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NEWSLETTER

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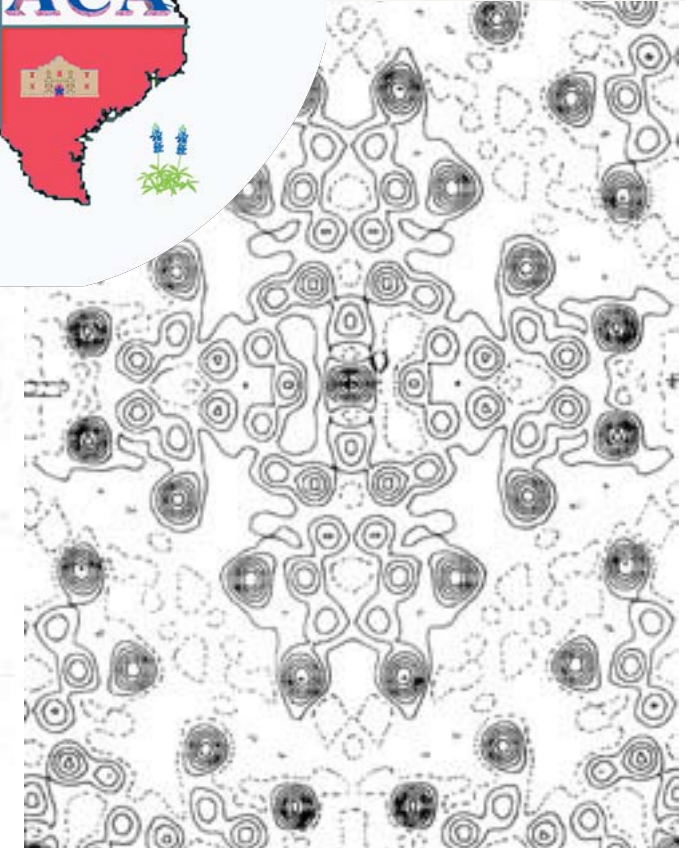
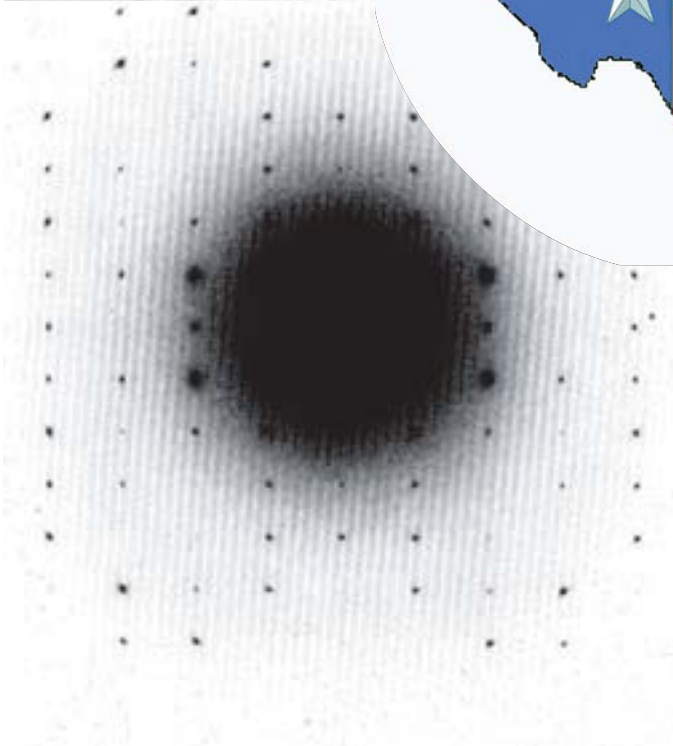


Table of Contents

President's Column 1-2
 Council News 2-3
 2002 Election Results 3-5
 Canadian Division News..... 6
 ACA Committee Reports 6
 2002 Patterson Award to Doug Dorset..... 7
 What's on the Cover 7
 News / Travel Awards Available 9-10
 2001 Fankuchen Award Address 11-17
 2001 Travel Awardees 19-21
 US National Committee for Crystallography 25-26
 September 11th Scholarship Fund 27
 ACA Corporate Members 28-30
 Protein Data Bank (PDB) Update 31
 Cambridge Data Bank (CCDC) Update..... 31-32
 2001 MacCHESS Users Meeting..... 34-35
 12th Annual Southwest Macromolecular Symposium..... 35
 59th Pittsburgh Diffraction Conference 37
 New OSTP Director 39
 Letters from Friends..... 39
 Contributors to ACA Funds 41-42
 Contributors to This Issue 42
 Meetings and Schools Calendar..... 43
 Positions Available..... 43-44
 Journals Available for Free 44

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

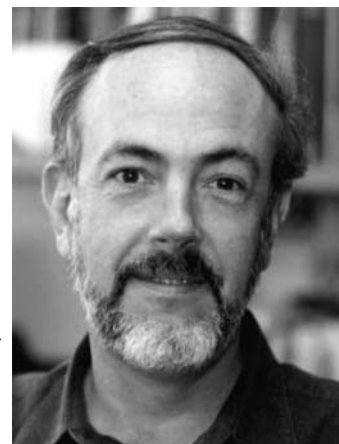
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Presidents Column

The September 11 tragedies at the World Trade Center and the Pentagon remind us once again how much we should value our security and freedom. In part, terrorism and hatred are fostered by isolation and intolerance. I was struck by a news report that well after the attacks and the subsequent launch of the US-led war on terrorism, perhaps not more than 5% of the Afghanistan population was aware of the 9/11 events. Crystallography is a universal science that unites many disciplines and like most other sciences, crystallography is represented in countries around the world. As scientists, we should be proud that interactions in our laboratories, international collaborations and scientific meetings often lead to friendships with individuals from other cultures which easily break down barriers and demonstrate the absurdity of radical intolerance and fanaticism. What can we do? Today, perhaps there is no better way to bring individuals together than through the common ground of scientific and technical interchange. Please go out of your way, either directly, or indirectly through continued casual interactions, to demonstrate trust, friendship and good will to all of your colleagues – both local and global - from different cultures. Tomorrow, after the current crisis has been resolved, perhaps governments around world, in seeking enduring peace and freedom, will look for completely new opportunities to break the cultural barriers that stand in the way of cooperation and mutual understanding. If that is the case, then those who lost their lives in September may not have died in vain.



ACA Council met this fall, at the Cincinnati/Northern Kentucky site of our meeting in 2003. We had an engaging tour of the city, met with the management of the spacious convention center where our sessions and vendor displays will be held, enjoyed breakfast and lunch in a fine setting which overlooked the city on the Ohio River, and had good discussions with our program and local chairs, Bobby Barnett and Jeanette Krause Bauer. At dinner, we toasted Louis Delbaere and Connie Chidester for their excellent contributions as members of ACA Council - Louis' term as Canadian Representative will end this year and as this year's Past President, Connie's term will end as well. We'll miss both of them.

The ACA thrives through the volunteer efforts of its membership. Certainly, one of the most demanding responsibilities that a member can take on is the editorship of the ACA Newsletter. Ron Stenkamp, who for sometime has shared this responsibility with Judith Flippen-Anderson, is now stepping down as co-editor and ACA Council wishes to express their profound gratitude to Ron for the 6 years of service and



**ACA Council Meeting,
October 2001:
Front row: Marcia Evans,
N. Rao, and Charlie Carter
Back row: Doug
Ohlendorf, Connie
Chidester, Bill Stallings,
Lee Brammer and Louis
Delbaere**

dedication that he has offered our organization in this capacity. Editorship of the Newsletter requires persistence, good taste and a lot of hard work. The quality of the Newsletter has remained high and subscription to the Newsletter clearly represents a significant benefit of ACA membership. Ron, thanks again for all your good work and support! Judy, you also deserve our continuing gratitude for your efforts and dedication! And, who will replace Ron? None other than Connie Chidester who previously served as our Newsletter Editor from 1991 to 1993. Connie, welcome back!

Finally, I am *very* happy to tell you that we have at last delivered on a key obligation that was my responsibility to fulfill during my year as VP: that wonderful town Chicago has been selected as the site of the ACA meeting in 2004 and Council is most pleased to announce that Bernie Santarsiero and Karl Volz, both from the University of Illinois at Chicago, will be our local co-chairs and that the program co-chairs will be Christer Aakeroy from Kansas State University and Marilyn Yoder from the University of Missouri, Columbia. Over the last two years, our meeting committee also visited Toronto and Salt Lake City and while a fit at these sites for 2004 was not possible, they remain on the list as good possibilities for future meetings. Special thanks to everyone who was involved in these activities.

As we move into a new year and I end my term as ACA President, I want to thank each and every one of you who contributed to the success of the ACA in 2001. The results from this year's election are in. I want to be first to welcome our new members to Council – David Rose will be joining us as the new Canadian Representative and Ray Davis as our new VP. I'm looking forward to 2002 and I know our new President Charlie Carter is looking forward to it as well.

See you in San Antonio,
Council News

The ACA Council typically holds day-long meetings three times a year, in Spring and Fall and just prior to the annual ACA meeting. Other Council business is conducted through discussion by email. A report on the Spring 2001 Council

meeting can be found in the summer *Newsletter*. The Council held its Summer 2001 meeting on July 20th, in Los Angeles directly prior to the ACA annual meeting. The ACA meeting also affords the opportunity for the Council to meet with all the ACA committees and with SIG officers. These meetings take place over breakfast and lunch on most days during the annual ACA meeting, as they did in LA.

Topics discussed at the main Council meeting included site selection and planning for the 2004 and 2005 meetings as well as preliminary discussions of potential sites beyond 2005. With follow up discussions at the Fall 2001 Council Meeting, and site visits by the ACA Meetings Committee (Marcia Evans, S. N. Rao & Judy Flippen-Anderson), it is anticipated that the venue and meeting co-chairs for 2004 can soon be announced. Council members were also given a preview of the new ACA web site design, being developed by T. J. O'Donnell. You will now see the new design upon accessing the web site at www.hwi.buffalo.edu/ACA/. Efforts are also underway to permit financial transactions, e.g. membership renewal, to be conducted securely via the web. Your feedback on whether you like the new format and comments on what you would like to see on the web site are encouraged.

Meetings with ACA Committees focussed on their activities over the past year. Annual reports from these committees should be available on the ACA web site. Some committees are more active than others; in some cases there has been an absence of communications between committee members. The ACA Council thus concluded that it should take a more activist role in promoting action by the committees during the year. This is particularly important early in the year when new members are beginning their terms. Thus a conference call will be initiated by the ACA President with each standing committee early each year.

In addition to hearing about their ideas for the 2002 meeting program and any other issues of concern, the Council discussed with SIG officers an idea to introduce a new award for junior investigators. Further details will be released once this proposal has had a chance to be fully developed. There has been much discussion among ACA Council members about encouraging

the SIGs to become actively involved in more aspects of the ACA. This is one such initiative.

The week of the Los Angeles ACA meeting concluded with a successful program planning meeting held on the afternoon of Thursday July 26th. The meeting was chaired by Wally Cordes, program co-chair for 2002, and included representatives from all SIGs as well as ACA Council members. It was used to finalize the program for the 2002 Meeting in San Antonio and afforded an opportunity for instant feedback from SIG representatives that should avoid clashes between sessions that have unfortunately arisen in the past. This planning meeting is part of an overall meeting planning strategy put into place by the ACA Council to encourage greater advance planning of meetings, and hopefully to strengthen meetings thereby. The meetings thrive not only on participation by attendees, but also on the willingness for individuals to organize sessions and to inform the SIG officers of what they topics they would like to see covered at upcoming meetings. We hope many of you will consider providing such input or volunteering your time.

The Fall 2001 Council meeting was held in Covington, KY directly across the Ohio river from downtown Cincinnati. The Council met with 2003 local and program chairs, Bobby Barnett and Jeanette Krause Bauer and worked on meeting budgets and planning issues. There was also an opportunity to examine the excellent facilities provided by the new Covington Convention Center and to sample the atmosphere of what promises to be an attractive riverside venue for the 2003 meeting.

Continuation of previous discussions of the ACA awards resulted in an effort to overhaul the award guidelines and to standardize the format of the citations for these awards. This should be completed in time for a vote at the Spring Council meeting. The Council initiative to introduce symposia associated with the award presentations is expected to get off to an excellent start with a 2.5-day symposium on electron diffraction and microscopy to honor Doug Dorset who will receive the 2002 Patterson Award in San Antonio.

As part of an IUCr effort to reach out to regions that are underrepresented in international crystallography, the ACA will be making a major effort to forge links with crystallographers in Central and South America. As part of this effort, funds are being made available to support crystallographers from these regions who may wish to attend the 2002 ACA meeting in San Antonio.

In an effort to make somewhat easier one of the more difficult tasks of ACA *Transactions* organizers, namely ensuring that speakers submit manuscripts for the *Transactions* Volume in a timely manner, the ACA Council has asked the ACA Office to assist. Thus, the office will in future send out letters of intent to be signed by those invited to speak in the *Transactions* symposia indicating their commitment to provide a manuscript by the time of the meeting.

The next scheduled Council Meeting will be in San Antonio on Friday May 24th, 2002 directly prior to the 2002 ACA meeting.

Lee Brammer, Secretary

ACA 2002 Election Results

Vice-President:

Raymond E. Davis

Canadian Representative to Council

David Rose

STANDING COMMITTEES

Continuing Education Four Year Term:

Marilyn M. Olmstead

Data, Standards, and Computing Four Year Term:

Jeffrey R. Deschamps

Data, Standards, and Computing Three Year Term:

Helen M. Berman

Communications Four Year Term:

Kay D. Onan

SIGs

Biological Macromolecules

Chair-elect: Vivien Yee
Secretary: Alice Vrieling

Fiber Diffraction

Chair: Tom Irving
Secretary/Treasurer: Jennifer Taylor

General Interest

Chair-elect: Alan Pinkerton
Secretary: Vivian Cody

Materials Science

Chair-elect: Charlotte Lowe-Ma

Neutron Scattering

Chair-elect: Thomas Proffen
Secretary: James Richardson

Service Crystallography

Chair-elect: Richard J. Staples

Small Angle Scattering

Chair-elect: Jinkui Zhao
Secretary/Treasurer: Pete R. Jemian

Small Molecules

Chair-elect: Brian Patrick
Secretary/Treasurer: Joseph Reibenspies

Young Scientist

Chair-elect: Kent Brown

Ray Davis - Newly elected ACA Vice-President

A native Kansan, Ray received a B.S. with Honors in Chemistry from the U. of Kansas. His introduction to crystallography came with his Ph. D. work with Al Tulinsky at Yale. He then spent two years with David Harker in Buffalo at Roswell Park Memorial Institute. In 1966, he joined Stan Simonsen and the rest of the faculty in the chemistry department at the University of Texas at Austin.

