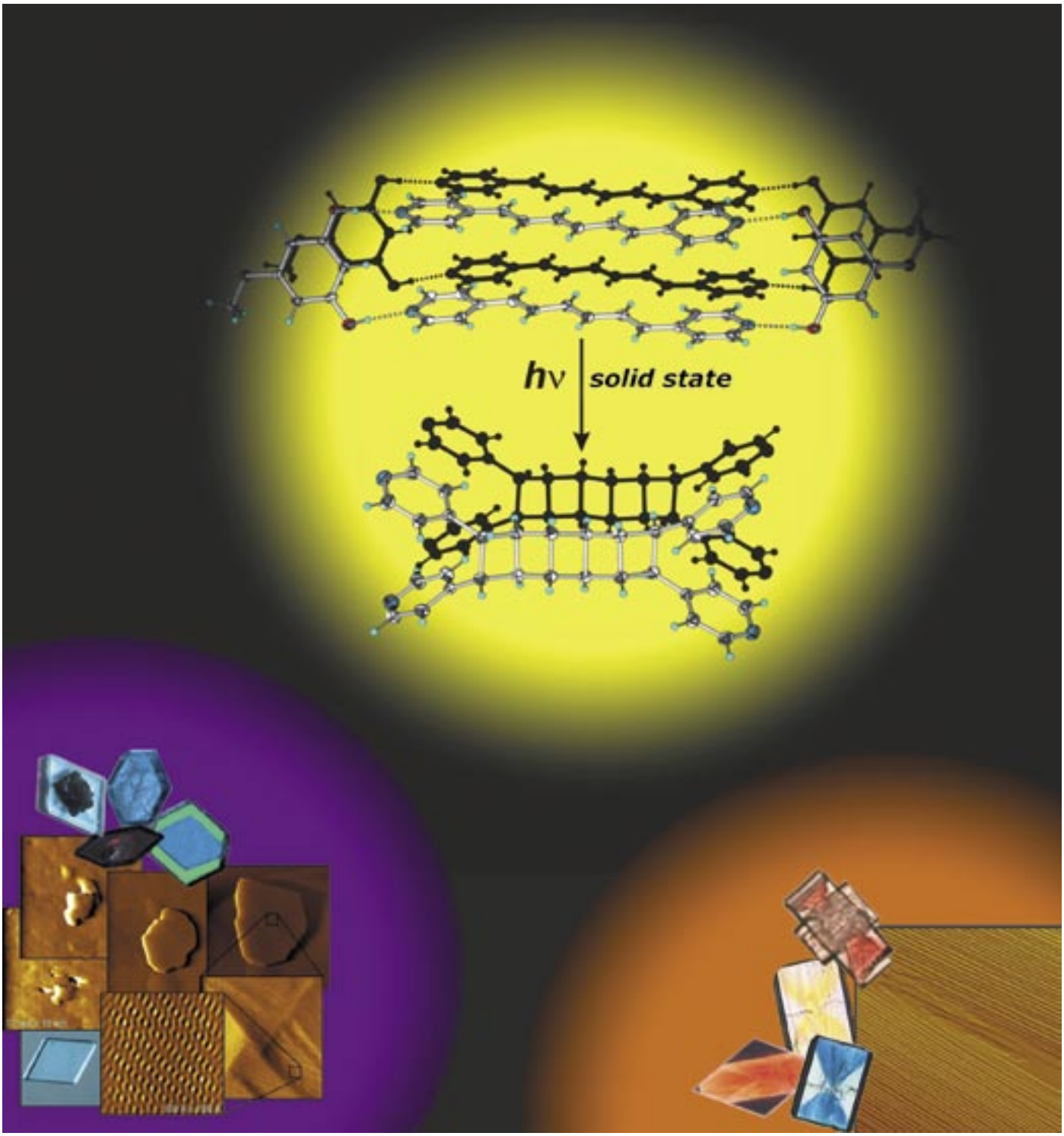
American Crystallographic Association

NEWSLETTER

Number 1 Spring 2004



Transactions Symposium

Chicago ACA Meeting July 17 -22

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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:

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President's Column

Greetings from your new president! In my first column, I want to share my vision of the ACA with you and ask your help for continuing its best traditions. First and foremost, the ACA is pivotal in organizing national meetings to bring together scientists interested in the latest research using x-ray diffraction methods. There are two facets to this role - organizing the best scientific program possible and choosing a great meeting site. The scientific program at each meeting reflects the hard work of the program chairs, numerous session chairs, and the active participation of members of the crystallographic community willing to share their latest research and to train younger scientists in the practical workshops. For the next meeting, I am especially grateful to Marilyn Yoder, Christer Aakeröy, Bernie Santasiero, and Karl Volz who have already spent many hours to ensure the success of the meeting. Ed Collins is program chair, and Khalil Abboud and Thomas Selby are the local chairs for the 2005 meeting, and their tasks have just begun.

The choice of meeting sites falls on the shoulders of the ACA Council members who wrestle with this task throughout the year. The ACA Council identifies sites that are in attractive locations, and then searches for a willing local chair and a suitable conferencing facility at a reasonable cost. Suggestions are always welcome, but I think each of the future meetings at Chicago 2004, Orlando 2005, will appeal to a broad cross section of the community. The sites for 2006 and 2007 are still under review. Suggestions for a site for 2008 are welcome.

The second role of the ACA is more subtle, but nevertheless, is one of its most essential features: to provide a professional network particularly for the younger crystallographers at the start of their careers. The meetings provide a welcome forum for the encouragement and recognition of research efforts through travel awards, poster awards and oral presentations, an opportunity to learn practical techniques in the workshops, and a chance to meet, not only peers, but senior investigators who become legends in their own time. To continue this tradition, I am hoping to reach out even more to the young scientists, to highlight their research through additional speaking invitations, to include them on important committees, and to find ways that make the ACA an even more attractive organization for networking with others in the field.

What can you do to help? ***Attend ACA meetings and recruit new ACA members!*** Everyone reading this column is already familiar with the ACA. I am guessing, however, that most do not realize that the ACA membership is dwindling, having decreased from 2031 in 1998 to 1732 in 2003. And this decline comes at a time when the practice of crystallography is expanding and assuming a more prominent national role in biomedical research. It seems as if many crystallographers take the ACA

for granted. Some renew their membership only when they attend meetings and learn of the discounted registration fee to ACA members. If, in fact, the shining traditions of the ACA are to be continued, then the ACA needs to expand membership in order to keep the meetings at interesting locales and to ensure that meetings will be scientifically vibrant, with a good mix of senior and junior crystallographers. So, do your part - attend the ACA meetings, pay your annual membership dues, and urge other crystallographers in your lab or at your institution to join the ACA.

Fran Jurnak

Call for Nominations for the 2005 Patterson Award

The Patterson Award was established to recognize and encourage outstanding research in the structure of matter by diffraction methods, including significant contributions to the methodology of structure determination and/or innovative application of diffraction methods, and/or elucidation of biological, chemical, geological or physical phenomena using new structural information.

The award, established in 1980, is given in memory of A. Lindo Patterson every three years, and consists of an honorarium plus travel expenses to accept the award and present a lecture at the Annual ACA meeting. Prior awardees include **Douglas Dorset** (2002), **Gerard Bricogne** (1999), **Christer Nordman** (1997), **George Sheldrick** (1993), **Michael Woolfson** (1990), **David and Liselotte Templeton** (1987), **Jerome Karl and Herbert Hauptman** (1984), and **Wayne Hendrickson** (1981).

James Stewart is chair of the Patterson Award Selection Committee; other members include **Wim Hol**, **Brian Patrick**, and **Janet Smith**. Nominating letters and supporting background documentation should be sent to the Chair, Prof Emeritus James M. Stewart, P.O. Box 472, McConnellsburg, PA 17233-0472, pastewart@operamail.com. The award recipient will be announced at the Chicago 2004 ACA meeting and the award and lecture will be presented at the Orlando 2005 meeting.

Guest Editorial:

John Helliwell is Professor of Structural Chemistry at the University of Manchester, UK and holds a joint appointment at the CCLRC Daresbury Laboratory, UK; He is also Editor-in-Chief of Acta Crystallographica.

John R. Helliwell

I am pleased to be invited to write this Guest Editorial for the *ACA Newsletter*. I wish to take the opportunity to explain the current thinking and activity of the IUCr journals. I am keen also to engage in dialogue over the challenges and opportunities that we face; my email is **john.helliwell@man.ac.uk**

Today's innovation fuels tomorrow's science and discovery. In our own field we see many fine examples of innovation leading to expanded capabilities. Among these we may highlight: the acceleration in the capabilities of modern laboratory equipment; the excellent instrumentation within the central synchrotron radiation and neutron facilities; the increasing number and power of software packages; and new methods. A major outcome is the prodigious output of the world's crystal structure determination laboratories today.

As a publisher of seven titles the IUCr relies on the team of volunteer scientists comprising 11 Section and Main Editors and over 100 Co-editors, who generously give of their time and expertise. The technical editing operation is at Chester, UK, with an outstanding team of 20 staff led by the Managing Editor, Peter Strickland. The IUCr is a learned-society publisher, and is not motivated by profit maximization. However, as an active publisher, the IUCr needs to operate with a financial surplus to ensure the viability and resilience of its commercial operations, invest for future growth and support the IUCr's educational activities. It makes every effort to provide the best possible value for money. It also has very broad responsibilities in serving the world's crystallographers and in serving a full spectrum of expertise from the new-to-the-field to the most accomplished. As one measure of success, IUCr journals have occupied three of the top five ranking positions in crystallography for 2003, and have consistently occupied the top places. The overall publication times have been improved, and now range from 1 month (*Acta Crystallographica Section E*), 2 months (*Acta Crystallographica Section C)*, to 5 months for *Acta Crystallographica Sections A, B and D*. Judged by these parameters, it is clear that we are a high-performance force in science publishing and offer top quality service in a marketplace increasingly dominated by just a few publishers. The IUCr journals have reason to be proud, but we want to continue to improve our products and our services to the science of crystallography worldwide.

Until very recently science journal publishing has operated on income from subscriptions and with copyright transfer from authors to journals. In this way, journals can recoup costs of publication and of distribution. As we all know, however, the number of for-profit journals has risen sharply in recent years, putting financial pressures on libraries and impeding access by scientists throughout the world. Recently there has been a movement towards open-access models of publishing. Under a typical model of this type authors would make a payment to finance the free availability of their articles via the Internet to all readers of a journal, subscribing and non-subscribing. The IUCr and its journals' personnel feel that open access is highly desirable because it makes the fruits of research available to all. In January 2004 we began to experiment with an open-access model in our own operation; the first examples have now occurred (in *Journal of Synchrotron Radiation*). Although a charge is levied for making an article open access, authors unwilling or unable to choose open access are in no way excluded from publishing in IUCr journals, as these will contain a mix of both standard and open-access papers.

