AMERICAN CRYSTALLOGRAPHIC ASSOCIATION

NEWSLETTER

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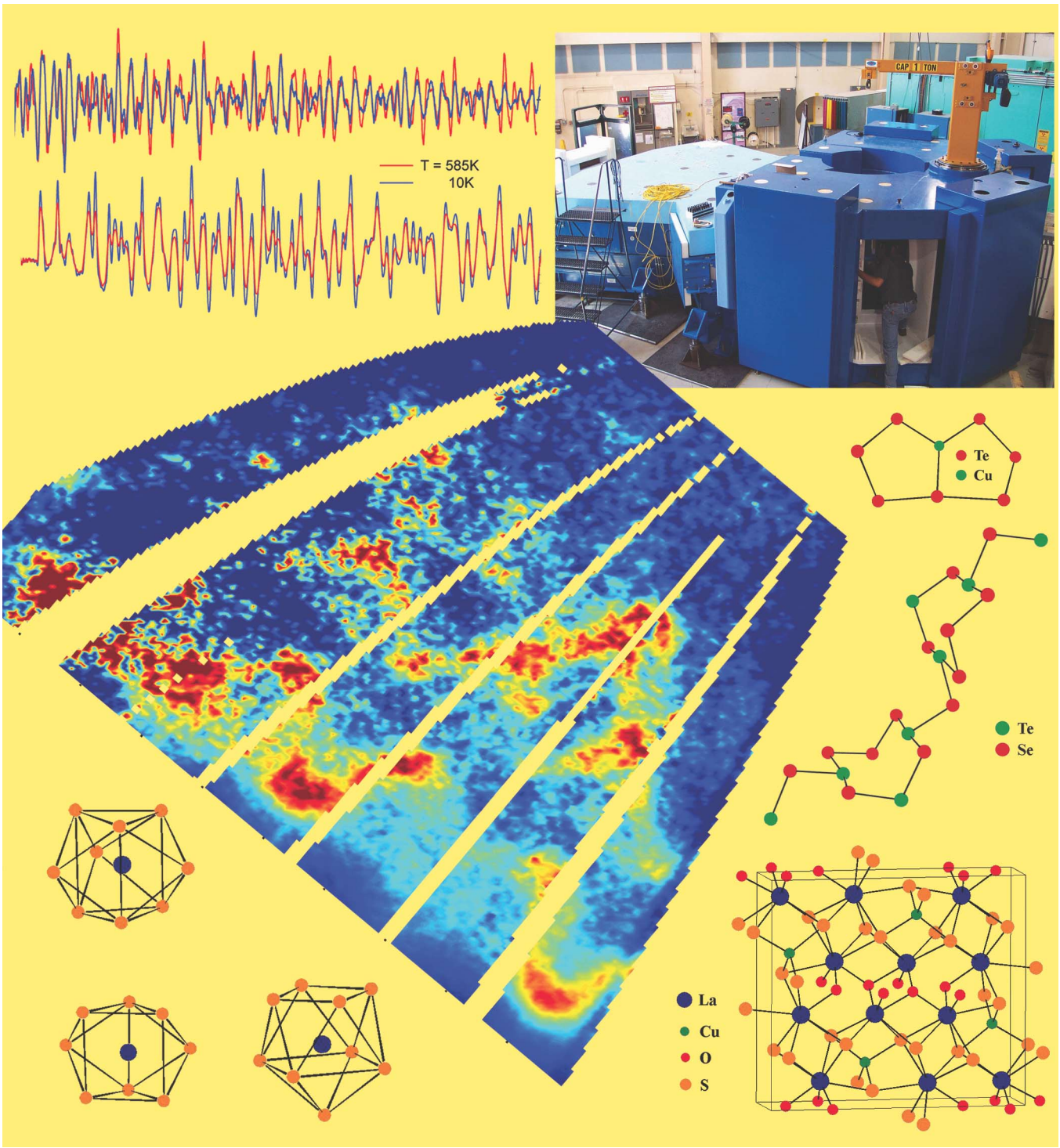

ACA 2003 - Covington, Kentucky
Buerger and Warren Award Symposia

Table of Contents

President's Column 1-2
Guest Editoral: Jon Clardy - Chair, USNCCr 2
News from Canada & Latin America 4-5
Index of Advertisers 5
News of Crystallographers / Web Watch 6
Pittsburgh Diffraction Conference - October 2003 6
Ed Lingafelter (1914 - 2003) 8-9
Henri Levy (1913 - 2003) 9
Mary Mrose (1910 - 2003) 10
Candidates for ACA Offices - 2004 12-18
ACA Balance Sheet 20
Database Updates - CCDC / NDB / PDB 22-23
ACA 2003 - Travel Awardees / Sponsors / Exhibitors 26
Neutron Protein Crystallography Station 28-29
Neutron Protein Crystallography Call for Proposals 29
Ferguson Symposium 31
Contributors to This Issue 31
West Coast Protein Workshop 32-33
ICDD Spring Meeting & Awards 35-36
Mid-Atlantic Protein Conference 39-41
ACA Corporate Members 41
Book Reviews 43-44
What's on the Cover 46
Furture Meetings 48
Positions Available 48

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President's Column

Let's get the bad news out of the way first. As you can see from the balance sheet in this newsletter, ACA's financial "bottom line" has been hit by the sustained economic doldrums we have all been enduring. Thus, nearly every matter discussed by ACA Council at its May meeting was necessarily viewed through the lens (or should it be the grating?) of fiscal prudence. Nevertheless, ACA remains committed to its core mission to "promote interactions among scientists who study the structure of matter at atomic (or near atomic) resolution". Thus, central scientific and educational objectives retain our foremost attention (the scientific program of our annual meeting, summer courses, encouragement and support of our student and younger members, our continued support of our hemispheric colleagues, to mention a few), while less necessary expenditures are being trimmed (e.g., don't plan to make breakfast or lunch of the coffee breaks in Covington). The insight and leadership of our financial officer, S. N. Rao, and our treasurer, Doug Ohlendorf, in this complex financial arena are much appreciated in these delicate and trying times.

Our continued gratitude goes to those many members who contribute, in excess of dues, to specific programs of the ACA. It will soon be possible to earmark contributions (whether for a specific fund or for undesignated use) as being in memory or in honor of individuals.

I am happy to note the reappearance in new form, after a hiatus of one year, of the ACA Summer Courses. This year's schedule includes two courses – one just before our Northern Kentucky ACA meeting, July 12-26 at the Illinois Institute of Technology, and one immediately following the ACA meeting, August 3-13 at Indiana University of Pennsylvania. I express ACA's appreciation to the teams headed by Andy Howard and Bryan Craven, respectively, for the huge effort in planning and executing these important affairs.

We are saddened to note in this issue the passing of our colleagues Mary Mrose, Henry Levy, and Ed Lingafelter (the latter two served as President of our association).

Elsewhere in this issue are the statements of candidates for offices and standing committees of the ACA. We are all grateful, not only to the nominating committee, headed by Winnie Wong-Ng, but also to those who agreed to stand for election.

And now – on to Northern Kentucky, where an absolutely superb meeting is planned (thanks to Bobby, Jeanette, and their committees). Meeting highlights will include the presentation of major ACA awards – the Bertram A. Warren Diffraction Physics Award to Takeshi Egami, the Martin J. Buerger Award to James Ibers, and the (new) M. C. Etter Early Career Award to Julia Chan, along with the scientific symposia that celebrate these awards,

and the announcement of next year's recipients of the Fankuchen and Trueblood Awards. Other major symposia in Covington are the transactions symposium on Biological Neutron Diffraction (organized by Gerry Bunick and Leif Hanson) and a special symposium on time-resolved diffraction in chemistry and biology (organized by Phil Coppens and Keith Moffat). As you can see on the meeting website (www.che.uc.edu/aca/index.html), this meeting has more than 500 abstracts, about evenly split between oral and poster presentations. The big scientific challenge for meeting attendees will clearly be the decision which sessions to attend and the regret at those necessarily missed. The exhibit show this year features 40 vendors (an all-time high), and I know attendees will support them by visiting their booths. And the social program that the local committee has planned will provide the opportunity for the pleasant interaction that is an indispensable part of every ACA meeting.

I look forward to seeing you there.

Ray Davis

Guest Editorial

At the start of the year, four new members (Phil Bourne, Ken Downing, John Parise and Cheryl Klein Stevens) joined the US National Committee on Crystallography (USNC/Cr). Jim Kaduk began a three-year term as Vice-Chair, and I began a three-year term as Chair. To the overwhelming majority of crystallographers, this change—and really any change—at the USNC/Cr is of little interest because they know nothing about the committee and its purposes. Some years ago when I was first asked to stand for election to the USNC/Cr, I must admit that I had no idea what the committee actually did.

The USNC/Cr is organized by the National Research Council to serve as a liaison between the US crystallographic community and the International Union of Crystallography (IUCr), the International Council on Science (ICSU), and the international scientific community. Some of the committee's duties are clearly spelled out. For example the committee selects the US delegates to the triennial IUCr General Assembly held along with the IUCr Congress. Many of the committee's tasks are less clearly defined. For example the committee, along with other bodies, is asked to suggest suitable candidates for various IUCr positions—IUCr Executive Committee, editors and co-editors of IUCr journals and the International Tables, and IUCr commissions.

The committee has fifteen elected members, three ex-officio members representing the ACA, and three nonvoting members representing the American Association for Crystal Growth, the ICDD, and the Microscopy Society. Representatives from the National Research Council attend our meetings on occasion. The complete roster of the USNC/Cr was listed in the Spring *Newsletter* and can be found on our website (www.sdsc.edu/Xtal/USNCCr/USNCCr.html). You can see how well it represents our personal diversity, the breadth of our scientific interests, and the variety of our institutional homes. The committee works only because its members are willing to donate their time and efforts to make it work. If you have any suggestions for new members, programs, or problems, please write to me (jon_clardy@hms.harvard.edu), or any other member of the committee.

Crucially important issues in international science are shared by all of the US national committees. In the last few years the National Research Council has organized meetings for all the national committee chairs to share their thoughts on problems and opportunities for the US in international science. Increasingly, those meetings have highlighted a growing concern about the access of foreign scientists to US laboratories, schools, and meetings. In short, the focus is on visa problems. By now, we have all heard the complaints of students who couldn't begin their studies in a timely fashion, visiting scientists who are afraid to visit their home countries for fear of not being allowed to re-enter the US, or foreign colleagues who did not get visas in time to attend a US meeting. All of these raise troubling issues about the free circulation of scientists.

Some organizations have released public statements deploring the situation. The American Chemical Society, for example, urged "swift federal action" expressing its concern that "the increasing number of delays and denials of visas to international students, scientists, and engineers will ultimately affect scientific progress and U.S. prosperity." At a recent Congressional hearing, the Chair of the House Science Committee, Sherwood Boehlert (R, NY) declared, "the current situation is untenable." He went on to say that backlogs in the visa system are "unnecessarily impeding the flow of foreign students and scholars" who are a "vital source of new ideas and perspectives". In response, Representative Ralph Hall (D, Texas) suggested that more American-born students be "enticed ... to pursue science and engineering careers" as a way to lower the demand for visas.

The administration's position was most clearly stated by John Marburger, the Director of the Office of Science and Technology Policy, in an address to the American Association for the Advancement of Science. He noted "Most of the current delays and backlogs are related to our efforts to screen applicants more rigorously." He went on to state that the current problems with the system are understood and that the agencies are working to correct them. Perhaps the most useful comment he made was his encouragement for "a better knowledge among all parties regarding how the visa system works, and what are its objectives. ... Students and visiting scientists need to get accurate information from their institutions and collaborators about how and when to apply for visas. We can all help make the system work better." His entire address can be found at www.ostp.gov/mtml/jhmAAASvisa.pdf.

The National Academy has set up a very useful site (www.nationalacademies.org) for obtaining just that information. In addition to accessible and authoritative visa information, the site also provides a visa survey to help monitor scientific mobility and spot trends that impede the free flow of scientists. If you, or someone you know, has a visa problem, I encourage you to visit the site.

Jon Clardy

HAMPTON

News from Canada

1. A new international initiative in structural genomics has recently been announced. The collaboration, funded by the Wellcome Trust, GlaxoSmithKline, Genome Canada, Canadian Institutes of Health Research and the Ontario government, will be based at the University of Toronto and at Oxford University. Directed by Al Edwards in Toronto, the consortium plans to provide at least 350 novel proteins to the public database over the next three years, with funding totaling approximately Can$100 million (about US$65 million). For more details, see www.newsandevents.utoronto.ca/bin4/030404aa.asp

2. CanadaQuirks: CIHR In this item, your correspondent attempts to clarify Canadian terms, organizations, issues, etc. that might be of interest to the crystal community.

CIHR, the Canadian Institutes of Health Research, is now the primary Federal Government arm for granting funding for basic health research. Evolving from the former Medical Research Council (MRC), the CIHR has Institutes to drive funding and research in certain areas of interest (to the government as well as to scientists). These include, among others, Cancer, Circulatory and Respiratory Health, Immunity and Infection, Aboriginal Health, Gender and Health, Genetics (which is home for much of the Structural Biology) and, most interesting to me, Aging. Unlike the NIH (I think), individual operating grant applications are reviewed by a central peer review process and, once approved for funding, assigned to an Institute. Each Institute also has some funds for special Calls for Proposals, Workshops, and other programs. While the amount of funding available to CIHR has increased significantly over the old MRC, the research mandate has spread this money over a broader scope. For more information and a full list of Institutes, see www.cihr.ca.

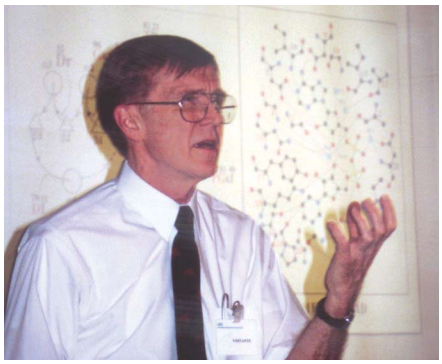
3. Any contributions to future Canadian reports are welcome to drose@uhnres.utoronto.ca. News from outside your correspondent's geographical and/or technical areas is especially welcome, as are requests (from anywhere) for items for CanadaQuirks. Let's not get personal, though!

David Rose

XVI Meeting of the Brazilian Crystallographic Association - March 2003 – São Carlos, SP, Brazil.

More than 100 members of the Sociedade Brasileira de Cristalografia (SBCr) gathered in March 2003, at the Physics Institute of the São Carlos campus, Univ. of São Paulo, for the 16th time since the Society was founded in 1974.

The meeting was preceded by a two-day workshop on "Data Collection and Data Treatment Strategies using Area Detectors" . The workshop program organizer and main lecturer was Zbigniew Dauter (Brookhaven), who discussed, among other subjects, Data Collection Strategies, International Tables Made Clear and Index, Integration and Scaling of Data. His enthusiasm was such that he was also involved in the hands-on sessions in the afternoon, with the collaboration of Igor Polikarpov, Javier Ellena and J.R. Sabino, from the IF-SC/USP.



The opening lecture on "Ion Gating and Selectivity in Gramicidin A" was delivered by William Duax, IUCr President.

This was the first time a high ranking official of the IUCr attended a meeting of a crystallographic society in Latin America, which made it a very special occasion.

Oral and poster sessions included 75 presentations on Biomolecules, Thin Films, Small Molecules, Diffraction Theory, Methods and Instrumentation, Powder Diffraction, Crystallographic Teaching, and Synchrotron Radiation Applications. One of the highlights was the presentation by Richard Garrat (IF-SC/USP) showing his injection molded plastic components kits for building 3D molecular models of protein structures.