I had known Ray and Stan through ACA meetings before joining the department, but have had the pleasure of working with Ray as a colleague since 1974. Ray's early research in small molecule crystallography was in the areas of aromaticity and organometallic structures, including his definitive structural evidence for bond localization in metal- π complexes. His more recent work has focused on packing arrangements and interactions in molecular crystals and on methods of crystal engineering, particularly those involving approximate symmetry. The structural and database aspects of this crystal packing research are augmented by video-assisted thermomicroscopic, powder diffraction, and calorimetric studies. His work with Joel Bernstein extending the Etter graph-set methodology for categorizing hydrogen-bond patterns is widely recognized.

Ray has received many teaching awards at UT Austin and has always strived to involve undergraduates in his research. He is active in curricular matters at all levels of the University and is coauthor of widely used college and high school chemistry texts. In recognition of his excellence in teaching, Ray was selected in 1995 as an inaugural member of the University's Academy of Distinguished Teachers, and currently holds the position of "University Distinguished Teaching Professor."

Ray has been an active and loyal member of the ACA for nearly 40 years. He and his wife Sharon attend most ACA meetings. He has served on many ACA committees and was a member of the local committee for the Austin ACA meeting (1987) and is local co-chair for ACA 2002. He is also Co-Director (with Joel Bernstein) of the 35th Crystallographic Course to be held in Erice, Italy in 2004 (Polymorphism, Solvates, and Phase Relationships). He was on the original editorial board of *Structural Chem.*, and currently serves in that capacity for *Cryst. Eng.*

Ray is a strong proponent of service and education and he will work to insure that ACA meetings continue to be valuable (and enjoyable). I was also pleased to see him emphasize that we need to make our members, and others, aware of our crystallographic history, and the multitude of contributions crystallography makes to many areas of science. The ACA is fortunate to have him as its next VP. Please join me in congratulating him on his election and wishing Ray well in this new position.

Marv Hackert

David Rose - Canadian Representative to Council

As a longstanding member of the ACA, David brings a wealth of experience to the position of Canadian Representative. A native of Buffalo, he completed his bachelors degree in Biophysics at the University of Pennsylvania in 1977. He then moved overseas to continue his studies at the University of Oxford where he received his D.Phil. in 1981. His work in Sir David Phillips' lab on antibody structure remains as one of his major research interests to this day. Upon the completion of his degree, David returned to the US for a postdoctoral position in Greg Petsko's lab at the MIT. In 1984, he joined the crystallography group at the National Research Council of Canada in Ottawa, eventually progressing to the status of Group Leader. He moved to his current position at the University of Toronto / Ontario Cancer Institute in 1991, where he is now a Professor in the Department of Medical Biophysics, and Senior Scientist of the OCI.

Much of his recent work has centered on the molecular recognition of carbohydrates by antibodies and carbohydrate binding proteins, and on the mechanism of oligosaccharide hydrolysis by glycosidases. His elegant studies of trapped covalent intermediates retaining beta-glycosyl hydrolases have led to fundamental insight into the mechanism of catalysis by this class of enzymes, and this work comes around full circle to the pioneering work on lysozyme by his mentor, David Phillips. A recent contribution has been the 1.7Å structure of the Golgi Mannosidase II, a 1,044 residue enzyme that folds into a single monolithic domain. This enzyme is a target for the development of anti-cancer agents, an area he is currently pursuing.

David is known as an engaging, accessible man with a knack for making anyone feel at ease (as long as they can stomach bad puns). He leads by example, and in addition to his scientific record, he is an especially effective teacher and administrator. As the graduate secretary in his home department of Medical Biophysics, his great empathy is made obvious by the steady stream of graduate students who come to him for advice and guidance. He is a dual US/Canadian citizen, and if nothing else, this should make his travels across the border just a tad easier.

Gil Prive

News from Canada

1. Canadian Light Source (CLS)

The protein crystallography beamline developer Pawel Grochulski is now resident at the CLS and will continue with the design and construction of the PX beamline for the CLS. A Letter-of-Intent has been submitted for a second PX beamline. Jim Britten from McMaster University has been organizing a small molecule beamline team, whose task it is to define the scientific goals and operational parameters of the proposed Small Molecule Single Crystal Beamline. The proposal for this beamline is to be reviewed in February 2002. The Danfysik people will start assembling the booster components on October 26th and the commissioning of the booster ring will start at the end of this year. All magnets of the main storage ring have been ordered and will start arriving at the CLS soon. Currently the staff of the CLS consists of 61 people.

2. Research Agencies

The Federal Government has announced that it will provide a budget for the Canadian Institutes for Health Research (CIHR) in December 2001. An increase in this budget is anxiously anticipated and appropriate lobbying efforts increased substantially during November. The National Sciences and Engineering Research Council (NSERC) received an increase in budget and as a result has established a new program for Collaborative Health Research projects.

Louis Delbaere

ACA Communications Committee Report 23 July 2001

The activities of the Communications Committee since the St. Paul ACA Meeting have encompassed a broad range of issues. Two of them deal directly with the use and development of the ACA web site.

1. Upgrade of the ACA web site.

The Committee was asked to participate in a redesign of the ACA web site. Our input on the design of an upgraded web site was solicited via conference call with the ACA office and T. J. O'Donnell and Jay Budai, the designers hired by ACA to perform the web site upgrade. The Committee was also involved during the redesign process, providing opinions via electronic mail on trial designs, and testing features of versions of the upgraded web site.

2. Educational Links on the ACA web site.

The Committee was charged with developing a listing of links to existing sites relevant to crystallographic education and training. The list of links to educational sites currently available from the ACA web site is reasonably extensive. Howard Jones, a member of the ICDD, is heading a similar effort with regard to the ICDD web site. The Committee has made contact with Mr. Jones with the intention of initiating a joint effort to identify useful crystallographic educational web links which are not yet available from either web site.

3. "Web Watch" column in ACA Newsletter.

Committee members were asked to identify web sites of interest to crystallographers and briefly summarize their content. The intention is that the web sites and summaries would form the basis of a recurring "Web Watch" column in future issues of the ACA Newsletter.

4. Keeping crystallographic books "in print".

The ACA, through the Communications Committee, must make a strong effort to keep books of crystallographic interest "in print". One way to facilitate this is to establish a library in the ACA office. Donations to this library, particularly of out-of-print books, will be solicited in calls for book donations in future issues of the *ACA Newsletter* and on the ACA web site.

5. Press conferences at ACA Meetings.

One of the charges of the Communications Committee is to help the local committee organize press conferences at ACA annual meetings. To this end, the Committee is exploring the development of a "press kit" that would contain information about the ACA, scientific advances involving crystallography and the particular meeting. The kits would be used to publicize the ACA and crystallography to the local press of a meeting's host city, leading hopefully to regional, and possibly national, press coverage of future ACA meetings.

F. J. Rotella

Electronic Balloting – Year 2

Electronic balloting was authorized by the ACA membership in 1999. Last year was the first year the ACA implemented electronic balloting, and 219 (approximately 37%) out of 597 ballots were submitted electronically. This year there were many problems with regular mail. By now everyone should be aware of the anthrax incidents that occurred on the east coast. However, it wasn't until the ACA election that the extent of the problem became obvious. To help members get their votes in on time the ACA office in Buffalo sent out an e-mail message to all members reminding them of the option to vote online and the deadline for the election. At the Naval Research Laboratory in Washington DC we still haven't received our paper ballots and balloting in the election is now closed! Hopefully all members that wanted to vote in the election were able to do so.

The turn out for this year's election was 481, down about 20% relative to last year's turnout. The number of ballots cast online was 216 – essentially unchanged since last year. There were still some minor problems with electronic balloting. All problems reported to me were corrected and, as far as I know, anyone that wanted to vote online was able to do so. You can expect to see some changes in the online ballot next year to further improve the process. If you didn't use the electronic ballot in this election please consider it next year, it saves you postage and simplifies the counting process. Any comments or suggestions on the electronic ballot or other web issues can be sent to deschamps@nrl.navy.mil.

Jeff Deschamps

2002 ACA Patterson Award to be presented to Doug Dorset

The Patterson Award is awarded to Douglas L. Dorset for his fundamental contributions to quantitative electron crystallographic structure determination at atomic resolution. He developed methodology for the optimal collection of data within the constraints of the accepted dynamical diffraction theory for electrons. He pioneered the application of modern direct methods for crystallographic phase determination for electron diffraction magnitudes. He developed this method in spite of widespread skepticism, based on the belief that dynamical and multiple scattering effects would render electron diffraction intensities useless for the determination of unknown crystal structures. He solved a wide range of organic, macromolecular and inorganic structures from electron diffraction data on a quantitative basis and in doing so showed the validity and utility of direct methods in phasing electron diffraction data.



Douglas L. Dorset was born in southeastern Pennsylvania on August 29, 1942. He attended Juniata College majoring in Chemistry and received his Ph.D. degree in Biophysics from the University of Maryland in 1971 with Dr. Albert Hybl. He joined Dr. Donald Parson's electron crystallography laboratory at Roswell Park Cancer Institute that year and in 1973 moved to the Medical Foundation of Buffalo – now the Hauptman-Woodward Medical Research Institute – where he headed the Electron Diffraction Department and did the fundamental work for which he is being recognized.

In the face of those who said that electron diffraction data could not yield quantitative results, he argued long and hard that the problems of dynamical scattering and multiple reflections could be overcome and that electron diffraction data could yield *ab initio* structure determinations. He was responsible for bringing the work on electron crystallography of Vainshtein and Zvyagin carried out in Moscow to the attention of a larger western audience. He developed techniques to overcome the problems of the missing cone of data, dynamical scattering, radiation specimen damage and sample problems. His breadth of applications included polymers, waxes, zeolites, fibres, cholesterol derivatives, solid solutions of paraffins and proteins at low resolution. He was the first to carry out an *ab initio*

solution of a membrane protein structure using electron diffraction data at 6 Å resolution. He has also published on model validation using least-squares methods. In 1995 he published "Structural Electron Crystallography," the definitive text on the subject.

Some of his accomplishments in the area of quantitative *ab initio* crystal structure determination from electron diffraction intensities and electron micrographs are:

1. Established conditions for measuring 'quasi-kinematical' electron diffraction data given well-known constraints of electron scattering theory, thus ensuring feasibility of structure analysis. Improved methods for specimen preparation to obtain optimal crystal orientation. Methods for data collection in selected area diffraction experiments. Method for approximate *a priori* correction of multiple-beam dynamical scattering.

2. Pioneered use of direct phasing methods for analysis of experimental electron diffraction structure factor magnitudes; determined optimal methods for such analyses, given multiple scattering perturbations to the data.

3. Adapted methods for structure refinement (Fourier or minimally constrained least squares) from x-ray crystallography; determined limitations to the use of refinement procedures and pioneered the incorporation of data corrections.

4. Important collaborative work on the high-resolution imaging of organic crystals with 'low dose' techniques, pushing back the previously conceived limitation imposed by radiation damage.

He is presently one of the Co-editors of *Acta Crystallographica*, Section A and Chairman of the IUCr Commission on Electron Diffraction.

Last year Doug joined Exxon – now ExxonMobil – to pursue his interests in multicomponent organic solids. His methods development opens the field of structure determination to nanocrystalline materials which are not accessible via single crystal or powder x-ray methods. This should prove to have a large impact on academic as well as industrial problems.

Patterson Award Committee: Jane Griffin, Chair; Philip Coppens, Dave Duchamp and Andy Howard

What's on the Cover

The cover illustrations were provided by Doug Dorset.

Upper right: structure of isotactic polypropylene beta phase determined from 3-D electron diffraction data.

Upper left: Omp-F porin structure determined by electron crystallography.

Lower left: polybutene-1, form III electron diffraction pattern.

Lower right: potential map for copper perchlorophthalocyanine determined from electron diffraction data by direct methods.

The ACA History Committee

The ACA History Committee is an ad hoc committee consisting of Jenny P. Glusker, chair (jp_glusker@fcc.edu), Bryan Craven and Hugo Steinfink. Our charge is to recommend how ACA can preserve and display our historical treasures before they are discarded. We identify these treasures as: 1. papers, photographs, documents and 2. apparatus.

We would like the assistance of ACA members in initially setting up a database with information on where collected works and papers of crystallographers are stored (hopefully already in an archive, library or museum) so that this information can be made available. We are also anxious to find out if there are any papers, audio or video tapes that should be preserved that do not yet have a home. It is not seen as practical for ACA to collect old apparatus, but we plan to approach some museums about this once we know what is available.

Since individual reminiscences of crystallographers are invaluable for maintaining a history of this branch of science we also solicit these, probably for a volume like that of "Crystallography in North America." ACA members are urged to contact the chairman with any of the information solicited above.

Jenny Glusker

Carol Brock Named to the Governing Board of the Cambridge Crystallographic Data Centre

In May 2001 Jenny Glusker stepped down as the U.S. member of the Governing Board and this position is now filled by Carol Brock of the University of Kentucky. The Board meets in Cambridge twice a year.

Robert Cooper Taylor (1917-2001)

Robert Cooper Taylor, professor emeritus of chemistry at the University of Michigan, passed away Sept 27th, 2001 after a short illness. In recent years he served as departmental historian and maintained the departmental alumni records.

Taylor received a BA degree from Kalamazoo College in 1941 and a PhD from Brown University in 1947. From 1942-45 he was employed as a research chemist on the Manhattan project. He joined the chemistry department at Michigan in 1949 where he served until his retirement in 1987. From 1967-86 he was associate chairman working with three successive chairs. He was also director of the Chemistry Division, Merit Information Center at the University 1972-1989.