The area of science publishing includes a variety of general discussion fora. The IUCr takes part in many of these activities. For example, it participated in the international conferences on trends in electronic publishing organized by the International Council for Science (ICSU) and UNESCO. It also plays an active role within the International Council for Scientific and Technical Information (ICSTI) and the Committee for Data (CODATA), and the Association of Learned and Professional Society Publishers (ALPSP). The IUCr has championed the need for deposition and accessibility of primary science data, in our case coordinates and diffraction data. Data validation has also been a major theme; here the crystallographic information file (CIF) and its macromolecular version (mmCIF) have led the way. Other publishers of papers containing structural data have adopted these methods. Our point of view and approach as a learned-society, not-for-profit publisher, have recently found an unexpected channel of communication. The UK Parliamentary Science and Technology Committee is conducting a general inquiry into scientific publications; we can hope and expect that a submission that we have made of our views and activities will impact this inquiry in a positive way.

It is worth giving a précis of the seven titles in the IUCr journals suite (see box for full titles and Editors). The growth of the journals spans a history of more than 50 years, with a phylogenetic tree of several branches! Theoretical papers addressing the foundations of crystallography are published in *Acta Crystallographica Section A*. *Section B* publishes comprehensive studies in structural chemistry and in structural condensed-matter physics. *Section C* specializes in the rapid dissemination of high-quality studies of novel and challenging crystal and molecular structures, while *Section E* is our electronic-only structural journal; it provides a simple and easily accessible publication mechanism for the growing number of inorganic, metal-organic and organic crystal structure determinations and allows very rapid publication of short structural reports. *Acta Crystallographica Section D* publishes methods and novel biological structures and also crystallization papers. Apparatus and methods papers are published in *Journal of Applied Crystallography*. Synchrotron radiation instrumentation, methods and novel applications papers are published in *Journal of Synchrotron Radiation*. These journals are demonstrably successful by a variety of metrics, such as the number of articles and pages published, their high citation impact ranking, and the fact that they carry very few corrigenda. They are also in the black financially. The biological crystallization and structure specialities we think warrant a new journal for high throughput results, and we are considering the launch of a new Section of *Acta Crystallographica* for these papers.

There are still major challenges in the structures field. For example the growth of so-called 'black box' crystal structure analysis, has, via highly automatic CCD diffractometers and widely available, excellent, and easy to use structure analysis software, broadened the community and accelerated the flow of structures being determined even further. This is especially true in chemical crystallography, which has a very high volume of data depositions. It is becoming increasingly true in biological crystallography. High-quality acceptance standards have now become the norm, recognizing of course that difficult categories of poorly diffracting samples remain, and must be accommodated. Some structures go on to more detailed investigation, e.g. by time-resolved or temperature-resolved techniques.

How does it work out overall? Let us look at chemical crystallography. The data on the R-factors and data-to-parameter ratios of all the structures in 2002 for *Acta Crystallographica Sections C and E* show similar distributions, suggesting that both the not-so-high throughput and the high throughput crystal structure determinations are reaching similar high standards. We also have found that the auto-validation checks are generally accepted by the crystallographic community, and the consistency of standardized validation checks is appreciated. Researchers not only take the checks in their stride; they have now become a matter of routine. Getting these checks done by the authors themselves before submission is also important and enables our Co-editors and referees to concentrate instead on the science quality and commentary.

To sum up, the IUCr journals must keep up with the pace of change and influence change where we can. Firstly we are introducing open access for sound reasons of principle and we will continue to adapt the policy so that it is right for all we serve. Secondly, we are extending the monitoring of citation impact as a parameter to understand, for example, its relevance among various types of articles. Impact factor analyses are now such a necessary fact of life in modern academe that we cannot avoid using them. In the UK these data determine publication policy guidance to university staff. Thirdly, the accelerating trend toward dominance of online publication demands that we secure the long-term preservation of information in digital form in ways that both complement databases and guarantee success for internet search engines. The IUCr journals have always evolved to meet new challenges and will rise to those ahead. Are our approaches to meeting the latest challenges the ones you would choose? I welcome comments on the points raised in this article, on any new ways that you see to improve what we do and how we do it, and on future directions that you foresee.

John Helliwell

Section Editors for *Acta Crystallographica:*
Section A: Foundations of Crystallography
Prof. Dieter Schwarzenbach

Section B: Structural Science
Prof. Carol Brock

Section C: Crystal Structure Commun.
Prof. George Ferguson

Section D: Biological Crystallography
Prof. Ted Baker & Dr. Zbyszek Dauter

Section E: Structure Reports Online
Prof. Bill Clegg & Dr. David Watson

Journal of Applied Crystallography
Editor: Prof. Gernot Kostorz

Journal of Synchrotron Radiation
Main Editors: Prof. Ake Kvick
Dr. Dennis Mills & Prof. Toshiaki Ohta

MacArthur Fellowship to Amy Rosenzweig

Last October Amy Rosenzweig, Northwestern University, received one of the 24 "genius" awards for 2003 given by the John D. and Catherine T. MacArthur Foundation. The prestigious $500,000 MacArthur Fellowships are unusual in that they are given to a wide range of artists, writers, scientists, academics and social activists, and that the recipients can do as they please with the grant.

Amy uses x-ray crystallography to study the structural mechanisms for the metabolism of metals in living cells. Transition metals such as copper, iron, and zinc play critical roles in the catalytic activity of many enzymes, but they can also be toxic if they accumulate out of control. Aberrant metal metabolism has been identified as the critical factor in such diseases as Menkes syndrome, Wilson's disease and familial amyotrophic lateral sclerosis, and may represent an important element in Alzheimer's and prion diseases. Among other recent projects, Rosenzweig and her colleagues have explored the role of magnesium in beta-lactam formation; understanding this reaction will be important for overcoming resistance to penicillins and cephalosporins.

Amy received a B.A. (1988) at Amherst College and a Ph.D. (1992) from the Massachusetts Institute of Technology. She was an NIH Fellow at Harvard Medical School and the Dana Farber Cancer Institute before joining Northwestern U. as Assistant Professor of Biochemistry, Molecular Biology, and Cell Biology, with a joint appointment in the Dept. of Chemistry (1997). In 2002, she was promoted to Associate Professor.

NIGMS Protein Structure Initiative

The National Institute of General Medical Sciences (NIGMS) plans two announcements (RFAs) next month for the next phase of the ***Protein Structure Initiative (PSI)***. The pilot phase of the PSI ends in the fall of 2005 and NIGMS has planned the subsequent phase with two parts. Large-scale centers will focus on the production of unique proteins and methodology and technology development to lower costs and increase success rates. Specialized centers will focus on the development of methodology and technology for classes of challenging proteins, especially membrane proteins, small complexes, and proteins from human and other higher eukaryotes. The RFAs will be described in more detailed in the summer *ACA Newsletter*.

2004 Shull Prize to J. Michael Rowe

The Neutron Scattering Society of America (NSSA) announced January 12th that the first **Clifford G. Shull Prize in Neutron Science** will be awarded to **Dr. J. Michael Rowe** of the National Institute of Standards & Technology (NIST) Center for Neutron Research (NCNR) for his seminal vision, leadership, and contributions to the field of neutron scattering.

The prize, which recognizes outstanding research in neutron science and leadership promoting the North American neutron scattering community, was established at the inaugural American Conference on Neutron Scattering (ACNS) in 2002 to honor Clifford G. Shull, who received the Nobel Prize in 1994 with Bertram Brockhouse. The prize and $5000 honorarium will be awarded at the 2004 ACNS, June 6-10, in College Park, MD (**www.ncnr.nist.gov/acns**).

Mike Rowe and Cliff Shull in 1995

Early in his career, Mike Rowe was at the forefront of research on the dynamics, structure and fundamental properties of materials, including influential work on hydrogen in metals, orientationally disordered solids and monatomic liquids. In addition, he has made significant contributions to the development of inelastic spectrometers and other instruments that utilize cold neutrons and is a leader in the design of the latest generation cold neutron sources, including the most efficient hydrogen cold source currently operating in the world at the NCNR. Mike's talents and his profound impact on American neutron science go far beyond his individual contributions to research and instrumentation. Through his leadership and engineering creativity over the past 15 years, the NCNR has become the most important and widely used neutron facility thus far developed in the United States. Mike received his PhD in 1966 from McMaster University where he worked with Bertram N. Brockhouse. He worked at Argonne National Laboratory prior to joining the National Bureau of Standards (now NIST) in 1973.

PSI Protein Structure Initiative

Call for Nominations for Etter Awards

The ***Margaret C. Etter Early Career Award*** recognizes outstanding achievement and exceptional potential in crystallographic research demonstrated by a scientist at an early stage of their independent career. The award was established to honor the memory of Margaret C. Etter (1943-1992), who was a major contributor to the field of organic solid-state chemistry. She had a love for people, for science, and especially for people who do science, that we honor. Given annually, the award consists of an honorarium plus travel expenses to accept the award and present a lecture at the ACA meeting. The First Etter Early Career Award was presented at the 2003 ACA meeting to **Julia Chan**. Because the 2005 ACA meeting will be a spring meeting nominations are being solicited for both 2004 and 2005.

Scientists involved in crystallographic research in the broadest sense will be eligible for the award. Nominees must be no more than 10 years beyond the awarding of their Ph.D. degree, not including career breaks, and must have begun their first independent (not postdoctoral) position within the past 6 years. Nominees employed in tenure-track academic positions must not yet have received tenure. Nominations must include as a minimum a nomination letter clearly indicating the accomplishments of the individual since beginning their independent career and assessing their future potential. Additional supporting letters and a c.v. may be provided but are not requirements. Self-nominations are not permitted. Nominees may be employed in regular academic positions, as service crystallographers, in industrial positions or in government laboratory positions.

Margaret C. Etter Student Lecturer Award. Each ACA Special Interest Group (SIG) may select one student to receive an award and to present a lecture in one of the sessions organized by that SIG. Selections are based upon submitted abstracts and are independent of whether the student presenter originally requested an oral or poster presentation. Award winners are determined by the elected officers of the SIGs. Students who are selected receive a monetary award of $250, which is independent of any requests for support via the ACA Travel Awards. The nominee must be a student at the time abstracts are submitted. The 2003 winners were **Monica Allain, Firas Awwadi, Peter Chupas, David Lodowski,** and **Jennifer Padilla**

Nominations for all awards should be sent to the ACA Director of Administrative Services, Marcia Colquhoun marcia@hwi.buffalo.edu.

From "The Snowflake, Winters Secret Beauty" by Kenneth Libbrecht and Patricia Rasmussen; see Books, p 25.

Patricia Rasmussen Collection, © Rasmussen 2002

British Amorphous Materials SIG

Members of the former ACA Amorphous Materials Special Interest Group may be interested to learn that a Structure of Amorphous Materials Special Interest Group has recently been formed by the (British) Society of Glass Technology (SGT), to provide a valuable forum for the discussion and presentation of issues of current interest and significance in areas relating to the structure of any non-periodic material. All those actively engaged or interested in this research field are encouraged to join the SIG, whose first meeting will be held in conjunction with the Annual Meeting of the SGT at the University of Liverpool, UK. (21st – 24th April 2004). Membership of the SIG is independent of that of The Society of Glass Technology, but those from North America may like to know that the SGT has a thriving North American Section. It is also hoped that the SIG can be involved in organizing a joint session on amorphous materials at a future ACA Annual Meeting, for the benefit of its American members. The SIG membership fee is £15 (free to members of the SGT) and application forms, together with further information on both the SIG and the Society's activities (including the North American Section) can be found online at ***www.sgt.org***

Adrian Wright

Fellowships at Hunter College and CUNY

Gene Center Fellowship Program: $25,000 plus tuition and health insurance. Awarded to outstanding entering graduate students who are U.S. Citizens or permanent residents.