The meeting was sponsored by three Brazilian funding agencies (FAPESP, CNPq and CAPES) and two commercial companies Dairix-RIGAKU and Bruker AXS.

Iris Toriani

Index of Advertisers

American Magnetics ---------- 36
ATPS, Inc ---------- 46
Bruker/Nonius ---------- Inside Front, 37, 44
DataCentric Automation ---------- 14
deCODE Genetics ----------11
Discovery Partners International -------- Inside Back
Diversified Scientific ---------- 39
Geonic Solutions, Inc. ---------- 30
Gilson, Inc. ---------- 19
Hampton Research ---------- 3
MAR USA ---------- 24,25
NASA Inst. Structural Biology ---------- 27
Oxford Cryosystems ----------21
Rigaku/MSC, Inc. ----------. Outside Back, 7
Rigaku/Osmic, Inc. ---------- 34
RoboDesign International Inc.---------- 47
Tri Tek Corporation ---------- 42
Veeco Instruments ---------- 45
Wyatt Technology Corporation ---------- 17
Xenocs ---------- 4

National Academy of Sciences

The US National Academy of Sciences elected 72 new members and 18 foreign associates from 11 countries at the 140th annual meeting of the Academy in April. A number of crystallographers were among the newly elected members.

US members:

Martha L. Ludwig, Univ of Michigan, Ann Arbor

Robert M Stroud, Univ of California, San Francisco

Foreign associates

Janet Thornton, EBI, United Kingdom

Ada Yonath, Weizmann Inst., Israel

ECA Prize 2003 to Professor Carmelo Giacovazzo

The European Crystallographic Association has announced that the third European Crystallography Prize will be awarded t Prof. Carmelo Giacovazzo of the University of Bari, Italy. Prof. Giacovazzo is being recognized for his major theoretical and practical contributions to the solution of the phase problem in a wide spectrum of applications.

The European Crystallography Prize, which includes a monetary award as well as a certificate of recognition, will be presented during the Opening Ceremony of the upcoming 21st European Crystallographic Meeting to be held in Durban, South Africa, August 24-29, at which Prof. Giacovazzo will describe the work for which he is being honored.

Members of the European Crystallography Prize Committee, who were appointed by the Executive Committee of the European Crystallographic Association are: Davide Viterbo (Coordinator), Italy; Leonid Aslanov, Russia; Boris Kamenar, Croatia; Åke Kvick, France; Dino Moras, France; Jochen Schneider, Germany; and Xavier Solans, Spain. Prof. Giacovazzo was born in Locorotondo (Bari), Italy and studied Physics in Bari. He is Full Professor of Mineralogy at the University of Bari and Director of the CNR Institute of Crystallography. After a first period dedicated to the study of defects in minerals, he has devoted his research interests to the development of Direct Methods for the solution of the phase problem. His main theoretical contributions are the Representation Theory and several probabilistic formulae for the estimate of structure invariants and seminvariants. From a practical point of view he has directed and coordinated a research group for the implementation of widely used computer programs for the solution of crystal structures not only from single crystal data but also from powder diffraction data. More recently he has developed new and powerful methods for solving ab-initio macromolecular structures using data collected at atomic resolution. He has also provided a new probabilistic approach for the location of heavy or anomalous scatterers in SIR-MIR-SAD-MAD techniques and for the subsequent phase estimation.

2003 Pittsburgh Diffraction Conference and Call for Nominations for the Sidhu Award

The Pittsburgh Diffraction Society is pleased to announce that the next conference will be held in New Brunswick, NJ at the Rutgers University Inn from October 30 through November 1, 2003. The symposia are "Macromolecular Complexes of Biological Interest", "The Single Crystal – Powder Diffraction Interface" and "Teaching Diffraction to Undergraduates". There is a reception and poster session on October 30 and a banquet and award ceremony on October 31, during which the Sidhu Award will be made. Nominations are herein requested for this award, which is made in honor of Professor Surhain Sidhu, to a scientist within 5 years of the PhD who has made an outstanding contribution to crystallography or diffraction. For further information and to submit nominations, please email (emge@rutchem.rutgers.edu) or send mail to: Thomas J. Emge, Dept. of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey, 610 Taylor Road, Piscataway, NJ 08854

Crystallography Web Watch

Crystallograpic Associations - A number of other crystallographic associations have their own web sites. Check out what the rest of the world is up to. Here are a few to get you started: Solvenia (rcul.uni-lj.si/~fn01leban/slkr/index.html), Czech Republic and Slovakia (www.xray.cz/xray/cryst.htm), Australia and New Zealand (www.sca.asn.au/), and Egypt (www.geocities.com/egyptiansca/).

Crystallographic course work and notes - A nice collection of notes on various crystallographic topics can be found via the "About" page (chemistry.about.com/msub51.htm). Another good source of links is the BUBL website from the University of Strathclyde, Glasgow, Scotland (bubl.ac.uk/link/c/crystallography.htm).

Mineralogy - The Univerisity of Wűrzburg has a set of annotated links to internet resources, especially for mineralogists, (www.uni-wuerzburg.de/mineralogie/links.html). Another source of mineralogy information is the Mineralogy Database (webmineral.com/).

IUCr Commission on Crystallographic Teaching - has written a series of pamphlets, each dealing with a specific crystallographic topic at a specific level. The emphasis is on a particular teaching approach and there may well be, in time, pamphlets giving alternative teaching approaches to the same topic. (see www.iucr.org/iucr-top/comm/cteach/pamphlets.html).

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

The Communications Committee will be holding an open meeting at this years' Annual Meeting (Sunday, July 27th, at lunchtime). Be sure to stop by to learn what we're doing and to make your own suggestions!

John Sack

Rigaku/MSC

Edward C. Lingafelter (1914-2003)

The death of our colleague, mentor, teacher, and friend, Professor Edward Clay Lingafelter saddened his many students and friends, but also brought back many happy memories of his loving and talented tutoring, given so unstintingly to us all. Ed died on April 7 at the age of 89. His wife of 65 years, Roberta, preceded her husband in death by one day, having died on April 6. She was 87 years old.

Ed was awarded the Ph.D. degree in chemistry by the University of California at Berkeley in 1939 where he distinguished himself, gained a broad knowledge of chemistry, and developed an assured confidence when faced with un-anticipated questions. For example, when he was preparing for his Ph.D. qualifying exam, it was customary to schedule a preliminary meeting with the Advisory Committee to lay out for the candidate what would be expected in the exam. At this preliminary meeting, Ed was startled when the members of the committee began asking the tough questions expected on the qualifying exam itself. Ed recalled that on the very first question, he struggled to come up with a partial answer. Then, having gotten through that, he gained sufficient confidence to formulate a satisfactory answer to the second question and went on to an unqualified "pass" of the exam! It remains uncertain whether Ed or the committee erred in their expectations for the meeting, but it seems unlikely, considering Ed's personality and character, that he misunderstood what the meeting was about. During his graduate studies at Berkeley, Ed became interested in X-ray diffraction and spent some time at The California Institute of Technology in Pasadena where X-ray crystallographic studies were well advanced. This introduction proved to be a blessing for many of us who later had the good fortune to work for and with him.

After completing his studies at Berkeley in 1939, he located a temporary position in the Department of Chemistry at the University of Washington in Seattle. Thus began his life's work. The appointment involved aiding Professor Tarter in his studies on surfactants using classical physical chemical techniques. In view of Ed's interest in X-ray crystallography, he initiated diffraction studies on these compounds. To that end he was able to obtain the basic equipment for the study of single crystals. The equipment, mainly supplied by The California Institute of Technology, was delivered in the late summer of 1942 and within weeks was producing beautiful rotation photographs of single crystals of long-chain sulfonates, detergents whose properties were being studied by other means in the department.

Because of the very serious academic disruptions of World War II, the enrollment at UW had decreased from about 11,000 in 1939 to about 4500 in 1945 at the end of the war. Thus it was that X-ray crystallographic studies could not continue until after the war. At the time, progress in molecular structure determination based on single crystal X-ray diffraction data was extremely slow because of the laborious computations, mainly by gear driven desk calculators. However, the era of electronic computers came to UW and to crystallography there in the early 1950s. The first crystallographic work was done on the accounting machines of the UW administration on a third shift arrangement. Soon after, however, Ed played a key role in acquiring the first electronic computers available to faculty and students at the UW. He was one of six members of a committee appointed by the Graduate School in the autumn of 1953 that arranged for an early IBM machine which became operational April 1, 1955. Then in 1957 it was replaced by the first stored program, drum memory machine on campus, an IBM 650. This was about 1000 times faster than hand calculations. The IBM 650 was displaced in 1960 by the very large, at the time, IBM 709 possessing 0.19 MBytes of memory and a 600 Byte operating system. Ed was active not only in acquiring these machines, but in supporting them from his research funds as each successive generation of machines came on line.

The early structures worked on at the UW were the sodium salts of n-alkane sulfonates and related paraffin-chain structures. During the decade of the 1950s, as more graduate students chose crystallographic problems, Ed's interests turned to the structures of metal complexes. Throughout the rest of his career, he and his students determined the structures of many organometallic complexes of both practical and theoretical interest. In this work he gave training and guidance to 39 graduate students and a score of post-doctoral students. The training in chemistry and crystallography was above reproach, but there were also great moments in the ethics of science. One memorable occasion was when, just as the UW group had managed to determine it, the structure of a zinc chelate appeared in *Acta Crystallographica*. At that time the group was in the process of checking a bond lengths and angles program. The bond lengths and angles reported in the paper were very different from those that Ed expected, so the structure from the literature was used as a test case for the new program. The student doing the programming reported that something was wrong, he couldn't get the same results as those published. Ed sat down at the desk in his very characteristic way and looked at the results. In what seemed like an instant he said

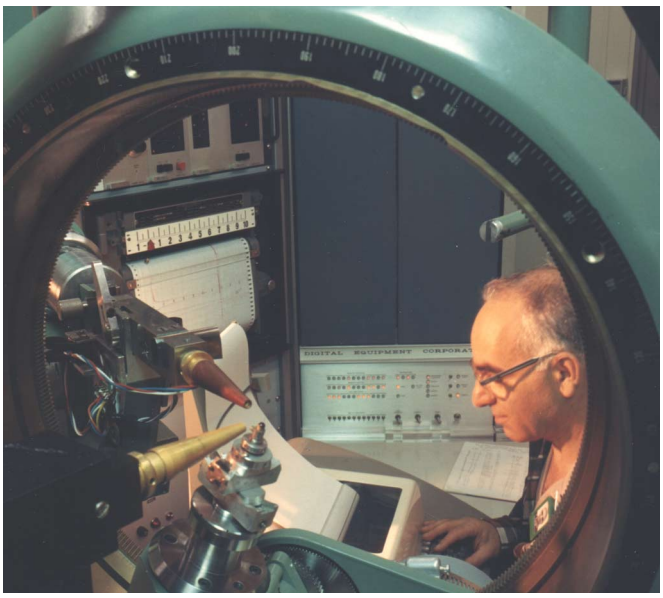
"They've used β* for β." Then, instead of firing a letter off to the journal, he wrote to the author of the paper, pointing out the error, and suggesting they publish the correction as co-authors. It was a wonderful example of his magnanimous nature.

During most of his career, Ed carried a fairly heavy teaching load. He is remembered by his students as an inspiring lecturer, not only in crystallography, but in other areas of chemistry as well. At the same time that he was teaching he assumed rather heavy administrative duties, serving half-time as Associate Dean of the Graduate School of the UW from 1960-1969. His lectures, and his method of managing courses were always exceedingly well organized and he knew exactly the right level at which to "pitch" a course. Therefore, he would go to the junior level Physical Chemistry class and then move into the Chemistry for Nurses class and get commendation from those disparate groups, and then come back to the graduate students and shift attention appropriately. As his Berkeley exam foretold, he had the knowledge and gift to deliver the answers just right. But above all he cared about the training of students and his concern was palpable.

For most of his career, Ed Lingafelter was active in the ACA, attending most national meetings and serving as President of the ACA in 1974. He also served as Co-editor of Acta Cryst., 1975-1981, and he served on many committees for the National Science Foundation. He continued to be active in both teaching and research, reaching mandatory retirement in 1984 at the age of 70. The temporary appointment in 1939 turned into tenure and finally retirement after 45 years at UW. Even after retiring, Ed continued in research as co-author on a number of papers and continued to help students and colleagues.

Jim Stewart, Lyle Jensen and Ron Stenkamp

Henri A. Levy (1913-2003)



It is with sadness that we inform you that Henri A. Levy (BS, 1935; PhD, 1938, Caltech) died on March 25, 2003 following a short illness. Born on September 12, 1913 in Oxnard, California, he studied chemistry and physics at Caltech under Linus Pauling, staying on as a postdoctoral fellow in Pauling's lab after receiving his doctorate to begin his career in crystallography. In 1943, he moved to Oak Ridge National Laboratory (ORNL) where he continued research for many years, even after his initial retirement in 1975. Originally working on highly radioactive materials related to the war effort, he returned to studying the crystallographic structure of molecules following the war. Ernest Wollan and Clifford G. Shull had recently shown that neutron beams from the ORNL Graphite Reactor were diffracted by crystals in ways very similar to X-rays. Working with Selmer W. Peterson, he took advantage of the fact that neutron diffraction experiments could locate the positions of hydrogen atoms with much greater precision than X-ray studies. They took the lead in pioneering work on hydrogen containing crystals, such as potassium hydrogen fluoride, urea, maleic acid, and water (ice). The structures of all these materials involve significant hydrogen bonding. The unique properties of water and ice are largely the result of hydrogen bonding. Indeed, the Antarctic Place-Names Committee honored him, along with others who had worked on water and ice, by naming Levy Island in Antarctica's Crystal Sound after him. As the reactors at ORNL became more powerful and more sophisticated, he and his co-workers took the lead in developing computer-controlled instruments for making diffraction measurements, and they developed computer programs for processing the data. The experimental and computational methods that they developed have had a profound impact on the way structures of large molecules are studied today. Following his official 'retirement' in 1975, he continued research as a consultant to ORNL and as a Professor at the University of Tennessee. During this time, he turned his attention to solving the three-dimensional structure of large biological molecules, devoting much of his efforts to tomography of electron microscopic images of transcribing and replicating chromatin, in collaboration with Don and Ada Olins. He belonged to numerous professional societies, serving as President of the American Crystallographic Association in 1965 and as a delegate to the International Union of Crystallography for several years. He is survived by his wife of many years, two children, three grandchildren, and numerous siblings, cousins, nieces, and nephews. The family requests that any memorials be in the form of contributions to IJAMS Nature Center, PO Box 20518, Knoxville, TN 37940; and the Southern Appalachian Highlands Conservancy, 34 Wall St., Suite 802, Asheville, NC 28801.

David Levy and Bill Busing

Mary E. Mrose (1910-2003)

Mary E. Mrose was a mineralogist, a crystallographer and a teacher. She was also a bonsai enthusiast for whom the International Pavilion (www.bonsai-nbf.org/international/mrosepavilion.htm) at the National Bonsai and Penjing Museum at the National Arboretum in Washington, DC (www.bonsai-nbf.org/nbpm/index.htm) is named.

T*he followed appeared as a news item at the time she was honored in 1995.* She was born in 1910, one of eight children of Emil W. and Mary M. Mrose. Her first career was that of teacher. After certification from the State Normal School at Salem, Massachusetts in 1931, she was one of three in a class of seventy five to obtain a teaching position. For the next fourteen years she taught history, geography and civics, and occasionally mathematics and English, at the junior high school level.