His research on the structure and force fields in boron compounds was seminal in character. He was one of the earliest to understand how the computer was completely revolutionizing structural chemistry and vibrational spectroscopy. He was a fellow of the AAAS and was appointed assistant editor of the ACS journal *Inorganic Chemistry* when it was launched in the

1960s. He was the US Editor for the 6th, 7th and 8th editions of the *World Directory of Crystallographers*.

During Taylor's years as associate chair of the department he continued to teach the mandatory physical chemistry lab course. His office assigned all graduate student instructors and graders as well as processed fellowship and research assistant appointments. He came to personally know every student in the department over this period, a claim unique in the department. Given his combined expertise in computers and interest in people, he set up a computerized alumni database and was devoted to maintaining it during retirement. He became a departmental history expert with considerable insight back to the early 1900s. Each year, he assisted in writing the departmental newsletter. He leaves a brother, two sons and three grandchildren.

University of Michigan / University Record

Travel Awards

The Jeffrey Award

A fund established in memory of George A. Jeffrey will be used to assist outstanding graduate students to attend the Congresses of the International Union of Crystallography. The first award(s) will be made at the Geneva IUCr Congress (August, 2002). Applications are invited world-wide. These must be from graduate students in good standing at the time of the Congress. Applications must include:

- (1) A one-page letter explaining the student's background and any special circumstances in support of the application.
- (2) Letters of recommendation from the student's mentor and from one other person familiar with the student's crystallographic abilities and background. The mentor should state the expected date for the student's graduation.
- (3) A one-page biographical sketch of the student.
- (4) Copies of any reprints, preprints or abstracts in which the student is an author.
- (5) An abstract with the student as first author, which has been submitted for the program of the Geneva IUCr Congress.
- (6) The student's e-mail address.

The original and two copies of the application (in English) should be mailed to Prof Bryan Craven, Chemistry Department, Indiana University of Pennsylvania, Indiana, PA 15732, USA. It must be received no later than March 1, 2002. Applications will be judged by Profs Craven, Helen Berman (Rutgers University) and Martin Caffrey (Ohio State University). The important criteria will be the scientific excellence of the student's research, the student's financial need and the student's proficiency in English which is the official language of the Congress. The Jeffrey Award will cover at least the student's registration fee and the cost of student housing.

USNCCr Awards for the 2002 IUCr Congress

The US National Committee for Crystallography (USNCCr) will award a minimum of \$20,000 in travel grants next year from its own funds, and is working with NASA and ICDD in anticipation that the total amount available for travel awards will be between \$40K-\$50K! Directions for applying for these awards were published in the Fall issue of the *ACA Newsletter*. More information about applying for these travel awards can be had by contacting Kathryn Ely (ely@burnham-inst.org) or at the USNCCr web site www.sdsc.edu/Xtal/USNCCr/USNCCr.html.

AAAS Travel Awards

The AAAS Directorate for International Programs announces the Women's International Science Collaboration (WISC) Program for 2001-2003.

Supported by the U.S. National Science Foundation (NSF), this program aims to increase the participation of women in international scientific research through travel awards to locations around the world. The awards are to foster new research partnerships between U.S. scientists and colleagues overseas.

****Both male and female scientists are eligible to apply****

Men and women scientists who have their Ph.D. or equivalent research experience are eligible to apply. Graduate students (Ph.D. candidates) are also eligible, if they will be conducting research in an established Ph.D. program in the U.S. and will be traveling with their Ph.D. advisor and will serve as co-PI on future proposals.

For further information on fields eligible for funding, please visit the NSF website at www.nsf.gov or contact one of the AAAS administrators listed below.

Application deadlines are January 15 and July 15, 2002.

For further information and region-specific guidelines, please visit www.aaas.org/international/wiscnew.shtml or contact the appropriate AAAS administrator:

Central and Eastern Europe, Newly Independent States (NIS) of the former Soviet Union: Karen Grill, kgrill@aaas.org, (202) 326-7027

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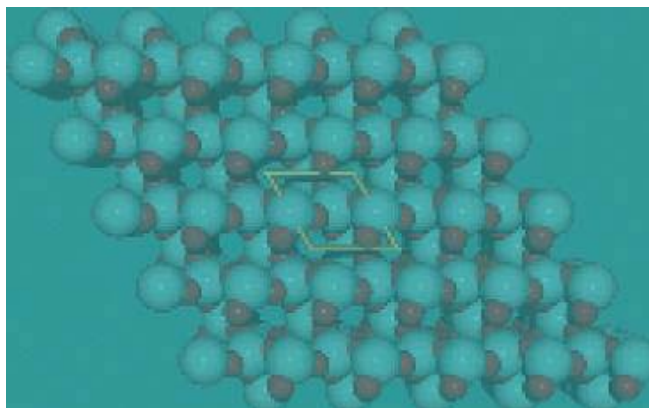
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The ACA website has a brand new look - check it out at

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Fankuchen Award 2001 - Address by James McDonald Stewart - Los Angeles - July 24, 2001

“O wad some power the giftie gie us
 To see oursels as others see us!
 It would frae monie a blunder free us,
 And foolish notion:
 What airs in dress an’ gait wad lea’e us,
 And ev’n devotion!”

R.Burns (To a Louse, on seeing one on a Lady’s Bonnet at Church)

Since my father was born in Scotland, I was raised with Burn’s pithy observations ringing in my ears. Therefore, when I read Jon Clardy’s announcement published in the ACA newsletter with nothing about my blunders or my foolish notions I was as nonplused as when, earlier, a call came from Connie Chidester and Winnie Wong-Ng that I was to appear here today. Not withstanding all the kind words I’m sure there are those out there who see me as the louse.

It is a totally unexpected pleasure for me to be at this ACA meeting here in Los Angeles in the year 2001. I am deeply grateful for the opportunity to participate again in a society whose activities I truly believed I had left forever. My thanks go to all those who have honored me by remembering activities of long ago.

Professor Isadore Fankuchen

However, before I say any more about that, I wish to remind you of the man for whom this award is given: Isadore Fankuchen. Professor Fankuchen lived from 1904 until 1964. In that time crystallography advanced from concept to application. One of his greatest contributions was destined to be that of introducing and teaching the use of crystallography to many students from around the world. I was not privileged to know him. I studied under E. C. Lingafelter at the University of Washington in Seattle. One of Lingafelter’s graduate students in the early fifties was Bruce Brown. Bruce came to UW from Brooklyn Polytechnic Institute. He recalls Fankuchen having both Braggs on campus to give lectures. He also recalls “Fan’s” enthusiasm for telling that Dorothy Hodgkin was able to resolve the penicillin structure while the organic chemists were still contemplating their tarry residues.

Chapter XVIII in *Physical Methods in Organic Chemistry*, page 1073-1108 (1949) provides an excellent example of Fankuchen’s eclectic grasp of diffraction methods illustrates his determination to include as many workers as possible in the correct use of X-ray diffraction for the determination of structure. In this concise summary he lucidly covers from powder diffraction to proteins. Working with Professor J. D. Bernal before the second world war (1937) he pursued the characterization of proteins by diffraction. He published on a “concentrating” monochromator made from a crystal of pentaerythritol in that same year. Right up until the time of his

death he applied his talents and enthusiasm to the subject he loved. It is with this daunting remembrance that I have come here today to tell you something of my own contributions to crystallography and those events, those mentors, colleagues, and students who made it possible.



I. Fankuchen (1904 - 1964)

A powerful influence in all our endeavors is the application of the work of the Braggs, of Ewald, of von Laue, and of all the others who come before us in our discipline. In the case of crystallography the availability of computers was key to making possible larger and larger scale calculations and the automation of data gathering. The excitement of seeing the application of these techniques in solving structures is a powerful motivating force. It represents a small step toward satisfying the wish expressed in Tennyson’s *Flower in the Crannied Wall*:

Flower in the crannied wall,
 I pluck you out of the crannies,
 I hold you here, root and all, in my hand,
 Little flower — but if I could understand
 What you are, root and all, and all in all,
 I would know what God and man is.

It makes us all want to share, just as Fankuchen wanted to share, those insights that crystallography can provide.

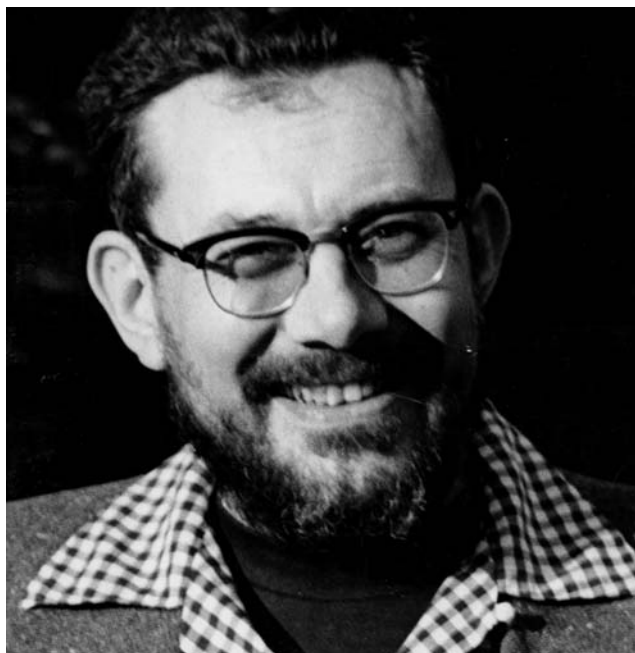
Grace, a difficult concept in the world of science

The events that I will detail in this lecture are imbedded in an extensive human matrix, namely all the people who so generously supported the effort that brings me here today. First, was the blessing of coming into the Lingafelter group. Second, was being “led” into crystallography. To be given the blessing of playing a small supporting role in the development of crystal structure analysis is a gift that I prize. It led to many other opportunities and has given me a wonderful life. Third, was the privilege of being able to have many interpersonal relationships while “doing” science and making a living. I attach a list of the names of those that I can recall at this time who gave me the ability to facilitate putting together XRAY and XTAL for use in the crystallographic community. The obvious ones are my mentors and teachers who had the patience to see that I got it right. Then there were the colleagues who contributed programs and increased the scope of the “library.” Those who used the programs and documentation and then critiqued them so that they could be improved were also of great help, as were graduate students who suffered the slow development and rejoiced in the excitement of the successes, and the bright undergraduates who helped with much of the maintenance, bookkeeping, and distribution work. During the various stages of my activity, the support that I received from several universities, many government agencies, and the people who worked in those places was phenomenal. Because of people’s interest in XRAY and XTAL I was privileged to travel the world and learn more about what was needed to do crystallographic computations. However, without a doubt, for me, it was the interactions with the people who built and used the system that I treasure most. It was through their effort that “it” all came together. It is through their effort that I am privileged to speak to you today. In effect I am the spokesman, singled out, to acknowledge this award for all of us who contributed to the effort.

XRAY and XTAL

A focus of this presentation is the anecdotal history of the XRAY and then XTAL system of crystallographic computer programs. These computer codes served many crystallographers around the world over the years. The XTAL system is still extant at www.crystal.uwa.edu.au as a Free Software Foundation offering by the Crystallographic group, led by Professor Syd Hall at the University of Western Australia. XTAL3.7, edited by S. R. Hall, Roeli Olthof-Hazekamp, and D. J. du Boulay can be downloaded from the internet!

Since forgetting is reputed to be a simple first order kinetics phenomena, I will say essentially nothing about the details of the collection of earlier programs, their structure and function. If the half life of our memories is six months then a quick calculation shows that I now remember 6×10^{-8} of what I learned in 1953! So it would be foolhardy to try to impress an audience currently immersed in the science with how to “do” crystallographic computing today. Moreover, it will be interesting to see if I can coherently compress 48 years into this short presentation.



Professor Ed Lingafelter circa 1956

The beginnings

For me the development of crystallographic computer codes began in 1953 at the University of Washington in Seattle. When I came to UW from Western Washington College of Education in Bellingham it was my intention to be an analytical chemist. To say that I was naive, is to understate an understatement. I chose UW because it was only 90 miles from Bellingham. Offers from U. Chicago and Syracuse and the prospect of crossing the Cascade mountains was too daunting. In fact, at that time, I thought of Spokane as a major eastern city. When I met with Professor Paul Cross, the head of the chemistry department I announced that I would like to be an “analyticker.” To which he replied: “We have enough analytical chemists. Professor Lingafelter has a job for you as a micelle chemist.” Being born in the year 1931, being fully aware of the Calvinist concept of being “led,” having just married Bernice Dorren the Saturday before, and hearing the word “job,” I willingly signed on with the Lingafelter group.