Bridges to the Doctorate program provides 2 year transition support from Masters to Ph.D. programs in Biology, Biochemistry, Biomedical Sciences, Chemistry and Physics; $8,400/year plus full tuition, equipment and travel allowance.

Biophysics Training Grant: $16,500/year for two years plus tuition and health insurance.

Gertrude Elion Fellowship for Women in Chemistry: $15,000/year plus tuition for two years.

Minority Biomedical Research Support: $13,500/year plus tuition and $800 travel allowance for Master's students, $18,000 plus tuition and $800 travel allowance for Ph.D. students.

Minority Access/Graduate Networking (MAGNET) fellowships: ***President's/Humana Fellowship (***4-year $16,000/year plus full tuition.) ***President's Dissertation Year Fellowship:*** $18,000 plus full tuition.)

Also, ***Postdoctoral Research Fellowships for Minorities Underrepresented in the Sciences.***

For details see website of *The Center for Study of Gene Structure and Function:* **http://sonhouse.hunter.cuny.edu/genecenter/admission.html** or contact: **gemeda@genectr.hunter.cuny.edu**; (212) 650 3957

Lisa Keefe
ACA Council Secretary

Highlights of Fall Council Meeting

The ACA Council met October 16-17, 2003, at the Four Points Sheraton Hotel in Chicago, IL. All Council members were present and in addition Karl Volz, Co-Local Chair for the 2004 meeting in Chicago, met with the Council to present his report on the 2004 meeting plans.

Past President ***Ray Davis*** reported on the 2003 meeting in Covington, KY. The meeting was a huge success, both financially and scientifically. The major awards, with symposia built around them, and the new awards were well-received. At the business meeting it was decided to add to the ballot the proposal to remove the requirement for supporting signatures for membership applications.* The Latin American Initiative was discussed, particularly visa problems for foreign visitors to the ACA meeting. The last Council meeting in Covington, held with all those involved in planning future meetings, was perceived to be very helpful. It was noted that the role of the SIG's should be clarified and that the SIG's should be advisory to the program chairs. A report was received from Bryan Craven on the summer school. *Canadian Representative* ***David Rose*** reported on the Canadian National Committee Award and requested that a statement be inserted in the mail to Canadian members regarding donations. Council agreed to the request.

Treasurer ***Douglas Ohlendorf*** reported that because the 2003 meeting was profitable, he could project a revenue neutral budget for 2004. General discussion about meeting costs, including registration fees, ensued. Discussion followed regarding whether or not to have food at coffee breaks. Food is extremely costly! In fact, the cost of food is much more than the cost of the science (reimbursements and waivers). If food is served, then from where does the money come? Exhibitor fees or donations? Vendors could be given the opportunity to sponsor food at poster sessions. An increase of $100 to the exhibitor fee for 2004 (to be reviewed next year) was also discussed.

Karl Volz presented an update on planning for the 2004 Chicago meeting. Rao offered to negotiate the A/V costs with the Hyatt office in Washington, and this was agreed upon. Cost estimates for holding the banquet at the Field Museum indicated it would be too expensive; after some discussion Council decided to move the banquet to the Hyatt Hotel. There are no good options for lodging for students, and therefore Karl suggested that students should be encouraged to share rooms. Council agreed that this should be advertised. After further discussion, it was decided to set registration fees at $330.

Council met again on Friday morning, and again discussed meeting plans. Possible sites for 2006 and 2007 were discussed without reaching any conclusions. A request for support for students to attend Gordon Conferences was endorsed. The amount of support will be decided upon after further negotiations.

Executive Officer ***Bill Duax*** reported on Headquarters expenditures, proposed budget, and ideas for reducing expenses. A suggestion that program and abstract books might be mailed only upon member request and at the expense of the member will be considered. A motion to move the *Transactions* to electronic format for publications from #36 onward was approved. Ideas for the ACA web site were discussed. **Rao** suggested a photo gallery of Nobel laureates in crystallography on the ACA web site, and this was approved. It was suggested that the YSSIG might be interested in participating in a web site chat room and employment bulletin board. Alumni stories could be posted, for example. **Fran Jurnak** suggested that the SIGs be encouraged to invite a senior scientist to present in their sessions. The Latin American Initiative was discussed. ACA bylaws allow for any National Crystallographic Association that has at least 20 members and regularly elected officers to apply for Affiliate Membership in the ACA. **Bill Duax** proposed policies for executing this, and Council voted to adopt the proposed policies.

In other business, dates for the 2004 Summer School were approved and Etter award guidelines were discussed and approved. **Charlie Carter** requested support from ACA for the protein crystallography school organized by scientists in Cuba and a second crystallography workshop in Havana. The organizers would like help to defray the expenses for the lecturers to participate. **Ray Davis** suggested donating the CDs and videos from the ACA summer schools.

Lisa Keefe, ACA Secretary

**** Editor's note: This proposal passed in the November election.***

Index of Advertisers

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Crystallography Web Watch

The ACA Communications Committee welcomes a new year with the continuation of our Web Watch column. Current committee members are: **Jeanette Krause, Kay Onan, Louis DelBaere** and **Cathy Drennan**. However, the entire crystallographic community is invited to become *members through participation*. If you come across any crystallography or science sites that you think your fellow crystallographers and scientists could find useful or entertaining, we would like to hear from you. Please email the web address and a brief description to **Jeanette Krause** (**jeanette.krause@uc.edu**) Meanwhile, the following sites may be of interest.

George Phillips Jr. has put together a nice site listing crystallographic software at: **phillips-lab.biochem.wisc.edu/tools.html**. Software developed by this group (including downloads) is listed at: **phillips-lab.biochem.wisc.edu/software.html**

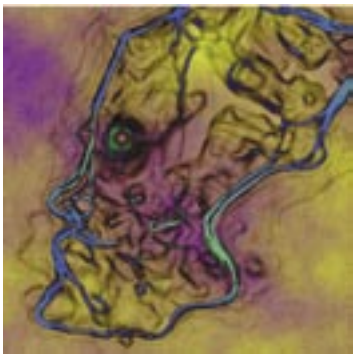
ALB Crystallography site (**sdpd.univ-lemans.fr/index.html**) gives a number of links to software and tutorials related to powder diffraction and more.

CaRIne (**pro.wanadoo.fr/carine.crystallography**) is PC-format software for use in teaching crystallography and for research in materials science, chemistry and earth sciences.

A number of links to crystallography/education sites as well as science in general can be found at: **paloweb.com/Science/Physics/Crystallography/Education/**

NASA provides a number of educational products including a classroom activity for growing protein crystals from Brazil nuts at: **spacelink.nasa.gov/Instructional.Materials/NASA.Educational.Products/.index.html**

UK Center for Materials has put a nice website together at: **www.materials.ac.uk/resources/browse.asp**. Just browse under *Materials Keywords* and you will find a broad collection of educational resources related to materials science, crystallography, chemistry, physics and much more. ***The Center recently sponsored an Art in Science photo competition. Below, a 3rd prize winner, "Face in the Dark 1", by Lars Rose. See description at: www.materials.ac.uk/photocomp/***



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From "The Snowflake, Winters Secret Beauty" by Kenneth Libbrecht and Patricia Rasmussen; see Books, p 25.

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Harold W. Wyckoff (1926 - 2003)

Harold W. Wyckoff, Professor Emeritus of Molecular Biology and Biochemistry at Yale University, died on Thanksgiving Day, November 27, 2003, of pancreatic cancer. He was the husband of Andrea Wyckoff, father of Richard and Benjamin Wyckoff and the late Elizabeth Wyckoff, and grandfather of three: Jillian, Robin, and Nina Elizabeth. Harold (Hal) was born in Niagara Falls, NY. He was President of the ACA in 1980. For a number of years he was a member of the Board of The Orchestra of New England, which often performs at Battell Chapel in New Haven. Hal was a fellow of Berkeley College, served on many national committees, and for 50 years authored publications of interest to the medical community. The list of his publications starts with a paper in 1952, when he was still a graduate student at MIT, and includes editing *Methods in Enzymology:* Vol. 114, 115, in 1985.

Hal did his undergraduate work in physics at Antioch College (B.S. 1949) and obtained a Ph.D in biophysics from MIT in 1955. His area of interest was mainly x-ray diffraction. At the time he started graduate work at MIT no structures of proteins or nucleic acids had yet been determined. As an NIH postdoctoral fellow in Cambridge, England, Hal worked and published with both Aaron Klug and Francis Crick, continuing the work on DNA which he had started for his Ph.D. thesis. In addition to his DNA studies he also worked with Kendrew and Perutz and their colleagues on myoglobin. At this time, in lieu of an academic post, Hal went to work in industry as a research physicist and group leader in the American Viscose Corporation, a position he held for about six years. His work there was mainly devoted to chemical high polymers such as polyethylene.

Hal joined the Molecular Biology and Biochemistry (MB&B) department at Yale in 1963 and served on the faculty for 30 years, teaching and pursuing his research interests. As he did not have a preset research program when he arrived, Fred Richards suggested that they team up to find out what could be done about determining the structure of ribonuclease. Fred and Hal worked on a chemical mutant that Fred had discovered and which differed from the wild type enzyme by the absence of a single peptide bond. The significance of this difference had much to do with scientific politics. David Harker and colleagues had been working on ribonuclease A for years but Hal and Fred wanted the answer now. In those days crystallographic ethics demanded that one did not work on someone else's protein, but since this was (marginally) a mutant and therefore a "different" protein, Hal and Fred decided that it was okay. Hal, together with a stellar group of graduate students, solved the structure of ribonuclease-S in a dead heat with Harker. This was the first protein structure determined at Yale and the third protein structure (after myoglobin and lysozyme) to be determined by x-ray diffraction of crystals.

During this period (1962-1968) MB&B attracted junior faculty, a number of whom were interested in x-ray based procedures. Since the equipment was expensive, the department decided to pool resources and started what has been known ever since as the CORE Laboratory. Since Hal knew every aspect of the required instrumentation, he became the defacto leader of the CORE. Hal, and the technical staff he assembled, produced one of the most effective facilities of this kind in the U.S. The main faculty users were Harold Wyckoff, Donald Engelman, Frederick Richards, Peter Moore and Thomas Steitz. The acronym is obvious, and it has been WERMS for the last 30 years.

The structure and function of enzymes was always Hal's primary interest. He believed that the catalytic mechanisms of enzymes and the basis of their kinetics could only be understood with structural data on wild type molecules, mutants, and complexes, together with chemical studies. He also thought that molecular evolution could best be understood with models of some of the variants in hand. In his later years the emphasis of Hal's research shifted to muconolactone isomerase and to alkaline phosphatase, a much larger protein than ribonuclease-S.