While teaching, she earned an M.A. in Geography from Boston University and a B.S. in Education from the State Teachers College in Salem, where she later taught earth science, geography and education. She also studied at the New England Conservatory of Music and became an accomplished pianist.

Moving toward her second career, Mary studied geology at Boston University and Radcliffe College. In the 1940s, after a year's stint as an industrial chemist, she taught geology at Boston University, at the same time serving as research assistant in the Harvard Department of Mineralogy. There she was involved in the preparation of Volume 11 of the 7th edition of Dana's System of Mineralogy, the bible of the field.

Her second career began in earnest in 1953, when she joined the U.S. Geological Survey in Washington, D.C. Until her official retirement in 1983, her activities at the Survey included X-ray studies of minerals; field work in New Hampshire, South Dakota, Arkansas and California; and authorship or co-authorship of seventy three articles, including papers in which she described and named nineteen new minerals. One of many honors and awards bestowed upon her was the designation of a very rare mineral from Moctezuma, Mexico, as "Mroseite" in recognition of her valuable contributions to mineralogy. She was an active member of the International Centre for Diffraction Data for thirty years and was a member of mineralogical and geological societies in the United States, Canada, Great Britain and Ireland, and France.

Her third career, which began after her retirement from the Geological Survey, was with the National Institute of Standards and Technology where, as a guest worker, she compiled data for an update of Crystal Data: Determinative Tables and a companion database, which was published by the International Center for Diffraction Data.

Mary Mrose's lifetime avocation had been the identification of trees. In 1991, she became a volunteer in the library of the U.S. National Arboretum which afforded her many opportunities to add to her impressive knowledge and introduced her to the fascination of bonsai.

David Garvin & Mary Ann Orlando (September 1995)

Beyond 1995 things pretty much remained the same for her until macular degeneration stopped her from driving. She continued at both NIST and the Arboretum until approximatey three years ago, depending on others for transportation so therefore a little more sporadically than before. But about two to three years ago, due to other health problems, she pretty much gave up going anywhere. However, she was always a source for Polish recipes. She was so excited when someone brought her some pigs feet because then she could make her special "cold feet" (I can't begin to reproduce the Polish name). She never missed Wall Street Week on PBS and she certainly could wax indignant about current affairs! Her generosity is legend and her spirit was indefatigable. Her body may have deserted her but she was mentally sharp as a tack and was fun to talk to right up to the end.

Judy Konnert (April, 2003)

deCODE

Louis T. J. Delbaere
Vice-President

Professor of Biochemistry, Canada Research Chair in Structural Biochemistry, University of Saskatchewan, Saskatoon, Saskatchewan, S7N 5E5, Canada.

Education**:** B. Sc. Chemistry, University of Manitoba (1965), Ph. D. Chemistry, University of Manitoba (1970). PDF University of Oxford (D. C. Hodgkin/K. Prout, 1969-71), PDF University of Alberta (R. U. Lemieux/M. N. G. James, 1971-73).

Professional Activities**:** Member Communications Committee of the ACA 2003-6; Member IUCr Commission on Synchrotron Radiation 1999-2005; Member IUCr sub-committee on Union Calendar 1999-2005; Vice-Chair Canadian National Committee for the IUCr; Chair, Canadian Delegates, XIXth International Union of Crystallography Congress and General Assembly Geneva (Switzerland) 2002; Member, International Advisory Board, 3rd International Conference, Inhibitors of Protein Kinases, June 22-28, 2003, Warsaw, Poland; Chair Protein Crystallography Beamline Team, Canadian Light Source 1999-2003; ACA Council Canadian Representative 1999-2001; Member Canadian Institutes of Health Research Senior Investigator Awards Committee 2001-2; Chair Phosphotransfer Session International School of Crystallography of Molecular Biology, Erice, Sicily 2000; Canadian Delegate IUCr Congress and General Assembly Glasgow (Scotland) 1999; Program Chair ACA Annual Meeting Arlington (Virginia) 1998; Canadian Institutes of Health Research Regional Director for Saskatchewan 1997-2001; Member National Cancer Institute of Canada grants panel 2001-2; Medical Research Council of Canada Grants Panel, Member 1991-93 & 1999 and Chair, 1994-96.

Research Interests**:** Crystallographic studies of phosphoenolpyruvate carboxykinase to examine the active site residues and the mechanism of catalysis for both ATP-dependent and GTP-dependent enzymes. Additional projects concern the structure and function studies of other important enzymes. This research involves the use of synchrotron radiation, so extensive use will be made of the on-site Canadian Light Source after the facility is functioning in 2004.

Statement: For four years I was directly involved with ACA Council, first of all as Program Chair of the Annual Meeting in Arlington, Virginia and subsequently as the Canadian Representative on Council. I was recently elected to the ACA Communications Committee. Last year I was re-appointed as a member of the IUCr Commission on Synchrotron radiation and as a member of the IUCr sub-committee on Union Calendar.

The ACA must cover all areas of crystallography so we must continually strive to have jointly-supported sessions with other societies that use crystallographic techniques, highlighting the multidisciplinary nature of our branch of knowledge.

All crystallographers should find themselves at home in the ACA. Synchrotrons are being used for diffraction of macromolecules, small molecules, fibers and powders, so there is a common x-ray source for these areas. In addition many methods, including computational methods, overlap different fields of crystallography.

We must encourage our younger colleagues to present their work at ACA meetings. Graduate students often present their first papers at ACA meetings; we should continue to support them to attend these meetings and to provide a significant number of travel awards for this purpose.

Structural genomics initiatives should produce an enormous amount of data and it is important that these data be as reliable as possible, available to the general scientific community and yet allow the protection of relevant intellectual property rights.

It is important to continue to reach out to our colleagues in Central and South America and support some of these researchers to participate in symposia at ACA Annual Meetings because the ACA represents all of us as a Regional Affiliate of the IUCr.

Education in crystallography is very important and the ACA should continue to support efforts such as the Summer Courses in Small Molecule Crystallography and Macromolecular Crystallography.

I am honored to be asked to stand for election as Vice-President and would strive to maintain the custom of service to all members of the ACA.

Howard Einspahr
Vice-President

Formerly, Research Fellow and Director, Bristol-Myers Squibb Pharmaceutical Research Institute, Princeton, New Jersey, recently retired.

Education: BA, Chemistry, Rice University (1964); PhD, Chemistry, University of Pennsylvania (1970) with Jerry Donohue; postdoctoral research fellow, California Institute of Technology (1970-1972) with Dick Marsh.

Professional Activities: Co-Editor, *Acta Crystallographica Section D* (1997-present); U.S. National Committee for Crystallography (1998-present); Space Studies Board, National Research Council, National Academy of Sciences (2001-present); Chair, Macromolecular Biotechnology Strategic Planning Committee, NASA (2001-present); Chair, General User Program, Industrial Macromolecular Crystal-

lography Association, Advanced Photon Source (1995-2003); American Crystallographic Association Service Award (1991); *ad hoc* Member and Chair of peer review panels for NIH (1987-2000) and NASA (1992-2003).

Research Interests: My first significant steps in science were as a small-molecule crystallographer, but during an extended stay at the University of Alabama at Birmingham, begun as a postdoc with Charlie Bugg, I had the good fortune to team with Bud Suddath and others to determine the structure of pea lectin. It was during this time that I became interested in experiments to evaluate the utility of microgravity in the study of protein crystal growth. It was also during this time that, along with the rest of the lab, I became interested in applications of macromolecular structure for drug design. In the mid '80s, Keith Watenpaugh and I joined the Upjohn Company to provide structures for its drug design programs and I continued this work when I joined BMS in the early '90s. All this is by way of explaining that my current research interests are structural biology, macromolecular crystal growth, and drug design. Most recently, I have been particularly interested in the nuclear hormone receptors as targets for drug design.

Statement: For as long as I've known it, the ACA has tried to serve the full range of diffraction and structural science interests. This has been one of its strengths and one of its challenges. The evolution of the SIG system has provided an excellent mechanism for assisting this mission by fostering the nucleation of new communities of scientific interest and by assuring that all the constituents within the ACA are heard by its leadership and are served effectively. The SIGs have also provided important opportunities for a committed membership to participate meaningfully in the organization and to identify and develop successive generations of new leaders. The ACA must continue to evaluate the success of its programs to assure that it fulfills the needs of the broader community while effectively serving the needs of its principal constituencies. This includes monitoring the health and welfare of our national facilities, journals, and databases, which are vital to our continued progress and to assuring the impact and utility of our results. It also means playing an important part in supporting education initiatives that will help to identify and nurture the young scientists that are our future. Finally, we belong to the American Crystallographic Association and we have evolved to serve the scientists in two American countries and to do it well. Recently, however, we have seen the first steps toward widening the community we serve to countries in Latin America. I think that is the right path toward the future and I urge the ACA to continue its leadership in this direction.

Alicia M. Beatty, Communications Committee

Assistant Professor of Inorganic Chemistry, Department of Chemistry, Mississippi State University.

Education: B.S. Chemistry, University of Missouri - St. Louis, 1989. Ph.D. Inorganic Chemistry, Washington University, St. Louis, MO, 1994 Post-doctoral work with Christer Aakeroy, Kansas State University.

Professional Activities: 2003 Chair-elect, ACA Service Crystallography SIG (Chair, 2004). Session Chair: Crystal Engineering Symposium, ACA Annual Meeting, San Antonio, TX, May, 2002. Member: ACS, ACA. Reviewer: ACS, RSC, IUCr journals.

Research Interests: Synthesis of novel crystalline materials through hydrogen-bonded assembly of organic and coordination complexes, especially clay mimics and magnetic materials.

Statement: "Listen, or your tongue will make you deaf." (Native American proverb).

"Ten people who speak make more noise than ten thousand who are silent." (Napoleon Bonaparte).

Normally we don't think of ourselves as having to strike a balance between Cherokee and Napoleonic philosophies. However, communication does go both ways. The ACA, which communicates through many electronic and print outlets, must figure out what it is that the ACA wishes to communicate to its members, to the scientific community, and to the public (i.e. to listen) and then figure out how best to communicate (i.e. to speak). It would be my pleasure to serve on the Communications Committee, which is concerned with our mouthpieces to the world. I would add my voice to the ten, while trying not to go deaf.

Cathy Drennan, Communications Committee

Cecil and Ida Green Assistant Professor of Chemistry, Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, 02139.

Education: A.B., Chemistry, Vassar College (1985); Ph.D. (with Martha L. Ludwig), Biological Chemistry, University of Michigan (1995); Post-doctoral (with Douglas C. Rees), California Institute of Technology (1996-1999).

Professional activities: Organizing committee of 19th Enzyme Mechanisms Conference (2003-2005); Editorial board of *Biochemistry & Molecular Biology Education* (2000-present); P.I., NIH-funded Undergraduate Summer Research Program in Macromolecular Interactions, MIT (2002-present); Chem Dept coordinator

Data Centric Automation

for MIT Science & Engineering Program for High School Teachers (2002-present); Assoc member, NASA-Penn State Astrobiology Research Center (1999-present); Organizer of first undergraduate events for American Society for Biochemistry & Molecular Biology (ASBMB) (1996-2000); Human resources committee member, ASBMB (1996-2000); High school teacher, Scattergood Friends School, West Branch, IA (1985-1988); Member, Am Cryst Assoc; Am Soc Biochem & Molecular Biol; Am Chem Soc; Soc Biol Inorg Chem.

Research Interests: Crystallographic studies of metalloproteins required for nucleotide & vitamin biosynthesis, methyl transfer reactions, DNA repair, the regulation of cellular metal uptake, and metallocluster assembly.

Statement: It is an honor to be nominated as a candidate for the Communications Committee. As someone who began my professional life as a high school teacher, I have had a long-standing interest in public outreach and in the effective communication of scientific ideas and results. I look forward to participating in the organization of press conferences, contributing to the preparation of crystallographic research reviews, and assisting in the coordination of ACA publications. If elected, my experience with publications of the American Society for Biochemistry and Molecular Biology will be useful in fulfilling my obligations.

Simon Billinge, Continuing Education Committee

Department of Physics and Astronomy, 4263 Biomed. Phys. Sciences Building, Michigan State University, East Lansing, MI 48824.

Candidates for ACA offices in 2004

The Nominating Committee has selected the following candidates for the 2003 elections for ACA offices in 2004.

Vice-President: Louis Delbaere and Howard Einspahr

Committees**:**

Communicatons: Alicia Beatty and Cathy Drennan

Continuing Education : Simon Billinge and Scott Misture

Data Standards a & Computing : Brian Toby and Ward Smith

2003 Nominating Committee

Winnie Wong-Ng (Chair), Bill Stallings and Victor Young

Canadian Division

Chair: Jim Britten and Bob McDonald

Secretary: Pawel Grochulski

2003 Canadian Division Nominating Committee
David Rose and Gary Enright

To nominate write-in candidates for any of these offices write to the ACA Secretary: Lisa J. Keefe, IMCA-CAT, Sector 17, Bldg. #435A, Advanced Photon Source, Argonne National Laboratory, 9700 South Cass Ave., Argonne, IL 60439 (Fax: (630) 252 0521)**.** Letters must be received by September 15, 2003 and must be signed by 5 supporting ACA members and include a signed statement by the candidate describing his or her qualifications. Nominations for Canadian Division officers must be made by members living in Canada. Statements from all candidates will be included with the ballots which will be sent to all members in October 2003.

Education*:* University of Oxford, BA Materials Science (1986), University of Pennsylvania, Ph.D. in Materials Science and Engineering (1992)

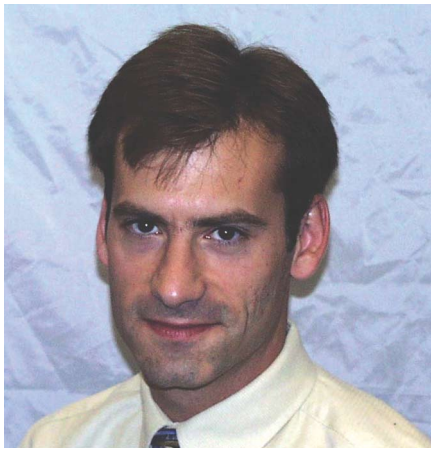
Professional Activities: Member: American Physical Society, American Crystallographic Association, Neutron Scattering Society of America. Chair: *ACA* Neutron scattering SIG (2001-2002), *Workshop, From Semicondutors to Proteins: beyond the average estructure,* Traverse City, MI, August 2001, *Workshop, Local Structure from Diffraction,* Traverse City, MI, July 1998. Secretary*: - Neutron Scattering Society of America* (2003 -) .Organizer*: - Symposium, Electronic Oxides: Properties and Applications,* CFMR Spring Symposium , Michigan State University, April 1997. Co-organizer : *B. E. Warren Award Symposium* at the ACA meeting, Cincinnati, July 2003, *Workshop, Real-space Pair Distribution Function Methods* at the meeting Neutrons In solid state Chemistry and the Earth Sciences Today and tomorrow (NICEST), Oak Ridge, TN, March 2003, *Symposia, Impact of Scattering on Nanoscience and Nanotechnology* and *From Structures to Materials Science,* ACA meeting, San Antonio, TX, May 2002, *Workshop, Real-space Pair Distribution Function Methods,* ACA meeting Los Angeles, July 2001, *Symposium, Microstructure and Texture of Real Materials,* at the XVIIIth IUCr Congress, Glasgow, Scotland, August 1999.