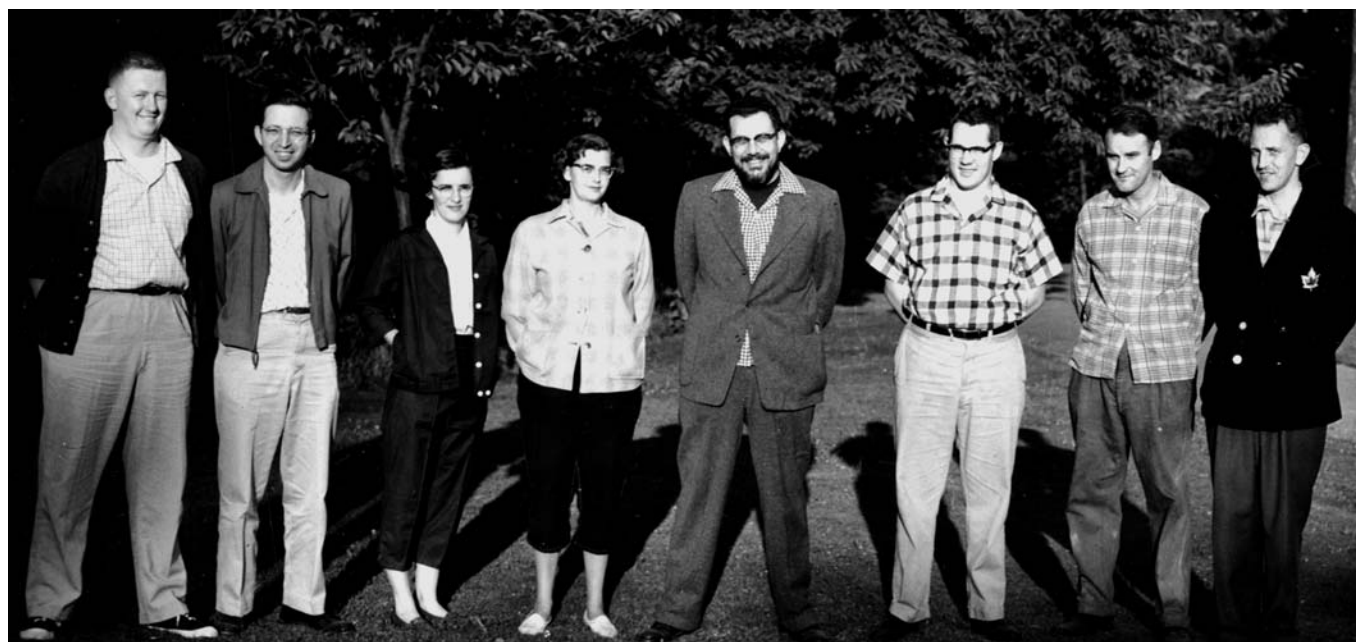
After a stint of work on an apparatus to measure the vapor pressure lowering of soaps, I began to insinuate myself into the, to me, vastly more interesting activity of crystal structure analysis. Not only was the idea of “finding atoms” appealing but there was also the opportunity to see how one could use the UW Business Office tabulating machines to do Fourier transforms. Professor Lyle Jensen, Professor Joe Kraut, and their groups from the medical school were in close contact with Professor Lingafelter’s group in the chemistry department and had an arrangement which allowed the use of the IBM 604 calculating punch and the IBM 402/407 accounting machines. Once I saw these machines I asked to be allowed to wash my hands

of colligative properties of soaps and instead do structure determination on transition metal chelates. These structures were particularly nice to do since very often the heavy atom lay on the center of symmetry in a space group such as $P2_1/c$. As I remember (10⁸) I managed one projection by Beevers-Lipson strips before the university acquired an IBM 650 drum machine. Lyle Jensen became the master programmer of this machine, at that time, a wonderful computer. This machine gave me my first real opportunity to be included in some of the crystallographic programming for the group. Upon graduation I went east to do post doctoral work with Professor Preston Harris at The Ohio State University of Agriculture and The Mechanical Arts in Columbus. There I worked on the structure of explosives such as RDX. At OSU we had access to a 650 on which to use the Washington programs and a new IBM 704 which was completely void of any crystallographic software. It seems ludicrous, in this day and time, to remember how many hours I spent writing machine code to read a card, nine edge first, face down, into the machine and translate the punches therein into binary numbers stored in memory. It was on the IBM 704 that STARTX, the first program of XRAY was coded. For those of you who like the history of crystallographic computing, I recommend Professor Durward W. J. Cruickshank's "Reminiscences of X-Ray Structure Analysis" in *Advances in Molecular Structure Research*, Volume 6, pages 1-47 (2000). The description of the use of a teakettle for a carriage return repair will please your mind. That paper lays out many of the serious considerations that we, eight time zones away in Seattle, were contemplating and applying in the development of the XRAY system.

The conception of the XRAY system

The actual details of XRAY and XTAL development can be seen in articles from a series of books on crystallographic computing that resulted from computing schools sponsored by the International Union of Crystallography (IUCr). For instance: *Crystallographic Computing*, the proceedings of an International Summer School organized by The IUCr Commission on Crystallographic Computing and held in Ottawa, 4 to 11 August 1969. Edited by F. R. Ahmed with co-editors S. R. Hall and C. P. Huber.

After completing my work at OSU I needed to find a "real" job. A postdoctoral appointment is not the most secure way to keep shoes on the baby, and by this time there were two of them requiring the cobbler's product. My good fortune was that I was given a one year appointment back at UW. It was in the year 1960. By that time UW had an IBM 709; the tube version of the IBM 7094. It put me back in contact with the Lingafelter/Jensen/Kraut groups. One of the members of the Kraut group was Darrell High. He is a programmer's programmer who finally finished a degree in biochemistry but has spent his working life on programming for Burroughs and Compaq. He and I began first philosophizing, then programming a systematic set of programs all interconnected by common file formats to supersede the ones originated by the combined groups as well as some other codes imported from groups in the greater crystallographic community. We were also determined that all the codes must be space group and setting independent.



Lingafelter group circa 1956 (Jim is 3rd from the right)

The basic plan was to set up a consistent method of delivering data to the programs in cards of specified formats, to store the data in a “binary data file” on magnetic tape that was to be accessed by all programs, to make the binary data file cumulative so that card data input was minimized as a structure was solved and refined, and to build a library of mutually interdependent, well documented, programs to be used for the solution and publication of structures determined by diffraction. Stated like this in the year 2001 it seems so trivial that you may wonder what in the world brings me here today. Moreover, John Rollett at Oxford, Busing and Levy at Oak Ridge, and others in other places were setting out on the same track. However, to appreciate the fundamental problem of building such systems I ask you to think for a moment about computing conditions in the present. The word processor upon which I’m typing the draft of this presentation offers 23 different ways to store the

the campus, but in the Washington, DC area there were many computers and crystallographers. Through contacts in the region and by returning to UW each winter break and summer session for about eight years the system continued to develop. During that time the UM also set up a Computer Science Center with an IBM 7094. However, there was another problem that became apparent to me in trying to help other labs with their calculations. That was the problem of transportability. In those early days, where every machine cycle and storage register was precious, there was great disparity in the structure of the various machines. Operating systems, bit patterns, word sizes, instruction sets, assemblers, compilers, character codes, and storage media all were different on most of the major makes and models of computers. This made for interesting challenges. XRAY was designed to look consistent to the crystallographer but it was not consistent as far as machines other than IBM were concerned.

Listing of some of those who helped in some ways, large and small, in the production of XRAY and XTAL.

Alden, R.	Engelhardt, L.	Le Page, Y.	Prince, E.
Ammon, H. L.	Flack, H. D.	Levy, H. A.	Robertson, B. E.
Appleman, D.	Freer, S.	Lingafelter, E. C.	Santoro, A.
Baldwin, J.	Furey, W. F.	Machen, Pella	Schenk, H.
Barton, R. J.	Glanville, J.	Marr, H.	Schwarzenbach, D.
Bartsch, U.	Hall, S. R.	Martin, K. O.	Spackman, M.
Blanc, E.	Hawkins, Eleanor	Maslen, T.	Spadacinni, N.
Boonstra, E.	Hendrickson, W.	Mauer, F. A.	Stewart, J. M.
Braun, R.	Hermans, J.	Merom, Rina	Subramanian, V.
Brown, B.	Hester, J.	Mighell, A.	Takeda, H.
Busing, W. R.	High, D.	Morosin, B.	Wald, J.
Carson, M.	Holden, J. R.	Munn, R. J.	Wang, H.
Chastain, R.	Holland, Debra	Norden, Amy	Watts, P.
Collins, D. M.	Jarski, Mary Ann	Norden, Trina	Watenpau, K.
Davenport, G.	Jensen, L. H.	Nucci, Anne	Willis, Jean
DeCamp, W.	Keefe, W.	Nucchi-Vogel, Stefanie	Zhang, Y. M.
Dickinson, C.	King, G.	Olthof-Hazekamp, Roeli	
Doherty, Ruth	Konnert, J.	Pagoaga, K.	
Dreissig, W.	Konnert, Judith	Plastas, H.	
Du Boulay, D.	Kraut, J.	Plastas, Linda	
Egert, E.	Kruger, G.	Preston, H.	
	Kundell, F. A.		

document; starting with “ANSI (Windows) Delimited Text” and ending with “WordPerfect Compound File.” Standards are hard to make and harder to enforce, especially so on Turing machines being used by individuals whose “good sound reasoning” dictates that it be done their way!

The problem of hardware and operating system differences

The next factor that influenced the design of XRAY was that in the fall of 1961 I received a faculty appointment at the Department of Chemistry at the University of Maryland in College Park, UMCP. There was at that time no computer on

When Darrell High and I started, we wrote the “driving” routines in FORTRAN. But, because we believed that we must have optimum efficiency, we expended considerable time writing and checking some marvelous assembler language code for the IBM 709 which was still valid on the IBM 7094, but useless on the CDC, UNIVAC, Burroughs, and other machines. Moreover, during the time the people who wrote FORTRAN compilers were getting better and better at producing excellent optimizing compilers. The end of machine assembler code came one summer at Seattle. I gave Bob Braun, one of Ed Lingafelter’s graduate students the assembler version of our structure factor program and asked him to translate it into FORTRAN. He came back shortly with a little

deck that ran only 10% slower than the assembler version. That did it. From there on we used assembler code for just a few arcane subroutines such as getting times and dates from the local operating system.

The next problem to be dealt with was the very loose FORTRAN standards at that time. CDC FORTRAN looked a lot like IBM FORTRAN and simple programs usually worked well on either machine, but each vendor provided “interesting enhancements” to basic FORTRAN that were not transportable from platform to platform. To complicate the problem further, the vendors used different word sizes, e.g. 60 bits for CDC, 36 bits for IBM, and different internal character codes. In the beginning the various vendors either ignored or fought such things as ASCII.

PIDGIN FORTRAN as an aid to transportability

All these factors led us to code the crystallographic programs in what we called PIDGIN FORTRAN. This change meant that XRAY63 which was essentially written for the IBM machines had to be cleaned up and rewritten in PIDGIN FORTRAN. This of course meant that we sacrificed some efficient code for IBM in order to accommodate CDC, UNIVAC, Burroughs, etc. for codes that produced nearly identical results on all the vendor’s machines, but required minimal modification to the symbolic codes. I do not wish to imply by this abandonment of assembly language and use of a “simplified language containing vocabulary from two or more languages” that we were unmindful of trying to produce the most efficient codes we could invent. However, we could already see that the machines were getting faster and faster and that there were computer scientists working on FORTRAN and other language standards and that writing in the lowest level languages cost too much time and effort when what we felt was needed was working, transportable codes for doing crystallography without every crystallographer needing to be a line by line programmer. Even though we wrote in PIDGIN FORTRAN we did expend considerable thought to the algorithms that would give us the most compact, best and quickest results. In addition we tried to write codes so that as more memory became available the codes would run for larger and larger structures without modification. Looking back to the IUCr sponsored book *Crystallographic Computing Techniques* which followed the summer school held in Prague in 1975, I find that I was talking, among many other things, on the efficiencies to be gained by using “one dimensional” arrays in writing FORTRAN codes. Immediate access storage, what is now called RAM, was limited. The “really big” 5 M\$ machines like the IBM 7094 or the UNIVAC 1108 had 32k of 36 bit words. In PC terms that amounts to roughly 0.2 MB of RAM so we struggled to make the best use we could of what we had available. For those of you who have been raised in this era of high security operating systems, you may be amused that the early operating system on the IBM 7094 required 100 words (600 bytes) of storage. The whole 32k words were so precious to us that we would roll the operating system to a tape, load XRAY from our tape, proceed to calculate our Fouriers or Fcs,

ending by restoring the original OS from our scratch file. There were times when the machine operators were not amused by this use of “their” machine since none of their console commands short of a “cold start” would stop the hx + ky + lz from pressing forward. However, in defense, I’ll tell you that, more often than my wife likes to recall, we were the second and third shift operators followed by being first shift chemistry instructors.

RATMAC the next step in transportability

An example of our efforts at finding good algorithms is the way in which XRAY was metamorphosed into XTAL. At one of the IUCR summer schools I met Syd Hall. Each of us had been working on writing code to produce all the triplets for doing direct methods. My post doctoral student, Roger Chastain, had generated an excellent code that was very fast, Syd had generated a code that was equally fast but used an entirely different algorithm. On comparing how it was done in each case we realized that the methods were quite different, but could be used in combination. Thus began a long collaboration that lasted till I faded away at UMCP and Syd took up the care and feeding of XTAL from his base at UWA in Perth.

Syd and I met on several occasions and decided that XRAY could be drastically improved upon by another rewriting. A colleague of mine at UMCP, Bob Munn, was a great fan of Brian Kernighan at Bell Labs in Murry Hill, NJ. Munn brought the book *Software Tools* by Brian W. Kernighan and P. J. Plauger Addison-Wesley (1976) to our attention. This book describes a preprocessor, RATFOR with a MACRO processor that allows programs to be written in a C like structured language. The programs thus written were then preprocessed by RATFOR into FORTRAN for compiling. In addition the MACROS could be used to hold all the unresolvable conflicts among the various machines available to us. We went to see Kernighan and he declared RATFOR and the MACRO processor “in the public domain.” The computing group at Bell Labs developed UNIX and C among other things. We then set out to translate XRAY into what we named RATMAC and to add all new crystallographic programs in this dialect of FORTRAN. In his paper referred to earlier, Cruickshank mentions that the crystallographic community in Great Britain thought ALGOL was better than FORTRAN and that FORTRAN was probably not the best way to go. It may be that our enthusiasm for RATFOR was also short sighted. But it surely solved many of the transportability problems that PIDGIN FORTRAN left unresolved.

Crystallographic Computing 2001

In the present time I see and read and am amazed by what all of you are accomplishing in structure analysis. The advent of higher and higher speed machines with huge storage capacities programmed in more and more productive ways, the availability of synchrotron radiation sources, the automation of data gathering, the production of stunning graphics, and all the other advances since I left the field are beyond anything I

would have predicted. The most wonderful accomplishment is what has happened in macromolecular crystallography. Keith Watenpaugh has told me that from the genome project it is now proposed to clone hundreds of proteins every year and determine their structures by diffraction. One path to achieve this remarkable goal is shown by workers following Wayne Hendrickson's use of selenomethionine in place of methionine in proteins. This can reduce the initial phasing problem to a direct methods solution for the heavy atoms, a problem solvable with programs such as George Sheldrick's SHELX system <http://shelx.uni-ac.gwdg.de/SHELX/>. Perusal of the Protein Data Bank site <http://www.rcsb.org/pdb/> shows that there are already thousands of determined macromolecular structures and many pieces of software to accomplish the goal. I believe Fankuchen approves.