Hal had a full and rewarding life of successful research. His colleagues of all ages owe much to his kindness and much of the success of their own programs stems from his help and advice. He will be sorely missed by the MB&B faculty and the Yale community.

(adapted in part from notes by Fred Richards, edited for the MB&B Newsletter by William Konigsberg)

(The photograph is courtesy of the American Institute of Physics.)

Arthur von Hippel (1898 - 2003)

Arthur R. von Hippel at age 100; (photo taken by his grandson, Jonas A. Kahn (www.jonaskahn.com)

Arthur R. von Hippel, a pioneer in the field of materials science, died at the age of 105 on December 31, 2003, after a brief illness. Born in 1898 in Germany to an academic family, von Hippel studied physics and then joined the physics institute headed by Nobel Prize recipient James Franck. He married Franck's daughter Dagmar in 1930. In 1933, after Hitler came to power, von Hippel left Germany and, after working at the Niels Bohr Institute in Copenhagen, joined MIT in 1936. At MIT, he created the Laboratory of Insulation Research, which made critical contributions to the development of dielectric materials for radar during World War II, earning von Hippel the President's Certificate of Merit in 1948. Although not himself a crystallographer, he was a beloved teacher and mentor to many who became crystallographers, including four past presidents of the ACA, Robinson Burbank, Howard Evans, Robert Newnham, and Sidney Abrahams.

In recognition of his contributions to materials research, the Materials Research Society established the von Hippel Award as its highest honor in 1976 and named von Hippel as the first recipient. The inaugural award recognized von Hippel as a pioneer in the study of dielectrics, semiconductors, ferromagnetics, and ferroelectrics and as an early advocate of the interdisciplinary approach to materials research, as exemplified in his laboratory, where scientists worked cooperatively to solve the mysteries of materials from the atomic to the microstructural level.

Von Hippel's example substantially furthered the science of materials. The publication of his books *Dielectrics and Waves* (John Wiley & Sons, New York, 1954) and *Dielectric Materials and Applications* (the Technology Press of MIT and John Wiley & Sons, New York, 1954) pulled material from courses von Hippel taught in which he brought together physicists, chemists, engineers, manufacturers, and users as they learned to communicate with one another. He later published two visionary books, *Molecular Science and Molecular Engineering* (the Technology Press of MIT and John Wiley & Sons, New York, 1959) and *The Molecular Designing of Materials and Devices* (MIT Press, Cambridge, MA, 1965). In a tribute to von Hippel's 100th birthday, Markus Zahn, Professor of Electrical Engineering at MIT, noted that the M.C. Escher woodcut, *The Thinker,* "showing a man in a foolscap contemplating a 'screwy' model in puzzled confusion" was made for the latter book. Zahn recalled that "von Hippel had a friendship with M.C. Escher because he felt a relationship with Escher's art and molecular designing"

At the time of von Hippel's official retirement in 1964, numerous groups from his laboratory joined in forming the new MIT Center for Materials Science and Engineering, with a von Hippel reading room in recognition of the professor's contributions. After retirement, von Hippel continued researching and teaching, even connecting materials with the field of biology, as discussed in his last publication in 1979, *From Atoms Toward Living Systems* (*Materials Research Bulletin* 14, p. 273).

Von Hippel's outspokenness and defense of the underdog made him beloved by his students but not always by the engineering establishment. His amused comment on being notified of his election to the National Academy of Engineering in 1977 was, "it appears that my friends have outlived my enemies." His teaching style was warm and humorous, and he frequently helped students in need. For the last 65 years of his life, von Hippel lived in Weston, Massachusetts. He always greatly enjoyed time with his family, and time spent in the mountains of New Hampshire, walking and skiing. He and his wife, Dagmar, who died in 1975, are survived by five children: Peter, Arndt, Frank, Eric, and Maianna; 11 grandchildren; and seven great-grandchildren.

(adapted from the MRS website. See ***http://www.mrs.org/gateway/2004/vonhippel/,*** *and links therein.)*

Rosemary C.E. Durley (1948 - 2003)

Rosemary Durley (nee Belford) was born in Edinburgh, Scotland in 1948, and grew up in Belfast, Northern Ireland. Rosemary received a B.Sc. degree from Bristol University in 1968, and then moved to Birkbeck College, London where she earned a master's degree. She went on to do research on crystal structures at University College, London with Jackie Truter and received her Ph.D. in 1973. She was appointed Assistant Professor at the University of Saskatoon, Canada in 1974, where she continued her research as well as teaching chemistry. After taking time off to raise two children, she returned to academia at Washington University, St. Louis, Missouri in 1988 to work with F. Scott Mathews. She used x-ray crystallography to study the crystal structures of enzyme complexes involved in oxidation-reduction pathways and related redox co-factors. In particular, she studied the mechanism of flavocytochrome redox complexes and methylamine dehydrogenase redox chain complexes. She had many publications in this field and made many presentations. In 2000 she retired due to chronic illness. She passed away on December 29, 2003. She is survived by her husband, Richard, and two children, Alison and Stephen.

Scott Mathews

Democracy in the Imperfect World: Local Crystallography of Crystals with Disorder

Adapted from the Warren Award lecture presented at the 2003 ACA meeting by Takeshi Egami, University of Tennessee and Oak Ridge National Laboratory

It is a great honor and pleasure to receive the 2003 B. E. Warren Diffraction Physics Award of the ACA. I see this award not as an award to me as an individual, but to my whole group, i.e. past and present students, postdoctoral fellows and visitors, who believed in the new approach, in spite of earlier objections from the field. While main-stream crystallographers start with the assumption of lattice periodicity to study the structure of a crystal, we took an opposing, local approach without the assumption of periodicity. This is because the modern crystalline materials we focus on are becoming more and more complex. Even when they are nominally crystalline, their atomic structure usually has significant deviations from the average lattice structure, and these deviations are almost always responsible for interesting properties of the solids.

Determining the details of these deviations is an important component of structural characterization today. Traditionally these deviations were treated by extending the conventional methods; small displacements are commonly described in terms of the Debye-Waller factor, large displacements by partially occupied sites, and chemical disorder by atoms with a chemically averaged scattering factor. However, such pseudo-periodic models represent not-so-subtle departures from physical reality, and could lead to serious misunderstanding of the physical and chemical origins of the phenomena in the material. In order to describe these deviations from perfect periodicity more rigorously and capture their physical implications we need to be freed from the restriction of periodicity, and adopt other non-crystallographic approaches represented by the method of atomic pair-density function (PDF).

The assumption of periodicity means regarding each atom as equivalent. This resembles the bureaucratic, militaristic or dictatorial approach of regarding complex human society as a collection of bodies that can be numerically represented by numbers, disregarding individuality. In materials as well, when they are complex the assumption of periodicity may not be warranted. It is individual variation that makes society interesting. If everybody shares the same opinion all the time the world will be simpler and more peaceful, but will be completely boring. To examine such complex systems the crystallographic approach that views the system from outside is less effective. A much more meaningful, democratic and humanistic alternative is to take the local view, from the position of each atom. While war statistics certainly helps one to grasp the scale and economical impact of the war, great novels such as *War and Peace*, *All Quiet on the Western Front*, or *For Whom the Bell Tolls*, tell us much more vividly what really happens at a human level. The local crystallography represented by the PDF method is such an approach.

B. E. Warren (1902 – 1991) was the most prominent pioneer in the field of diffraction studies of non-periodic matter and deviations from periodicity. He was one of the very earliest researchers to study the structure of non-crystalline materials and diffuse scattering due to lattice vibration by x-ray diffraction. His numerous and brilliant achievements, which culminated in his well-known textbook, include proving the random network model of Zachariasen for glassy silica and B_2O_3, and establishing various approaches we now use in studying materials with disorder, such as the Warren-Krutter-Morningstar approximation and the Warren-Cowley order parameter for short-range compositional order. I met him only once, 25 years ago at a conference at Yorktown Heights. He was already a nicely aged retired professor, but I was struck by his young mind and the keen pleasure of discovery he showed even at that age. He has been my source of inspiration ever since.

The method he used most frequently was the PDF analysis, based upon the idea

by Debye. The PDF, $\rho 0g(r)$, describes the distribution of the separation, r, between two atoms in the system, and can be obtained from the structure function, $S(Q)$, where Q is the diffraction vector ($= 4\pi sin\theta/\lambda$, θ is the diffraction angle and λ is the wavelength of the probe), by a simple Fourier-transformation. Theoretically the Fourier-integral has to be calculated up to infinite Q, but in reality the wavelength of the probe sets the upper limit of Q, since $Q < 4\pi/\lambda$. Terminating the integral prematurely results in spurious oscillations called termination errors. The PDF method suffered the stigma of termination errors for a long time. That is why we met strong opposition when we started to use this method for the study of crystals. However, this is now much less of a problem due to the advent of synchrotron based radiation sources, such as pulsed neutron sources and synchrotron radiation sources: They provide strong short wavelength radiation that significantly extends the limit of the Fourier-integral. Also their high intensity dramatically reduces statistical noise.

Since the PDF is the direct Fourier-transform of $S(Q)$, it is applicable on any material, as long as $S(Q)$ is isotropic. Thus it is applicable to crystalline powders or polycrystalline solids without texture. Actually Warren first applied the PDF analysis on crystalline powder (rhombic sulphur) before applying it on glasses and liquids. But since x-rays with the shortest wavelength available at that time were molybdenum Kα radiation (E = 17.44 keV), his data extended only to Q_{max} = 9.8 Å^{-1} and the accuracy was not great. This probably drove him to apply the method on non-crystalline materials.

If the crystal is perfectly periodic, the Bragg peaks contain all the information needed to determine the structure, so that simply applying Fourier-transformation does not add any new information. However, if the material is less than perfectly periodic the PDF provides *more* information than the analysis of the Bragg peaks, since *S(Q)* includes the diffuse scattering intensities as well as the Bragg peak intensities. Note that the data for a conventional crystallographic analysis are in the form of a set of finite number of Bragg peak positions and intensities. On the other hand the *S(Q)* is a *continuous* function of a variable *Q*. In the conventional analysis the data points in-between the Bragg peaks are considered to be the "background" and are discarded, while they are retained in the PDF analysis since they contain important information on diffuse scattering. Thus the PDF utilizes the *total* intensity of probe particles scattered from the sample. For this reason we call S(Q) the *total scattering structure function,* and the PDF method the *total scattering method.*

While there are many other local probes, such as the EXAFS method or NMR, their range is mostly restricted to nearest neighbors. In contrast the range of the PDF method is much wider, limited only by the *Q* resolution. It can determine the local structure on the continuous length-scale from the short-range (< 5Å) to medium-range (5 -20 Å), to nano-scale (20 - 100 Å). In particular the range from 5 to 100 Å is very difficult to be probed by any other methods. This gives the PDF method a distinct advantage in studying nanometer scale phenomena. The NPDF of the Lujan Center of Los Alamos National Laboratory, which was recently upgraded with funding from the National Science Foundation, the Department of Energy and university matching by a group I headed, is the first neutron diffractometer specifically designed for the PDF analysis of crystals.* It has a high *Q*-resolution ($\Delta Q/Q = 1.5 \times 10^{-3}$), which allows the PDF to be determined up to 200Å, successfully bridging the gap between local probes and crystallographic methods. Its large back-scattering detector banks provide a high data collection rate even at short wavelengths, extending Q_{max} to over 40 $Å^{-1}$.