Research Interests: Local structure property relationships of disordered crystals and nanocrystals using advanced x-ray and neutron diffraction techniques. Atomic Pair Distribution Function method applied to complex materials. Single crystal diffuse scattering and total scattering

studies. Studies of charge localization and nanoscale inhomogeneous electronic states in complex electronic oxides. Studies of semiconductor alloys and microporous materials. Local structure of biologically relevant molecules and materials in the excited state. More information about my research, (p)reprints, and a complete publication list, can be found at http://www.pa.msu.edu/cmp/billinge-group.

Statement**:** How are crystallographers educated? With the demise of Crystallography Departments at universities in the US this is a relevant question. Crystallographic methods mostly are taught in a rather *ad hoc* way, folded into solid state chemistry and physics courses and introductory biochemistry courses. Graduate students also learn through hands-on work as part of their Ph.D research. This situation suggests a central role that the ACA can (and does) play in the education of crystallogaphers by conducting workshops at ACA meetings, providing a forum for talks on crystallographic education, and publishing monographs and textbooks (this is mostly handled bu IUCr). This is an aspect of life as a crystallographer that I support and have participated in by running hands-on workshops at ACA meetings and elsewhere.

Scott Misture, Continuing Education Committee



Assoc. Professor of Materials Science, NYS College of Ceramics at Alfred University, 2 Pine Street, Alfred, NY 14802

Education: Ph.D. in Ceramic Science, Alfred University, 1994

Professional activities: Member of ACA, American Ceramic Society, Materials Research Society, Electrochemical Society. Subcommittee Chair of the ICDD Denver x-Ray Conference Organizing Committee, Member Executive Committee, Spallation Neutron Source and HFIR Users Group.

Research interests: Ionic and mixed conduction in ceramics, electroactive ceramics, glass processing and surfaces of glass

Statement: As a former chair of the Materials SIG, I have a working knowlege of the operation of the ACA and look forward to participating in the Continuing Education Committee.

Ward Smith, Data Committee

Protein Crystallographer, GM/CA Collaborative Access Team, Advanced Photon Source, Argonne National Laboratory, Argonne, IL 60439.

Education: B.S. Chemistry, University of Illinois (1971), Ph.D. Biological Chemistry, University of Michigan (1977).

Research Interests: Structure and function of biological macromolecules, structure-based drug design, protein crystallography, x-ray diffraction hardware and software, application of synchrotron radiation in macromolecular crystallography.

Statement: The continued development and implementation of standards in crystallography is a critical component of improving communication. This is particularly true in macromolecular crystallography as rapid methods of data collection and structure solution are incorporated into structural science. The implementation of publication standards and deposition policies has helped ensure the continuing impact of structural information. Managing the large amounts of data and making these data available in a useful way is crucial to maximizing the value of structural science, both in public and industrial settings. Crystallography has always been a discipline blessed with a significant amount of freely available software. Preserving and enhancing this resource is important. Maintaining a high level of quality and easy availability of structural results will be challenging in the new world of high throughput macromolecular crystallography. I look forward to serving on the Committee, if elected, working to help improve development and implementation of data standards, to encourage the continuing development of methods and to work to enhance the communication of all aspects of structural science to a broad audience.

Brian Toby, Data Committee

Research Chemist and Leader, Crystallography Team, NIST Center for Neutron Research, National Institute of Standards & Technology, Gaithersburg, MD 20899-8562.

Education: B.A., Chemistry, Rutgers University (1980). Ph.D., Physical Chemistry, California Institute of Technology (1986). Research Associate/Lecturer in Takeshi Egami group, University of Pennsylvania (1988-1990)

Professional Activities: ACA: several SIG Chair positions, and organized several sessions at meetings; IUCr: former member COMCIF and Neutron commissions; ICDD: member and former taskgroup chair.

Research Interests: Structure determination from neutron and synchrotron powder diffraction; neutron Laue diffraction methods; improvements to NIST's neutron powder diffractometer, currently the highest resolution & most versatile in the USA; Rietveld and powder diffraction

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software.

Statement: If elected to the Data, Standards & Computing Committee, I will [ab]use that authority to pursue a goal: to convince the ACA to create an award to honor crystallographers who create and publically distribute software. Freely-distributed software has traditionally been vital for our research, but in many areas of crystallography, this work is not funded. The ACA needs to demonstrate the importance of software within crystallography.

Canadian Division

Jim Britten, Chair

Assistant Professor, Department of Chemistry, and Brockhouse Institute for Materials Research McMaster University, Hamilton, ON, Canada.

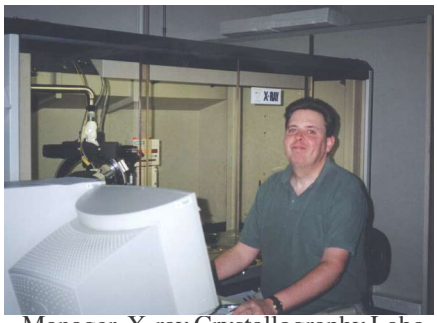
Education: BSc., St. Francis Xavier (1977); PhD., McMaster (1984); NSERC PDF, U. de Montreal; Killam PDF, Dalhousie

Professional Activities: Member of ACA; Secretary, Canadian Division of the ACA (1998,1999); Chair, Service Crystallography SIG (1997); Member of Canadian Institute for Synchrotron Radiation (CISR); Beamteam Leader for Small Molecule Crystallography Beamteam at the CLS; Beamteam Member for Powder Diffraction Beamteam at the CLS; Member of the User Advisory Committee at the CLS; Member of the Beamline Advisory Committee for the CLS; Member of SCrAPS

Research Interests: Service Crystallography; Synchrotron X-Ray Diffraction; Microcrystals; Ab Initio structures from powder diffraction; Texture analysis; Stress/Strain Analysis; Charge Density Analysis; Incommensurate Structures; Twinned Structures; Thin Film Analysis.

Statement: This is an exciting time for crystallographers in Canada. The Canadian Light Source will be operational this year, and the Macromolecular and XAFS beamlines will be commissioning early next year. The new Canadian Center for Advanced X-Ray Diffraction Studies will build an undulator beamline for powder and single crystal diffraction experiments, with future bending magnet lines for service crystallography and SAXS. The CLS will be a focal point for crystallography in Canada. At the laboratory level, CFI funding has greatly improved the instrumentation available to crystallographers. The Canadian Division of the ACA should have a role in improving communications between researchers, in facilitating access to our new resources, and in showcasing Canadian research at the international level. As Chair of this group, I would do my best to make this happen.

Robert MacDonald, Chair



Manager, X-ray Crystallography Laboratory, Chemistry Department, University of Alberta, Edmonton, Alberta T6G 2G2, Canada

Education: B.Sc. (Chemistry, 1984), Memorial Univ. of Newfoundland; Ph.D. (Inorganic chemistry, 1991), Univ. of Alberta; Post-doctoral fellowship (supervisor A. D. Hunter, 1991), Univ. of Alberta.

Professional activities: Member of ACA since 1992.

Research interests: Small-molecule service crystallography.

Statement: Crystallography in Canada continues to evolve as a front-line characterization technique. If elected as your representative I will be honoured to represent the interests of our community to ACA council.

Pawel Grochulski, Secretary

Staff Scientist at Canadian Light Source Inc. and Adjunct Professor of Biochemistry, Univ. of Saskatchewan, Saskatoon, Saskatchewan, S7N 0X4, Canada.

Education: M.Sc. Physics, Technical Univ. of Lodz, Poland (1979), Ph.D. Physical Chemistry, Technical Univ. of Lodz (1988), D.Sc. Physical Chemistry, Technical University of Lodz (1994).

Professional Activities: Member of ACA.

Research interests: Macromolecular crystallography; structure–based drug design; synchrotron radiation and X-ray optics.

Statement: My crystallographic education began in small molecule crystallography, extended to macromolecular crystallography and widened to include synchrotron radiation. In almost all my professional career as a protein crystallographer, I have been a user of various synchrotron facilities. Since I joined the Canadian Light Source (CLS), I have learned how to provide crystallographic services to users frequently unfamiliar with such techniques. I believe that my previous experience will allow me to address the needs and concerns of users of our Canadian Macromolecular Crystallography Facility (CMCF) at CLS. If elected, I will do my best to fulfill the duties of the secretary of the ACA's Canadian Division.

GILSON

AMERICAN CRYSTALLOGRAPHIC ASSOCIATION, INC.
BALANCE SHEET - December 31, 2001 and 2002

	CURRENT FUNDS		TOTAL	
	Unrestricted	Restricted*	All Funds	
			2002	2001
ASSETS				
Current Assets:				
Cash	52,302		52,302	58,702
Investments	253,829	300,498	554,327	766,296
Inventory	3,600		3,600	3,600
Total Current Assets	309,731	300,498	610,229	828,598
Fixed Assets:				
Computers and Printers	6,500		6,500	6,500
Office Equipment	1,300		1,300	1,300
Accumulated Depreciation	0		0	-0
Total Fixed Assets	7,800		7,800	7,800
TOTAL ASSETS	317,531	300,498	618,029	836,398
LIABILITIES & FUND BALANCE				
Liabilities:				
Deferred Dues Income				0
Total Liabilities	0		0	0
Fund Balance:				
Unrestricted	317,531		317,531	500,655
Restricted		300,498	300,498	335,743
Total Fund Balance	317,531	300,498	618,029	836,398
TOTAL LIABILITIES & FUND BALANCE	317,531	300,498	618,029	836,398

* Current Balances in individual restricted funds - as of December 31, 2002

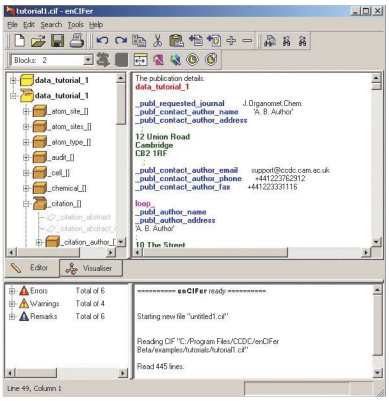
Buerger Award	31,208
Etter Award	53,853
Fankuchen Award	57,333
Patterson Award	30,456
Pauling Award	25,800
Supper Award	9,300
Trueblood Award	25,268
Warren Award	25,099
Wood Science Writing Award	42,181

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

OXFORD CRYO

Update from the Cambridge Crystallographic Data Centre (CCDC)

Currently, the Cambridge Structural Database (CSD) contains over 290,000 structures, including the February and April data updates, available to subscribers via the Web, and a target of 300,000 structures will be close by the time of next full CSD System release in November 2003. As the number of CIFs deposited with the CCDC continues to rise exponentially, it is appropriate that April saw the release of the long-awaited CIF editor: *enCIFer* (version 1.0) from the CCDC. enCIFer is available for free download for *bona fide* research purposes from: **www.ccdc.cam.ac.uk/prods/encifer/index.html.**



The CIF (Crystallographic Information File) is now the standard means of information exchange in crystallography. An increasing number of journals require CIF depositions to be associated with new papers, and some generate papers for publication directly from CIFs. It is also the (much) preferred way of submitting data to the CSD. Being text files, CIFs can be manually edited or amended, and if this is not done correctly, programs designed to read and interpret CIF data will encounter problems. It is for this reason that *enCIFer* has been written.

enCIFer provides an intuitive interface which, having finished a crystal structure refinement, allows you to add information, *e.g.* bibliographic data, crystal properties, etc., safely to the resultant CIF without corrupting the strict syntax, giving rise to a format compliant file. Additionally, *enCIFer* has been designed to suit expert and novice CIF editors alike. Feedback from beta-testers has been encouraging, so please try it in your laboratory and let us know what you think (support@ccdc.cam.ac.uk).
Single and multi-block CIFs can be edited using enCIFer permitting:

- Location and reporting of syntax/format violations using the current CIF dictionary
- Correction of these syntax/format violations
- Editing of existing individual data items or looped data items
- Addition of new individual data items or looped data items
- Addition of certain standard additional information via two data entry wizards:
    - Publication wizard – basic bibliographic information required by most journals and databases that accept CIF deposition files
    - Data wizard – chemical, physical and crystallographic property information that enhances a CIF for journal or database deposition
- 3D visualisation of structure(s) in a CIF

Many journals have arrangements whereby the CIF is deposited with the CCDC before the paper is submitted for publication. The CCDC also accepts *Private Communications* for structures for which formal journal publication is not envisaged. Full details about both data deposition schemes can be found on the CCDC website: www.ccdc.cam.ac.uk/conts/depositing.h

Karen Lipscomb and Susan Robertson

The Nucleic Acid Database Update

On April 25, 2003 -- the 50th anniversary of the discovery of DNA -- the Nucleic Acid Database (ndbserver.rutgers.edu) released an updated and expanded version of its website. After a period of community testing through a beta test site, the NDB features a new look and layout, a greatly revised new Atlas, a new database that includes x-ray and NMR structures, and a new search engine. The new NDB site graphics and layout have been created to enhance navigation through the site. There are nine main sections -- Atlas, Deposit, Download, Search, Reports, Education, Standards, Tools and Links -- available from the navigation link at the top of most NDB pages. A site index shows the entire NDB site at a glance. The expansion and redesign of the NDB Atlas includes: pages for NMR structures; more descriptive structure categories; improved graphics, and further information about each structure.

The Atlas is divided into x-ray and NMR structures at the top level, and then into further categories (such as DNA Junctions and Viruses). The top level page for each includes images for each structure listed. A text-only index option is also available.

The images used in the Atlas are part of the new graphics features used at this site. Pictures which emphasize nucleic acid features were created by 3DNA software (Xiang-Jun Lu and Wilma Olson, Rutgers). Secondary structure pictures are now available for RNA structures. These pictures were created by software developed by Huanwang Yang (Rutgers) in collaboration with Fabrice Jossinet (CNRS), N. Leontis (Bowling Green University), and Eric Westhof (CNRS). RNAML files which were used to create the RNA pictures can also be downloaded. (RNAML: http:///smi-web.stanford.edu/projects/helix/pubs/rnaml/) Links to structure factor files and links to tables of derivative data are now available. Derivative data tables include nucleic acid backbone torsions, base pair parameters, base pair step parameters, and hydrogen bonding classification. Base pair and base pair step parameters are based on "A Standard Reference Frame for the Description of Nucleic Acid Base-pair Geometry" (Olson et al., *Journal of Molecular Biology* (2001) 313: 229 - 237). Hydrogen bonding classifications are based on the Saenger classification (Wolfram Saenger, *Principles of Nucleic Acid Structure*, Springer-Verlag New rk Inc. 1984) and on the Leontis/Westhof classification (Leontis and Westhof, *RNA* (2001) 7:499 - 512).

Much of the NDB Atlas reengineering work done was done as part of the NDB Summer Research Project (2002) where undergraduate students from Bryn Mawr College and Rutgers worked closely with the NDB staff.

In addition to the regular NDB query and reporting options, a new beta NDB search tool is available to query a new database that contains nucleic acid containing structures from NMR and X-ray crystallographic studies. The new database is based upon the PDB mmCIF Extension Dictionary available from deposit.pdb.org/mmcif/.

The new beta search allows queries of x-ray structures, NMR structures, or both. Query fields are divided into categories: General Information, Experimental Type, Sequence, Biomolecule, Nucleic Acid Modifications, and Structural Features. This beta Search page is currently under development. New query fields will be activated once they have been tested.

Once a search results set is obtained, users have two choices. First, users can click on an ID in the results set which will direct them to the Atlas page for the entry. Second, users can select IDs of interest and generate pre-defined reports for information such as Base Pair Parameters.

User comments on this beta search engine should be sent to ndbadmin@ndbserver.rutgers.edu.