Ozymandius and the Zen of crystallographic computing

To conclude this presentation it is necessary for me to describe how Shelly's Ozymandius came into XRAY. (Figure 6. Ozymandius) For those of you who have not used XTAL, I need to explain that sometimes, on the unpropitious occasion of a user committing an error in using the system, the error exit to the programs will randomly produce a message from a file of messages which treat errors philosophically. This began on the IBM 709 at UW. It was my custom in those early days to head to Seattle from College Park as soon as finals were over in December in order to use the Christmas break for computing. On one New Years Eve I was sitting at a table, probably puzzling over why a hexagonal space group wasn't computing right, when I realized that I was all alone in the roar of the machine room. At that moment I had the revelation that what I was doing had a certain arrogance of ambition that reminded me of Ozymandius. I determined to find and reread Shelly's great commentary and moreover put a copy in the system so that when bad things happened in the course of a calculation, and depending on the time used and a random number generated, it would print out. Over the next years I found or was given more quotes that seemed appropriate to the collection. This was, of course, just a different kind of arrogance, but it gave some of us comic relief. Not always, however! Once a graduate student got Emerson's "One of the benefits of a college education is to teach the boy its little avail." He disappeared for three weeks! In another case an undergraduate wanted a little programming exercise and I gave him a "B.C." cartoon which showed a man setting out to dig a cave in a mountain. The cartoon character draws a doorway on the mountain, places his chisel on it, strikes the doorway, and with one onomatopoeic "ZAK" the whole mountain falls down leaving the doorway standing. This was in the days of output by line printer and all that got into the Ozy collection was a page size "ZAK!" Unfortunately, I was told later, zak is a very low Dutch word for a foolish person and a lady Dutch professor/crystallographer managed to draw the "lucky number" one day. It then became my turn to be Zak of the day. It is my prayer that this day has not been another.

James Macdonald Stewart

OZYMANDIUS

I met a traveller from an antique land who said...
Two vast and trunkless legs of stone
Stand in the desert... near them, on the sand,
Half sunk, a shattered visage lies, whose frown,
And wrinkled lip, and sneer of cold command,
Tell that its sculptor well those passions read
Which yet survive, stamped on these lifeless things,
The hand that mocked them, and the heart that fed:
And on the pedestal these words appear...
'MY NAME IS OZYMANDIAS KING OF KINGS
LOOK ON MY WORKS YE MIGHTY AND DESPAIR!'
Nothing beside remains, round the decay
Of that colossal wreck, boundless and bare
The lone and level sands stretch far away.

P. B. Shelley

ACA Travel Awardess for LA Meeting

As a recipient of a travel grant I have prepared this letter to summarize my participation at the ACA 2001 Annual Meeting.

Often in research I get the impression that I am working on projects that are of interest to no one other than myself. Although many times this is indeed true, the ACA annual meeting always provides an excellent opportunity to interact with individuals with similar interests. I found several talks, as well as posters, whose content was the basis for several vigorous discussions both at the conference and again at home. In particular I found Qun Shen's talk on Triplet- phase data collection extremely interesting.

Los Angeles is great place for a meeting. I never pass up a chance to eat my body weight in pupusas and the Grand Central Market, a five minute walk from the hotel, provided just that.

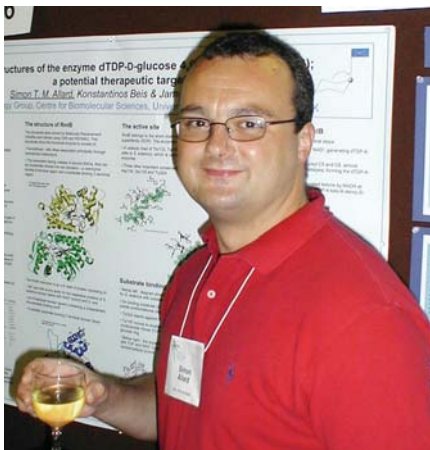


Jeffrey Roach (U. North Carolina)

This was my first time in Los Angeles and the first time in a hotel with over 1400 rooms; which was more imposing I don't know!

The meeting was excellent and not only introduced me to many new techniques

and structures but also enabled me to put faces to names I had heard so many times before whilst working on my Ph.D. There were many talks I enjoyed, but with a background in microbiology and infectious diseases, I found the talk on prion proteins and the crystallographic evidence for a possible mechanism for prion protein aggregation particularly fascinating.



Sunday evening saw the first poster session which included my poster entitled "Crystal Structures of the enzyme dTDP-D-glucose 4,6-dehydratase (RmlB); a potential therapeutic target". This concerns the second enzyme in the dTDP-L-rhamnose pathway (specifically RmlB). The pathway is found in many pathogenic organisms but not humans and thus represents a possible therapeutic target. We have solved the structure of the enzyme in complex with substrate and a number of ligands, enabling us to propose a complete mechanism for this important enzyme. The session was busy but it gave me the chance to explain my work to a number of people including one group who were working in the same area. Later on in the week, I was able to explain my work to a slightly larger audience when I gave a small talk on my poster. The evening also gave me the opportunity to discuss various postdoctoral positions and chat with fellow Ph.D. students from the USA and Canada. The day was rounded off at the California Pizza Kitchen for the Mentee/Mentor Dinner and more informal discussions concerning structural work

and problems with protein solubility!

Monday was the day I found most revealing as it included the *Transactions* symposium on high throughput crystallography. These talks were highly informative but also made me realize for the first time just how much money was being put into areas such as structural genomics. The automation now available, especially concerning robots which can now grow your protein, purify it, crystallize it and mount in on the synchrotron beam line is amazing. Add to this programs like Arp/Warp and it seems like the future of crystallography will be to merely press a button. However, one couldn't help but feel that all the difficult proteins, i.e. those that were insoluble and membrane proteins were being somewhat neglected in the structural genomics camp.

All in all the conference was a real eye opener and well worth the long trip over the Atlantic. I am extremely grateful at having been given the chance to attend such an interesting meeting.

Simon T. M. Allard (The University of St Andrews)

The grant from ACA helped me to participate in the 2001 meeting and especially it has the great impact that it helped me get another grant from Oscar Öflunds stiftelse to cover the rest of my travel expenses to this meeting and also to one other meeting. This happened because I was able to inform them that I had received a travel grant from ACA before they selected the recipients of their grants.

This meeting was my second ACA meeting so I had some kind of idea what to expect but even so this meeting exceeded my expectations. The local organizers had done a great job.

I am currently doing neutron crystallography studies on proteins. The workshop: Neutron Diffraction Studies of Macromolecules was very interesting for me, so thanks to Gerry Bunick, Leif Hanson and John Helliwell that this field of crystallography was so well represented even though not many scientists are doing neutron crystallography on proteins.



I was also able to listen to lots of interesting talks. Sometimes I just had difficulty choosing between sessions which were going on at the same time, which is of course much better situation than when I cannot find any really interesting talks. This is often the situation in other meetings where majority of talks are dedicated to small molecules and physics or molecular biology.

It was also nice that I was able to present my poster in this meeting. I also found lots of interesting information and ideas from other posters.

I also enjoyed many well-organized social events and I also appreciated that these events were not options for lectures. California was a nice place to visit.

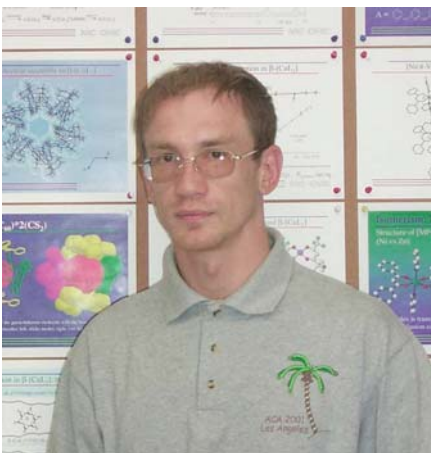
Vesa Tuominen (Turku Centre for Biotechnology)

The conference was a great opportunity, to meet the authors of papers that I admire. The structural genomic talks instilled me with a sense of opportunity, while at the same time was humbling. As Taylor and Kennard have shown with small molecules, the structural insight gained from an extensive database is invaluable and I look forward to being able to access an expanded protein database. I was also encouraged to see the automation of some of the mundane tasks of crystal screening. However, the discussions of the necessity to remove the human element in the pipeline were quite disconcerting.



Paula Lario (McGill University)

It was my first ACA meeting, and my first participation in an American meeting at all. I have been a long time in crystallography but it is only at the meeting that I personally met a number of outstanding men who brought the science of crystallography to its current horizons. I especially appreciate the friendly atmosphere and easy interaction that prevailed at the conference and that is inherent to the whole ACA community



Both the scale and content of the conference were great. One could not attend all lectures that I wished to. I really enjoyed the entire Supramolecular Structure and Engineering symposium as well as many lectures on other topics. I also reviewed or discussed many posters and attended most exposition sites.

Yet the greatest opportunity for me was to present our results and ideas on a new class of metal-organic frameworks we currently explore at the National Research Council of Canada. Started in 1997 from a single discovery at the Steacie Institute for Molecular Sciences, the research has led to dozens of useful host receptors incorporating chelated metal complexes, hundreds of new supramolecular materials and several new ideas contributed to Crystal Engineering. This is why I am especially proud to receive the Margaret Etter Award. I would be happy to believe that my attendance at the conference was as useful to the society as it was useful to me.

Dmitriy V. Soldatov (Steacie Inst. for Molec. Sci, NRC)

I would like to send my most sincere thanks for providing the partial financial support which allowed me to attend the ACA 2001 meeting held at Los Angeles. The participation in the meeting was a great experience and helped me to get acquainted with recent developments in the field of crystallography. The most interesting part of the meeting in my point of view is the development of the crystallographic methods. Crystallographic software such as Shake And Bake, SHELXS, SHARP, SOLVE, ARP/WARP, REFMAC, O, etc. made crystal clear approaches to solve the complicated macromolecular structures in a user friendly automated manner. The approaches of Gerard Bricogne's and Peter Kuhn's are very promising. However, challenging crystallographic problems will still override the automation of crystal structure determination and need crystallographer's skills. No matter what the state of experimental technology to solve the phase problem, the understanding of the crystallography concepts such as reciprocal lattice, Ewald sphere, space groups, symmetry, twin laws, phase problem are necessary and require three dimensional imagination. J.P. Glusker's illustrations helped me a lot in understanding and her approach to teaching crystallography to the students are most fascinating part. The other part of the meeting I liked most is the way structural biologists are utilizing

crystallography as a tool to look at the function of macromolecules. Moreover, the numerous oral and poster presentations were very useful. The meeting was well organized and attended by over 1000 scientists, which helped me to get interaction directly with American crystallographers.



Babu A. Manjasetty (Univ. California, Santa Cruz)

The 2001 ACA meeting in Los Angeles was my first, and I would like to take this opportunity to express my appreciation for being a part of this important event. Also, I am extremely grateful to have been a recipient of the ACA travel grant which helped make my attendance possible. I found the seminars to be informative and intriguing. In addition to the educational merits of the conference, I enjoyed the opportunity to socialize and network with my colleagues and peers. Getting to know those in the crystallographic community is a very positive experience for my career.

Aside from the seminars and social functions, my poster presentation allowed me to gain many fresh perspectives and to engage in some very beneficial dialogue about my research. The experience was an invaluable one. This meeting was one of the highlights in my career and I look forward to furthering my relationships and educational opportunities at the next meeting. Thank you again.



Shorena Nadaraia (University of Missouri - Columbia)

Attending the 2001 ACA conference in Los Angeles this past summer was a wonderful experience. It was great to be able to see the diversity of crystallographic research around the country and to gain a better understanding of the future of the field. In addition to learning from the posters and presentations, I enjoyed being in LA for the week and meeting many people. Having just received my B.A. in May 2001, giving my first professional presentation at this conference was a very exciting and incredible experience. It was a chance for me to share work I had done, as well as to gain new insights into some of the problems that I encountered with my research. I want to thank everyone involved for a great and successful conference!



Anne E. Fischer (College of Wooster)

Future ACA Meetings

2003

Covington Convention Center, Northern Kentucky (greater Cincinnati) - July 26-31



Jeanette Krause Bauer (program chair - jeanette.krause@uc.edu) and Bobby Barnett (local chair - barnett@pg.com)

2004

Hyatt Regency, Chicago, Illinois, July 17-22. Bernie Santarsiero and Karl Volz (both at the University of Illinois) at Chicago will be the local co-chairs. Christer Aakeroy (Kansas State) and Marilyn Yoder (U. of Missouri, Kansas City) will co-chair the program committee.

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Images from the Mentor Mentee Dinner in Los Angeles



U.S. National Committee for Crystallography (USNCCr) – November 11, 2001



Jack Marburger, White House science adviser, joins USNCCr at its fall meeting

Front: Attendees Bill Duax (IUCr Exec. Comm.), Winnie Wong-Ng (sec.-treas.), Marv Hackert (Chair), Jack Marburger (Dir., OSTP), Katherine Kantardjieff, Peter Buseck. Middle: Charlie Prewitt (ICDD), Bill Stallings, Alex Chernov (AACG), Kathryn Ely, John Spence, Tamae Maeda Wong (NRC), Lonny Berman, Bob Sweet. Back: Bing Jap, Charlie Carter, Doug Ohlendorf, Ian Robinson, John Parise, Jon Clardy (Vice-chair), Jeff Post (attending but not in photo is Howard Einspahr).

The fall meeting of the USNCCr opened with Marv Hackert thanking the departing members Peter Buseck, Bing Jap, Ian Robinson and Cynthia Stauffacher for their service. The nominating committee chaired by John Parise reported that Joel Brock (Cornell), Jim Kaduk (BP Amoco), Marilyn Olmstead (UC-Davis), and Ron Stenkamp (U. Washington) have been elected members of the USNCCr for the 2002-2004 triennium.