While the synchrotron based radiation sources have greatly alleviated the problems with the PDF method, there is still room for improvement, including the problem with the inelastic correction. They will be discussed in a paper in the proceedings published in *Z. Krystallographie*. The same paper also discusses some highlights of the progress made in my group in the past two decades on the PDF study of disordered crystals.

This talk is dedicated to my extended group, namely my former and present students, postdoctoral fellows, visitors and collaborators, who are too numerous to name here. Today the Rietveld refinement is the mainstream method of structural analysis by powder diffraction. However, I am old enough to remember that initially it was seen to be an exotic, unreliable method, and it took some time before the method was accepted and widely practiced. It is my sincere hope that the PDF method will follow a similar course and become widely used in the near future. Hopefully the 2003 Warren Award will accelerate this process. I also acknowledge the national facilities, such as IPNS, MLNSC of LANSCE, NSLS, APS, ISIS and ILL, for providing critical services and x-ray or neutron beams, and the funding agencies, the National Science Foundation in particular, for supporting this endeavor over many years. Lastly but not the least, I thank my family, particularly my wife, Sayuri, for allowing me to pursue the scientific dream that included many days away from home.

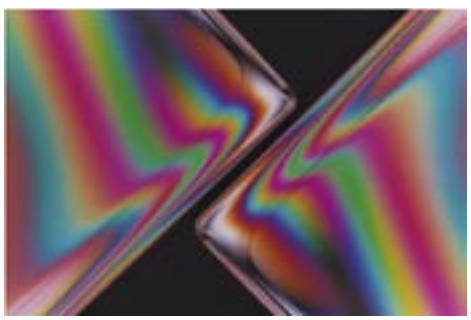
*For details contact Thomas Proffen: tproffen@lanl.gov; tel. 505-665-6573.

Takeshi Egami

News from Canada

Niagara Crystallography Meeting: This annual meeting of crystal scientists from the Niagara region – Buffalo, Hamilton, Toronto, London, Kingston, Rochester (formerly called BHT) - was held in Hamilton on November 21st, 2003. As usual, the format was a morning workshop session from an international expert in an emerging technology, followed by a social/lunch period and an afternoon of talks from trainees in the participating laboratories. This year's workshop was led by **Randy Read**, from Cambridge University, on maximum likelihood methods, particularly as applied to molecular replacement. The afternoon consisted of talks from **Peter Stogios** (Privé lab, OCI, Toronto), **Melanie Adams** (Jia lab, Queen's University, Kingston), **Rachael Summerfield** (Junop lab, McMaster University) and **Yuri Lobsanov** (Howell lab, Hospital for Sick Children, Toronto). There were also introductory talks from new PIs in the region, **Joseph Widekind** (Rochester), **Alba Guarne** (McMaster) and **Hong Ling** (Western Ontario). It is fascinating to watch the growth of the field in this region: this year's attendance was over 100. Financial support was provided by PENCE, MAR USA, and Bruker Biosciences. On November 20th, preceding the meeting, **Randy Read** gave a talk in Toronto highlighting his exciting results with the serpin complexes, and visiting with local scientists.

David Rose



"Photoelectric Stress Pattern in Transparent Plastic Moulding" by Robert Anderson won 1st prize, Materials Concepts, in the Art in Science Competition. See Web Watch Column, page 10, for website that has description of the photo.

The Fabric of the Cosmos: Space, Time, and the Texture of Reality by **Brian Greene**, Alfred A. Knopf, New York, NY (2004), hardcover, 576 pp.,$18, ISBN 0-375-41288-3

Brian Greene received his undergraduate degree from Harvard University and his doctorate from Oxford University, where he was a Rhodes Scholar. He joined the physics faculty of Cornell University in 1990, became a full professor in 1995, and in 1996 moved to Columbia University where he teaches physics and mathematics. His previous book, *The Elegant Universe* was a Pulitzer Prize finalist. Greene explains with clarity and enthusiasm recent developments in superstring and M-theory. He uses imaginative, sometimes humorous analogies to provide insight into the eleven-dimensional "multiverse," of M-theory. In the final chapter he discusses progress toward reconciling the understanding of quantum gravity that comes out of loop quantum gravity theory (which starts big and trys to embrace the small) with the understanding of quantum gravity derived from string theory (which starts from the small and moves to include large scale gravity). He also asks and discusses tantalizing questions such as: How much entropy can a black hole have? Could the universe be a hologram? Is the geometry of space fundamental, or are there different equally valid geometries from different perspectives? Finally, an appendix with 46 pages of notes helps answer the questions of the more"mathematically inclined" readers.

The Third Man of the Double Helix: The Autobiography of Maurice Wilkins by **Maurice Wilkins,** Oxford University Press, Oxford, UK, (2003), hardcover, 274 pp., $27.50. ISBN: 0-198-60665-6.

In the 50th anniversary year of the DNA discovery, Maurice Wilkins at last tells the story his way. This book tells how he showed his colleagues the x-ray picture that gave them their crucial insight, and about his interactions with Rosalind Franklin, the researcher who actually created the picture, and who also received very little credit for her role in the discovery. ***(From Book Description, Amazon.com).***

In his review in ***Science,* Dec. 19, 2003, Robert Olby** says: "Like Watson's autobiographical accounts, the book is intensely personal. We are made privy to relationships and events many would leave in the past. But the tone is strikingly different from that of *The Double Helix*. It is considerate, forgiving, and often apologetic." . . . . "Wilkins describes his relationship with (Rosalind) Franklin very clearly, contrasting his sensitive and diffident character with the strength and confidence of hers. He also provides four significant revelations about this much-discussed history: (i) The idea of putting Franklin to work on DNA was suggested by Wilkins. (ii) In January 1952, Cambridge chemist John Kendrew suggested that Wilkins work with his colleagues, Watson and Crick. (iii) Watson and Crick invited Wilkins to co-author their discovery paper to Nature (but they did not invite Franklin). (iv) When Franklin left the Unit, Randall (Wilkins' boss) asked to join the team Wilkins had been assembling to work on the structure of DNA"....."The emotion in *The Third Man* is contained, but beneath the surface there still lies resentment at a collaboration at King's College refused and an opportunity missed."

Isaac Newton by **James Gleick**, Pantheon Books, (2003), hardcover, 288 pp., $16, ISBN 0-375-42233-1

James Gleick is an author, reporter, and essayist. His books on science *Chaos: Making a New Science* (Viking; Penguin, 1987) and *Genius: The Life and Science of Richard Feynman*, Pantheon, 1992) - were Pulitzer Prize and National Book Award finalists. "The best and most original part of Gleick's book is the description of the young Newton in his first five chapters. Gleick's account is based on a detailed study of the manuscript notebooks that Newton kept as a student in Cambridge, recording his many false starts and digressions as he groped his way towards an understanding of the laws of nature. In these notebooks we see him, not yet possessing words to express the concepts such as force and momentum that would allow him to formulate the laws precisely, and not yet possessing the mathematical tools of differential and integral calculus that would allow him to deduce the consequences of the laws. To reach his fundamental insight that the laws of nature can be expressed as differential equations, he had to simultaneously guess the laws and invent the mathematical language of calculus in which to express them. The notebooks record his successes and failures as they happened, not reinterpreted in the light of later discoveries." ***(From a review by Freeman Dyson in the New York Review of Books, July 3, 2003.)***

Elements of Synchrotron Light for Biology, Chemistry, and Medical Research by **Giorgio Margaritondo,** Oxford U. Press, New York, (2002), 260 pp., hardcover,$100, ISBN 0-19-850930-8: paper, $55, ISBN 0-19-850931-6

Written for practicing scientists and undergraduate students in the life sciences, medical research, and chemistry, this volume describes synchrotron sources and free electron lasers. It also details the instrumentation and techniques related to these technologies. As an introduction to the subject, the book emphasizes basic concepts and keeps mathematical formalism to a minimum**.** ***(Book News, Inc.®, Portland, OR)***

This book is structured by a two-level presentation including a simple descriptive treatment and slightly more in-depth discussions of specific topics. The first-level treatment covers the notions, terminology and techniques that are required to use a synchrotron facility. The book is therefore an ideal first step for all those considering the use or beginning to use synchrotron light for their work. Topics include basic functioning mechanisms of synchrotrons and free electron lasers; description of sychrotron-based techniques in x-ray imaging and radiology; spectroscopy; microscopy and spectromicroscopy; EXAFS; crystallography; and microfabrication. ***(From Book Description, Amazon.com.)***

Editor's note: see Physics Today, March, 2004, p.83 for a more complete review by Sol M. Gruner, Cornell Univ.

Einstein's Clocks, Poincaré's Maps: Empires of Time, by **Peter Louis Galison,** W.W. Norton & Company, NY, (2003), hardcover, 389 pp., $24, ISBN: 0-393-02001-0

Peter Galison is Mallinckrodt Professor for the History of Science and of Physics at Harvard University. He is a recipient of a MacArthur Fellowship and the Max Planck Prize, and won the Pfizer Prize for the Best Book in the History of Science for his previous book *Image and Logic*.

At the beginning of the 20th century, just as industry and government were anticipating the imminent coordination of time around the globe, says Galison, the notion of time and the ability to coordinate two clocks at a distance, were being demolished in the nexus of physics, technology, and philosophy.***(From Book News, Inc.®, Portland, OR***

In his review in *Science,* December 19, 2003, M. Norton Wise says: "Galison has produced an easy-reading but penetrating book. *Einstein's Clocks, Poincaré's Maps* brings the story of time to life as a story of wires and rails, precision maps, and imperial ambitions, as well as a story of physics and philosophy."

The Snowflake. Winter's Secret Beauty by **Kenneth Libbrecht**; photography by **Patricia Rasmussen**. Voyageur, Stillwater, MN, (2003). 112 pp. $20, ISBN 0-89658-630-8.

The Snowflake combines the superb photography of Patricia Rasmussen with an in-depth account of the science of snow crystals, as told by Caltech physics professor Kenneth Libbrecht. It takes you into the winter clouds to examine the birth and growth of snow crystals, revealing the mystery of why no two snowflakes are alike. Includes a richly illustrated guide to the many types of snowflakes and the weather conditions that produce them. ***(From Book Description, Amazon.com)***.

Kenneth Libbrecht's website on snowcrystals: **www.its.caltech.edu/~atomic/snowcrystals/** was featured in the *Web Watch* column of the fall 2002 *ACA Newsletter*. This is a beautiful book!