Christine Zardecki

Protein Data Bank Update

The Protein Data Bank will be exhibiting at the ACA Meeting in Northern Kentucky at which we will sponsor our first PDB Poster Prize to recognize a student poster presentation involving macromolecular crystallography. The prize will also be awarded at the meetings of the other IUCr Regional Associates - the Asian Crystallographic Association (AsCA), and the European Crystallographic Association (ECM)--as well as at the IUCr Congress itself. Each award will consist of two educational books; this year's prize will be signed copies of *Biochemistry - Vol I* by Donald and Judith G. Voet, and *Introduction to Macromolecular Crystallography* by Alexander McPherson. Winners will be announced on the PDB web site and in the PDB, ACA, and IUCr newsletters.

PDB dinner included a surprise birthday cake to mark a decade rollover for director Helen Berman. PDB members shown are from left to right: Gary Gilliland, Zukang Feng, Padma Vedanthi, Phoebe Fagan, Richard Kreuter, Judy Flippen-Anderson, Helen Berman and John Westbrook.

The Protein Data Bank has more than 20,000 entries in the current release. In the first quarter of 2003, approximately 1,200 structures were deposited to the PDB. 76% of all of the structures received during this period were deposited with a "hold until publication" release status; 9% were deposited with a specific hold date; and 15% were deposited with a "release immediately" status. 85% were the result of x-ray crystallographic experiments; 11% from NMR.

Several new features are available for testing from the PDB beta website at beta.rcsb.org/pdb/. The View Structure section of the Structure Explorer now offers still ribbon images of the assumed biological unit(s) for structures, where relevant, in addition to static images of the asymmetric unit. The interactive molecular viewers available from this page continue to provide a variety of ways to visualize the asymmetric unit. Links to the coordinate files that are used to generate the biological unit images are also accessible here, as well as from the Download/Display File section of the Structure Explorer.

Curated (Beta) mmCIF Files: The Download/Display File section of the Structure Explorer pages on the beta website now provides links to view or download curated mmCIF files. These files include remediated data from the Data Uniformity Project (www.rcsb.org/pdb/uniformity/). The files follow the latest version of the mmCIF dictionary supplemented by an exchange dictionary developed by the RCSB and the MSD-EBI. This exchange dictionary can be obtained from deposit.pdb.org/mmcif/.

The curated mmCIF files for a set of query results can be downloaded by selecting the Download Structures or Sequences option from the pull down menu at the top of the Query Result Browser page.

Curated mmCIF files for all PDB structures are available in gzip (.gz) format at ftp://beta.rcsb.org/pub/pdb/uniformity/data/mmCIF.gz/. UNIX-compressed versions of these files (.Z) remain available at ftp://beta.rcsb.org/pub/pdb/uniformity/data/mmCIF/.

Redundancy Reduction Cluster Data: The results of the weekly clustering of protein chains in the PDB are now available for beta testing at ftp://ftp.rcsb.org/pub/pdb/derived_data/NR/. These clusters are used in the "remove sequence homologs" feature on the PDB web sites. Files that list the clusters and their rankings at 50%, 70% and 90% sequence identity are available. Smaller rank numbers indicate higher (better) ranking. Chains with rank number 1 are considered to be the best representative of their cluster. The contents of these files and the details of the clustering and ranking are further described at ftp://ftp.rcsb.org/pub/pdb/derived_data/NR/README and www.rcsb.org/pdb/redundancy.html. Comments on these new features are appreciated and may be sent to notify@rcsb.org.

Weekly PDB news is available from the PDB home page at www.pdb.org/.

Christine Zarkecki

MAR USA

MAR USA

ACA 2004 - Travel Awardees

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NASA INST STRUCT BIO

The Neutron Protein Crystallography Station at Los Alamos

The new PCS (Protein Crystallography Station) at Los Alamos has just successfully completed its first cycle of operation as a user facility at the neutron spallation source. This article, which overviews the station and reports some preliminary data collection results, accompanies a call for proposals for the second cycle.

Neutron diffraction is a powerful technique for locating hydrogen atoms and water molecules. Hydrogen atom positions and the coordination of water molecules cannot be directly determined using x-ray diffraction at resolutions typical for most protein crystals. Most PCS experiments so far have been concerned with locating functionally important hydrogen atoms to determine detailed enzyme mechanisms for the design of better drugs. However, investigations of hydrogen bonding and hydration have also been carried out. The PCS is also used for membrane and fiber diffraction.

Spallation neutron sources are a new arena for protein crystallography in the emerging era of proteomics. Spallation neutrons have a time-dependent wavelength structure that allows time-of-flight (TOF) techniques to be used to collect time (wavelength) resolved Laue diffraction data using all of the available neutrons. The PCS is the only neutron protein crystallography resource in the U.S. and the first in the world to be built at a spallation source.

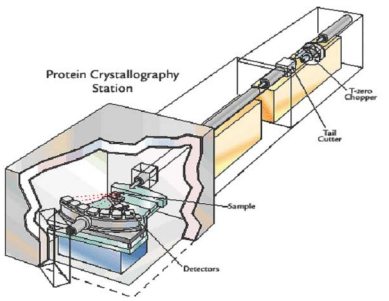


Figure 1. A schematic layout of the PCS.

The PCS is located on flight path 15 at the Lujan Center, figure 1. Pulses of neutrons with a wavelength band of 0.6Å to 5Å travel 28m through vacuum pipes with collimation inserts and beam-shaping devices that optimize the beam for high counting rates and low backgrounds at reasonable instrument resolutions. The vacuum pipe is tightly surrounded by heavy shielding until it reaches the sample position, where the shielding opens up to a large cave. In the cave, a kappa-circle goniometer moves the crystal through a number of orientations, recording a wavelength-resolved Laue pattern on a large detector at each setting. A complete data set requires between 12-30 crystal settings depending on crystal symmetry. A nitrogen cryostream cooler is used for low temperature data collection. An 8T super-conducting magnet can be used to orient membrane and fiber samples. The front cover of the *ACA Newsletter* no. 4 winter 2002 features a view inside the cave and also a Laue pattern collected during a user experiment. A customized version of the software d*TREK (Molecular Structure Corporation) is used for data display and processing, figure 2.

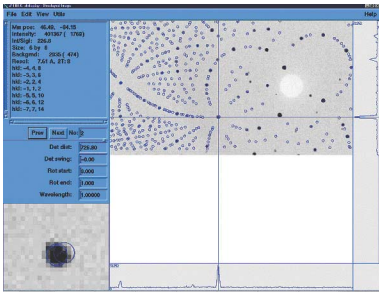


Figure 2. Analysis of data collected from insulin using d*TREK. The main display area shows the data as a Laue projection. The zoom display area (bottom-left) shows a cursor-selected reflection with superimposed circles representing starting and refined predicted positions. Horizontal and vertical line sections through the cursor position are shown along the borders of the main display area. The top-left display area contains statistical details about the cursor-selected reflection

The structure of human insulin was recently determined by neutron diffraction at the Japan Atomic Energy Research Institute (JAERI) (Maeda, M, Chatake, T., Tanaka, I., Osterman, A. & Niimura, N. (2003) "Crystallization of large single crystals of cubic insulin for neutron protein crystallography studies", submitted to *J. Synch.Rad.*, to be published as proceedings of ISDB 2003, Tsukuba, Japan.). Insulin can crystallize in space group $I2_13$, and is therefore ideal for testing the corrections applied to symmetry equivalent reflections recorded at different wavelengths in the wavelength-resolved Laue patterns. An experimental team from JAERI and the Bioscience Division collected data from one crystal setting for 16 hours on the PCS (λ=0.6Å-5Å; a=78.9Å; 4222 observed reflections; 1490 observed reflections with I/σ>2; 1006 unique reflections with I/σ>2 and d>2.1Å). A table of R_{merge} and completeness as a function of resolution indicates that a complete data set of sufficient resolution to locate individual hydrogen atoms (d~2.1Å) could be collected in ~10 crystal settings, equivalent to 6 days of beam time, Table 1. Significant data are found out to at least 1.8Å resolution indicating that a much higher resolution data set could be obtained over a longer period of time.

Table 1 R_{merge}, completeness (%C), and <I/σ> verses resolution for Human insulin. The cumulative R_{merge} and completeness are also given ($CumR_{merge}$, Cum%C). Only reflections with I/σ>2 are included in these calculations.

Res	No. Refs.	%C	Cum %C	R_{merge}	$CumR_{merge}$	<I/σ>
- 3.23	847	43.6	43.6	0.036	0.036	23.0
- 2.57	327	19.1	31.5	0.222	0.037	5.2
- 2.24	122	8.2	23.9	0.178	0.037	3.5
- 2.04	66	4.9	19.3	0.219	0.037	2.6
- 1.89	47	3.4	16.2	0.194	0.037	2.7
- 1.78	21	1.5	13.7	0.208	0.037	2.5

The protein D-xylose isomerase is an enzyme that catalyzes the conversion of D-xylose to D-xylulose and glucose to fructose by hydrogen atom transfer. One possible enzymatic mechanism is metal ion-mediated ionization of water, the metal being magnesium. The catalytic motif of a magnesium cation, a water molecule and an enzyme carboxylate group is common to many magnesium containing enzymes that are important in cancer research.

An experimental team from Oak Ridge National Laboratory (ORNL), Fox Chase Cancer Center, and the Bioscience Division collected data at 23 crystal settings on the PCS (Hanson, B.L., Langan, P., Katz, A., Li, X., Harp, J., Glusker, J., Bunick, G. & Schoenborn, B.P. (2003) "A Preliminary Time-of-Flight Neutron Diffraction Study of *S. rubiginosus* D-Xylose Isomerase [EC5.3.1.5]" *Acta Cryst. D,* submitted). The average collection time at each setting was ~20 hours ($P2_12_12_1$ a = 94Å, b = 100Å, c = 104Å; λ=0.6Å-5Å; 181,797 observed reflections; 62,692 observed reflections with I/σ > 2; 24,931 unique reflections with I/σ >2). Table 2, R_{merge} and completeness as a function of resolution indicates that the data set corresponds to ~2.1Å-2.0Å resolution (i.e. 50% complete in outer resolution shell). Significant intensities are observed out to a 1.5Å resolution, indicating that a much higher resolution data set could be obtained by recording for a longer period of time. From a preliminary 5Å-2.5Å neutron density map, shown in Figure 3, it is already possible to see that deuterium atoms have replaced labile hydrogen atoms. A detailed analysis of this data is underway at ORNL.

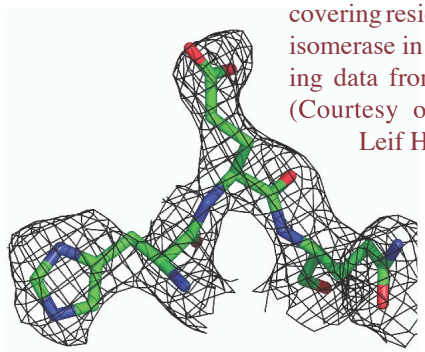


Figure 3. A slice of neutron density covering residues 220-222 in xylose isomerase in a preliminary map using data from 5A-2.5Å resolution (Courtesy of Gerry Bunick and Leif Hanson, ORNL).

Table 2 R_{merge}, completeness (%Comp), and <I/σ> verses resolution for xylose isomerase. The cumulative R_{merge} and completeness are also given ($CumR_{merge}$, Cum%Comp). Only reflections with I/σ >2 are included in the above terms. The completeness for all reflections without a I/σ threshold, %AllComp is given for comparison.

Resolution	No. Refs.	%C	Cum %C	%AllC	R_{merge}	$CumR_{merge}$
- 5.69	7,758	98.5	98.5	99.4	0.028	0.028
5.69 – 4.02	12,023	96.1	96.9	97.1	0.266	0.030
4.02 – 3.29	11,457	91.1	94.3	93.0	0.314	0.031
3.29 – 2.85	8,443	82.1	90.0	89.2	0.388	0.032
2.55 – 2.32	4,36 8	54.5	76.6	77.7	0.365	0.032
2.32 – 2.15	4,205	49.9	71.1	70.4	0.340	0.032
2.15 - 2.01	3,689	43.4	66.1	61.1	0.325	0.032
2.01 – 1.90	2,811	33.3	60.8	54.3	0.294	0.032
1.90 – 1.80	2,257	26.0	55.7	48.8	0.282	0.032

These results are among the first to be produced from this new tool for structural biology. The xylose isomerase result is significant in that, with a unit cell volume of ~1MA^3, it is by far the largest enzyme system to be studied to high resolution with neutrons. Data were collected from a number of proteins during the first user cycle and are currently being analyzed. The PCS has the potential to play an important auxiliary role in high throughput proteomics programs by providing unique information about the catalytic mechanism of newly discovered enzymes.

The PCS is funded by the Office of Science and the Office of Biological and Environmental Research of the U.S. Department of Energy.

Paul Langan and Benno P. Schoenborn.

Neutron Protein Crystallography - Call for Proposals

The new **PCS** (Protein Crystallography Station) at Los Alamos has just completed its first successful year of operation as a user facility and is now inviting experimental proposals for the second user cycle. The DOE-OBER funded user facility is the first **PCS** in the world to be built at a spallation neutron source, the first to use Time-of-Flight Laue techniques and the only neutron crystallography resource for structural biology in the U.S. Beam-time is free and is allocated twice a year through a call for proposals and a peer review process.

This new tool for structural biology will play an auxiliary role to high throughput Proteomics programs by providing detailed information about the mechanism of newly discovered enzymes. Although most protein structures are determined using x-rays, the position of hydrogen atoms and the coordination, sometimes even the position of water molecules, cannot be directly determined at resolutions typical for most protein crystals. Hydrogen atoms are the primary motive force in most enzymatic processes. Neutron diffraction is a powerful technique for locating hydrogen atoms even at resolutions of 2A-2.5Å and can therefore provide unique information about enzyme mechanism, protein hydrogen and hydrogen bonding.

For information about the **PCS** and experimental requirements: Contact Paul Langan (langan_paul@lanl.gov) or Benno P. Schoenborn (schoenborn@lanl.gov).

For more information about the proposal process: Contact lansce_users@lanl.gov, LANSCE User Office, MS H831, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, or visit lansce.lanl.gov/userfs/proposals/index_prop.html

Important Dates:

Issue of second call: August 4, 2003

Proposal Deadline: September 2, 2003

GEONIC SOLUTIONS

George Ferguson Honored at Dublin City University, April 10, 2003

A meeting was held in the Research & Engineering building at Dublin City University on the topic of 'Chemistry and Crystallography' in honor of George Ferguson, University of Guelph Emeritus Professor, Guelph, Ontario, Canada and Honorary Professor at the University of St. Andrews, Scotland.

The meeting was comprised of two sessions generously sponsored by the School of Chemical Sciences (Professor Malcolm Smyth, Head and Dean of the Science & Health Faculty) and Bruker Nonius Limited (Marcus Winter). Some 40 participants were present from several countries including Canada, U.K. Switzerland, the Netherlands, Germany, Spain and Ireland.

The meeting was organized by John F. Gallagher and Frankie Anderson (School of Chemical Sciences and National Institute of Cellular Biotechnology, DCU). The meeting was opened by John Gallagher who welcomed everyone to Dublin and especially George and Lorna Ferguson.

John Low (Dundee & Aberdeen) gave a very interesting talk on his own career and his interactions with George Ferguson spanning some 30 years. They interacted especially in the areas of hydrogen bonding, co-crystals and polymorphism, in collaboration with Chris Glidewell (St. Andrews) and researchers at the University of Jaen, Spain. John also produced some pictures of (menacing) Scottish folk in a variety of tartan kilts. (Was this to inspire fear in the local Irish?) John's talk was an excellent introduction to the other talks and he surpassed everyone also in the wardrobe department when it came to the dinner (think tartan and leather!)