USNCs: The USNCCr represents U.S. crystallographers in the IUCr through the National Academy of Sciences and the National Research Council, and is one of about 25 such USNCs. Each USNC maintains close ties to U.S. professional societies while seeking to promote international scientific cooperation and U.S. participation in international science.

White House Science Adviser: A highlight of this fall’s meeting was the presence of Dr. Jack Marburger, recently confirmed Director of the Office of Science and Technology Policy, and White House Science Adviser. His remarks addressed five questions we had asked him to discuss with our committee, namely:

- 1) How will funding and the justification/ priorities for funding in the sciences change in light of the incidents of September 11th?
- 2) What changes and restrictions can we anticipate for those who work with “bio-hazardous” materials? Should researchers be concerned about this list expanding or getting too vague to the point where research involving “select agents” can no longer be carried out in university laboratories, but only in government laboratories? What can we do to help?
- 3) We are concerned about the overall support for research

in the physical sciences as well as the life sciences. Often innovation in technology springs forth from the physical sciences and many such researchers often switch to other fields and make important contributions to their new fields. How can we support increases for the physical sciences?

4) Our committee is concerned about openness in science, both in publication and in scientific communication with peers in other countries. What can we expect in terms of restrictions in travel to meetings abroad? Will visa permits be tightened?

5) What policies do you foresee regarding patenting of crystal structures (and genes) derived from naturally occurring specimens?

Dr. Marburger addressed each of these questions and generally impressed the committee with his knowledge of and approach to these issues. He spoke of crystallography as an “enabling” science at the interface of many exciting fields such as drug development, proteomics, and nanomaterials. He encouraged us to work with his office to create a more informed environment to help the public appreciate how science works and benefits our society. He stressed the need for us to better communicate the importance of not just our findings but also the role of the underlying technologies and national resources that support our successes in research. He expressed concerns about balance in funding and the need to foster the enabling technologies as well as support efforts directed towards the end-products of research. On the “select agents” issue, he commented that it will be important to develop procedures to control the access to biohazardous materials and urged each of us to work with our respective institutions to create a dialogue as to how this can best be implemented. On the travel issue, he noted that President Bush is reaching out to other countries to promote more global solutions to problems. He also said that we should not anticipate much change in travel restrictions to other countries. On the foreign visa issue, he stated that in light of the events of 9/11, we can expect increased scrutiny of foreign visas and improved efforts to track foreign students once they are admitted into the United States. On the patent issue, he noted that it is not a scientific issue other than its possible impact to inhibit science in affected areas.

IUCr matters: The next IUCr meeting will be in Geneva, Palexpo Congress Centre, August 6-15, 2002. One of the functions of the USNCCr is to nominate individuals for various committees and commissions of the IUCr. Bill Duax is currently on the Executive Committee. The USNCCr has written in support of Bill’s nomination as the next President of the Executive Committee, with Judith Flippen-Anderson proposed as a candidate for regular member. Another function of the USNCCr is to elect the U.S. delegates to the IUCr General Assembly. Delegates must be permanent residents of the U.S. who are active in research or education related to crystallography but need not be a current member of the USNCCr. For next year’s IUCr meeting in Geneva, the U.S. delegates will be Marv Hackert (chair), Jon Clardy, Judy Flippen-Anderson, Bill Stallings, and Bob Sweet, with Charlie Carter, Abe Clearfield, Howard Einspahr, James Kaduk, and Ian Robinson

serving as alternates.

Travel Awards: Our Research and Travel Support Subcommittee, co-chaired by Howard Einspahr and Kathryn Ely, has been very busy preparing for next year’s round of travel grants for young scientists to attend the Geneva IUCr meeting. The USNCCr voted to award a minimum of \$20,000 in travel grants next year from its funds, and is working with NASA and ICDD in anticipation that the total amount available for travel awards will be between \$40K-\$50K! Further information on these travel award applications is available from Kathryn Ely, this Newsletter, or on our web site.

Latin American Initiative: The USNCCr has initiated a program to help promote crystallography in Latin American countries. This effort has many aspects including travel assistance and joint sponsorship of symposia. The ACA has set aside travel funds to help Latin American crystallographers attend next May’s ACA meeting in San Antonio. The USNCCr voted to allocate up to \$5000 in travel assistance for Latin American crystallographers to attend various crystallographic schools or workshops in the U.S. Bob Sweet attended a workshop at the LNLS synchrotron in Campinas, Brazil.

Education: Our education subcommittee co-chairs, Ian Robinson and Cynthia Stauffacher, are working with their counterparts in the ACA to provide web-based materials on crystallography for not only students of crystallography, but also for K-12 students as well. We also have started discussions about the need for a publicity brochure at the level appropriate for the general public, and of even participating in the making of a film for public television. Katherine Kantardjieff has done a survey of crystallography course offerings at many universities. Wally Cordes is organizing a special symposium on ‘How to teach crystallography’ for the San Antonio ACA meeting and a similar symposium is planned for the IUCr meeting in Geneva.

Other areas: The USNCCr also has subcommittees on Crystallographic Databases (PDB, PDF, NDB, CSD), Research Resources (light and neutron sources, computational resources), Publication Standards and Ethics, and an Interdisciplinary Committee with representatives from the AACG (Chernov), ICDD (Prewitt), and MSA (Glaeser). Alex Chernov reported that the AACG will hold a joint meeting with the ACA meeting in San Antonio. Charlie Prewitt reported that the ICDD Board of directors announced that Tim Fawcett has accepted the offer to be the next Executive Director and that ICDD has a new relational database for the Powder Diffraction File (PDF 4).

The next regular meeting of the USNCCr will be held on May 25, 2002 in San Antonio, TX. If there are any issues you would like the USNCCr to address, please contact the Chair (m.hackert@mail.utexas.edu) or the Secretary (winnie.wong-ng@nist.gov). The committee currently consists of 15 regular members, 1 representative from the IUCr, 3 ACA representatives, plus representatives from AACG, MSA, and ICDD. See our web site for a list of current members and more information about the USNCCr: <http://www.sdsc.edu/Xtal/USNCCr/USNCCr.html>

Marv Hackert, Chair USNCCr

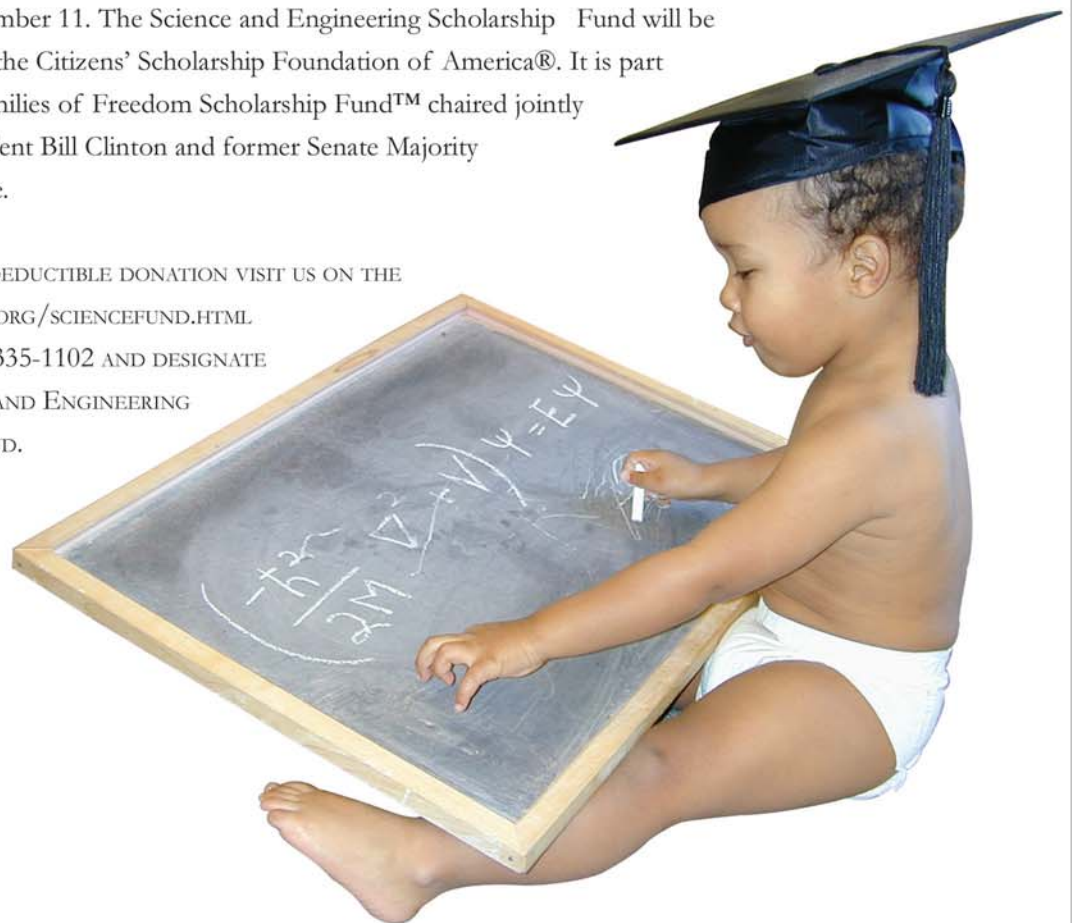
SEPTEMBER 11TH

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In response to the tragedy of September 11, dozens of organizations representing more than a million scientists and engineers have established a Science and Engineering Scholarship Fund.* Donations to the Fund will support the science and engineering education of dependents of those who were killed or injured on September 11. The Science and Engineering Scholarship Fund will be administered by the Citizens' Scholarship Foundation of America®. It is part of an overall Families of Freedom Scholarship Fund™ chaired jointly by former President Bill Clinton and former Senate Majority Leader Bob Dole.

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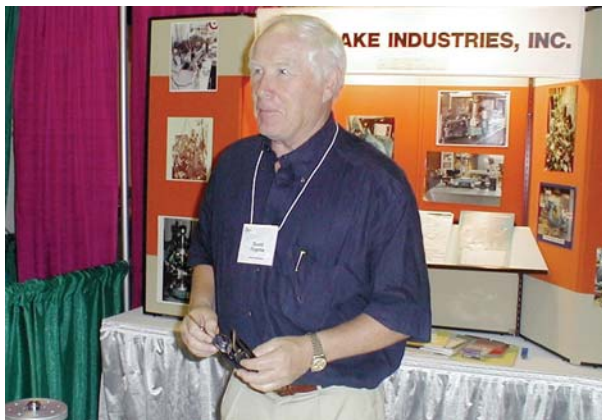
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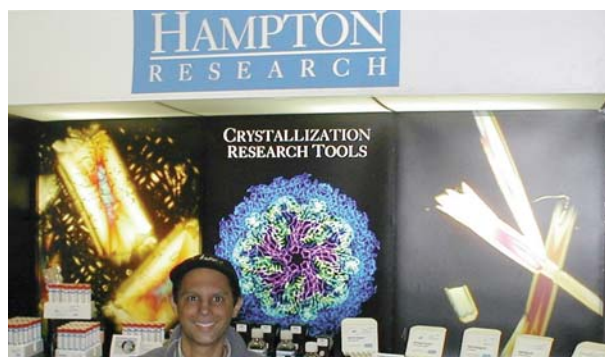
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Where would we be without them - Marcia Evans, Vanessa Vair and Patti Coley receiving the ACA's thanks at the banquet in Los Angeles as K. C. Cole, Bill Duax and Henk Schenk look on with approval

Protein Data Bank



At the booth in LA: Front - TN Bhat, Helen Berman, Narmada Thanki, and Kyle Burkhardt. Back - John Westbrook, Christine Zardecki and Gary Gilliland.

As this *Newsletter* goes to press, more than 16600 entries are released in the Protein Data Bank and more than 3000 structures have been deposited this year. Of these depositions, approximately 80% were determined by X-ray crystallography. 89% are proteins, 6% are nucleic acids, and 5% are protein-nucleic acid complexes. 72% were deposited with a release status of HPUB; 13% HOLD; and 15% release immediately.

For existing (legacy) entries and recently released entries, the PDB has made standardized files in mmCIF format available as part of the Data Uniformity Project. For these entries, inconsistencies between the specification of the chemical sequence and sequence that is from the coordinate records have been resolved. Another focus of this work was to include in the mmCIF data files the results of prior uniformity processing of individual PDB records. The standardized data for records such as compound name, citation, and source organism were previously accessible from the PDB database, but this information was not available in all of the data files. The mmCIF data files include the integration of all of this information, as well as additional macromolecular names and synonyms from related SwissProt sequence database entries. These files, which follow the latest version of the mmCIF dictionary (see <http://deposit.pdb.org/mmcif/>), are available from the PDB beta FTP site at

<ftp://beta.rcsb.org/pub/pdb/uniformity/data/mmcif/>. An application program called CIFTr was made available at <http://deposit.pdb.org/software/> for translating files in mmCIF format into files in PDB format.

For searching the entries in the PDB database, an option that allows users to select a subset of structures from which homologous sequences have been largely removed is now available from the primary PDB Web site and its mirrors. This option, which is available from all PDB search interfaces, filters subsets of structures that match a particular query. The default threshold for sequence similarity removal for queries from the home page or SearchLite is 90%; SearchFields provides the

option of selecting either 50, 70, or 90% similarity as cut-off values. Users can toggle between the complete set of results and the reduced subset by using the options menu at the top of the Query Result Browser. Further information about this new feature is available at www.rcsb.org/pdb/redundancy.html.

These features and further information about the Protein Data Bank are available at www.pdb.org. Questions and comments may be sent to info@rcsb.org.

Christine Zardecki

The Cambridge Structural Database (CSD): A quarter of a million crystal structures and rising..