Annual Review of Biophysics and Biomolecular Structure, Vol. 32, **R.M. Stroud, W.K. Olson, M.P. Sheetz, *eds.,*** Annual Reviews, Palo Alto, CA, (2003), 533 pp., $180.00, ISBN0-8243-1832-3

Twenty contributions represent the current state of research in biophysics and bimolecular structure. Specific papers focus on topics such as protein analysis, electrostatic interactions, transport kinetics, nucleic acid recognition, fluorescence microscopies and spectroscopies, mammalian cyclooxygenases, lipid rafts, x-ray crystallography, molecular recognition and docking algorithms, enzyme catalysis, the calcium pump, and liquid-liquid immiscibility. In addition to the subject index for this volume, cumulative indexes of authors and chapter titles for volumes 28 to 32 are also included. (***Book News, Inc.®, Portland, OR)***

*Note: Vol. 33 will be released in June, 2004***.**

Responsible Conduct of Research, by **Adil E. Shamoo,** and **David B. Resnik,** Oxford University Press, NY, (2003), 345 pp., hardcover: $65, ISBN 0-19-514845-2; paper: $30, ISBN: 0-19-514846-0.

Shamoo (applied professional ethics, U. of Maryland at Baltimore) and Resnick (medical humanities, East Carolina U.) present an introduction to the ethical issues in the use of humans and animals in research. Coverage ranges from broad issues relating to social responsibility, research funding, and freedom of inquiry to more specific topics such as ethical aspects of recording data in lab notebooks, experiment design, citing published works, and deciding authorship matters. While focused on biomedical research, coverage also includes topics applicable to most research-oriented disciplines.***(From Book News, Inc.®, Portland, OR)***

Putting Science in Its Place: Geographies of Scientific Knowledge, by **David N. Livingstone**, University of Chicago Press, Chicago, (2003), hardcover, 246 pp. $27.50, ISBN 0-226-48722-9. Livingston is a geographer and historian of science at Queen's University, Belfast, Northern Ireland.

Most scientists are well aware how "science affects place and, in turn, how place influences science. David Livingstone explicitly addresses this issue in ways that illuminate both scientific and political developments. Livingstone, a geographer and historian of science at Queen's University, Belfast, Northern Ireland, notes that credible knowledge is assumed not to bear the marks of place. He quotes an anonymous statement to the effect that 'it was the end for cold fusion when people decided that it 'only happened in Salt Lake City.' Yet, he adds, geographic context does affect scientific knowledge. Using historical examples drawn from the 16th through 20th centuries, Livingstone examines what he calls the venues, cultures, and movements of science." ***(from a review by Cristina Gonzalez in Science, Dec. 5, 2003.)***

Einstein in Berlin, by **Thomas Levenson**, Bantam Books, NY, (2003), 486 pp., hardcover: $18, ISBN: 0-553-10344-X, paper: Bantam, (2004), $11, ISBN: 0553378449

Thomas Levenson is an Emmy and Peabody Award winning documentary filmmaker whose credits include a two-hour biography of Einstein for the PBS series *Nova*. He has written two previous books, *Measure for Measure: A Musical History of Science* and *Ice Time: Climate, Science, and Life on Earth.*

In the spring of 1913 two of the giants of modern science traveled to Zurich. Their mission: to offer the most prestigious position in the very center of European scientific life to a man who had just six years before been a mere patent clerk. Albert Einstein accepted, arriving in Berlin in March 1914 to take up his new post. In December 1932 he left Berlin forever. "Take a good look," he said to his wife as they walked away from their house. "You will never see it again." In a book that is both biography and the most exciting form of history, here are eighteen years in the life of a man, Albert Einstein, and a city, Berlin, that were in many ways the defining years of the twentieth century. ***(From Book Description, Amazon.com.)***

Everything's Relative : And Other Fables from Science and Technology, by **Tony Rothman,** John Wiley & Sons, NY, (2003), 288 pp. $25, ISBN: 0-471-20257-6

Tony Rothman is a physicist and writer. He is the author of seven other critically acclaimed science books and a frequent contributor to leading science publications, including *Scientific American* and *Discover.* The publisher quotes Roald Hoffman, winner of the 1981 Nobel Prize in Chemistry: "If you were not a sceptic about the mythology of discovery, you will be one after reading Tony Rothman's fascinating book. It's an assemblage of compelling antistories, all eminently readable, to counter the stories scientists tell themselves, and then tell us. And that we...are all too eager to hear."

Combining a storyteller's gift with a scientist's focus, Tony Rothman breaks down many of the most famous "just-so" stories of physics, astronomy, chemistry, biology, and technology. His "truth-is-stranger-than-fiction" anecdotes include how: (i) Henry Young, the greatest American scientist after Benjamin Franklin, severed his friendship with Samuel Morse after not receiving proper credit for his key role in inventing the telegraph. (ii) Albert Einstein, one of the greatest twentieth-century physicists and a titan of science, misinterpreted his own highly celebrated theory of relativity. (iii) Neither James Watt, nor Robert Fulton, nor John Fitch, nor Simon Newcomen invented the steam engine - Captain Thomas Savary first invented the prototype for the steam engine back in 1698. (iv) More than 600 lawsuits were filed against Alexander Graham Bell after he took sole credit for inventing the telephone. ***(From the publisher's comments on the book jacket.)***

The Measure of All Things : The Seven-Year Odyssey and Hidden Error That Transformed the World, by **Ken Alder**, Free Press, paper: (2003),448 pp., $11, ISBN: 0-7432-1676-8; hardcover: (2002), 422 pp., $9, ISBN: B-0000-94P5-7

Ken Alder is an associate professor of history at Northwestern University. His first book, *Engineering the Revolution,* won the 1998 Dexter Prize for the best book on the history of technology.

Amidst the chaos of the French Revolution, two astronomers set out in opposite directions from Paris to measure the world, one voyaging north to Dunkirk, the other south to Barcelona. Their findings would help define the meter as one ten-millionth of the distance between the pole and the equator. *The Measure of All Things* is the amazing story of one of history's greatest scientific quests, a mission to measure the Earth and define the meter for all nations and for all time.

When Ken Alder located the long-lost correspondence between the two men, along with their mission logbooks, he stumbled upon a two-hundred-year-old secret. The meter, it turns out, is in error. Pierre-François-André Méchain, made contradictory measurements from Barcelona and, in a panic, covered up the discrepancy. The guilty knowledge of his misdeed drove him to the brink of madness, and ultimately to his death. Only then did his partner, Jean-Baptiste-Joseph Delambre, discover the truth and face a fateful choice: what matters more, the truth or the appearance of the truth? Should one perpetuate a small lie in the service of a larger truth? *The Measure of All Things* describes a quest that succeeded even as it failed. ***(From Book Description, Amazon.com. See also the review in Physics Today, July, 2003, by Bruce Stephenson.)***

Quantum Theory of Tunneling, by **Mohsen Razavy**,World Scientific, River Edge, NJ, (2003), 549 pp., paper: $48, ISBN 981-238-019-1; hardcover: $88, ISBN 981-238-018-3.

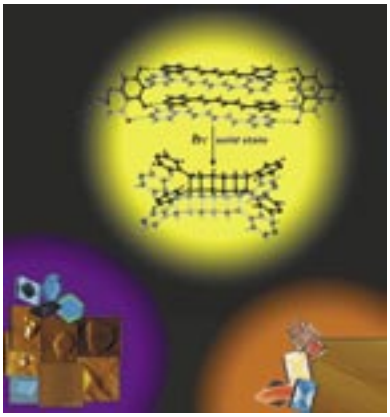
This graduate textbook results from a lecture course given at the Institute for Advanced Studies in Basic Sciences, Zanjan, Iran in the summer of 1999. It provides a comprehensive introduction to the theoretical foundations of quantum tunneling, stressing the basic physics underlying the applications. The topics addressed include exponential and nonexponential decay processes and the application of scattering theory to tunneling problems. In addition to the Schrödinger equation approach, the path integral, Heisenberg's equations and the phase space method are all used to study the motion of a particle under the barrier. Extensions to the multidimensional cases and tunneling of particles with internal degrees of freedom are also considered. Furthermore, recent advances concerning time delay and tunneling times and some of the problems associated with their measurement are also discussed. Finally, some examples of tunneling in atomic, molecular, nuclear and condensed matter physics are presented. ***(From Book Description, Amazon.com.)***

A Short History of Nearly Everything, by **Bill Bryson,** Broadway Books, New York, (2003), 559 pp., $27.50, ISBN 0-7679-0817-1.

Bill Bryson's previous books include *A Walk in the Woods, I'm a Stranger Here Myself, In A Sunburned Country,* and *Bryson's Dictionary of Troublesome Words.*

Confessing to an aversion to science dating to his 1950s school days, Bryson here writes for those of like mind, perhaps out of guilt about his lack of literacy on the subject. Bryson reports he has been doing penance by reading popular-science literature published in the past decade or two, and buttonholing a few science authors, such as Richard Fortey (*Trilobite! Eyewitness to Evolution, 2000*). The authors Bryson talks to are invariably enthusiasts who, despite their eminence, never look on his questions as silly but, rather, view them as welcome indicators of interest and curiosity. Making science less intimidating is Bryson's essential selling point as he explores an atom; a cell; light; the age and fate of the earth; the origin of human beings. Bryson's organization is historical and his prose heavy on humanizing anecdotes about the pioneers of physics, chemistry, geology, biology, evolution and paleontology, or cosmology. To those acquainted with the popular-science writing Bryson has digested, his repackaging is a trip down memory lane, but to his fellow science-phobes, Bryson' s tour has the same eye-opening quality to wonder and amazement as his wildly popular travelogues. ***(From an Amazon.com Editorial Review by Gilbert Taylor, in Booklist. Copyright © American Library Association. All rights reserved.) See also the review by Orla Smith in Science, Feb. 13, 2004..***

Images from the Transactions Symposium on Crystals in Supramolecular Chemistry
to be held at the 2004 ACA Meeting July 17 - 22



Applications of Crystal Design session, Yellow Background: A depiction of the synthesis of a 5-cyclobutane ladderane from ***Leonard R. MacGillivray, Tomislav Frii*** and the late ***Xiuchun Gao***, University of Iowa. Ladderanes are so named because they contain a series of fused cyclobutane rings that may impart unique electronic properties or serve as spacers to separate metals or functional groups for a potential new class of optoelectronic materials. Natural ladderanes having three or five fused cyclobutane rings were discovered in 2002, and are known to serve as membrane lipids in ammonium-oxidizing bacteria that participate in nitrogen cycling in the oceans. A template-directed solid-state strategy to preorganize molecules that can then be photodimerized to form targeted compounds was developed for ladderanes. The template is formed by cocrystallizing trans-bis(4-pyridyl)polyenes with 5-methoxyresorcinol. The resorcinol holds the ends of two polyene molecules together through hydrogen-bonding interactions, then UV irradiation "zips" the molecules into a ladder structure. (adapted from *Angew. Chem. Int. Ed.*, **43**, 232 (2004), and *Chem & Eng. News*, **82**, no.1, 13 (2004).

Crystal Growth Mechanism Session; Orange Background: Uric acid crystals grown in the presence of various natural pigments and/or synthetic dyes probes show oriented dye inclusions. The background image is an atomic force microscopy (AFM) topograph of uric acid (100). The unregulated crystallization of uric acid in the human body can lead to grainy precipitates in the renal tract and symptoms associated with the disease gout. ***Jennifer A. Swift*** and coworkers at Georgetown University investigate the mechanisms of uric acid crystallization using *in situ* AFM and spectroscopic methods. Dynamic AFM studies on single crystal surfaces provide information on molecular-level growth rates and mechanisms under simulated physiological conditions. Crystallization in the presence of a variety of synthetic dyes and/or natural pigments leads to uric acid crystals containing oriented dye inclusions. The orientation of the included dye provides a means to discern how impurities recognize and bind to the growing crystal surfaces. For additional information, see *J. Am. Chem. Soc.* **124**, 8630-8636 (2002) or *Chem. Mater.* **15**, 2718-2723 (2003).