Malachy McCann (Maynooth) outlined his research over the past 25 years. He emphasized the importance of crystallography in coordination chemistry, and especially with regard to some manganese derivatives which have demonstrated effectiveness both as overly active detergents and in the treatment of common afflictions. We are left wondering about the tale of some students trying to climb in a chemistry professors bedroom window in the early hours of the morning after a research colloquium (and under the influence!).

Volker Bohmer (Mainz) gave a first class account of some macrocyclic derivatives, notably calix[n]arenes, and also recounted his collaborations with chemical crystallographers, including George, over the years. The importance of crystallography in macrocyclic chemistry was stressed.

Des Cunningham (Galway) discussed some current research on main group chemistry derivatives including Sn, Pb, Sb and discussed the influence of the role of halogen...halogen contacts on their 2-D and 3-D structures.

Gillian Holmes and Sean Conway (IUCr, Chester) gave an up to date account of recent developments in the Journals section of the IUCr in Chester and outlined some future plans.

Pat McArdle (Galway) gave an engaging talk about crystallography in Galway over the past two decades and the various adventures which Des and himself got up to in promoting crystallography, often in situations without much external funding. The Galway group has gone from strength to strength in many areas of chemical crystallography over the past two decades. The development of the OSCAIL (open in Gaeilge) programs over the past decade was outlined as well as some indepth forays into the world of FORTRAN programming. This was one of the most enetertaining talks that I have listened to in quite some time and one I would certainly like to hear again.

Trevor Spalding (Cork) gave an entertaining talk on several borane derivatives, from complexes to clusters. Reactivity and conditions were explored to explain how tweaking certain reactions can produce quite different isomers and products. This talk nicely wrapped up the chemistry and crystallography talks and served to underline how important and intertwined are the two fields.

The talks were followed by a presentation by John Gallagher on behalfof the participants to both George and Lorna.

Lorna and George Ferguson waiting for the arrival of the remaining guests to the dinner in his honor

The meeting dinner was held at Pacific Restaurant from 7:30 onwards until very late. The meeting was a great success judging by the smiles on everyones faces as the dinner crept into the wee hours (or was that the wine talking!). A special thanks is due to everyone who made the meeting such a great success.

John Gallagher

Contributors to this Issue: *Paul Anderson, Alicia Beatty, Simon Billinge, Jim Britten, Bill Busing, Charlie Carter, Connie Chidester, Jon Clardy, Ray Davis, Louis Delbaere, Cathy Drennan, Takeshi Egami, Howard Einspahr, Marcia Evans, John Gallagher, David Garvin, Pawel Grochulski, Jim Ibers, Xianjui Ji, Lyle Jensen, Judy Konnert, Paul Langan, David Levy, Karen Lipscomb, Bob Macdonald, Terry Maguire, Carla Mattos, Scott Misture, Mary Ann Orlando, S Narasinga Rao, Susan Robertson, David Rose, John Sack, Benno Schoenborn, Ward Smith, Ron Stenkamp, Jim Stewart, Brian Toby, Iris Toriani, Josh Warren, and Christine Zardecki*

16th West Coast Protein Crystallography Workshop, March 23-26, Asilomar Conference Center, Pacific Grove, California.

As has been the tradition at this meeting since its beginnings, nearly all of the talks were given by students and post-docs. The meeting was organized by John Tainer and Libby Getzoff from The Scripps Research Institute, and they assembled a fine program that focused on methods and techniques. For details concerning the program, please see the workshop website at http://www.wcpcw.org/.

One of the many magnificent views of the Pacific ocean at Asilomar

The meeting started on Sunday evening with a session on crystallization methods. The techniques described included the design of proteins to enhance their function and crystallization (Sherry LaPorte, UCSF), the use of an automated incubation chamber to set up and monitor crystal growth experiments (Rhett Affleck, Discovery Partners International), and the use of microfluidics and small volumes for crystallization experiments (Kyle Self, Fluidigm Corp; J.M. Berger, UC-Berkeley). Peter Nollert (DeCode Biostructures) gave a live demonstration involving coupled pipettes to quickly set up cubic phase crystallization experiments for membrane proteins. The final talk in the session, by Sheryl Tsai (Stanford and UCSF), described high throughput methods applied to studies of polyketide synthases.

On Monday, speakers from the national and synchrotron laboratories in the Bay Area described their efforts to automate various steps in macromolecular crystal structure analyses. Nicholas Sauter (Lawrence Berkeley Natl. Lab) summarized methods used at ALS for automated crystal screening. Tim McPhillips (SSRL) showed components of the Collaboratory for Macromolecular Crystallography that will eventually automate nearly all of the steps in a crystal structure determination. Ken Frankel (LBL) described a new beamline at ALS that will support crystallographic data collection as well as small-angle scattering measurements. He pointed out that analysis of how people use their beamtime shows that 85% of the time is used in non-data collection activities. Efforts to improve the time actually used for data collection are underway.

Diffraction methods were covered in the next session. Kathy Gelato (UC-Davis) talked about her use of anomalous scattering from deoxybromouridine to solve the structure of a Holiday Junction. She reported a split anomalous dispersion density for the bromine possibly connected with radiation damage. Ana Gonzalez (SLAC) then described her investigations of the relationship between radiation damage and the number of wavelengths used in MAD experiments. Her conclusion is that two-wavelength MAD experiments are optimal for reducing radiation damage while providing strong phase information. The use of chromium radiation from a rotating anode source was described by Joe Ferrara (Rigaku/MSC). He provided three examples (thaumatin, trypsin, and glucose isomerase) where good phases were obtained using anomalous dispersion from calcium or sulfur with the chromium source. The final talk in the session by Carsten Ryttersgaard (UCLA) showed what you can learn about your diffraction pattern by generating an average reciprocal lattice unit cell. Subcells missed by auto-indexing programs become apparent if the average cell is generated from the data frames. Streaking and spot shape information can also be obtained this way.

The evening session on space groups and phasing generated considerable discussion. The session started with a talk by yours truly (RES) on some structures deposited in the PDB with questionable space group assignments. Following that, Susan Heffron (UC-Irvine) described an interesting case in her studies of polygalacturonase where the initial analysis of the diffraction pattern indicated an orthorhombic space group (Rsym =0.047), but the structure was really monoclinic. The molecule has a beta-helix structure and this contributed to the pseudo-symmetry. The use of sulfur anomalous scattering to phase T4 lysozyme at atomic resolution was described by Blaine Mooers (Univ. of Oregon). He used the ACORN program and a series of cysteine mutants of T4 lysozyme to study the effects of different sulfur arrangements. Tzanko Doukov (MIT) presented the structure of carbon monoxide dehydrogenase/acetyl-coenzyme A synthase including the complex iron, nickel, copper center. Eric Lansdon (UC-Davis) then described a bromide soaking experiment used to solve the structure of APS kinase. The final talk in the session was given by Rob Grothe (UCLA) on methods being developed to obtain structural information from oriented polycrystalline samples.

The talks on Tuesday morning focused on structure analysis and interpretation methods as well as motion and conformational changes in macromolecular crystal structures. Debnath Pal (UCLA) gave the first talk summarizing software developed for archiving information from crystallization trials and for validating structures. Peter Muller (UCLA) described a bond valence method for identifying metal atoms in macromolecular structures. Use of a graphics program (Modelzilla) that allows the combination of molecular graphics and geometric modeling was shown by Sean Hennessy (Scripps Research Institute). He also showed examples of colored molecular models generated using 3-d printing techniques. The next presentation by Jingtong Hou (UC-Berkeley) covered mathematical approaches useful for investigating protein fold space. Principal component analysis of selected folding classes of proteins permits the sorting of

molecules in fold space and supports speculation concerning the evolutionary connections within that space.

Nobuyuki Ota (UCSF) described a method called multi-conformation simulated annealing pseudo crystallographic refinement (MCSA-PCR) that can be used for computational docking studies of flexible ligands in flexible binding pockets. Extraction of information from ultra-high resolution studies bearing on intermolecular interactions and equilibrium dynamics was the topic covered by Ulrich Genick (Brandeis). The following talk by Ursula Ramirez (Northwestern) described the structural detail concerning ligand conformations that can be obtained from a 1.1 Å resolution study of the Ffh GTPase domain. Ho-Leung Ng (UC-Berkeley) then summarized a series of structures of calmodulin bound to peptides from calmodulin-binding proteins. Analysis of the set of structures is not sufficient to explain the entropic components of the binding energies.

Dave Teller, Dale Tronrud and Dick Brennan enjoy the California sun during a coffee break

In keeping with the overall emphasis on techniques and methods at this year's workshop, the evening session consisted largely of presentations utilizing non-crystallographic information. Jeffrey Chao (Scripps Research Institute) presented the results of a joint NMR and x-ray crystallographic refinement of L30, a yeast ribosomal protein, and Lisa Craig (Scripps Research Institute) talked about her work on pilin using x-ray crystallographic and cryo-electron microscopic approaches. The use of atomic force microscopy in virus studies was covered by Alex McPherson (UC-Irvine), and Byron DeLaBarre (Stanford) showed how much structural information can be extracted from a low resolution (4.7 Å) study of valosin containing protein. The final talk in the session, by Seth Harris (UCSF), covered a mix of low- and moderate-resolution studies of Hsp90 heat shock proteins.

The final session on Wednesday contained a mix of talks on new structures and structure/function studies. Doug Davies (U. Washington) started the session with a talk on tyrosyl-DNA phosphodiesterase where he described several structures of the enzyme and various complexes (including those with vanadate and tungstate) that provide strong hints about the enzymatic mechanism. Jason Greenwald (Salk Institute) presented his work on bone morphogenetic proteins including the structures of BMP7 with its antagonist (Noggin) as well as a domain from its receptor (ActRII). Matthew Franklin (Genentech) then talked about the structure of human growth factor receptor with a neutralizing antibody that binds to part of the putative dimerization surface of the receptor. Dirk Zajonc (Scripps Research Institute) reported on the structure of one member of the CD1 family (CD1a) complexed with a sulfatide. CD1 molecules are cell surface receptors that present lipid and glycolipid antigens to T cell receptors.

The next talk by Andreas Förster (U. Utah) covered structural analyses of proteasome components and complexes that suggest what conformational changes are associated with proteasome activation. Jennifer Elam (U. Texas Health Science Center - San Antonio) showed the structure of metal-deficient mutants of superoxide dismutase and suggested how changes in the metal-binding loops might permit oligomerization of the protein. Accumulation of insoluble complexes of SOD is associated with familial amyotrophic lateral sclerosis. Walter Voegtli (UC-Davis) then presented a 2.3 Å resolution structure of actin interacting protein 1 showing that it consists of two seven-bladed beta-propellers in a clam-shell shaped structure. A model of the complex with actin filaments bound to actin depolymerization factor/cofilin complexes was also included. In the final talk, Chris Thanos (Sunesis Pharmaceuticals) discussed the binding of small molecule ligands to a "hot spot" on IL-2 where it interferes with the binding interface for the IL-2 receptor.

As in the past, many poster presentations were also given at the workshop. This year, corporate donations allowed the presentation of several poster prizes. Winners of these prizes (and their posters) were: Kinkead Reiling (UCSF) - Anisotropic Displacement Parameter-Based Clustering: Thermodynamic Binding Modes of HIV Protease Examined in a 1.09 Å Structure; Robyn Stanfield (Scripps Research Institute) - Using Epitaxially Twinned Data to Determine the Structure of the HIV-1 Neutralizing Antibody 447-52D; Cynthia Fuhrmann (UCSF) - Sub-angstrom Resolution Crystal Structures of Alpha-lytic Protease Reveal Novel Experimental Insight into the Mechanisms of Protein Stability and Proteolytic Catalysis, Kate Kavanagh (UC-Davis) - Mechanistic Insights from Substrate-bound Structures of *Pseudomonas fluorescens* Mannitol 2-Dehydrogenase, and Rebecca Page (Scripps Research Institute) - Shotgun Crystallization Strategy for Structural Genomics: Crystallization of the *Thermotoga maritima Proteome*.

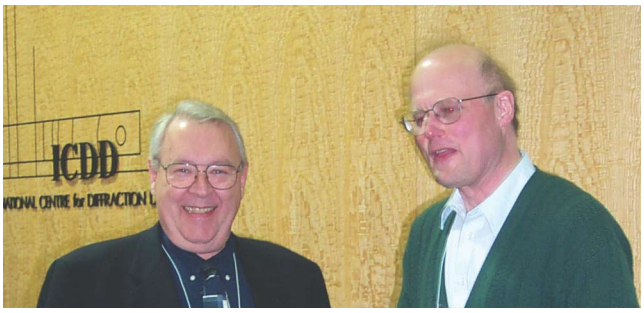
Ron Stenkamp

RIGAKU / OSMIC

ICDD's Annual Spring Meeting - March 17-21, 2003, Newton Square, PA

During the week of March 17-21, 2003, the International Centre for Diffraction Data (ICDD) welcomed its members and guests to the headquarters office in Newtown Square, Pennsylvania for its Annual Spring Meeting. For the first time in the ICDD's history, a new meeting format was introduced to maximize member interactions. A plenary session, a poster session, and a tour of historical Philadelphia were added to the typical schedule of committee, subcommittee, task group, and Board of Directors meeting.

A major announcement, delivered by Cam Hubbard, ICDD's Chairman, launched the meeting. In pursuing ICDD's long-term goal of supporting total pattern analysis, Cam announced a new collaborative agreement that was recently negotiated with Material Phases Data Systems (MPDS), distributors of the Linus Pauling File (LPF). This agreement will result in the incorporation of inorganic structural data (S-entry) from the LPF into the PDF-4 relational database, including atomic coordinates, crystallographic, and bibliographic data. Including this select LPF data will add new materials to the PDF database as well as provide complimentary atomic, crystallographic and bibliographic data to existing material sets. With integrated software, PDF-4 database users will be able to identify unknown materials and then quantify the components by either the Reference Intensity Ratio (RIR) method or Rietveld methods. The first collaboration product, scheduled to be released in 2005, will include the first 100,000 atomic coordinate data sets, visualization software, and enhanced digital pattern calculation in the PDF-4 database.



Peer interactions & networking… benefits of attending ICDD meetings! Left to right: John Faber and Jim Kaduk

The Plenary Session, Advances in Automated Phase Identification, was chaired by Tim Fawcett, ICDD's Executive Director. Leading experts in phase identification analysis discussed new technologies incorporated into today's integrated data analysis systems, and their expectations for the future. The plenary speakers, along with the titles of their presentations, included:

§ **Next Generation Developments in PDF-4 Design: Search, Search-Indexing and Data-Mining**
John Faber, ICDD, Newtown Square, PA

§ **Phase Identification at the Push of a Button: A Dream Come True?**
Martijn Fransen, PANalytical, The Netherlands

§ **Phase Identification Using Electron Backscatter Diffraction and Crystallographic Databases**
Joseph Michael, Sandia National Laboratories, Albuquerque, NM

§ **DIFFRACplus Search/Match**
Julien Nusinovici, Socabim, Paris, France

§ **Phase Identification Using Electron Back Scattering Patterns**
David Dingley, TSL-EDAX, United Kingdom

ICDD members and their spouses, families and guests stepped back in time to retrace the steps of one of the great scientists of all time, Benjamin Franklin, during a three-hour walking tour of historic Philadelphia. Participants experienced the life and times of Ben as they walked the same streets where Ben once walked. A guest appearance by Dr. Franklin culminated their journey through time.