Steve Maginn at the CCDC booth in LA

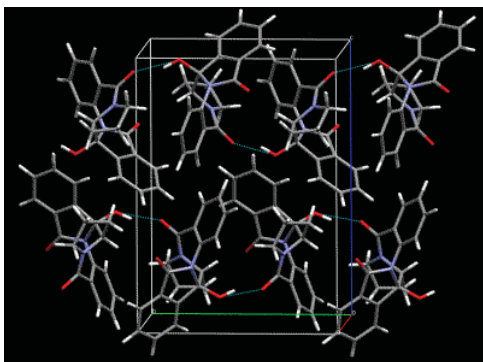
On 5 October 2001, the 250,000th crystal structure was archived to the CSD, marking another milestone in the ever-accelerating growth of the world's repository of small molecule organic and metal-organic crystal structures. The 250,000th CSD entry describes the structure of a photocyclization reaction product [A.G. Griesbeck, W. Kramer & J. Lex, (University of Koln, Germany), *Angew. Chem. (Int. Ed.)*, 2001, **40**, 577-579] and has been assigned the CSD reference code IBEZAQ.

This landmark in the history of the Cambridge Crystallographic Data Centre (CCDC) comes almost exactly 36 years after the inception of the CSD project in the Department of Chemistry, University of Cambridge, UK. From small beginnings – just a few hundred structures per year in the late 1960s – the CCDC has archived data for more than 20,000 small-molecule crystal structures during the past year, with nearly 85% of data now arriving electronically in CIF format via the Internet. Analyses of 25-year growth statistics predict that the CSD archive will contain 500,000 structures by 2010, assuming that existing methods of data generation, publication and data acquisition remain largely unaltered. Thus, the CCDC will process more information in the next decade than was processed in the previous 36 years of its existence.

The October 2001 release (5.22) of the CSD System was

mailed from Cambridge on 12 October. It contains a database of 245,392 entries, together with ConQuest 1.3, IsoStar 1.4, and the first release of Mercury - the new visualizer for the CSD. Mercury is also being made available for free download from www.ccdc.cam.ac.uk/prods/mercury, and will operate from CSD, CIF, mol2 and PDB formats. There are many additional features in ConQuest 1.3 and these, together with other details of the release, are summarised at www.ccdc.cam.ac.uk/support/522relnote.html). IsoStar 1.4 now contains 23,790 scatterplots of intermolecular interactions, 18,250 derived from the CSD, and 5,240 from PDB protein-ligand complexes.

In order to keep subscriber databases as up-to-date as possible, the CCDC will be trialling the web download of inter-release CSD entries with selected testers during the winter of 2001-2002. We aim to make this facility available to all subscribers from April 2002.



250,000th Structure - REFCODE = IBEZAQ

In line with a policy of making CSD information both more accessible and more valuable to the scientific community, the CCDC is also involved in a number of in-house and collaborative software developments, all of which make use of CSD information in various forms: SuperStar for investigating protein – ligand interactions, GOLD for protein – ligand docking, the Relibase+ database derived from the PDB and structured for examining protein –ligand interactions, and DASH for structure solution from powder diffraction data. All of these products are available for free evaluation, as described in www.ccdc.cam.ac.uk/prods/<productname>.

The CSD System and other CCDC products provide methodologies that are widely used in scientific research, and have so far been employed in more than 800 published projects. Full references and brief summaries of these papers are collected in a small database, DBUse, maintained by the CCDC and made freely available at www.ccdc.cam.ac.uk/dbuse.

The CCDC acknowledges and appreciates the cooperation and support received over many years from data depositors and journals, and from users of the CSD System and other products. We look forward to the future challenges of maintaining the CSD archive, and continuing to improve our services to the scientific community.

Frank Allen

ACA 2002 - San Antonio, Texas, May 25- 30



Wally Cordes (Program - wcordes@mail.uark.edu), Marv Hackert (Local - m.hackert@mail.utexas.edu), Ray Davis (Local - redavis@mail.utexas.edu) and Travis Gallagher (Program - travis.gallagher@nist.gov)

Advance Registration Deadline: April 5, 2002

Hotel Reservations: April 19, 2002

Additional information available on the ACA website - www.hwi.buffalo.edu/aca/

2001 MacCHESS Users' Meeting

Synchrotron users gathered once again at Cornell this past summer for the annual MacCHESS users' meeting. The focus of this year's meeting was "Obtaining Maximum Information from your Protein Crystals: Crystallization, Data Collection, Computing, Visualization and Refinement of Ultra High Resolution Structures". Organized by Dan Thiel, Marian Szebenyi and Richard Gillilan, the day-long meeting was held in conjunction with the Cornell High-Energy Synchrotron Source general users' meeting. Two of the nine speakers were new additions to the MacCHESS staff.

Quan Hao, new associate director of MacCHESS, spoke at the general CHESS users' meeting about his two *ab initio* phasing methods. The single-wavelength anomalous dispersion (SAD) method implemented in the computer program OASIS demonstrated that, by exploiting the anomalous signal at a single wavelength, direct methods can be used to determine phases at moderate (2.5 Å) crystallographic resolution for a large-size protein (5663 non-H atoms in the asymmetric unit). The second method utilized the low-resolution molecular shape determined from small-angle solution X-ray scattering data (SAXS) for the molecular search. The idea of locating a molecular shape in the crystallographic unit cell was tested with experimental diffraction data from two proteins. It is anticipated that the low-resolution phases calculated from the correctly positioned molecular shape can be used as a good starting point for phase extension.

The opening speaker of the morning, George DeTitta of the Hauptman-Woodward Institute, discussed his novel robotic crystallization operation. Drops of protein solution (as small as 0.1 ul) are combined with drops of test solution under oil in microarray plates. These batch crystallization experiments are observed over a period of 2-3 weeks by an automatic digital camera system. The final product is a database of 9000 images (snapshots of the wells at 6 time points) on CD which the user can scan for signs of crystallization. So far, software is best at recognizing empty wells, though crystal recognition is under development. Due to dead-volume requirements in the pipetting system, about 600 ul of protein solution at 10mg/ml are initially needed, several hundred of which are recoverable at the end of the run. The system is highly reproducible, with an accuracy of about 2% in drop volume. In all 1536 conditions can be screened at one time.

Gerard J. Bunick, University of Tennessee, spoke on the topic of crystal annealing. According to Bunick, annealing is no substitute for good cryoconditions, but may sometimes be used effectively to rescue crystals that might otherwise be discarded and to reduce overall mosaic spread. Apparent increases in resolution are most likely a result of decreased mosaic spread in high-resolution reflections. Effectiveness of annealing may also depend strongly on the method of crystallization. Crystals grown via dialysis (like ConA) may exhibit different types of defects than conventional crystals from hanging drops and may not be improved as much by annealing. The recommended procedure is to transfer flash-cooled crystals back into sealed

wells of mother liquor for no less than 3 minutes. Multiple applications of annealing on a single crystal are not recommended. Crystals that must be annealed on the loop should be allowed to fully thaw before restoring the cold-stream flow.

B. Leif Hanson, also from the University of Tennessee, introduced us to the use of helium cryostreams. Helium has a higher heat-capacity than nitrogen so crystals are cooled more rapidly in a helium stream of the same temperature. Less radiation damage, lower B factors and some increase in resolution has been observed. Cryosystem design is critical to proper performance. Crystals need to be very close to nozzle. Modified tools and handling techniques are also required.

Rob Thorne from Cornell University presented some work in progress on using x-ray topography to study annealing of flash-cooled lysozyme crystals. With unfocused x-rays, each spot in a diffraction pattern is an image of the crystal itself. Nearly perfect crystals at room temperature display a characteristically sharp image with every part of the crystal diffracting at the same angle. Flash-cooled crystals, however, have significant nonuniformities. Regions of defocusing are thought to be due to variations in the lattice spacing introduced by the cooling process. Thorne demonstrated that annealing performed on the crystal can actually restore uniform diffraction in the topography images. Thorne's annealings were performed in the cryostream rather than in a liquid drop as proposed by Bunick, nonetheless, these results offer strong new support to proponents of annealing.

Richard Gillilan, a new MacCHESS staff member, discussed his experience with oil as a cryoprotectant. Gillilan presented detailed studies of lysozyme comparing oil and a conventional cryoprotectant mix with bare unprotected crystals under various cooling scenarios. For this comparatively high-resolution experiment (about 1.1 Å) using high-luminosity synchrotron radiation, significant improvement in mosaic spread and resolution were observed for oil. Gillilan also reported that, contrary to the findings of Riboldi-Tunnicliffe and Hilgenfeld (*J. Appl. Cryst* **32**, 1003-1005 (1999)), his crystals of concanavalin A do not survive oil treatment. Other proteins are currently being examined. Part of the data processing for this work was performed using the OpenDX Crystal Modules (XTM), a novel data-flow style computing environment with advanced visualization capabilities. Gillilan described the general design and operation of XTM.



Bob Sweet (BNL) and John Nagle (Carnegie Mellon)

Dr K. R. Rajashankar of Rockefeller University spoke about his collaboration with Z. Dauter and M. Dauter on phasing crystal structures using rapid soaks in concentrated halide solutions. Typically 0.5-1.0M solutions of KBr or KI are allowed to diffuse into a protein crystal for a period of about 15-45 seconds. During this time numerous halide ions bind to the protein surface. Bromide and iodide ions apparently occupy the same sites in protein structures. Halide binding sites are also consistent among multiple copies of the protein within the unit cell. Though the iodine edge is not energetically accessible at many synchrotron lines, bromine is commonly accessible. Rajashankar presented an impressive list of structures solved by various groups using this method.

Mark Wilson from Yale (Brunger group) discussed rigid body refinement for multiple subregions of a molecule. The emphasis of this work is on disorder, rather than the usual focus of crystallography on ordered atoms. Data for Ca^{+2} bound calmodulin were collected at 1.0 Å resolution. Multiple conformer and translation-libration-screw (TLS) refinement strategies were introduced and used to characterize the unique flexibility of the protein. Wilson's study revealed extensive conformational heterogeneity at several different length scales in the protein and supports the recent view that the protein may be regulated principally at the level of its conformational dynamics.

Debashis Ghosh of the Hauptman-Woodward/Roswell Park Cancer Institute presented details of the acetyl xylan esterase structure (AXE) that diffracts beyond 0.80 Å resolution. The original structure was solved by the iodination method (Ghosh, et.al. *Acta Cryst.*, **D 55**, 779-784 (1999)). The current refinement used data to 0.85 Å. The tertiary structure is a doubly-wound α/β sandwich, with a central parallel β -sheet flanked by two parallel α helices on each side. Multiple conformations are quite frequent, about 15%. There are two catalytic states of the active site Ser and His. The experiment gives a glimpse of the transition state by obtaining a structure which mimics the tetrahedral intermediate. More details can be found in Ghosh, et. al, *J. Bio. Chem.*, **276**, 11159-66 (2001).

Martha Teeter, Boston College, finished the day with a lecture on high-resolution crystallography. With a crambin structure that diffracts to 0.54Å resolution, electron density can be seen in bonds as well as in atoms. Typically, 10% of sidechains in structures with resolution 1.4 Å or better exhibit multiple substates. Substates tend to be correlated with multiple side-chain shifts occurring in a concerted manner. Shifts of bound waters can clarify small shifts in side-chains. Often water molecules appear doubled as a result of these shifts. Teeter stressed the important role of water molecules in mediating interactions between biomolecules.

Previous MacCHESS meetings covered membrane protein crystallography and structural genomics. Suggested topics for 2002 may be forwarded to the organizers (reg8@cornell.edu). These meetings are made possible through the support of NIH NCCR grant RR-01646.

Richard Gillilan & Marian Szebenyi

12th Annual Southwest Macromolecular Symposium, Texas A&M, November 3, 2001

It takes dedication to spend a glorious autumnal Saturday telling and listening about crystallography, but 50 hearty seekers and expositors gathered from Louisiana, Oklahoma, and Texas for the twelfth annual SouthWest Macromolecular Symposium on the Texas A&M University campus. In addition to presentation of recent results and discussions of methods and experimental details (cf. titles + abstracts at our web site: www.tamu.edu/struct/SWMS-2001/SWMS-01.html), the highlight of the symposium was a presentation and discussion by the Gulf Coast Protein Crystallography Consortium (GCPCC) of the plans for the regional synchrotron MAD beamline on the campus of Louisiana State University, Baton Rouge, which is expected to be up and running by next spring.

The symposium was financially supported by Bruker - Nonius and Rigaku/MSC, Inc.



Scott Dodd, Henry Bellamy, and Marvin Hackert discussing plans for the forthcoming ACA meeting in San Antonio. Scott is assistant beamline manager and Harry is beamline manager of GCPCC; Marv is chair of the USNCCr and co-chair of the San Antonio ACA meeting.



Joe Ferrera (Rigaku/MSC, Inc.), Ed Meyer (SWMS organizer) and Bog Stec (Rice University) during the coffee-break at the poster session.

**The 59th Pittsburgh Diffraction Conference,
Oct 25-27, 2001, Covington, KY**

The conference was held overlooking the Ohio River and downtown Cincinnati. We were thrilled to have with us a 'very special friend of the Pittsburgh Diffraction Society' and our Guest of Honor—**Maureen Jeffrey**. Along with Maureen were her family Denis and Susan (daughter) Slevin, Paul (son) and Paulette Jeffrey and Jeff (grandson) and Kelli Slevin.

Banquet festivities included presentation of the awards:

Sidhu Award for the best contribution to crystallography/diffraction by a young investigator: **Larry Shapiro**—'Finding Protein Function Through Structural Genomics'

Chung Soo Yoo Award for the best poster by a graduate student—difficulty in the decision-making resulted in two awards: **Jeff Habel**—'Sulfur-ISAS Simulation Study' and **Michael Lufaso**—'Evaluation and Prediction of the Crystal Structures of Single Octahedral Cation and Ordered/Disordered Multiple Octahedral Cation Perovskites using the Software Program SPuDS'

A special **Service Award** was given to **Nathan Coker** in recognition of his outstanding contributions above and beyond the 'Call of Duty!'