Crystal Growth Mechanism Session; Purple Background: The desire to control the size, shape and quality of crystalline layers grown on the surface of other crystals requires insight into how chemical additives influence the kinetics of crystal growth. Toward this end, ***Tzy-Jiun M. Luo*** and ***G. Tayhas R. Palmore,*** Brown University and ***John C. MacDonald,*** Worchester Polytechnic Institute have studied the effect of 4-methylimidazole on the growth of crystals composed of bis(imidazolium 2,6-pyridinedicarboxylate) M (II) dihydrate where M (II) = Cu (II), Ni (II), Co (II), Zn (II), and Mn (II). It has been found that both the morphology and the kinetics of growth of these crystals can be controlled precisely by the amount of 4-methylimidazole added to the growth solution. Shown in the lower left of this figure is a blue, rhombohedral-shaped crystal of bis(imidazolium 2,6-pyridinedicarboxylate) Cu (II) dihydrate. The (100) face of this crystal was imaged *in situ* during its growth from solution using AFM (atomic force microscopy). The sequence of AFM images reveals both two-dimensional nucleation and dislocation mechanisms of growth. Higher resolution AFM images reveal a screw-dislocation with steps advancing in four different directions (lower right image) and the lattice spacing of the (100) face (lower middle image). By combining information gained from x-ray crystallography and *in situ* AFM studies of this isostructural series of metal complexes, a quantitative method for selecting crystal facets and crystal morphologies has been developed to produce crystalline templates upon which a second or third crystalline layer can be grown. Examples of crystals produced by this method are shown at the top of the figure to illustrate controlled morphology, selective faceting, and epitaxial layers grown on crystalline templates.

From left: Bill DeGrado, Douglas Rees, Jenny Glusker, Stephen Lippard, Catherine Drennan, Amy Rosenzweig

Metals in Biology: A Symposium in Honor of Jenny Pickworth Glusker

On December 12, 2003, the Fox Chase Cancer Center in Philadelphia held a symposium in honor of Jenny Pickworth Glusker, who retired from her position as Senior Member at Fox Chase in June 2003. Jenny is a past president of the ACA and was the founding editor of *Acta Crystallographica Section D*, and remained Editor of *Acta D* from 1993 through the end of 2002.

Jenny has had a long and distinguished career in crystallography. She comes from a medical family - both her parents were physicians. She went to Somerville College, Oxford for her BA, and as an undergraduate performed her research "Part II" year with Sir Harold Thompson on infrared spectroscopy, where she met her future husband Donald Glusker, who was there as a Rhodes Scholar. Jenny continued at Oxford as a graduate student, working on the crystal structure of the hexacarboxylic acid derivative of Vitamin B_{12} with Professor Dorothy Hodgkin from 1953-1955. Another derivative of B_{12} had been partly solved in Hodgkin's lab, and Hodgkin deliberately did not tell Jenny the details of the structure. When Jenny's model of the structure was finished, it agreed with the other B_{12} structure, and sealed the case for x-ray crystallographic determination of molecules as large as B_{12}. Jenny's work contributed to Dorothy Hodgkin's Nobel Prize in 1964.

Jenny with ymposium organizers Roland Dunbrack & Anna O'Connell

Jenny with (at left) her daughter Ann, her son Mark, and (at right) her daughter Kathy.

After Oxford, during 1956 and 1957, Jenny was a post-doctoral fellow in the lab of Linus Pauling at CalTech. Finding two academic jobs at one institution was nearly impossible at that time, since few institutions would hire women faculty. So the Gluskers moved to Philadelphia where Donald Glusker took a job at Rohm and Haas, and Jenny started post-doctoral work with Lindo Patterson, who had been at the Institute for Cancer Research (later part of Fox Chase Cancer Center) since 1949. In 1966, Patterson died of a cerebral hemorrhage, and Jenny took over as principal investigator in crystallography at Fox Chase, rising to Senior Member in 1979.

Jenny is the author of many papers on the structures of small molecules and proteins. This work ranges from her work on B_{12} to the mechanism of the enzyme aconitase in the Krebs cycle (the "ferrous" wheel mechanism now given in textbooks), the structure and mechanism of the enzyme xylose isomerase, the structures and mode of action of many carcinogenic small molecules, and the interactions of metals with proteins deduced from statistical analysis of small molecule and protein crystal structures and *ab initio* calculations. She is also the author of several textbooks that have been standards in the field of crystallography for many years. She has dedicated much of her time to the teaching of crystallography worldwide.

Editor's note: Jenny also originated the ACA Newsletter, and edited it for many years.

We were very fortunate to have five accomplished scientists as speakers at the meeting. All of the speakers had in common an interest in the role of metals in protein structure and function, which has been a lifelong interest in Jenny's research.

The first speaker was Catherine Drennan, an assistant professor of chemistry at MIT. Cathy led the audience through a family tree of five generations of women crystallographers, starting from Dorothy Hodgkin, Hodgkin's student Jenny Glusker, Jenny's student Miriam Rossi, a Professor at Vassar College, Rossi's student at Vassar, Cathy Drennan herself, and a young student of Cathy's currently studying at MIT. Cathy's talk was on *"Crystallographic Portraits of B12 and Adenosylmethionine-Radical Enzymes."*

The next speaker was Stephen Lippard, Professor of Chemistry and Chairman of the Chemistry Department at MIT, and a recent winner of the ACS Alfred Bader Award in Bioinorganic and Bioorganic Chemistry. His talk was titled *"Structural and Mechanistic Studies of Soluble Alkane and Arene Monooxygenases with Carboxylate-Bridged Diiron Centers."* Following lunch, Douglas Rees, Professor of Chemistry at CalTech and Investigator of the Howard Hughes Medical Institute spoke about his work on *"The Structural Basis of Biological Nitrogen Fixation."* Next, Bill DeGrado, Professor of Biochemistry and Biophysics at the University of Pennsylvania and winner of the 2003 R. Bruce Merrifield Award of the American Peptide Society, discussed his work on the *"De Novo Design of Metalloproteins."* The last speaker of the day was Amy Rosenzweig, Associate Professor of Biochemistry, Molecular Biology, and Cell Biology at Northwestern University. Amy received a MacArthur Foundation Fellowship in the fall of 2003*. Her talk was entitled *"Copper Binding Sites in Metallochaperones and Metalloenzymes."*

The symposium ended with a reception for those attending the meeting, followed by a dinner for invited guests, including Jenny's three children and their families, as well as many long-time friends from Fox Chase and elsewhere. We gathered to give a toast to Jenny's long and distinguished career and to a woman who is a kind and generous friend to all who know her. As Jenny is busy collaborating with a number of colleagues and writing more papers, we expect to enjoy her company for some time to come.

Roland L. Dunbrack, Jr., Fox Chase Cancer Center

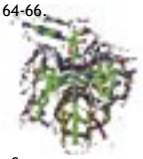
**** Editor's note: see Award notice, page 6.***

B12 Crystallographic Family Tree

Dorothy Hodgkin

1956: ***First structure of B_{12}***

Hodgkin, D.C., Kamper, J., Mackay, M.., Pickworth, J., Trueblood, K.N., and White, J.G.(1956) Structure of Vitamin B_{12}, *Nature* 178, 64-66.



Jenny Pickworth Glusker (Ph.D. student w/Dorothy)

1985: First structure of methyl B_{12}

Rossi, M., Glusker, J.P., Randaccio, L., Summers, M.F., Toscano, P.J. and Marzilli, L.G., (1985), The Structure of B_{12} coenzyme: Methylcobalamin studies by X-ray and NMR methods. *J. Am. Chem. Soc.* 107, 1729-1738.

Mirian Rossi (Postdoc w/Jenny)

1994: First structure of B_{12} bound to protein

Drennan, C.L., Huang, S., Drummand, J.T., Matthews, R.G., and Ludwig, M.L. (1994) How a Protein Binds B_{12}: A 3.0 Å X-ray Structure of B_{12}-Binding Domains of Methionine Synthase, *Science* 266, 1669-1674.

Cathy Drennan (undergraduate w/Miriam at Vassar College)

from left: Amy Rosenzweig, Cathy Drennan, and Jenny

X-Ray Diffraction Equipment Fire Sale!!!

Each of the following items are available for the grand sum of $0 (that is ZERO dollars) with the proviso given at the end of the descriptions.

* Rigaku RU200 rotating anode generator (circa 1984) with Cu target and Cr target. Ingersoll focussing mirrors are included along with all spare parts such as bearings and magnetic seal. The Cr target has only been slightly used. The system is in working order.

* Nonius FR571 Rotating anode generator with Mo target and slightly used Cu target. Spare parts (lots of fuses, tools, etc.) are included.

* Nonius FAST detector and kappa goniometer (heavy duty) with all parts including collimators, graphite monochromator, Microvax 3600 with VMS 5.5. and all software.

These items are available at no cost provided the taker(s) arrange and pay for packing and shipping. If the systems are not taken, they may be broken up and sold as individual parts. Inquiries should be directed to Dr. Jenny Glusker or Dr. H.L. Carrell at The Fox Chase Cancer Center, 333 Cottman Ave., Philadelphia, PA 19111 or by telephone at (215)728-2220.