A meet & greet by Ben Franklin was a highlight of ICDD's tour of historical Philadelphia. Left to right: Tim Fawcett, Ben Franklin, Cam Hubbard

Following the tour, a technical poster session, presenting a forum for members to discuss various interest areas and recent developments in x-ray diffraction, was held. The ICDD sponsored a mixer along with the poster session at the host hotel. Attendees enjoyed the fine food as well as the opportunity to network with peers. Watch for the publication of the poster abstracts in the June issue of *Powder Diffraction*.

The Technical Committee meeting, held later in the week, served as a summary of all subcommittee activities and included reports by ICDD's Regional Co-chairs in attendance: Nubuo Ishizawa, East Pacific Rim; David Taylor, United Kingdom; James A. Kaduk, North America; Evgeny Antipov, Newly Independent States; and Brian H. O'Connor, Indian Ocean Rim. The Technical Committee concluded with a presentation on "Transition Metal Oxides: Characterization and Energy Storage," given by Dr. W. Stanley Whittingham of the State University of New York at Binghamton, NY.

Interested in learning more about the ICDD? Please visit our website at www.icdd.com Better yet, plan to attend our meetings next year! The date of the 2004 Annual Spring Meeting will be March 22-26. Hope to see you there

Terry Maguire

Awards Announced at the ICDD Meetings

Distinguished Fellow Award: Frank McClune was named an ICDD Distinguished Fellow at the Annual Meeting of the ICDD Members held in March. Frank was honored for the continuous development and improvement of the Powder Diffraction File™ during his 34 years of meritorious service at the ICDD.Frank serverd as Managing Editor, Editorial and Production Manager, and for the last 19 years, as Editor-in-Chief.

Cam Hubbard presents an award to Frank McClune, recognizing his contributions and those of the entire ICDD staff, to the PDF

Frank nurtured the transition of the PDF® from cards and books into the PDF-4 family of relational database products available on CD-ROM and DVD. The PDF has grown tremendously in size and technical capability due to Frank's coordination with editorial task teams, cooperating database organizations, and the development of an extensive and rigorous editorial process. Frank will be formally honored during the Plenary Session of the 2003 Denver X-ray Conference.

ICDD members play an essential role in the development of the ICDD and its database products to meet the needs of the global scientific community. During the recent ICDD Meetings, several editors and consulting editors were recognized for their valuable contributions to the new PDF-4 family of products. This included editorial task teams that reviewed data quality, classification assignments, and criteria for Metals and Alloys, Zeolites, Ceramics, and Pharmaceuticals. The editorial results are incorporated into the product subfiles. The honorees are:Lawrence C. Andrews - Evgeny Antipov - Peter Bayliss - John Michael Bennett - Joel Bernstein - Lawrence R. Bernstein - Thomas N. Blanton - Jeffrey N. Dann - Albert Davydov - Catharine M. Foris - Richard F. Hamilton - Sergey Ivanov - Howard Jones - Shao-Fan Lin - Charlotte Lowe-Ma - William E. Mayo - Andrew M. McDonald - Howard F. McMurdie - Ronald C. Medrud - Scott Misture - Vladimir B. Nalbandya - Brian H. O'Connor - Susan Quick - David F. Rendle - Andrew C. Roberts - Albert Rohrman - Frank J. Rotella - Ann P. Sabina - Barry E. Scheetz - Deane K. Smith - Douglas L. Smith - Jan W. Visser - Peter L. Wallace - Winnie Wong-Ng - Peter Y. Zavalij.

Terry Maguire

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31st MidAtlantic Protein Crystallography Meeting – May 21-23, 2003, Durham, North Caolina

Duke University was the site of this year's conference, organized by Lorena Beese, Dan Gerwith and Jane Richardson. Over 190 participants attended, and were treated to an exciting mix of talks from faculty, postdocs, and students working on all aspects of biomolecular crystallography.

The opening session focused on the structural biology of cancer. Dan Leahy (Johns Hopkins) began the meeting with a presentation of several structures of HER family (epidermal growth factor) receptors. Like other receptor tyrosine kinases, HER proteins must dimerize in order to activate downstream signaling. The Leahy group's work reveals that the HER receptors accomplish this in a novel manner. Ligands bind to these receptors away from the dimer interface and cause a domain rearrangement "unsnapping" that exposes a previously occluded portion of the protein, which is necessary for protein-protein association.

John Sondek (UNC) followed with exciting new work from his group on guanine nucleotide exchange factors (GEFs) which activate the Rho family of signaling proteins. He showed a series of structures which, taken together, argue that the relative orientation of two conserved domains from these GEFs is relatively unconstrained. Additionally he presented compelling biochemical and structural evidence that one of these domains, the pleckstrin homology domain, plays an unanticipated role in Rho protein recognition, and by coupling this recognition to phospholipid binding could serve to target GEF activity specifically to membrane bound Rho targets.

Jim Hurley (NIDDK) rounded out the opening session with several informative structures of SET domain enzymes. These proteins irreversibly transfer methyl groups from S-adenosyl methionine donors to target proteins, and are best known for their role in chromatin remodeling and gene silencing. The Hurley lab used a structural genomics approach to identify a tractable SET domain protein from a large number of candidate organisms and constructs. The resulting crystal structure gives important insight into the high specificity of SET enzymes, and suggests a mechanism for controlling the number of modifications that a target lysine residue will undergo.

The Thursday morning sessions covered a wide range of topics that included exciting advances in the understanding of biological systems and significant sharing of "tricks of the trade" related to the technicalities of protein x-ray crystallography. The Love Auditorium in the LSRC building at Duke was nearly full, as the conference brought together prominent members of the protein crystallography community in the Mid Atlantic area of the US and a large number of students and postdocs. The session contained ten 15 minute talks, four of which were given by principle investigators. The other six speakers were graduate students or postdocs from various labs. The result was a well balanced mix of speakers from different stages in the academic ladder.

There were two talks dealing with the mechanism of biological function based on structural biology (multimeric organization of Hsp90 and the translocation of DNA duplex on DNA Polymerase I); a couple of structures that contained a previously unobserved fold (the *E. coli* outer membrane transporter BtuB and a hypothetical protein from *Haemophilus influenzae*); four talks focused on properties of protein binding sites (Nudix enzyme bound to CoA, Tcl1 oncoproteins and interactions with Akt, the binding of ubiquitin by Vps9p-CUE domain and structural determinants in binding promiscuity in the Pregnane X Receptor); and two new talks presenting crystal structures and comparing them to previously known members of a larger family.

Technically interesting observations included the use of post-crystallization soaking (PCS) of the Tcl1 oncoprotein crystals in high concentrations of sodium sulfate or in PEG solutions to substantially increase the diffraction quality of the crystals; the alanine dehydrogenase crystals lost a screw axis upon soaking in either samarium or iridium, going from the symmetry of space group $P2_12_12_1$ to that of $P2_12_12$, and the structure was solved using MAD data collected on the heavy atom derivatives; data for the apo Vps9p-CUE domain were initially collected to 2.3 Å resolution and improved to 1.7 Å resolution using a mutant where a methylated Lys was changed to Ala.

The afternoon session included five talks covering a wide range of fascinating new results. Hengming Ke (UNC), led off with a description of DJ1, a protein with a wide range of interesting associations. Originally isolated as a circulating antigen marking certain breast cancers, it has since been implicated as a regulatory

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subunit of an RNA binding protein. One mutation, L166P is associated with Parkinson's disease, and it appears to interact with several proteins that ultimately influence the activity of the androgen receptor. The structure itself is an alpha-beta-alpha sandwich, with close structural homologies to bacterial HSP31 and to a cysteine protease. It has two members of the Asp-His-Cys catalytic triad and is therefore unlikely to be a protease. The L166P mutation would likely disrupt a crystallographic dimer interface, which may account for its role in Parkinson's disease. Robert Rose (NCSU) presented structural data for a series of mutations, called MODY mutations, that lead to familial type II diabetes in a small percentage of patients. MODY mutations affect a protein called HNF-1, a regulator of transcriptional activation. Again, several of the mutants affect a subunit interface, which in this case also implicates a heterologous interaction with a second protein, DcoH, which is at the same time an enzyme and a transcriptional co-activator. This interesting story is enriched by the fact that there are two forms of the DcoH, which have different in vitro assembly properties with HNF-1. Intersubunit interactions apparently regulate the formation of the active coactivator via a metastable heterodimerization interface. Changsoo Chang, (NCI) then described the structure of interleukin 19, a novel 5-helix bundle cytokine related to IL10. Unlike IL10, however, IL19 apparently does not form the domain-swapped dimer, and therefore may not lead to homodimerization of its receptor. Mathew Miller (NIEHS) then presented the structural enzymology of β-lactam biosynthesis, including the structure of β-lactam synthetase and four complexes with inhibitors, intermediates and products. Among the surprises was that the manipulation of the pyrophosphate leaving group involved coordination of two Mg^{++} ions, not one as expected, and that the enzyme apparently retains the pyrophosphate throughout the catalytic cycle.

The final talk was yet another a wondrous tour de force from Zbigniew Dauter (NIH, BNL). He began by outlining the history of the various attempts to understand and control radiation damage. He then presented a careful description of the course of collecting twenty successive datasets from one cryoprotected thaumatin crystal, showing that there were systematic, monotonic amplitude changes that could not be attributed to unit cell changes. When imaged, these amplitude differences turned out to be the result of strikingly discreet changes – notably rupture of disulfide bridges, but also the loss of carboxyl groups and the consequent rearrangement of bound water sites. He concluded by showing that the rupture of the five disulfide bridges could be identified from the amplitude differences between early and late datasets, refined, and used to produce a remarkably clean electron density map! His moral: either don't overexpose or, if you do overexpose crystals, make use of the changes!

Workshop: Structural Genomics for the Rest of Us: The advancement and automation of single crystal X-ray diffraction is changing the way crystallographic experiments are conducted. A current focus of discussion among crystallographers is the impact of structural genomics on the development of high throughput, cost effective, and low-error methods for crystal structure determination.

Bob Petrovich (NIEHS) led the discussion of high-throughput bacterial expression using multiple expression systems (ECHO™ and Gateway™), tags (GST, His tag, and thioredoxin), and orthologs (*A. thaliana, A. gossypii, D. melanogaster, and C. elegans*). He pointed out that the Gateway™ system was less vector dependent and required fewer clones to get the same number of expressed proteins, that the solubility of expressed proteins was system independent but tag dependent, and that the ratio of soluble vs. insoluble expression was in the order of GST > His tag > thioredoxin. He also discussed several purification protocols in detail. Other expression systems to be considered include yeast, baculovirus, and insect cells. However, when nothing else works, one may have to turn to a mammalian expression system; Dan Leahy (Johns Hopkins) discussed mammalian expression reagents, amplification techniques, vectors, cell lines, transfection methods, equipment, and time scale. He emphasized that one needed to consider the factor of glycosylation at the very beginning of the experiment by mutating N-linked sites, using glycosylation-deficient cell lines, or enzymatic removal. He also shared with the audience his current favorite and successful methods in mammalian expression. For "the rest of us" who

are conducting interest/target-driven research, these expression systems should be able to produce pure protein of interest. The amount of protein, however, may be very small.

To screen large numbers of crystallization conditions with a small amount of protein, a robot has obvious advantages. Recent advancement of crystallization robots has brought about the Topas™ Crystallizer by Fluidigm Corp. Mike Lucero of the company discussed the theory and application of the crystallizer, which uses a system of pressure-driven flow valves manufactured in special elastomer on a small chip. The ability to screen 6,000 conditions with ~150 µl of protein in ~1 week sounds excellent, but currently each chip costs $600! Researchers will certainly be more interested in Topas™ if it becomes more cost effective. Aiming to be both high throughput and cost effective, direct crystallography, introduced in 2000 by Bi-Cheng Wang (UGA) uses native crystals and single wavelength x-rays and therefore eliminates some time-consuming and expensive intermediate steps such as heavy atom derivatization and SeMet labeling. He discussed the problems and proposed solutions toward a routine strategy of sulfur direct crystallography, and initiated the discussion of improving the signal/noise ratio by using chromium radiation. Joe Ferrara (Rigaku/MSC Inc.) presented the progress they have made, in collaboration with BC Wang, in the development of both hardware and phasing procedures for sulfur direct crystallography using chromium radiation with both in-house x-ray and synchrotron facilities.

Last but not least, Dave Richardson (Duke) addressed the validation and improvement of crystal structures by the use of all-atom contact analysis in a system of Process Quality Management, with which the errors in crystal structures are not only detected but also fixed at the lowest stage possible! Then the audience enjoyed a tour of their newly developed online service MolProbity, guided by its developer Ian Davis, a graduate student in the Richardsons' lab. Local chemistry and physics play critical roles in error detection and correction, which should not be too surprising. While pursing "real" structures, people should not forget that the three-dimensional structures of protein α-helix and double-stranded DNA were both correctly modeled first! It should not be too surprising, either, that the overall statistics (R and R_{free}) of a crystal structure are improved when the local errors are fixed.

Paul Sigler Prize: Sompop Bencharit from Matt Redinbo's laboratory at UNC was awarded the Sigler Prize for the best student poster entitled "Structural Basis of Heroin and Cocaine Metabolism by Human Carboxylesterase I".

Even the nearly constant rain, which wiped out the baseball game, could not dampen the participant's enjoyment of this very well organized conference. We all look forward to next year's meeting that will be held at Johns Hopkins University.

Charlie Carter, Xianjui Ji, Carla Mattos and Josh Warren

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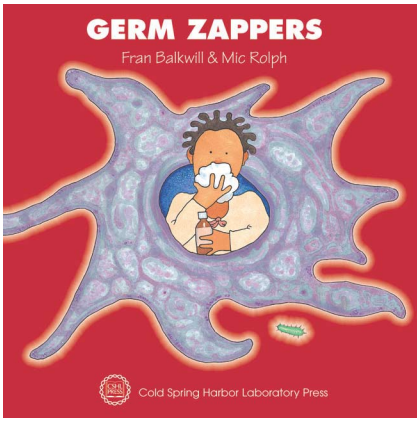
Enjoy Your Cells, Have a Nice DNA, Gene Machines, and Germ Zappers All four by Fran Balkwill and Mic Rolph, published by Cold Spring Harbor Laboratory Press (2002), paperback and hardcover. These four books are aimed at a youthful audience of around 9-12 years of age. The topics covered include different types of cells and the structure of DNA. DNA is a recurring topic, of course. The first three books are somewhat similar in fact because DNA figures prominently in each of them. Each book, however, examines a different aspect of DNA including its role in protein synthesis, cell division, reproduction, and growth and development of organisms. Germ Zappers is significantly different, covering the subject of the immune system.



The science content of the books comes from Fran Balkwill, Professor of Cancer Biology at Barts and the London Queen Mary's School of Medicine and Dentistry. Illustrations are the work of Mic Rolph, a graphic designer and illustrator. The books are designed to hold a pre-adolescent's attention while providing some pretty amazingly detailed science. Who knew that dendritic cells alerted the mighty lymphocyte squads? Or that the "Natural Killer" cells were a little like Dirty Harry ("make my day"considering their gratuitous ventilation of infected cells)? Mic Rolph's illustrations show his skill in drawing everything from menacing bacteria to babies, young people, dinosaurs, and the comparative insides of mice and humans.