Opening the 3-day scientific meeting was a full-day symposium on 'Exotic Uses of the CCD in Non-Standard Crystallographic Investigations' organized by Victor Young, Alan Pinkerton and John Parise. The symposium was opened with a very moving 'Tribute to Bob Sparks' given by Sue Byram. The session continued with advice on dealing with twins (Dieter Schwarzenbach, Simon Parsons, Maren Pink), solving structures from powder diffraction, charge density and high-pressure studies (Joe Reibenspies, Alan Pinkerton, Przemyslaw Dera), and lessons on *in situ* crystal growth (Simon Parsons). We were enlightened on new hardware and software features by the vendors (Joe Ferrara- MicroMax 002/RAPID and Chuck Campana-Simultaneous Integration for Twins a new feature in SAINT). Phil Coppens and Jonathan Hanson, experts in time-resolved crystallography, and Tim Graber (ChemMatCARS-Advanced Photon Source) opened our eyes to the world of synchrotron radiation and what that technology can do for general and specialized applications.



Exotic Uses of the CCD in Non-standard Crystallographic Investigations: Back - Victor Young, Joe Reibenspies, Maren Pink, Alan Pinkerton and Dieter Schwarzenbach. Front - Tim Graber, Sue Byram, Simon Parsons, Jonathan Hanson, Joe Ferrara and Phil Coppens

A special 2-day symposium on 'Intra- and Intermolecular Interactions' in memory of George Jeffrey was organized by Bryan Craven and Jeanette Krause Bauer. In this symposium, researchers representing the 'Good Old Days in Pittsburgh working with Jeff' mingled with 'the new generation of crystallographers and chemists' who were and continue to be influenced by George Jeffrey's work. A wide variety of topics were covered that spanned chemical, materials and macromolecular crystallography,



Intra- and Intermolecular Interactions Symposium in Memory of George Jeffrey: Jonathan Parquete, Richard Zaworotko, Anna Gudmundsdottir, Bryan Craven, John Finney, Miguel Garcia-Garibay, Carol Brock, Dave Stout, and Martin Caffrey.



Intra- and Intermolecular Interactions Symposium in Memory of George Jeffrey: Front - Paul Baures, Alfred French, John Rosenberg, Sine Larsen, and B. C. Wang. Back - Larry Shapiro (Sidhu Award winner), Chirster Aakeroy, Lee Brammer, Ned Seeman, Bryan Craven and Dieter Mootz

I would like to thank all those involved in the planning of this meeting; without you this meeting could not have taken place. Many thanks to the vendors for your financial support and to Marshall Wilson and the Department of Chemistry, University of Cincinnati for everything else needed to put the program together. Thank you to all the speakers and the participants for coming, especially in light of all that has happened in the past couple of months. See you all next year!

Jeanette Krause Bauer, PDS President & Conference Chair

New OSTP Director Offers Views on S&T

At the end of October, the Senate voted to confirm John H. Marburger to be the Director of the Office of Science and Technology Policy. Later, Marburger addressed the High Energy Physics Advisory Panel (HEPAP). His remarks offered good insight into his thinking and that of the President regarding science and technology policy and funding.

He touched on several topics during his presentation, the most important of which was the impact of the September 11 attacks. The attacks have had a “profound effect on the administration,” he said, recounting a meeting he attended with the President the day before. Bush made clear his commitment to winning this war, and views this as the mission of the administration, Marburger explained. His first message, Marburger told the panel, is that there has been a major change in “everything.” The key objectives of the federal government are now protecting people and reducing the possibility of future attacks.

As the scientific community interacts with Congress, “it is obligatory to acknowledge these changed circumstances” . Search for how you can help, he said. These changed circumstances will have implications, Marburger predicted, although no one fully knows what these changes will be. There will probably be less money for some programs, he said, and the need for planning will be greater. A “much crisper sense of priorities,” and “increased discipline” in budgeting will be needed, he said. Marburger described the Office of Management and Budget’s concerns about the distortion caused by earmarking, as well as the balance in funding for life and physical sciences. The important relationship between the physical sciences and life sciences is not widely recognized, he added.

Expanding upon his remarks about future S&T spending, Marburger thought that there could be “very serious” problems due to the significant funding needed to prevent future attacks, and because of the public’s concern about such attacks. Telling HEPAP that “I’m on your side,” he said “decisions about what to do next are going to be very, very difficult” for several years. Marburger said that recent reports about budgetary problems at the Large Hadron Collider “are not going to help.” “I don’t have a clear prediction of what will happen,” he added.

Turning to his interactions with the Office of Management and Budget, Marburger said he has a good relationship with OMB Director Mitch Daniels and OMB staff. He has also met with Gov. Tom Ridge on homeland security matters. OSTP is “waking up very rapidly,” Marburger declared, adding that there is a realization that there has been “a shortage of scientific presence” in policy formulation. The Bush Administration, he exclaimed, is taking a businesslike approach to budgeting, with an emphasis on results.

Marburger’s final advice to the panel was “take advantage of me and my office.” He urged that the scientific community keep in touch with his office, saying that its help was needed.

Richard M .Jones, AIP
fji@aip.org -www.aip.org/gov

Dear Friends and Fellow Crystallographers,

We are deeply shocked by the terrorists’ attack against America. We scientists are by Nature international and cannot understand or accept such a horrible tragedy.

We shall even more than before, continue collaborating together to promote our science in all countries, especially the underdeveloped ones. We strongly believe and are convinced that this is a very important contribution to the world’s peace.

With all our friendship,
Claude Lecomte, President, European Crystallographic Association

Dear Friends,

Yesterday we all were very much shocked by the horrifying pictures of New York and Washington. Unbelievable what happened; this catastrophe goes beyond any imagination. At the time the first news came in, my complete group was gathered and we first did not believe that the message could be true. However, it just appeared to be the befining of the terrorist’s attack and the day changed into one of the real balck days of history.

On behalf of the IUCr I want to express our sympathy n thee difficult days with the American people and in particular with all our colleagues in crystallography and their relatives.

Henk Schenk , President, IUCr

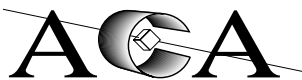
Metripol – A New Quantitative Approach To Analysing Strain In Transparent Materials

Oxford, UK - Metripol, an operating division of the Ferraris Group plc, has announced the development and launch of a new birefringence imaging microscope. This system - called the Metripol - lets scientists perform qualitative and quantitative measurements of strain on a wide variety of transparent microscopic specimens using a specially designed microscope and the Metripol software package.

The Metripol has already been used extensively is areas such as the study of strain in industrial diamonds, the analysis of collagen and hydroxyapatite distribution in bone and phase transitions in crystals. In fact, the microscope can be used to analyse any transparent materials where strain is of interest including crystals, liquid crystals, biological samples, amorphous materials and semi-amorphous materials.

It works by using filtered light together with a series of special filters, polarizers and a circular analyser. Images collected with this system can then be separated out into their different birefringence, orientation and transparency components which are normally superimposed in conventional polarising microscopy. Such images provide an enormous amount of useful information about the structure of birefringent transparent samples. Because the system is quantitative, accurate numerical values can now be assigned to these different components.

For more information visit www.metripol.com



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Thanks Ron!

Ron Stenkamp "retired" from editing the ACA Newsletter with the fall 2001 issue. He did a great job and was a pleasure to work with. The collaboration has ended but the friendship remains - lucky me!



Behind every great man is a greater woman -Ruth Clearfield, Celia Steinfink and Edith Hauptman at the banquet in Los Angeles

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2002 Denver X-ray Conference

The 51st Annual Denver X-ray Conference will be held 29 July - 2 August 2002 at the Antlers Adam's Mark Hotel, Colorado Springs, Colorado, U.S.A.

Following traditional format, the conference will include tutorial workshops on Monday and Tuesday, and technical sessions on Wednesday, Thursday and Friday. Exhibitions at the conference will run Monday through Thursday. The Plenary session at the 2002 DXC will be: Applications of X-ray Analysis to Forensic Materials.

For access to current conference information, please visit our web site at: www.dxcicdd.com. Additional information can also be obtained from: Denise Flaherty, Conference Coordinator, ICDD, 12 Campus Blvd., Newtown Square, PA 19073, Phone: 610-325-9814, Fax: 610-325-9823, E-mail: dxc@icdd.com.

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March 2002

4 - 7 - 10th Annual Meeting of the German Society for Crystallography (DGK), Kiel, Germany. www.ifg.uni-kiel/dgk2002

23-28 - 9th International Conference on the Crystallization of Biological Macromolecules. Jena, Germany. www.conventus.de/iccbm9/

25-28 - BCA Annual Meeting. Nottingham, UK. gordon.cryst.bbk.ac.uk/BCA/meets/BCAnew.html

May 2002

21-June 2 - 33rd Crystallographic course at E. Majorana Centre. erice, Italy. "From Genes to Drugs via X-ray Crystallography". www.geomin.unibo.it/orgv/erice/erice.htm.

August 2002

4-8 -ACCGE-14 -Fourteenth American Conference on

Crystal Growth and Epitaxy, - Seattle, Washington. The Conference will include Technical Sessions, a Vendor Exhibit, and a Short Course emphasizing all aspects of Bulk Growth, Epitaxy, Characterization, and Materials issues in Devices. There will also be a special symposium entitled "Celebration of 50 Years of Progress in Crystal Growth", chaired by Bob Feigelson (Stanford University) and featuring distinguished speakers whose work has had a major impact on progress in crystal growth. www.crystalgrowth.org.

6-15 - IUCr XIX - Congress and General Assembly of the International Union of Crystallography, Geneva, Switzerland.

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/

Protein Crystallographer - Tenure Track

Applications are invited for a tenure-track, full-time faculty appointment at the Assistant or Associate Professor level in the Institute of Materials Science and Department of Molecular and Cell Biology at the University of Connecticut. Applicants must have a doctorate degree in a biochemical, chemical or biophysical field and postdoctoral experience. The research area of interest is X-ray crystallography of proteins or protein/nucleic acids complexes, which will complement current research strengths in structural biology. The successful candidate will teach undergraduate and graduate courses in the Department of Molecular and Cell Biology and will be affiliated with the Polymer Program of the Institute of Materials Science. The successful candidate will be expected to establish a productive, extramurally funded research program. A part of the 28-member Department of Molecular and Cell Biology will soon expand into a new building adjacent to the Institute. The Institute is an interdisciplinary research facility that houses the 14-member Polymer Program and the X-ray diffraction facilities. The anticipated starting date is August, 2002. To apply, submit curriculum vitae, a brief statement of research and teaching interests, and arrange to have three letters of recommendation sent to: Search Committee #2, Institute of Materials Science, University of Connecticut, 97 North Eagleville Road, U-3136, Storrs, CT 06269-3136. Review of applications will begin after publication of this notice and will continue until the position is filled. We encourage applications from under-represented groups, including minorities, women and people with disabilities. (Search #02A170)

Macromolecular Crystallographer/Data Processing and Programming Specialist:

Area Detector Systems Corp. (ADSC) has an immediate opening for a Research Scientist with background experience in Molecular Crystallography and qualified in computer programming. The successful candidate will contribute to research on advanced software requirements used to analyze fine slice data used in the advancement of protein crystallography. This requires at least three years experience in Molecular Crystallography coupled with solid knowledge of C++ programming. Experience obtained either as a graduate student or in Post- Doctorate work is applicable.

ADSC is a privately held company founded in 1981 and is located in the sunny southern California area near San Diego. The company is an industrial leader that develops and manufactures CCD Detectors that are used in Synchrotrons worldwide in Protein Crystallography applications. Most recently, it has considerably increased the research and development activity with the support of major government grants. The company's web site is adsc-xray.com. Send your resume outlining your experience to: ADSC (c/o T.H. Hontz), 12550 Stowe Drive, Poway, CA, 92604 or e-mail to sales@adsc-xray.com.

Postdoctoral - Protein Crystallographer

There is an opening for a postdoctoral position in protein structure analysis and its implications in the Laboratory for the Structure of Matter at the Naval Research Laboratory, located in Washington, D.C. The research program would be collaborative with Drs. Jerome Karle, John Konnert and Jeffrey Deschamps. Our laboratory has two CCD area detectors, a network of graphics workstations, a 16 processor SGI Origin 3400 server and facilities for protein expression, purification and crystallization. The postdoctoral appointment could last up to three years and has the potential to lead to a permanent position. The salary would be approximately 55K. U. S. citizenship is required. Please send a C.V., including your experience in macromolecular structure determination, a letter describing your interests and the names and addresses of three references to Dr. Jerome Karle, Chief Scientist, Code 6030, Laboratory for the Structure of Matter, Naval Research Laboratory, Washington, D.C. 20375-5341. E-mail: williams@harker.nrl.navy.mil FAX: 202-767-0953

Wanted - Home for Lonely Books

The following journals are available for the cost of shipping:

J. Am. Chem. Soc. 1965-1976

Acta Crystallographica 1948-1969 (Bound)

Acta Crystallographica 1948-1971 (Unbound)

Al Tulinsky, Dept. of Chemistry, Michigan State University, East Lansing, MI 48824, Tulinsky@cem.msu.edu

Positions Previously Listed

Tenure Track Protein Crystallographer

A faculty position as Assistant Professor is available in Protein Crystallography in the Department of Biochemistry. Qualified candidates could be considered at the Associate Professor rank. This recruitment is part of an ongoing Structural Biology Initiative at Wake Forest University. Applicants should have a Ph.D. and postdoctoral experience. We seek an outstanding candidate who will establish a nationally competitive, independent research program in structural biology and will participate in graduate teaching. Excellent new facilities and generous start-up funds are being provided. Many opportunities for research collaborations are also available within the institution. Candidates are encouraged to seek additional information regarding faculty research interests, major instrumentation, and the Structural Biology Initiative at Wake Forest from our web site (www.wfubmc.edu/biochem/xray). Review of applications will begin as they are received and will continue until the position is filled. Applicants should submit a curriculum vitae and a statement of current and future research plans, and should have three letters of reference sent to: Dr. Leslie Poole, Protein Crystallography Search Committee, Department of Biochemistry, Wake Forest University School of Medicine, Winston-Salem, NC 27157. Wake Forest University is an Equal Opportunity Affirmative Action Employer.

ACA Nominating Committee for 2002

Chair - Tom Terwilliger
(terwill@telomere.lanl.gov)

Winnie Wong-Ng
(winnie.wong-ng@nist.gov)

Connie Chidester
(conniechidester@earthlink.net)

The committee requests suggestions from the membership for Society Officers and members of ACA Standing Committees for 2002 Elections.