems.com

DataCentric Automation
www.dcacorp.com

deCODE Genetics
www.decodegenetics.com

Diversified Scientific, Inc.
www.dsitech.com

Douglas Instruments Limited
www.douglas.co.uk

Fluidigm Corp.
www.fluidigm.com

Gilson Inc.
www.gilson.com

Hampton Research
www.hamptonresearch.com

Hewlett Packard Company
www.hp.com

MAR USA, Inc.
www.mar-usa.com

MARResearch GmbH
www.marresearch.com

Malvern Instruments
www.malverninstruments.com

Molecular Dimensions, Inc.
www.moleculardimensions.com

Neuro Probe, Inc.
www.neuroprobe.com

Oxford Cryosystems
www.oxfordcryosystems.com

Oxford Diffraction Ltd.
www.oxford-diffraction.com

Protein Data Bank
www.rcsb.org/pdb

Proterion Corporation
www.proterion.com

Rigaku/MSK, Inc.
www.RigakuMSC.com

Rigaku/Osmic, Inc.
www.osmic.com

Shamrock Structures LLC
www.shamrockstructures.com

Tecan
www.tecan.co

Tri Tek Corp.
www.tritek.com

*UOV/Biblioteca Universitaria
Oviedo, Spain*

Veeco Instruments
www.veeco.com

VizEveryWhere
www.vizeverywhere.com

Wyatt Technology Corp.
www.wyatt.com

Xenocs SA
www.xenocs.com

AUGUST 2004

- 2-6 **53rd Annual Denver X-Ray Conference**, Steamboat Springs, CO.
- 9-13 **14th International Conference on Crystal Growth (ICCG-14)**, Grenoble, France.
- 23-25 **4th Conference on Synchrotron Radiation in Materials Science**, Grenoble, France.
- 18-21  **High Pressure Commission Workshop on Crystallography at High Pressure.** University of Saskatchewan Canadian Light Source, Saskatoon, Canada.
- 24-26 **Satellite to ECM22: Crystallography at the start of the 21st century: Mathematical and Symmetry Aspects**, Budapest, Hungary.
- 26-31  **European Crystallography Meeting, ECM22**, Budapest, Hungary.

AUGUST / SEPTEMBER 2004

- 31-10 **Synchrotron Radiation Summer School**, Chester College and Daresbury Laboratory, UK.

SEPTEMBER 2004

- 2-5 **EPDIC-IX, European Powder Diffraction Conference**, Prague, Czech Republic.
- 15-18 **Structural Biology at Crossroads: From Biological Molecules to Biological Systems Conference Celebrating 30 years of EMBL**, Hamburg, Germany.

OCTOBER 2004

- 21-22 **SSRL 31st Annual Users' Meeting**, Stanford, CA.
- 28-30  **Pittsburgh Diffraction Conference**, Pittsburgh, PA.

NOVEMBER 2004

- 16-17  **Crystallographic Society of Japan 2004 Annual Meeting**, Osaka, Japan.
- 17-21  **The 3rd International Conference on Structural Genomics (ICSG 2004)** will provide a venue for discussing progress and visions for the evolving and rapidly expanding international structural genomics initiative. Washington, DC.

MAY 2005

- 19-29 **Evolving Methods in Macromolecular Crystallography**, 37th crystallographic meeting in Erice, Bruxelles, Erice, Italy.

MAY / JUNE 2005

- 28-2  **American Crystallographic Association Annual Meeting, ACA2005**, Walt Disney World Swan Hotel, Orlando, FL. **Local Chairs: Khalil Abboud, abboud@chem.ufl.edu, and Tom Selby, tselby@mail.ucf.edu; Program Chair: Ed Collins, edward_collins@med.unc.edu**

AUGUST 2005

- 18-23 **IUCr Computing School** (prior to IUCr Congress in Florence), in Siena, Italy.
- 23-31 **XX IUCr Congress**, Florence, Italy. Local Chair: Paola Paoli, iucr@iucr2005.it, Program Chair, Carlo Meali, www.iucr2005.it.

JUNE 2006

- 9-18 **The Structural Biology of Large Molecular Assemblies**, the 38th crystallographic course at the Ettore Majorana Centre, Erice, Italy.

JUNE 2007

- 7-17 **Engineering of Crystalline Materials Properties: State-of-the-Art in Modeling, Design, and Applications**, the 39th crystallographic course at the Ettore Majorana Centre, Erice, Italy.



FIRST ANNOUNCEMENT

Florence IUCr2005

XX International Union of Crystallography Congress and General Assembly

23-31 August 2005

Dear Colleague,

We have the pleasure of inviting you to the XX IUCr Congress for which an excellent scientific program is being planned. Thanks to the multidisciplinary of crystallography, presentations on the state of the art in a variety of subject areas will give you the opportunity to develop new fields of interest.

We are confident that the appeal of Florence, one of the most outstanding cities of art in the world, will do the rest, and that your visit will leave you longlasting, happy memories.

The Congress Citadel is in the center of the city, within walking distance of museums, churches and palaces of worldwide renown as well as of a great variety of hotels and restaurants. The second announcement with the final program will be circulated after the summer of 2004. Visit our web site (<http://www.iucr2005.it>) to get the latest news about the congress and to sign up for our mailing list.

Finally, do not hesitate to contact the congress secretariat for any further information. We look forward to welcoming you to Florence.

Yours sincerely,

Carlo Meali
Paola Paoli

www.iucr2005.it

SCIENTIFIC PROGRAM COMMITTEE		LOCAL ORGANISING COMMITTEE	
Carlo Meali, Chairperson, Italy		Paola Paoli, chairperson	
Silvia Benedetti, Italy Lee Bromberg, UK K. Byrappa, India William L. F. David, UK Roberto Fieschi, France Giuseppe Filippini, Italy Britt Johnson, USA Sven Kowmölzer, Sweden Fernando Lpez, Spain Claude Lecocq, France IUCr Office Yehoshua Karkas, Israel Yehoshua Karkas, Israel	Jennifer L. Martin, Australia Douglas H. Ohlendorf, USA John E. Parise, USA Dmitry Yu. Pushcharovskiy, Russia Anja Pyskalla, Austria Paolo Spedon, Italy Anthony L. Spek, The Netherlands Walter Steurer, Switzerland Adriana Zepari, Italy IUCr Secretariat Leonid A. Izrael, Russia	Members: Carlo Bazzicalupi Franco Cecchi Samuele Cioffi Irene Cini Massimo Di Niro Cristina Doni Cristina Faggi Maria Ferrarini Giulio Giori Stefano Giugliani Dante Nelli Marcello Melli Davide M. Passerio	Scientific Secretariat: Andrea Ienco Patrizia Rossi Annalisa Guerci Stefano Berrone Phone: +39 055 4796246/249 Fax: +39 055 4796242 E-mail: iucr@iucr2005.it ORGANIZING SECRETARIAT Newtours S.p.A. Phone: +39 055 5281111 Fax: +39 055 5281155 E-mail: Newtours@iucr2005.it