This reviewer enjoyed the task of reading these books and recommends them highly to anyone who knows of a receptive reader, whatever the age. *Reviewed by Paul Anderson*

International Tables for Crystallography, Volume D, Physical Properties of Crystals, edited by André Authier. Kluwer Academic Publishers, Dordrecht, Co-publication with International Union of Crystallography, Hardbound, ISBN 1-4020-0714-0, July 2003. This volume of the International Tables is concerned with the influence of symmetry on the physical and tensor properties of crystals and on their structural phase transitions. This role is very important in many different disciplines of the science of materials such as crystallography, elasticity, solid-state physics, magnetism, optics, ferroelectricity and mineralogy. Part 1 introduces the mathematical properties of tensors and of group representations and gives their independent components for each of the crystallographic groups. The software included in the accompanying CD ROM enables the irreducible representations of finite point groups in three dimensions (the 32 crystallographic groups and the groups of the quasicrystalline phases) and the independent components of a tensor of any rank for each of these groups to be determined. Part 2 is devoted to the symmetry aspects of excitations in reciprocal space: phonons, electrons, Raman scattering and Brillouin scattering. Part 3 deals with the symmetry aspects of structural phase transitions and of twinning. A prominent feature is the joint description of twinning and domain structures, which are usually presented in completely separate ways in handbooks of physics and mineralogy. The theory of structural phase transitions relates the symmetry characteristics of the transitions to their physical ones. The application of the symmetry principles that derive from this theory is illustrated by the tables on the CD ROM. The CD ROM also contains tables of tensor properties at any group-subgroup phase transition. *From the publishers web-site*

Particle Scattering, X-Ray Diffraction, and Microstructure of Solids and Liquids, Manfred L. Ristig, Springer (2003) 196 pages hardcover, ISBN: 3-540-44386-X. Interesting and new specific results of current theoretical and experimental work in various fields at the frontier of particle scattering and x-ray diffraction are reviewed in this volume. Special emphasis is placed on the study of the microstructure of solids, crystals and liquids, both classically and quantum mechanically. This gives the reader essential insights into the dynamics and properties of these states of matter. The authors address students interested in the physics of quantum solids, crystallography and material science as well as physical chemistry and computational physics. *From the publishers web-site*.

Fundamentals of Powder Diffraction and Structural Characterization of Materials, Vitalij Pecharsky and Peter Zavalij, Kluwer Academic Publishers, Boston, Hardbound, ISBN 1-4020-7365-8, May 2003, 744 pp. Fundamentals of Powder Diffraction and Structural Characterization of Materials provides an in-depth introduction to the theories and applications of the powder diffraction method for structure determination. The emphasis is placed on powder diffraction data collected using conventional x-ray sources, which remain primary tools for thousands of researchers and students in their daily experimental work. The book is divided into two parts: chapters one though three give essential theoretical background, while chapters four through seven guide the reader through practical aspects of extracting structural information from powder data. The book is supplemented by a compact disk containing experimental data collected from a variety of materials that are used as examples and in the problems offered at the end of every chapter. In addition color electronic versions of some 300 illustrations found throughout the book will be included. The book is designed for both the undergraduate and graduate students from materials science, solid-state chemistry, physics, geology, and literally any other science or engineering background, who demand structural information at atomic resolution. Key features: The book requires no prior knowledge of the subject, but is comprehensive and detailed, making it useful for both the novice and experienced user of the powder diffraction method. The book is useful for any scientific or engineering background, where precise structural information is required. The book comprehensively describes the state-of-the-art in structure determination from powder diffraction data both theoretically and practically using multiple examples of varying complexity. Particular attention is paid to

the utilization of Internet resources, especially the well-tested and freely available computer codes designed for processing of powder diffraction data. Comprehensive collection of the experimental data considered throughout the book is included on the compact disk. Electronic illustrations, included on the compact disk, may be easily used by instructors teaching the subject. *From the publishers web-site*.

Structural Bioinformatics, Philip E. Bourne and Helge Weissig, eds, John Wiley & Sons, ISBN: 0 471-20199-5, Paperback, 672 pages, February 2003. From the foreward: A must read for all of us committed to understanding the interplay of structure and function...[T]he individual chapters outline the suite of major basic life science questions such as the status of efforts to predict protein structure and how proteins carry out cellular functions, and also the applied life science questions such as how structural bioinformatics can improve health care through accelerating drug discovery." This book provides a basic understanding of the theories, associated algorithms, resources, and tools used in structural bioinformatics. The reader emerges with the ability to make effective use of protein, DNA, RNA, carbohydrate, and complex structures to better understand biological function. Moreover, it draws a clear connection between structural studies and the rational design of new therapies. *From the publishers web-site*.

Unusual Structures and Physical Properties in Organometallic Chemistry, Marcel Gielen, Bernd Wrackmeyer, and Rudolph Willem, eds., John Wiley & Sons, ISBN: 0 471-149635-9, 446 pages, June 2002 The principal idea of this volume is to offer a *Capita Selecta* of unconventional and thought-provoking topics in organometallic chemistry, presented by experts in each field. As intended, this approach leads either to reviews covering a specific uncommon class of organometallic compounds or to overviews which relate uncommon physical properties with various classes of organometallic compounds. The contributions are streamlined thus onto two main axes - unusual properties reflecting structures and bonding situations, on the one hand, and uncommon structural features or structure-reactivity relationships, on the other. Extensive cross-referencing of useful information is provided, making this volume accessible for people working in rather different areas of organometallic chemistry. *From the publishers web-site*.

Chemical Bond in Inorganic Chemistry, *I. David Brown, Oxford University Presss, ISBN: 0198508700, 288 pages, February, 2002*. The valence bond model is a description of acid-base bonding useful in fields such as materials science and mineralogy. This book outlines the theoretical basis of the model and shows how it can be applied to synthetic and solution chemistry. It emphasizes the separate roles of the constraints of chemistry and of three-dimensional space by analyzing the chemistry of solids. Many applications of the model in physics, materials science, chemistry, mineralogy, soil science, surface science, and molecular biology are reviewed. A final chapter explains how the bond valence model relates to and represents a simplification of other models of inorganic chemical bonding. *Book News, Inc., Portland, OR (booknews.com)*

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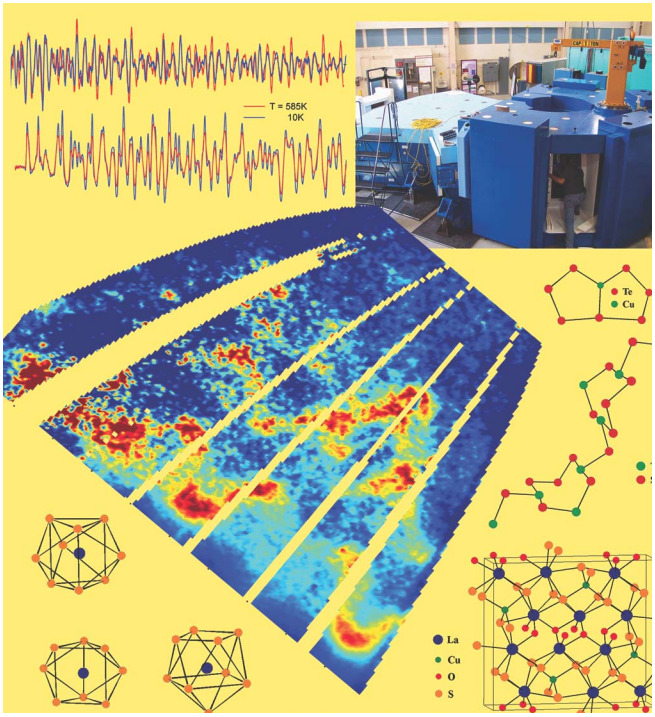
What's on the Cover



The images on the cover of this issue of the *ACA Newsletter* were provided by our 2003 award winners Takeshi Egami (Warren Award) and Jim Ibers (Buerger Award). They images were arranged by Connie Chidester.

Egami contributions: The photo in the upper right is a picture of the NPDF (Neutron Powder DiFfractometer), a pulsed neutron spectrometer at the Manuel Lujan, Jr. Neutron Scattering Center of the Los Alamos National Laboratory. It has recently been upgraded with new neutron detectors and is producing remarkable results. The person seen installing the neutron detectors is Dr. Thomas Proffen, the beam line scientist and project manager of the upgrade. Funding for the upgrade came from the National Science Foundation, Department of Energy, and five participating universities (University of Pennsylvania, University of California, Santa Barbara, University of Virginia, Michigan State University and State University of New York, Stony Brook). Since the upgrade, the data collection rate has been increased by a factor of five. This machine has the highest Q resolution among all the neutron powder diffractometer ($\Delta Q/Q = 0.0015$), and allows for high-resolution powder diffraction with Rietveld refinement, as well as the high-resolution atomic pair-density function (PDF) analysis.

The name (NPDF) has a double meaning of (Neutron-PDF machine). A PDF describes the distribution of distances between atoms in a sample, and is obtained by Fourier transformation of the diffraction data. Takeshi Egami feels that his selection for the Warren Award is largely based upon this use of the PDF technique on crystals with atomic or nano-scale complexity. The PDF technique has been widely used for the analysis of liquids and glasses, but he pioneered its use on crystals. In order to use the technique successfully on crystals the use of synchrotron based modern radiation sources, such as pulsed neutron sources and other synchrotron radiation sources, is critical. He has taken advantage of recent progress in these sources to apply the PDF method widely on various critical materials.

Two examples of the high-resolution PDF obtained by the NPDF are shown in the upper left corner of the cover. The sample is $LiNiO_2$ powder. The PDF underneath, range 1-50 Å, shows that at low temperature (10 K) the PDF has larger amplitudes than at 585 K. The top PDF shows the same data, over the range 100-200 Å. Only with the upgraded NPDF did it become possible to obtain the PDF over such a wide range of distances.

The interesting graphic in the center of the cover is a plot of the inelastic neutron scattering intensity against energy and momentum for a single crystal of the high temperature superconductor, $YBa_2Cu_3O_{6.95}$, at T = 110 K, obtained with the MAPS spectrometer at the ISIS of the Rutherford-Appleton Laboratory in the UK. This result was used to determine the phonon dispersion in this system (J.-H. Chung, et al., *Phys. Rev.*, B 67, 014517 (2003)), which suggested the possible role of phonons in the mechanism of high-temperature superconductivity.

Ibers contributions: The three molecules in the lower left corner illustrate various environments of Sm_5 Te_9: Tricapped trigonal prism (top), bicapped (lower left) and monocapped square prism (lower right). On the right side of the cover the top molecule is the anion $[Cu\ Te_7]^{-3}$. The middle molecule on the right shows a piece of the infinite chain found in $[Te_3Se_6]^{-2}$, and the bottom figure shows a unit cell for $La_3CuO_2S_3$.

ROBO DESIGN

JULY 2003

3-13 **ACA Summer Course in Macromolecular Crystallography,** Illinois Inst. of Technology, Chicago, IL. Contact Andrew Howard, **howard@iit.edu**

20-24 **The International Congress of Biochemistry and Molecular Biology**, Toronto, Ontario, Canada, **www.iubmb2003.org**

26-31 **American Crystallographic Association Annual Meeting, ACA 2003,** Covington, KY, Local Chair: Bobby Barnett. **barnettbl@cinci.rr.com**. Program Chair, Jeanetta Krause Bauer, **jeanette.krause@uc.edu.**

AUGUST 2003

3-13 **ACA Summer Course in Small Molecule Crystallography,** Indiana University of Pennsylvania, **Bryan Craven, craven@icubed.com; Charles Lake, lake@grove.iup.edu.**

4-8 **Denver X-ray Conference,** (sponsored by the ICDD), Denver marriott Tech Center Hotel, Denver, Co. **www.dxcidd.com**

10-13 **AsCA'03/Crystal-23,** Cable Beach Club resort, Broome, Western Australia. **http://www.broome2003.uwa.edu.au/**

14-15 **Biological Structure Workshop,** Cable Beach Club resort, Broome, Western Australia. (website above)

14-19 **Sagamore Meeting** (IUCr Commission on Charge, Spin and Momentum Densities), Cable Beach Club resort, Broome,Western Australia. (see website above).

24-30 **21st European Crystallographic Meeting,** Durban, South Africa , **http://www.ecm21-africa.co.za/**

SEPTEMBER 2003

1-4 **XIX Conference on Applied Crystallography**, Krakow, Poland. **crystalloraphy.us.edu.pl**

4-7 **Summer School on Polycrystalline Sturture Determination by Direct Methods,** Krakow, Poland. **crystallography.us.edu.pl**

2-6 **ECNS 2003 European Conference on Neutron Scattering,** Montpellier, France. Contact: R. Vacher, **rene@ldv.univ-montp2.fr**

3-7 **5th International Conference On Molecular Structural Biology (ICMSB2003),** Vienna, Austria. Conference Secretariat: Dr. Andreas Kungl, Austrian Chemical Society (GÖCH), **andreas.kungl@kfunigraz.ac.at**

8-13 **Aperiodic-2003**, Belo Horizonte, Brazil. Conference intends to promote the development of comon methods and nomenclature for the crystallographic investigation of aperiodic systems, including modulated structures, polytypes, incommensurate misfit or composite crystals and quasi crystals. **agora.grude.ufmg.br/aperiodic2003**

14-19 **Structure Solution from Powder Diffraction Data, SSPD'03;** Congress Center Academia, Stara Lesna, Slovakia. **http://www.sspd-03.sav.sk**

OCTOBER -NOVEMBER 2003

6-10 **Introduction & Advanced X-Ray Diffraction For Pharmaceutical Applications,** Danbury, CT

30-1 **Pittsburgh Diffraction Conference,** Rutgers University Inn, New Brunswick, NJ (see more info on page 6).

MARCH 2004

22-26 **ICCD Annual Spring Meeting**, Newton Square, PA

JUNE 2004

9-21 **Polymorphism: Solvates and Phase Relationships. and Electron Crystallography: Novel Approaches to Sturcture Determination of Nanosized Materials.** Erice, Italy. **www.crystalerice.org**

JULY 2004

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

MAY - JUNE 2005

28-2 **American Crystallographic Association Annual Meeting, ACA 2005,** WALT DISNEY WORLD SWAN Hotel, Orlando, Fl.

AUGUST 2005

17-22 **XX IUCR Congress,** Florence, Italy. Local Chair: Paola Paoli, **iucr@iucr2005.it,** Program Chair, Carlo Mealli. www.iucr2005.it

POSITIONS AVAILABLE

It is expected that the employers listed in this publication are equal opportunity employers who wish to receive applications from qualified persons regardless of age, national origin, race, religion, sex or physical handicaps. Please inform the Editor when the positions are filled, and of any positions that do not give opportunities to all applicants. Ads will appear in two successive newsletters unless the Editor is notified that the advertisement should be continued longer or discontinued earlier.

For the most up-to-date listings check the ACA Home Page under the Positions Vacant heading: **www.hwi.buffalo.edu/ACA/**

Previously advertised: Macromolecular postdoctoral

SUNY at Buffalo / Hauptman Woodward Medical Research Inst. Position available for macromolecular crystallographer. Must have experience in protein expression and purification; experience with construction of mutants is desirable; to work in Program in Proteomic and Genomic analysis of the short chain oxido reductase family of enzymes, especially members of the family linked to hypertension, cancer, Alzheimer's and polycystic kidney diseases. A new Ph.D.preferred with possibility of three years of support. The candidate would be encouraged to develop an independent project during the second and third year. Please send c.v. and three letters of reference to: Dr. William L. Duax, Dept. of Structural Biology SUNY at Buffalo, Hauptman Woodward Medical Research Inst., 73 High St., Buffalo, NY 14203.

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