The IV National Mexican Congress of Crystallography, Morelia, Michoacan, Mexico

The IV biennial National Mexican Congress of Crystallography was organized by the Society of Mexican Crystallography (SMCr) and was held in Morelia, Michoacan, Mexico from 10 to 14th November, 2003, at the Centro Cultural Universitario of the Universidad Michoacana de San Nicolas de Hidalgo. About 250 researchers, teachers, technicians, and students, from several universities, institutes, schools, and companies, in Mexico came to attend the meeting. The final program included 14 plenary lectures, 6 specialized invited lectures, 22 invited speakers, 21 oral presentations, 83 poster contributions, 7 courses, 5 workshops, of which 2 were addressed to high school students and younger children, and 3 commercial presentations. The topics covered in plenary lectures were: ***Superconducting Materials: The Last 30 years*** (**M. A. Alario y Franco, Spain**); ***Typomorphism in Minerals and its Meaning in Advanced Mineralogy*** (**M. Ostroumov, Mexico**); ***Introduction to the Program Fullprof: Refinement of Crystal and Magnetic Structures from Powder and Single Crystal Data*** (**J. Rodríguez-Carvajal, France**); ***Crystal structure and twinning crystallography in magnetic shape memory martensites of Ni-Mn-Ga*** (**N. Glavatska, Ukraine**); ***Macromolecular crystallography: current applications and future perspectives*** (**C. Abad-Zapatero, USA**); ***Structure of Outstanding Materials for Corrosion Control in the Oil Industry*** (**L. Martínez, Mexico**); ***The Association of Oxy-chlorides and Sulphates from the Boleo District, Municipality of Mulegé, Baja California Sur*** (**F. Escandón, Mexico**); ***Structure and Nanomechanics of Biomineralized Materials with the Atomic Force Microscope*** (**T. Schäffer, Germany**); ***A Method to Calculate the Ratio of BO_3 Triangles to BO_4 Tetrahedra in Borate Structures Derived by Crystal Chemical Reasoning*** (**E. Parthé, Switzerland**); ***Electronic Structure of Some 3d-coordination Compounds*** (**J. Kožíšek, Slovak Republic**); ***Image Reconstruction from Determination of Electron Exit Waves Applied to Sharp and Diffuse Interfaces*** (**H. Calderón, Mexico**); ***Impact of X-Ray Crystallography and Molecular Modeling in Drug Design*** (**M. Soriano, Mexico**) and ***A Study of Microstructural Effects by Powder Diffraction Using the Program Fullprof*** (**J. Rodríguez-Carvajal, France**). The courses given were: ***Crystal Chemistry*** (**E. Parthé, Switzerland**); ***Introduction to Crystallography*** (**A. Gómez, Mexico**); ***Nanostructures*** (**H. Calderón, Mexico**); ***Geochemistry of Minerals*** (**G. Villaseñor, Mexico**); ***Electronic Density*** (**J. Kožíšek, Slovak Republic**); ***Solid State Chemistry of Metallic Oxides*** (**M. A. Alario y Franco, Spain**); and **Small Angle X-Ray and Neutron Scattering** (**J. Palacios, Mexico**). Workshops were: ***Structures by Atomic Force Microscopy*** (**C. Segovia, Mexico**); ***Single Crystal Crystallography*** (**J. García-Díaz, Mexico**); ***Electron Nanodiffraction*** (**D. Acosta, Mexico**); ***Crystallography for High School Students*** (**L. Bucio, Mexico**); and ***Lottery Game on Materials for Kids*** (**P. Quintana, Mexico**).

With this meeting, the Mexican Society of Crystallography celebrated its fifth National General Assembly and the fifth Assembly of Delegates from several localities in Mexico representing Centers, Institutions, and Academies involved with crystallography. The Organizing Committee consisted of the General Committee: J. L. Boldú, President; R. Toscano, General Secretary; L. Bucio, Adjunct Secretary; V.M. Malpica, Secretary for Public Dealings; M.E. Villafuerte-Castrejón, Treasurer; E. Muñoz-Picone, First Voting Member; R. Rodríguez-Mijangos, Second Voting Member; and the Local Committee (Michoacan State): M.E. Contreras, Delegate; E.M. Alonso-Guzmán, J. Zárate, S.L. Bribiesca, G. Rosas-Trejo, M. Ostroumov, J. García-Díaz, J. Barreto, E. Huipe-Nava and L. Mondragón. In the course of its history, the Mexican Society of Crystallography has edited and printed approximately 30 notes concerning different topics in crystallography. These are mainly in the Spanish language, but a few are in English. They were produced as a result of the courses or lectures given during congresses, meetings, workshops and other events organized by the Society. The complete list of published notes can be consulted on our web page: **www.smcr.fisica.unam.mx**.

Lauro Bucio, Adjunct Secretary of the Mexican Society of Crystallography.

The ACA Summer Course in Small Molecule Crystallography, 2004

This course will be offered July 25 through August 4, 2004 at the Indiana University of Pennsylvania, in the town of Indiana located about 80 miles east of Pittsburgh. Each day there will be three lectures in the morning on single crystal and powder diffraction methods, followed by afternoon and evening workshops for problem solving, data analysis and for crystal structure determination. Attendees are encouraged to bring their own single crystal samples for x-ray data collection or powder samples for either x-ray or neutron data collection. Attendees are expected to have completed at least undergraduate courses in chemistry, physics and mathematics. No prior experience of x-ray crystallography will be assumed, but attendees are advised to read in advance ***Crystal Structure Analysis: A Primer,*** by Jenny P. Glusker and Kenneth N. Trueblood, Oxford Univ. Press (1985).

The organizers aim for a total of 30 attendees, who in past years have come from academia (students and faculty), government and corporate institutions, both in the U.S. and from abroad. Tuition will be $250. Student apartment housing at IUP (including breakfast and lunch) is available for a total of $350. Graduate student scholarships will be offered to about half those who attend. These will consist of a waiver of tuition and living costs. The scholarships will be awarded based on the student's (1) scientific ability, (2) expected benefits from the course and (3) skills in English. We encourage applications from Latin America.

Instruments available will be two Bruker-Nonius single crystal diffractometers (a CAD4 at IUP and a modern APEX instrument with CCD detector located at the University of Pittsburgh which will be electronically linked to the x-ray lab at IUP). Also available will be a Bruker-Nonius D8 powder diffractometer and a Rigaku Miniflex diffractometer in the x-ray lab at IUP. Attendees interested in sending powder samples for neutron data collection should contact Brian Toby before June 1 at brian.toby@nist.gov. There will be adequate computing facilities including access to the Cambridge structural data base and the ICDD powder diffraction data base.

The Course registration form can be obtained from the ACA web site at **http://www.hwi.buffalo.edu/ACA**. Completed forms must be received before June 1, 2003 by Bryan Craven, Chemistry Department, Indiana University of Pennsylvania, Indiana, PA 15705, USA or electronically by Charles Lake at **lake@grove.iup.edu.** Further information will be updated on the web site or can be obtained from **craven@icubed.com.**

We shall observe the basic policy of nondiscrimination and affirm the rights of scientists throughout the world to adhere or to associate with international scientific activity without restrictions based on nationality, race, color, age, religion, political philosophy, ethnic origin, citizenship, language, or sex, in accordance with the Statutes on the International Council of Scientific Unions. At this Course, no barriers will exist which would prevent the participation of bona fide scientists.

Bryan Craven and Charles H. Lake, Organizers.

ACA 2004, July 17-22, 2004 Hyatt Regency, Chicago, IL

Welcome to Chicago for a week of structural science and celebration! The Chicago ACA meeting promises to be full of stimulating science, fun and informative tours, and edifying workshops.

The ACA 2004 meeting agenda will include an on site workshop on ***CCP4/PDB Software Tools***, plus four synchrotron oriented workshops covering ***Hands-On MAD Phasing, Small-Molecule Methods,*** a ***General Introduction to the Synchrotron for Biologists***, and an all-day tour of the Advanced Photon Source and the Intense Pulsed Neutron Source, all to be held at the Argonne National Laboratory. Preregistration with APS is required.

Photo courtesy of Terry & Melody Howe.

2004 PROGRAM CHAIRS

Christer Aakeröy
aakeroy@ksu.edu
Marilyn Yoder
myoder@cctr .umkc.edu

Three Symposia will honor ACA Award recipients: The **Fankuchen Symposium** (**Prof. Alexander McPherson**); the **Trueblood Symposium** (**Prof. Richard E. Marsh**),and the **Supper Symposium** (**Prof. Nguyen-Huu Xuong**).

In addition, the ***Transactions* Symposium** on ***Crystals in Supramolecular Chemistry,*** organized by Alicia Beatty, will feature four half-day sessions: *Crystal Structure Prediction and Polymorphism; Crystal Growth Mechanism; Crystal Structure Design;* and *Applications of Crystal Design.*

2004 LOCAL CHAIRS

Bernie Santasiero **(bds@uic.edu)**
Karl Volz **(kvolz@uic.edu)**

This year we can renew old friendships, welcome new participants, and support our exhibitors at the ***Opening Reception*** in the East Riverside Exhibition Center at the Hyatt Regency Saturday evening. Other social events include the ***Mentor/Mentee Dinner*** on Sunday at the Blue Agave Mexican restaurant, and Monday's ***Young Scientist Mixer***. **Madeline Jacobs,** who directs the *C & E News* group of the ACS will receive the ACA Public Service Award at the ***Annual Awards Banquet*** on Wednesday evening, at the Hyatt Regency.

REGISTER EARLY! Deadlines:

Advanced meeting registration: June 01, 2004.

Advanced hotel registration: June 15, 2004.

See ACA Call for Papers for further details, or check out

http://www.uic.edu/orgs/aca2004/.

Chicago photos are courtesy of Terry & Melody Howe, ChicagoPhotography.com and the City of Chicago Office of Tourism.

ACA Meeting 2005 - Abstract Deadline December 15, 2004

to be held May 28 - June 2, 2005 at the Walt Disney World Swan Hotel, Orlando, Florida

Local Chairs:

Khalil Abboud, (at left)
Dept. Chemistry, Univ. of Florida,
(352)-392-5948; fax: (352)-846-2040
abboud@chem.ufl.edu

Thomas L. Selby, (center)
Dept of Chemistry
Univ. of Central Florida
Orlando, Florida 32816
Office: (407)-823-6752; Lab: (407)-823-1115
tselby@mail.ucf.edu

Program Chair:

Ed Collins,
Dept. Microbiol. & Immunology,
Univ. of North Carolina at Chapel Hill
Chapel Hill, NC 27599
(919) 966-6869; fax: 919 962-8103
edwardcollins@med.unc.edu

A few of the "204 things to do in Orlando" from
www.orlandoinfo.com/attractions/

1. *Go whale watching at Port Canaveral.*
2. *Paddle a swan boat on Lake Eola.*
3. *Smell the roses at Harry P. Leu Gardens.*
4. *Cast a line for bass fishing with a guide.*
5. *Marvel at Tiffany glass at the Charles Hosmer Morse Museum of American Art.*
6. *Canoe down a serene river.*
7. *Touch a stingray at SeaWorld Orlando.*
8. *Find Chief Osceola in mural at Celebration Hotel.*
9. *Count the manatees at Blue Springs State Park.*
10. *Airboat through the natural grasslands.*

photo courtesy of the Orlando/Orange County Convention & Visitors Bureau

Meeting Calendar

MAY 2004

13-16 **High Resolution Drug Design Meeting,** Bischenberg-Strasbourg, France, contact **podjarny@titus.u-strasbg.fr** *(see Fall ACA Newsletter, p 63)*

JUNE 2004

2-4 **13th Annual CCP13 / Fibre Diffraction Workshop** at ILL/ESRF, Grenoble, France

6-10 **American Conference on Neutron Scattering,** College Park, MD.

9-20 **Electron Crystallography: Novel approaches to Structure Determination of Nanosized Materials**, Erice, Italy. **www.crystalerice.org**

10-21 **Polymorphism : Solvates and Phase Relationships.** Erice, Italy. **www.crystalerice.org**

JULY 2004

11-16 **Gordon Conference on Diffraction Methods in Structural Biology,** Bates College, Maine

17-22 **American Crystallographic Association 2004 Meeting, Chicago, IL. Local Chairs: Bernie Santarsiero, bds@uic.edu; Karl Volz, kvolz@uic.edu; Program Chairs: Christer Aakeröy, aakeroy@ksu.edu; Marilyn Yoder, myoder@cctr .umkc.edu.**

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

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

OCTOBER 2004

21-22 **SSRL 31st Annual Users' Meeting**, Stanford, CA

MAY / JUNE 2005

28-2 **American Crystallographic Association Annual Meeting, ACA 2005, 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**